



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2025 – 11:29 PM EDT

PDB ID : 9MTR / pdb\_00009mtr  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site GGS-mutant Release Factor 1, and P-site fMEAAA KC-peptidyl-tRNA<sub>cys</sub> at 2.80Å resolution  
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.  
Deposited on : 2025-01-12  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

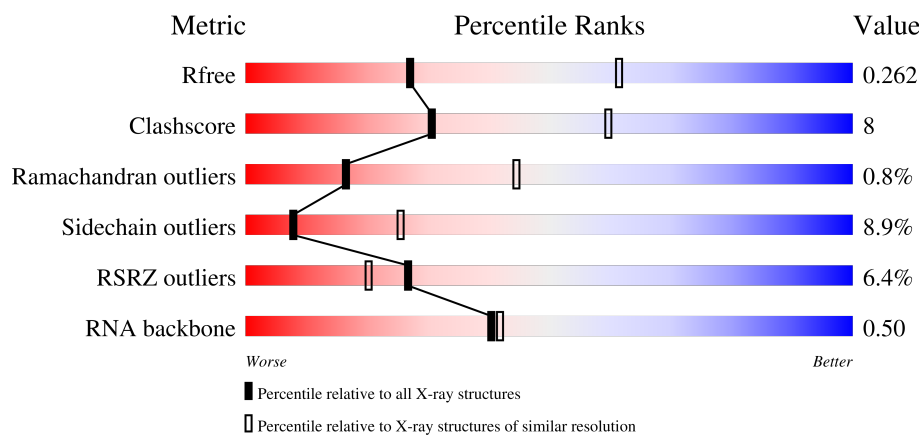
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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




























Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	



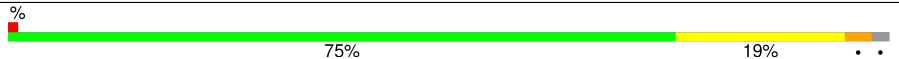
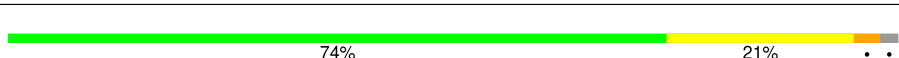
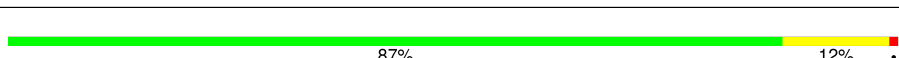
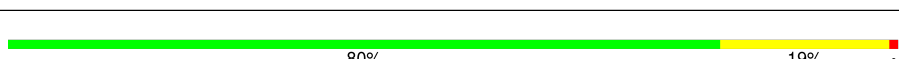
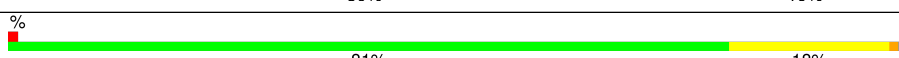
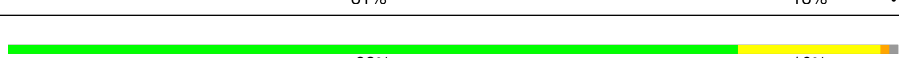
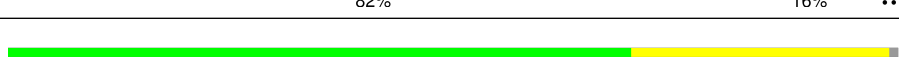

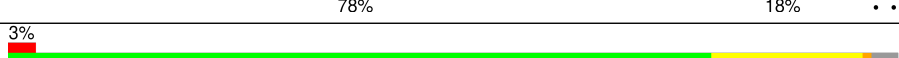







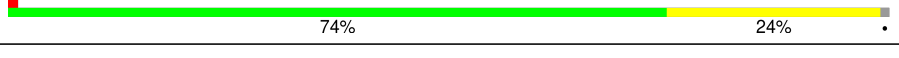
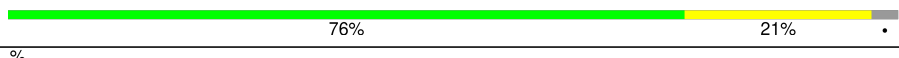

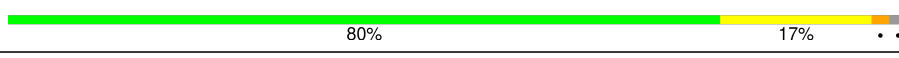



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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141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

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

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

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

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	74	
55	2x	74	
56	1z	7	
56	2z	7	

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	1A	4032	-	-	-	X
57	MG	1U	212	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			919	566	190	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			907	558	188	159	2			

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called CYS-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			
53	2v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1935	1196	359	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1953	1207	360	377	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1w	230	SER	GLN	engineered mutation	UNP P96077
2w	230	SER	GLN	engineered mutation	UNP P96077

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMEAAAKC-tRNA<sub>cys</sub> RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			
55	2x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMEAAAKC-tRNA<sub>cys</sub> Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	5	Total	C	N	O	S	0	0	0
			30	18	6	5	1			
56	2z	4	Total	C	N	O	S	0	0	0
			25	15	5	4	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1084	Total	Mg	0	0
			1084	1084		
57	1B	39	Total	Mg	0	0
			39	39		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1D	14	Total 14	Mg 14	0	0
57	1E	13	Total 13	Mg 13	0	0
57	1F	14	Total 14	Mg 14	0	0
57	1G	5	Total 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	3	Total 3	Mg 3	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	5	Total 5	Mg 5	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	12	Total 12	Mg 12	0	0
57	1V	8	Total 8	Mg 8	0	0
57	1W	5	Total 5	Mg 5	0	0
57	1X	6	Total 6	Mg 6	0	0
57	1Y	3	Total 3	Mg 3	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	12	2	Total 2	Mg 2	0	0
57	13	4	Total 4	Mg 4	0	0
57	15	9	Total 9	Mg 9	0	0
57	16	3	Total 3	Mg 3	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	221	Total 221	Mg 221	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	1	Total 1	Mg 1	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	1	Total 1	Mg 1	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1p	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	13	Total 13	Mg 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2A	835	Total 835	Mg 835	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	5	Total 5	Mg 5	0	0
57	2E	10	Total 10	Mg 10	0	0
57	2F	7	Total 7	Mg 7	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2O	3	Total 3	Mg 3	0	0
57	2P	1	Total 1	Mg 1	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	4	Total 4	Mg 4	0	0
57	2U	4	Total 4	Mg 4	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	2I	2	Total 2	Mg 2	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	4	Total 4	Mg 4	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	28	3	Total 3	Mg 3	0	0
57	2a	178	Total 178	Mg 178	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	1	Total 1	Mg 1	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2x	8	Total 8	Mg 8	0	0

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

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

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

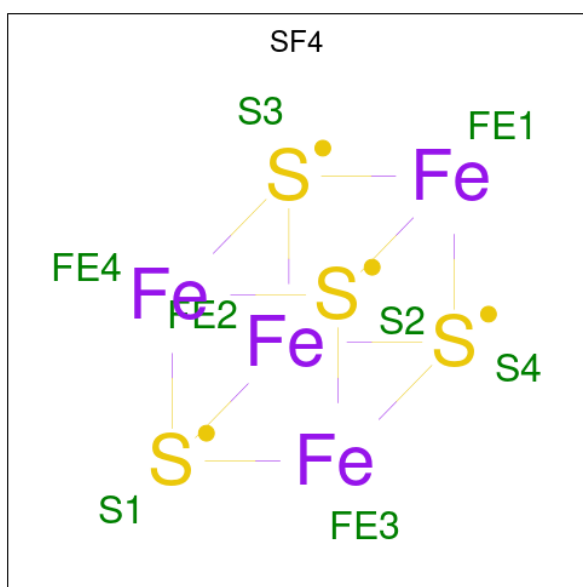
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total 1	Zn 1	0	0

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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:  $\text{Fe}_4\text{S}_4$ ).



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	1897	Total 1897	O 1897	0	0
61	1B	61	Total 61	O 61	0	0
61	1D	30	Total 30	O 30	0	0
61	1E	27	Total 27	O 27	0	0
61	1F	18	Total 18	O 18	0	0
61	1G	5	Total 5	O 5	0	0
61	1H	2	Total 2	O 2	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	8	Total 8	O 8	0	0
61	1O	6	Total 6	O 6	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	11	Total 11	O 11	0	0
61	1R	11	Total 11	O 11	0	0
61	1S	1	Total 1	O 1	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	13	Total 13	O 13	0	0
61	1V	6	Total 6	O 6	0	0
61	1W	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	10	Total 10	O 10	0	0
61	1Y	2	Total 2	O 2	0	0
61	10	9	Total 9	O 9	0	0
61	11	8	Total 8	O 8	0	0
61	12	3	Total 3	O 3	0	0
61	13	4	Total 4	O 4	0	0
61	15	7	Total 7	O 7	0	0
61	16	1	Total 1	O 1	0	0
61	17	8	Total 8	O 8	0	0
61	18	12	Total 12	O 12	0	0
61	1a	259	Total 259	O 259	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	2	Total 2	O 2	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	4	Total 4	O 4	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	3	Total 3	O 3	0	0
61	1w	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	25	Total 25	O 25	0	0
61	2A	1003	Total 1003	O 1003	0	0
61	2B	14	Total 14	O 14	0	0
61	2D	25	Total 25	O 25	0	0
61	2E	14	Total 14	O 14	0	0
61	2F	12	Total 12	O 12	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	3	Total 3	O 3	0	0
61	2P	7	Total 7	O 7	0	0
61	2Q	3	Total 3	O 3	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	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	2	Total 2	O 2	0	0
61	20	2	Total 2	O 2	0	0
61	21	10	Total 10	O 10	0	0
61	25	3	Total 3	O 3	0	0
61	27	2	Total 2	O 2	0	0
61	28	4	Total 4	O 4	0	0

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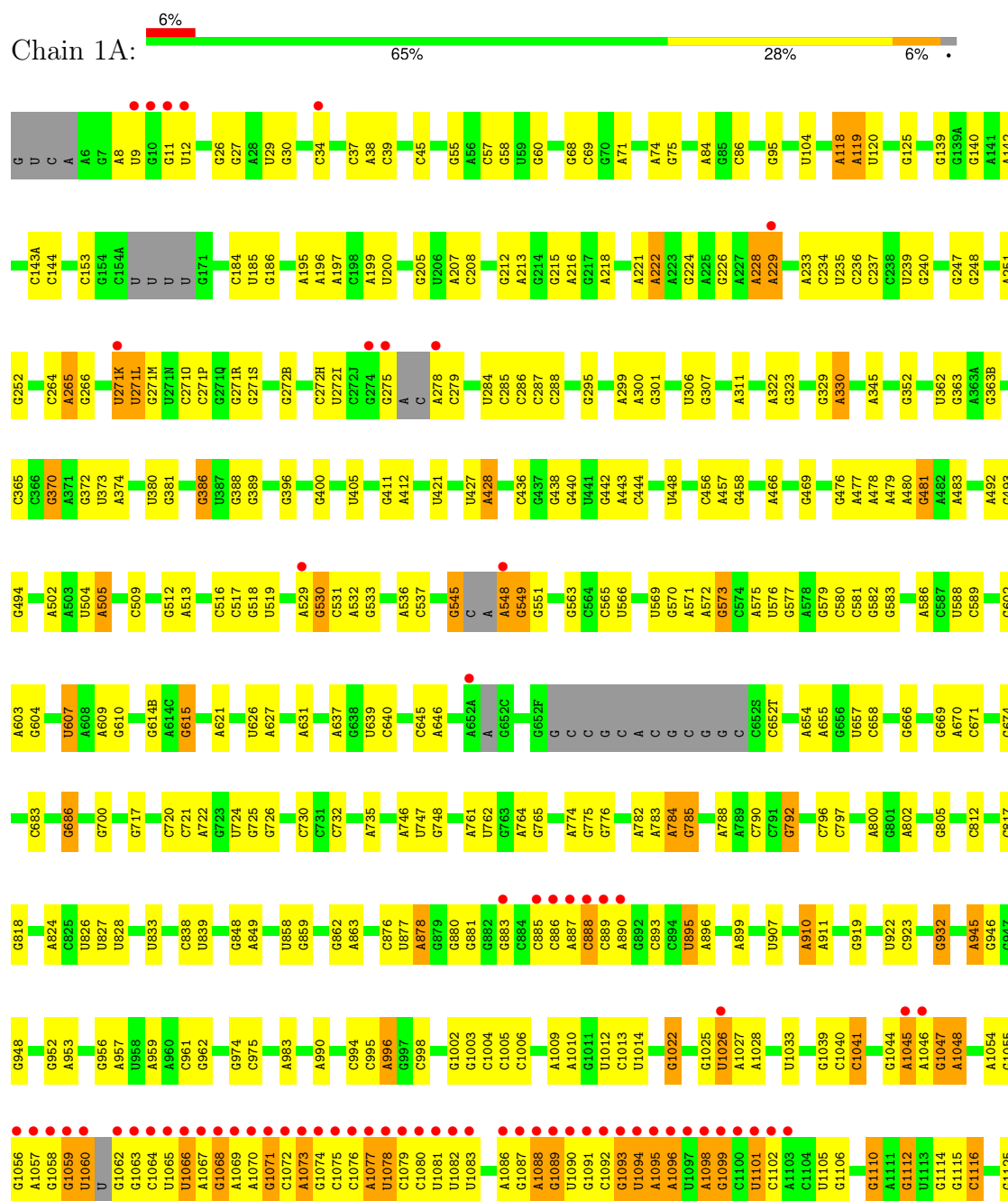
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total 1	O 1	0	0
61	2a	130	Total 130	O 130	0	0
61	2e	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2n	1	Total 1	O 1	0	0
61	2q	2	Total 2	O 2	0	0
61	2t	2	Total 2	O 2	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	1	Total 1	O 1	0	0
61	2x	14	Total 14	O 14	0	0

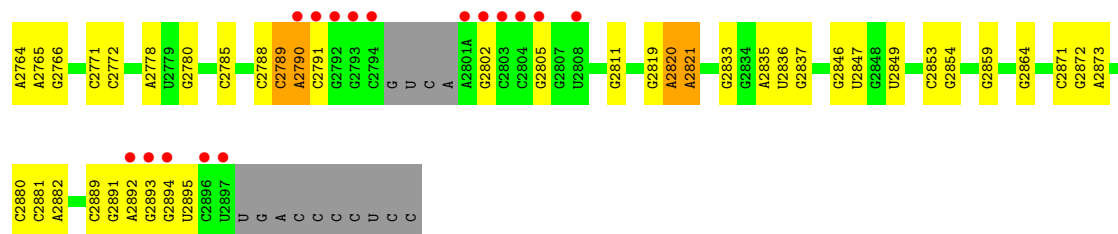
### 3 Residue-property plots

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

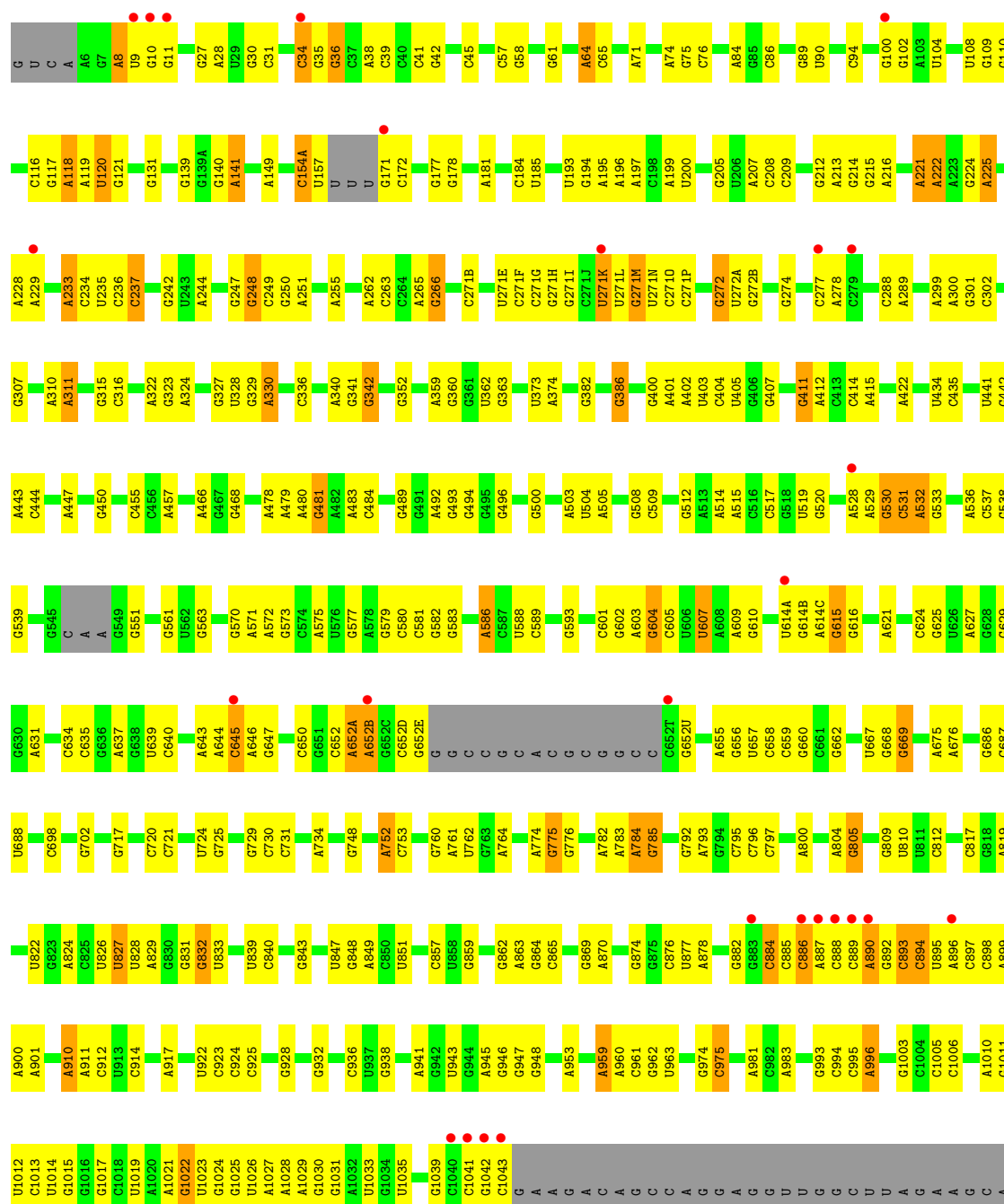
#### • Molecule 1: 23S Ribosomal RNA



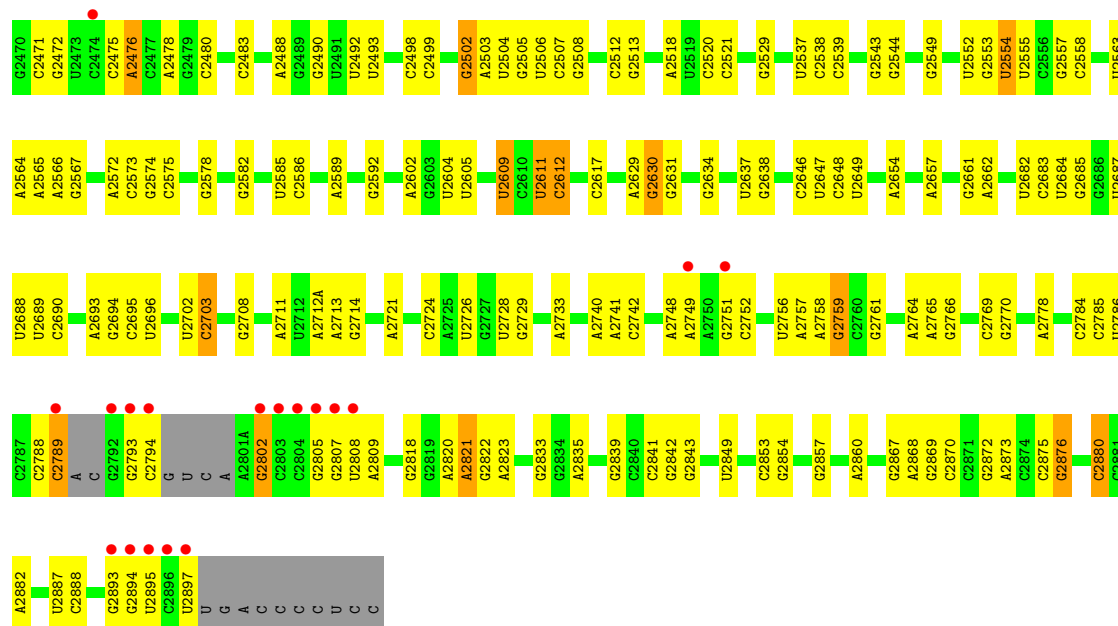




• Molecule 1: 23S Ribosomal RNA

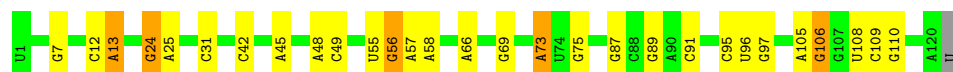






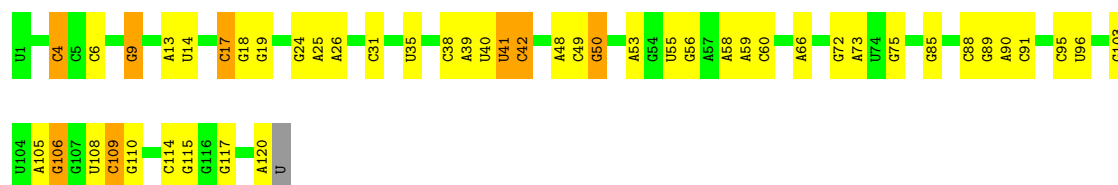
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 75% 20% . .



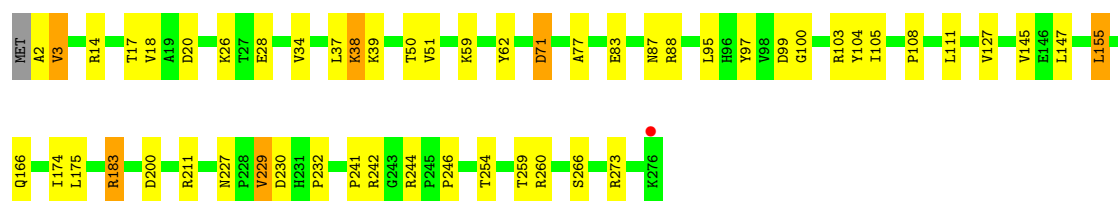
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 60% 33% 7% .



- Molecule 3: 50S ribosomal protein L2

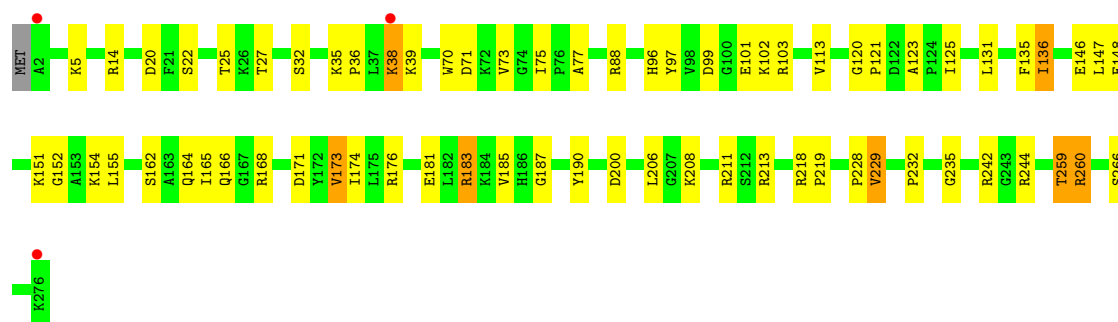
Chain 1D: 80% 17% .



- Molecule 3: 50S ribosomal protein L2

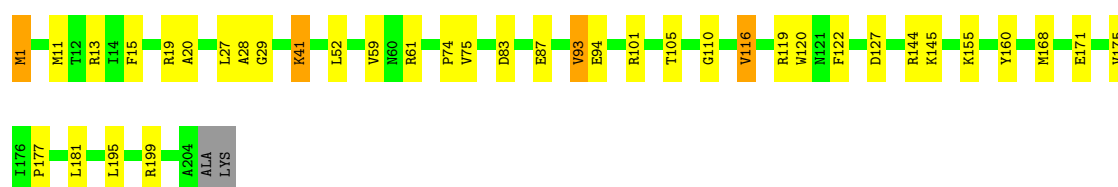
Chain 2D: 75% 22% .





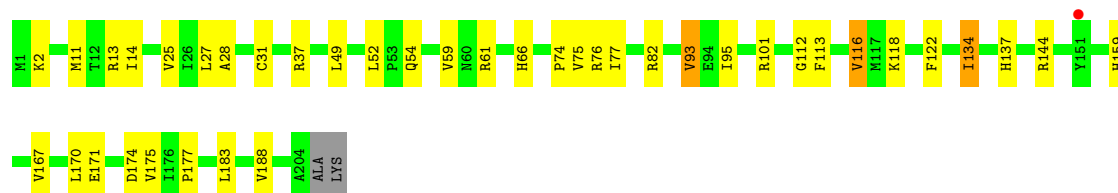
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 81% 17% ..



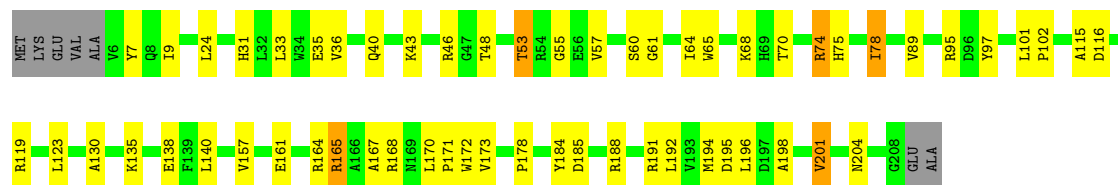
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 80% 18% ..



• Molecule 5: 50S ribosomal protein L4

Chain 1F: 69% 25% . .



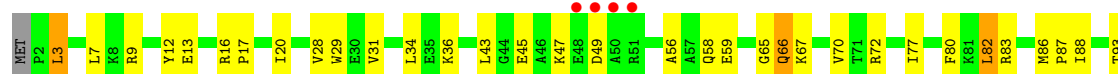
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 64% 28% 5% .





- Molecule 6: 50S ribosomal protein L5



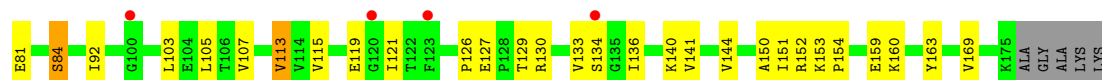
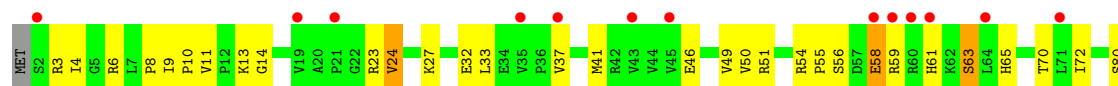
- Molecule 6: 50S ribosomal protein L5



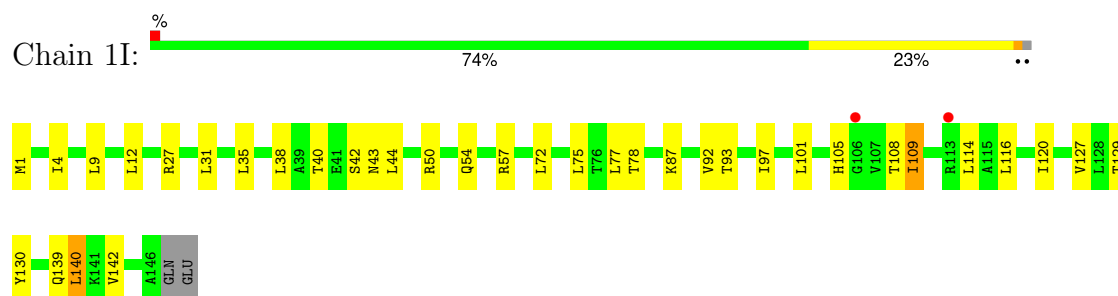
- Molecule 7: 50S ribosomal protein L6



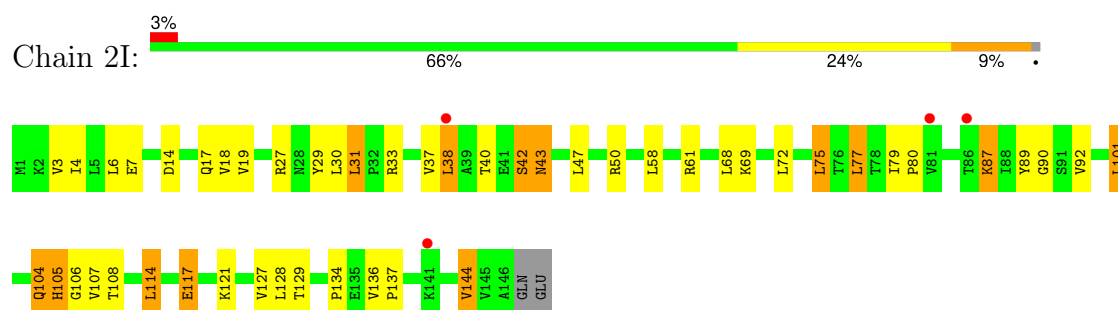
- Molecule 7: 50S ribosomal protein L6



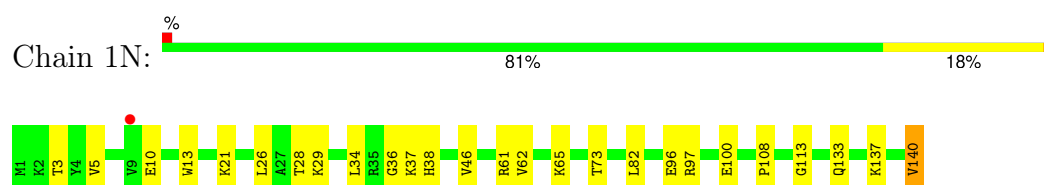
- Molecule 8: 50S ribosomal protein L9



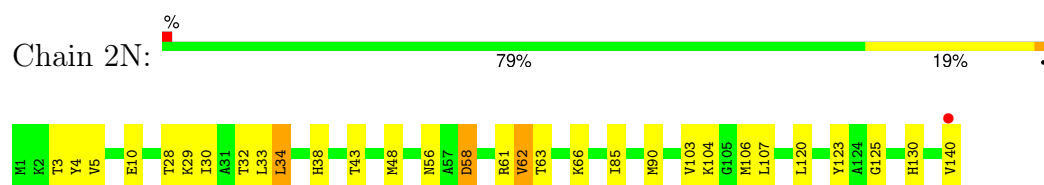
- Molecule 8: 50S ribosomal protein L9



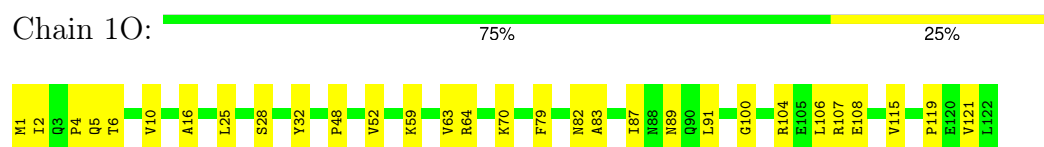
- Molecule 9: 50S ribosomal protein L13



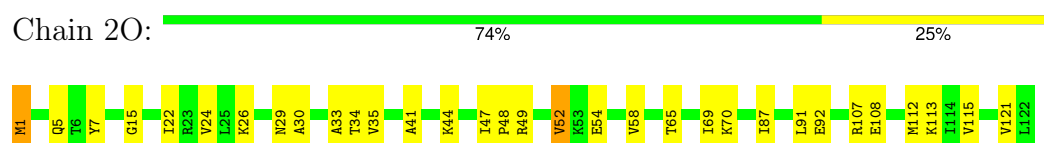
- Molecule 9: 50S ribosomal protein L13



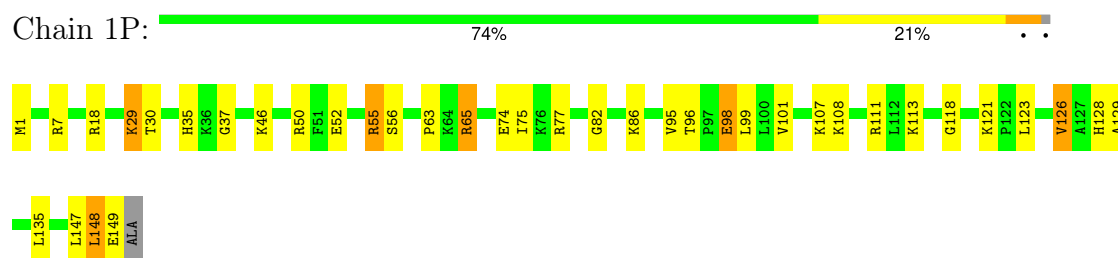
- Molecule 10: 50S ribosomal protein L14



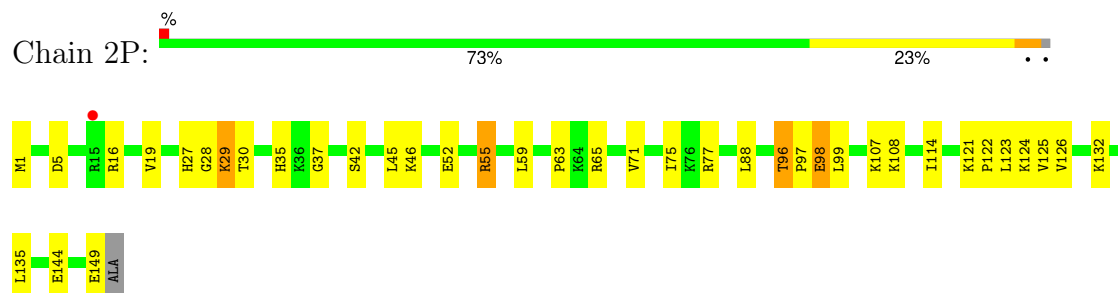
- Molecule 10: 50S ribosomal protein L14



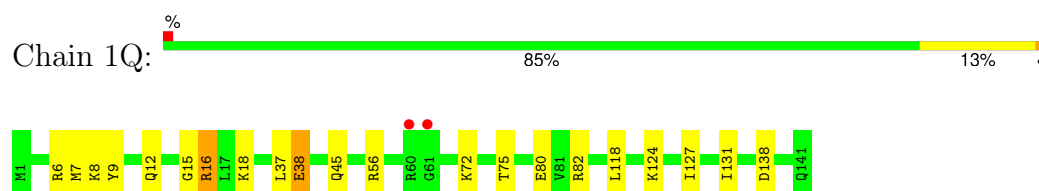
- Molecule 11: 50S ribosomal protein L15



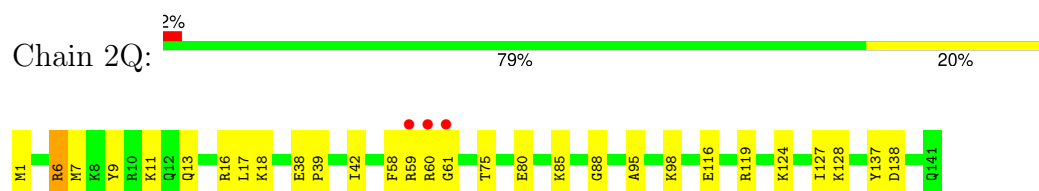
- Molecule 11: 50S ribosomal protein L15



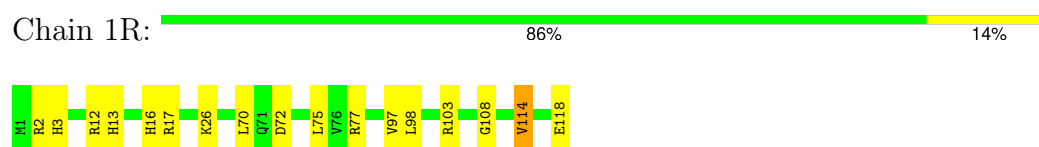
- Molecule 12: 50S ribosomal protein L16



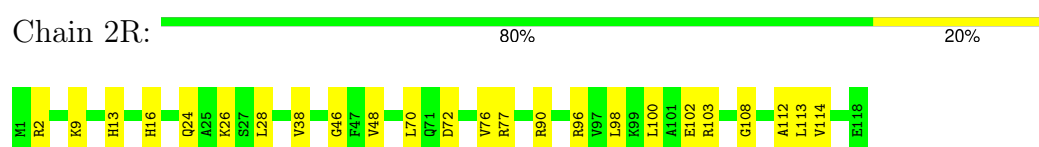
- Molecule 12: 50S ribosomal protein L16



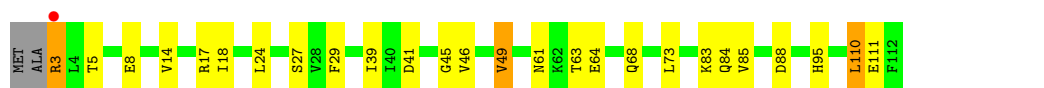
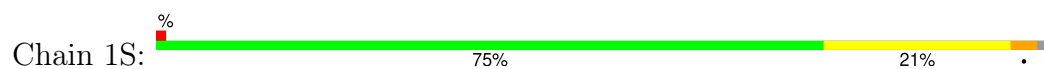
- Molecule 13: 50S ribosomal protein L17



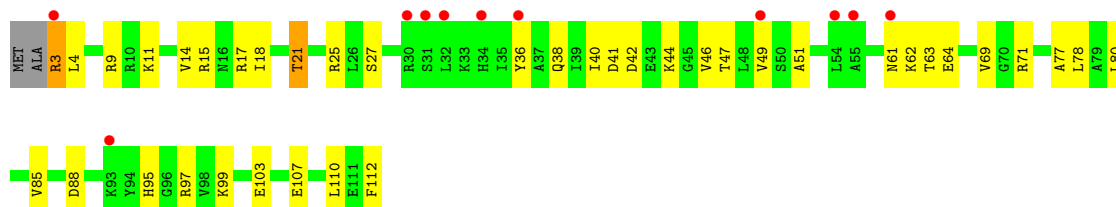
- Molecule 13: 50S ribosomal protein L17



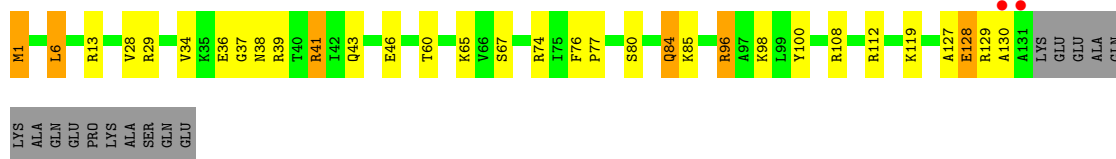
## • Molecule 14: 50S ribosomal protein L18



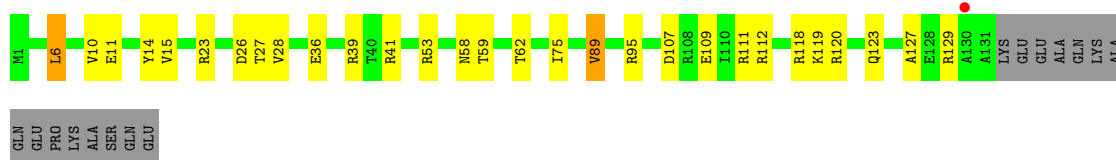
## • Molecule 14: 50S ribosomal protein L18



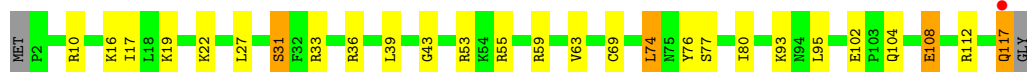
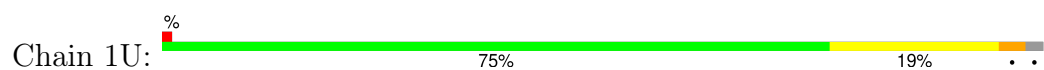
## • Molecule 15: 50S ribosomal protein L19



## • Molecule 15: 50S ribosomal protein L19

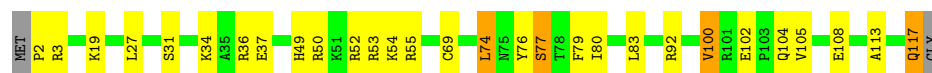


## • Molecule 16: 50S ribosomal protein L20



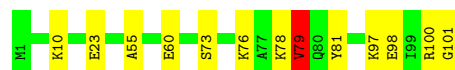
## • Molecule 16: 50S ribosomal protein L20





- Molecule 17: 50S ribosomal protein L21

Chain 1V: 87% 12%



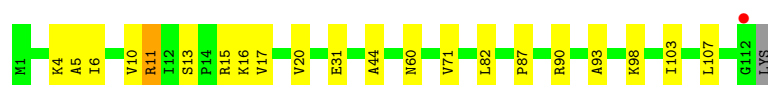
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 80% 19%



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 81% 18%



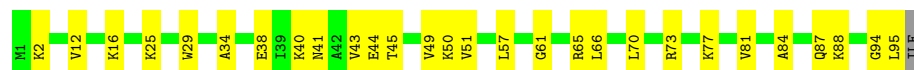
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 82% 16%



- Molecule 19: 50S ribosomal protein L23

Chain 1X: 70% 29%



- Molecule 19: 50S ribosomal protein L23

Chain 2X: 78% 18%

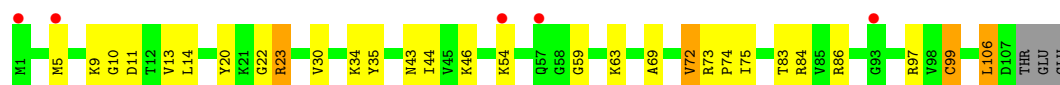


- Molecule 20: 50S ribosomal protein L24

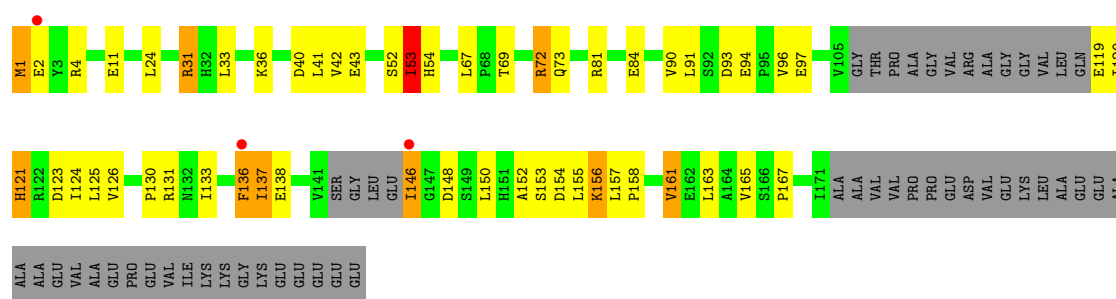
Chain 1Y: 79% 17%



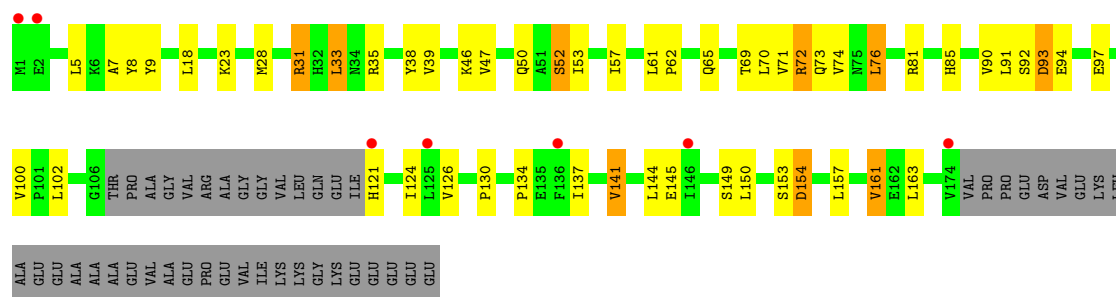
- Molecule 20: 50S ribosomal protein L24



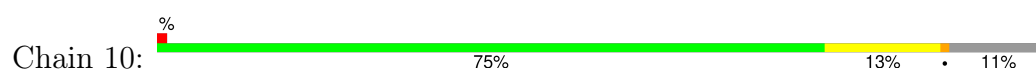
- Molecule 21: 50S ribosomal protein L25



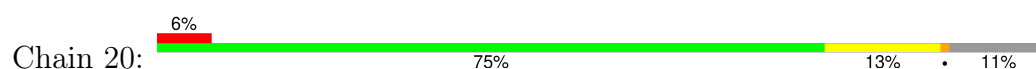
- Molecule 21: 50S ribosomal protein L25

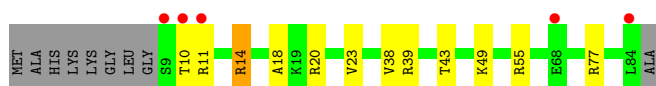


- Molecule 22: 50S ribosomal protein L27

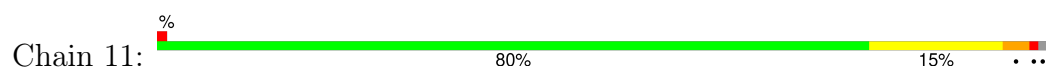


- Molecule 22: 50S ribosomal protein L27

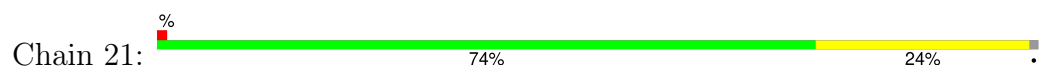




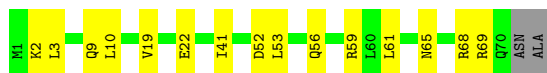
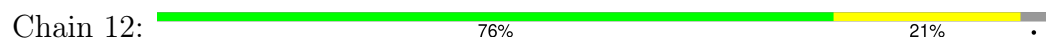
- Molecule 23: 50S ribosomal protein L28



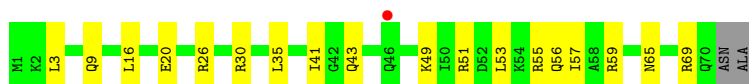
- Molecule 23: 50S ribosomal protein L28



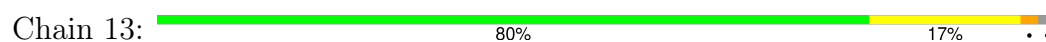
- Molecule 24: 50S ribosomal protein L29



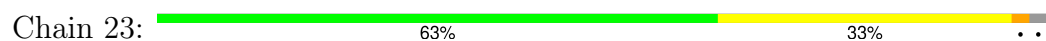
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



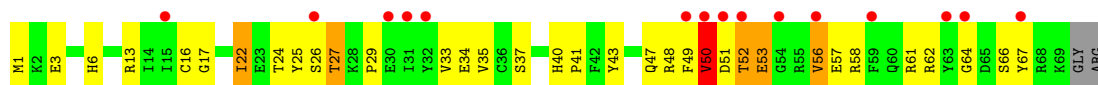
- Molecule 26: 50S ribosomal protein L31



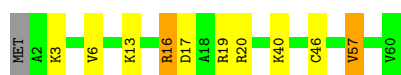
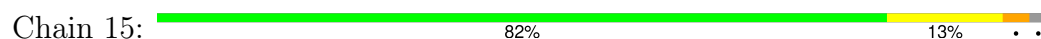




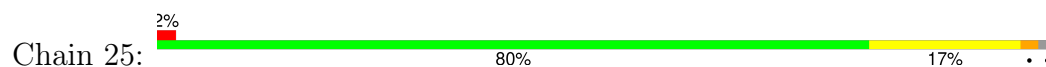
- Molecule 26: 50S ribosomal protein L31



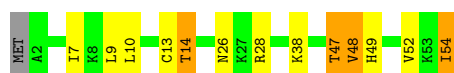
- Molecule 27: 50S ribosomal protein L32



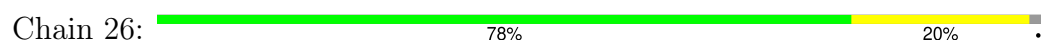
- Molecule 27: 50S ribosomal protein L32



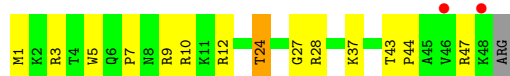
- Molecule 28: 50S ribosomal protein L33



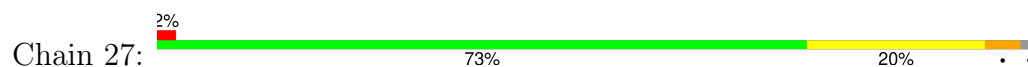
- Molecule 28: 50S ribosomal protein L33

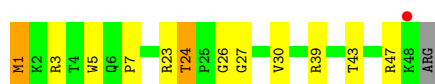


- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain 18: 82% 17% .



- Molecule 30: 50S ribosomal protein L35

Chain 28: 74% 25% .



- Molecule 31: 50S ribosomal protein L36

Chain 19: 81% 19%



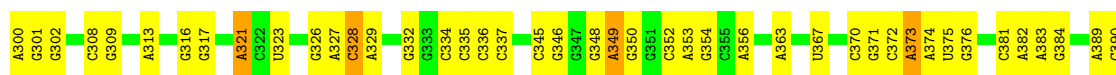
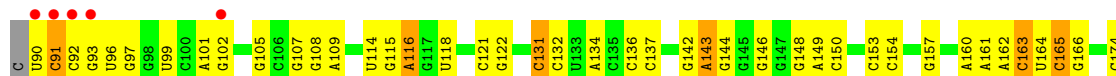
- Molecule 31: 50S ribosomal protein L36

Chain 29: 68% 32%



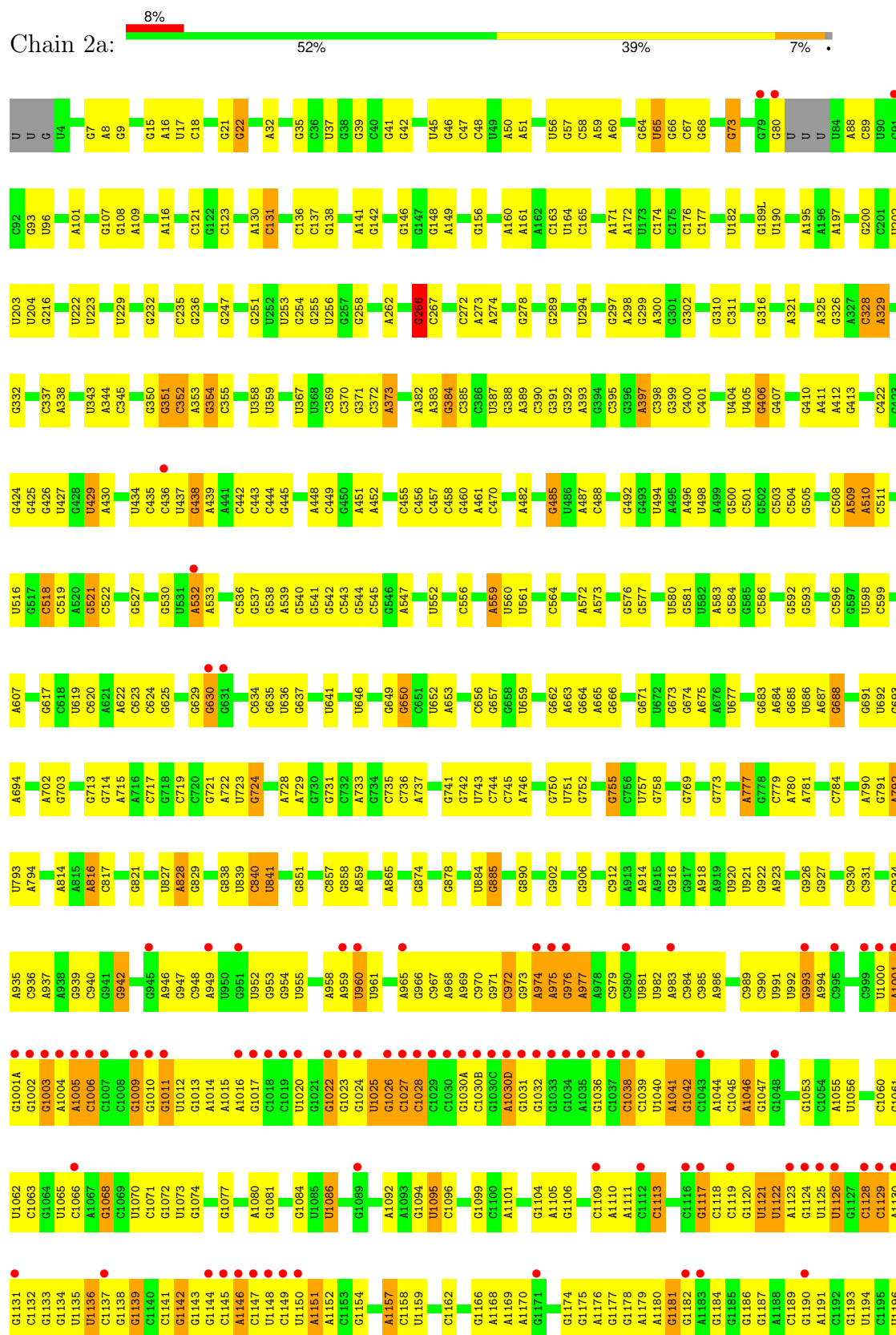
- Molecule 32: 16S Ribosomal RNA

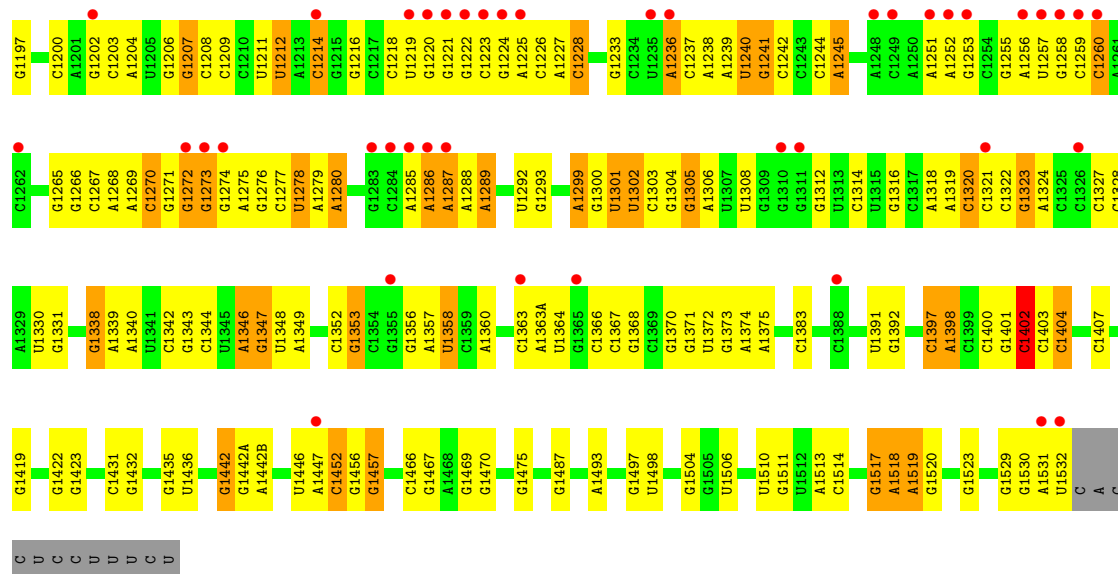
Chain 1a: 8% 52% 38% 9% .



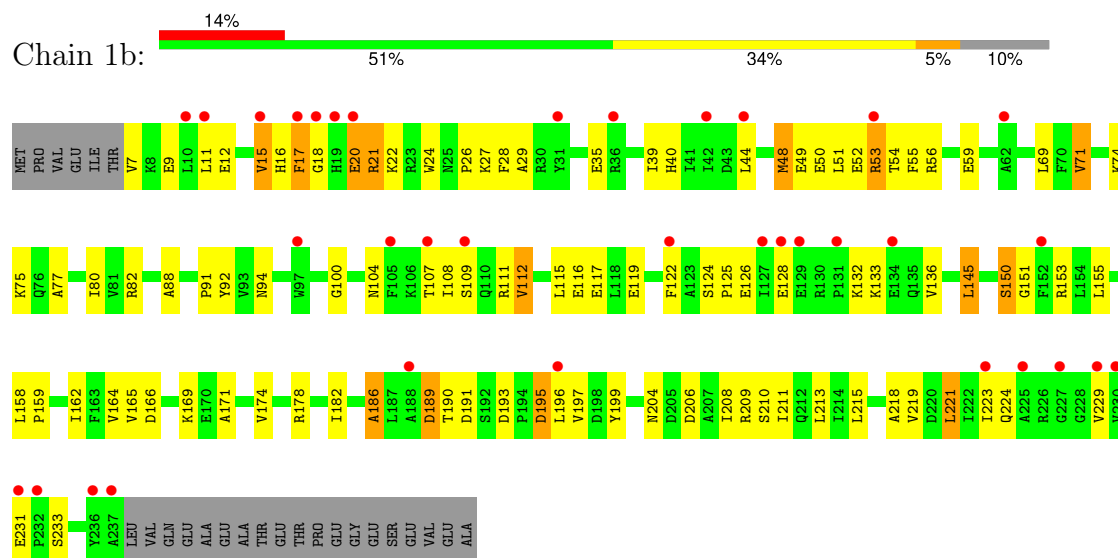


• Molecule 32: 16S Ribosomal RNA

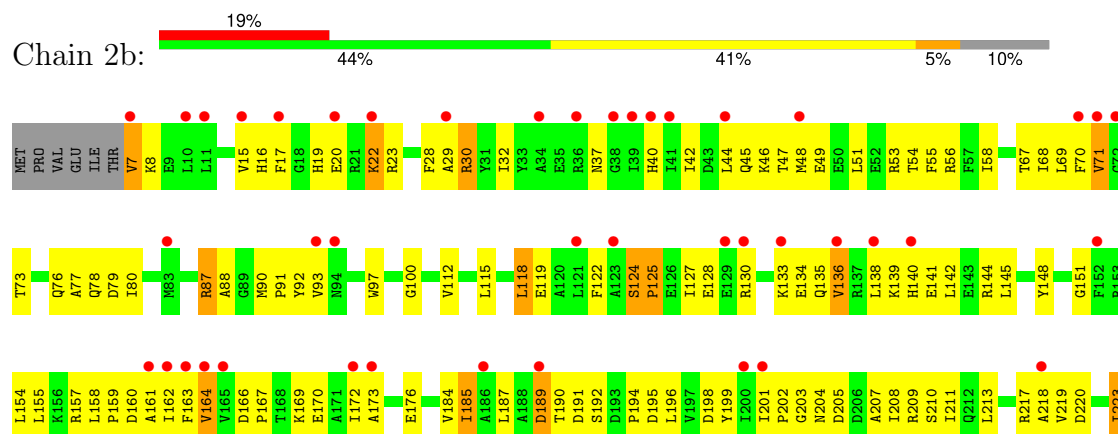




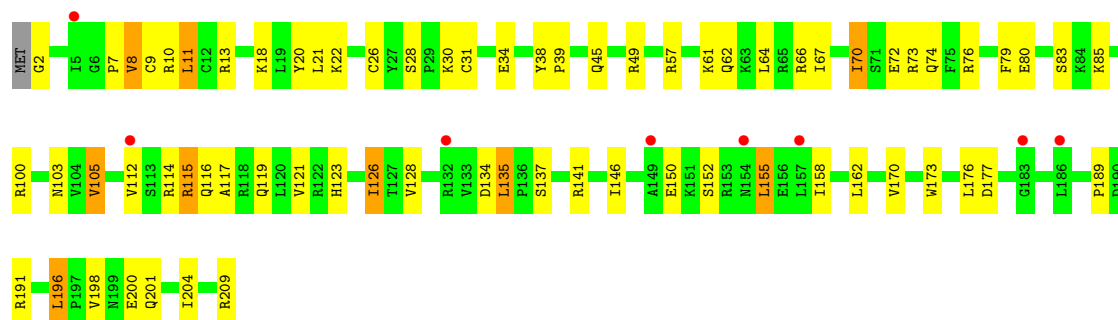
• Molecule 33: 30S ribosomal protein S2



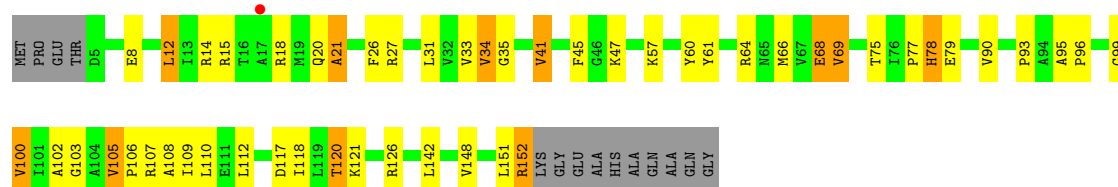
• Molecule 33: 30S ribosomal protein S2



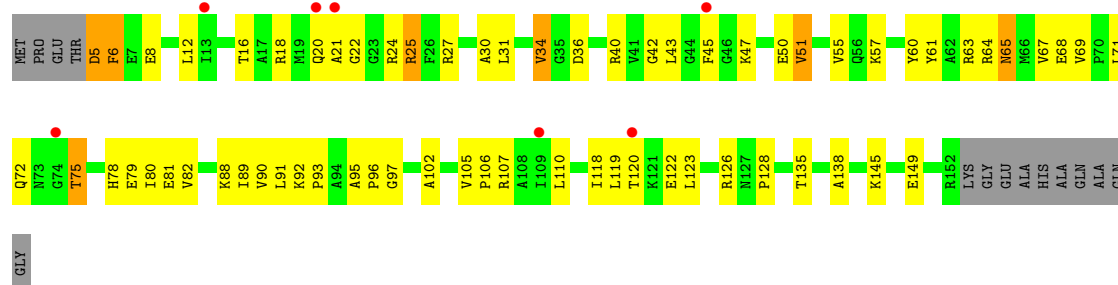




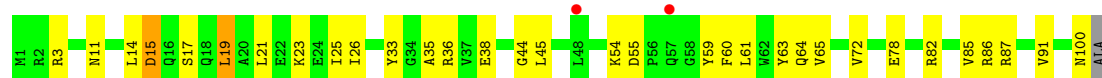
- Molecule 36: 30S ribosomal protein S5



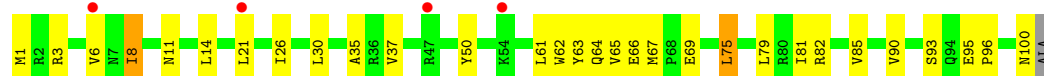
- Molecule 36: 30S ribosomal protein S5



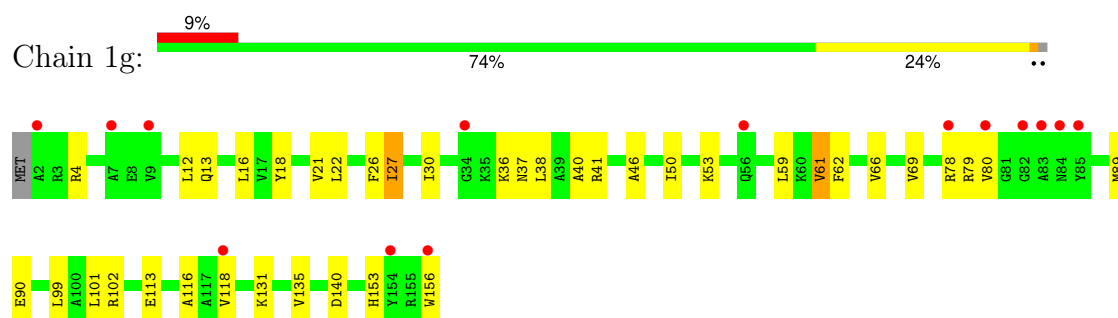
- Molecule 37: 30S ribosomal protein S6



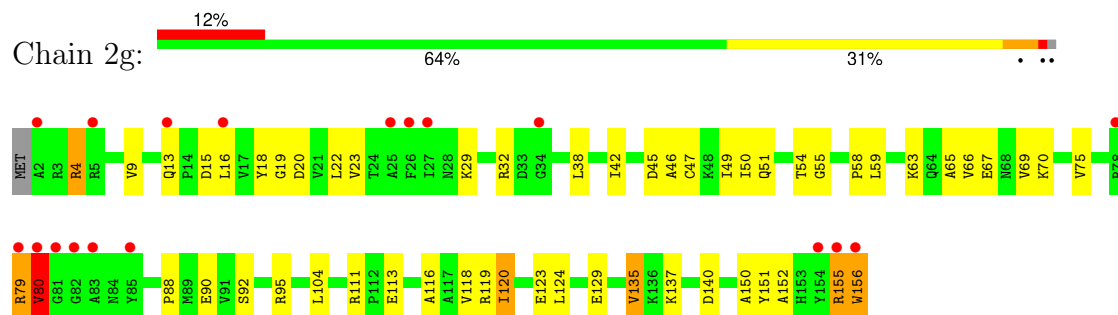
- Molecule 37: 30S ribosomal protein S6



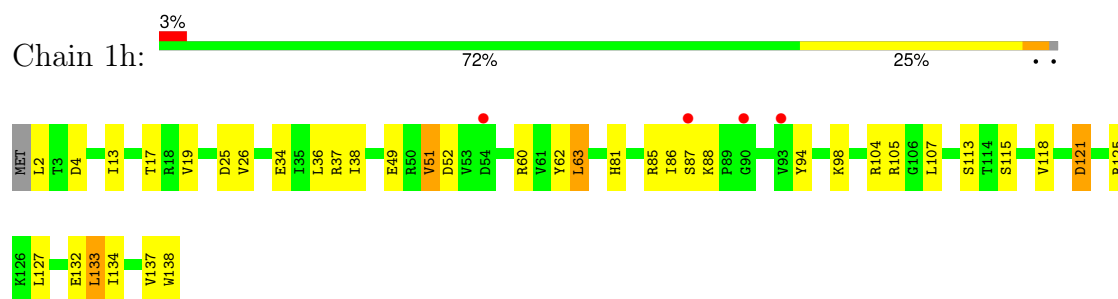
- Molecule 38: 30S ribosomal protein S7



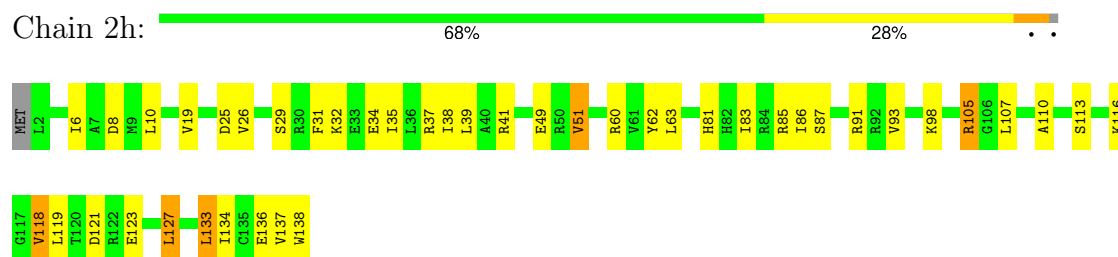
- Molecule 38: 30S ribosomal protein S7



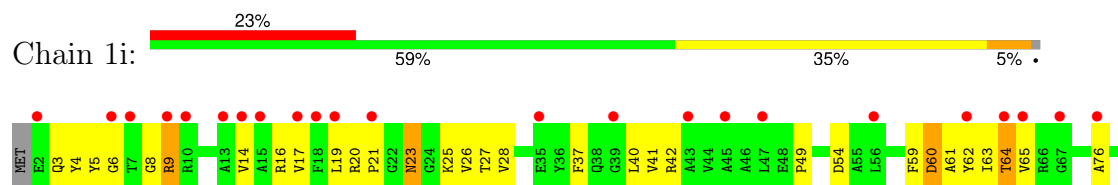
- Molecule 39: 30S ribosomal protein S8



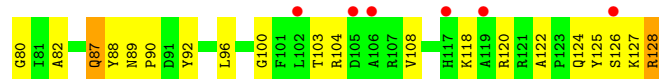
- Molecule 39: 30S ribosomal protein S8



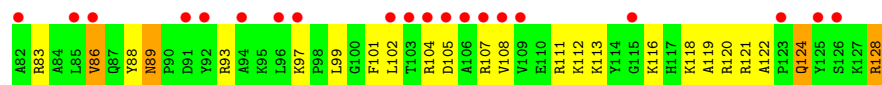
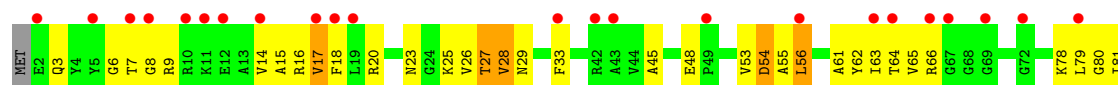
- Molecule 40: 30S ribosomal protein S9



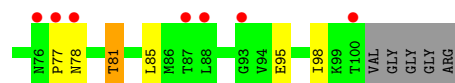
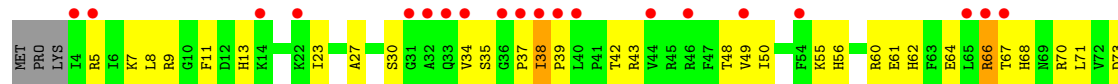




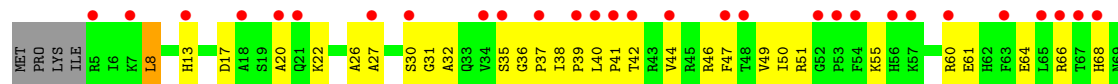
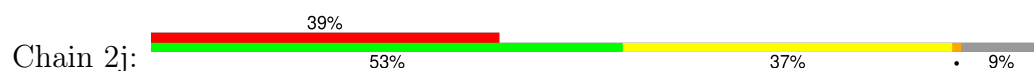
- Molecule 40: 30S ribosomal protein S9



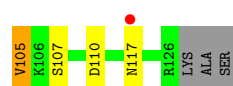
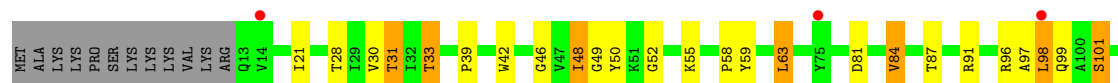
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

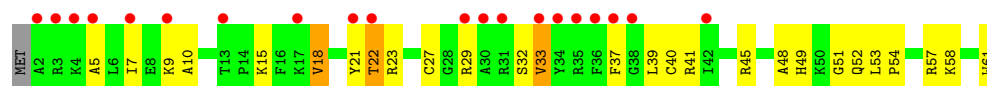




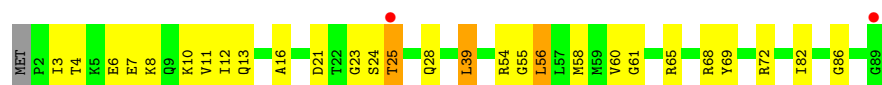
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



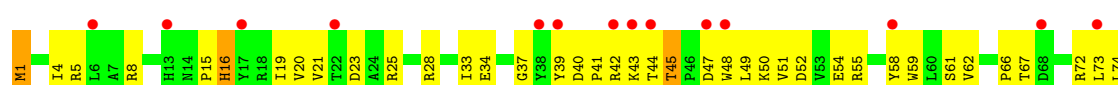
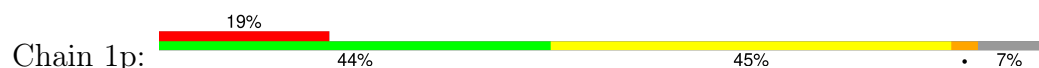
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

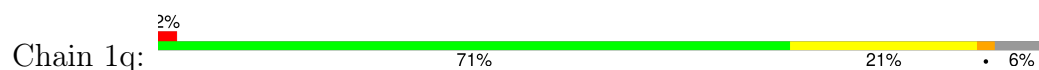


- Molecule 47: 30S ribosomal protein S16





- Molecule 48: 30S ribosomal protein S17



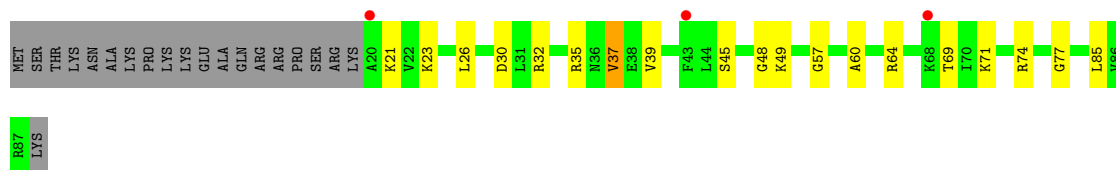
- Molecule 48: 30S ribosomal protein S17



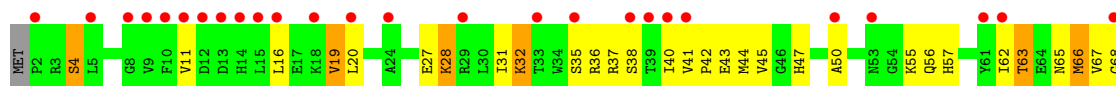
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

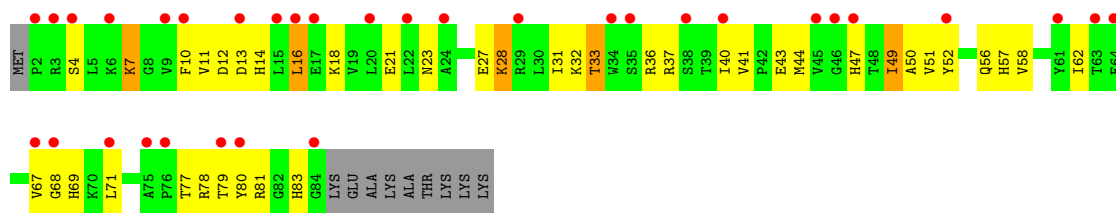


- Molecule 50: 30S ribosomal protein S19

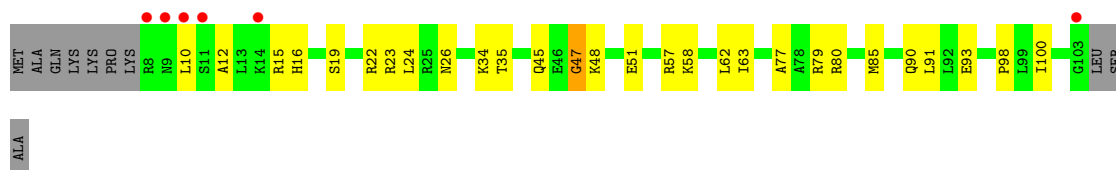


- Molecule 50: 30S ribosomal protein S19

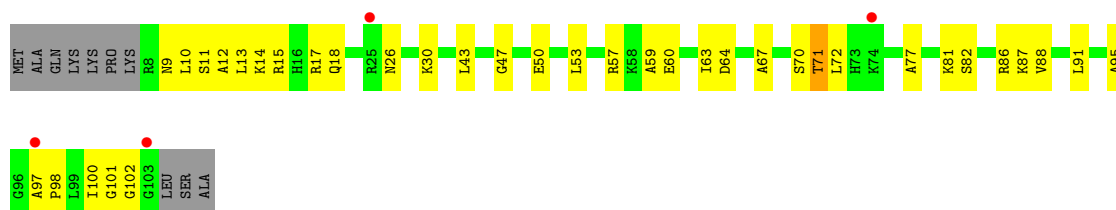




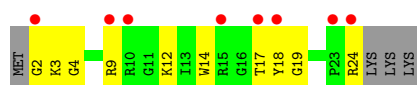
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



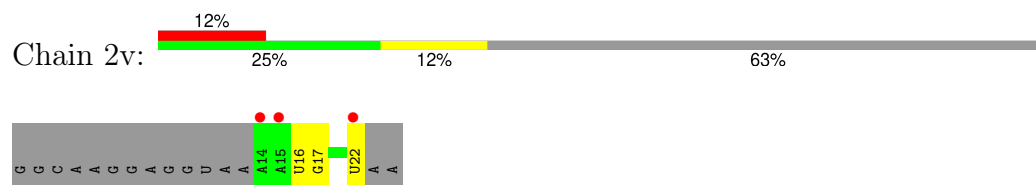
• Molecule 52: 30S ribosomal protein Thx



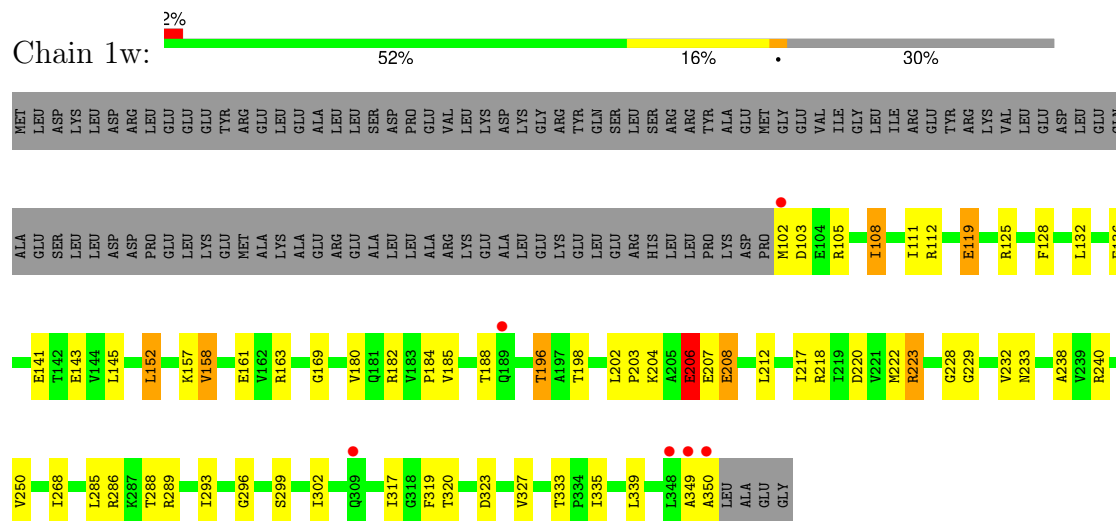
• Molecule 53: CYS-Stop mRNA



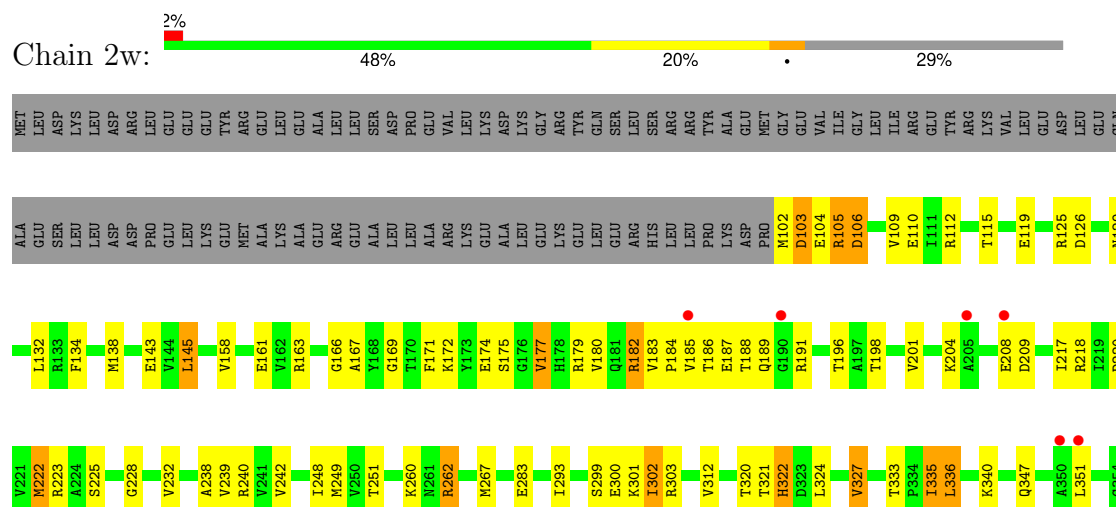
- Molecule 53: CYS-Stop mRNA



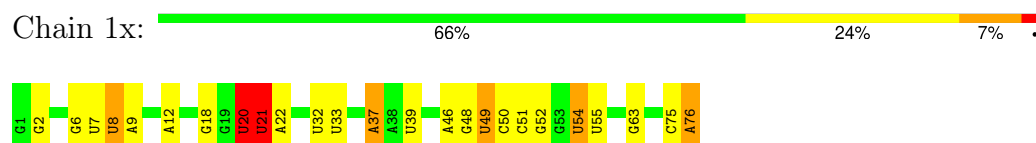
- Molecule 54: Peptide chain release factor 1



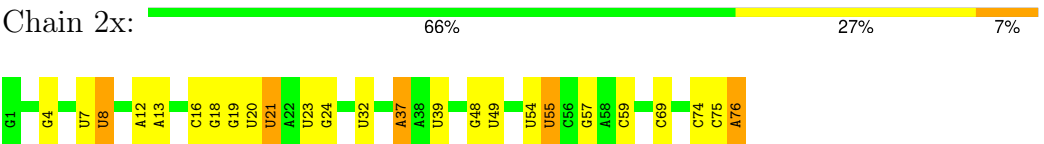
- Molecule 54: Peptide chain release factor 1



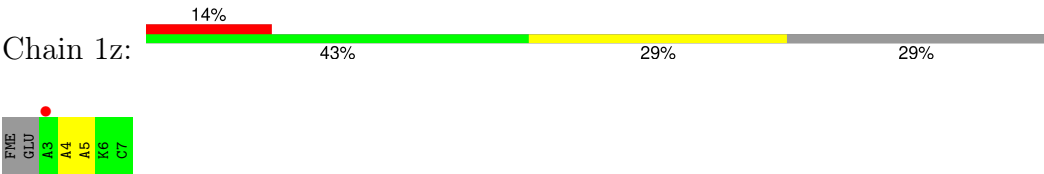
- Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part



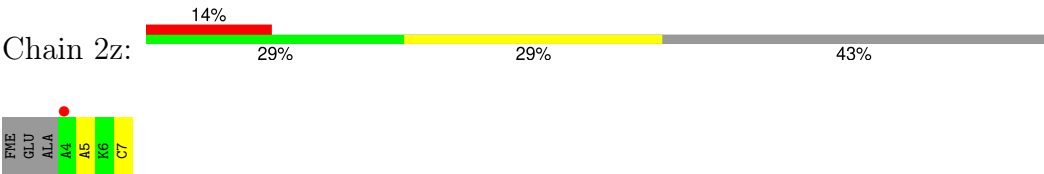
- Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part



● Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part



● Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.01Å 450.19Å 622.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.56 – 2.80 69.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (69.56-2.80) 97.5 (69.56-2.80)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.217 , 0.264 0.216 , 0.262	Depositor DCC
$R_{free}$ test set	71679 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	296656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, M2G, 8AN, MIA, 0TD, ZN, UR3, 4SU, 5MU, OMG, SF4, MG, G7M, 2MA, 5MC, PSU, H2U, MA6, OMC, 2MG, K, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.29	0/69011	0.45	1/107720 (0.0%)
1	2A	0.22	0/67295	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.33	0/4487
3	1D	0.27	0/2186	0.48	0/2944
3	2D	0.24	0/2186	0.47	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.50	0/2193
5	2F	0.20	0/1615	0.41	0/2188
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.38	0/1834
8	1I	0.21	0/1112	0.42	0/1514
8	2I	0.19	0/1079	0.43	0/1475
9	1N	0.26	0/1144	0.43	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.26	0/943	0.47	0/1269
10	2O	0.22	0/943	0.46	0/1269
11	1P	0.28	0/1152	0.54	0/1533
11	2P	0.21	0/1152	0.44	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.21	0/883	0.44	0/1176
14	2S	0.21	0/880	0.44	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.20	0/977	0.40	0/1301
17	1V	0.27	0/782	0.45	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.28	0/764	0.55	0/1025
19	2X	0.22	0/764	0.50	2/1025 (0.2%)
20	1Y	0.26	0/819	0.47	0/1095
20	2Y	0.22	0/819	0.47	0/1095
21	1Z	0.22	0/1267	0.49	0/1717
21	2Z	0.22	0/1299	0.47	0/1763
22	10	0.26	0/612	0.51	0/816
22	20	0.19	0/612	0.42	0/816
23	11	0.27	0/762	0.46	0/1014
23	21	0.22	0/762	0.39	0/1014
24	12	0.25	0/590	0.42	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.28	0/474	0.48	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.23	0/565	0.61	2/761 (0.3%)
26	24	0.24	0/545	0.49	0/737
27	15	0.28	0/469	0.53	0/635
27	25	0.23	0/469	0.47	0/635
28	16	0.25	0/460	0.49	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.32	0/426	0.52	0/561
29	27	0.25	0/426	0.49	0/561
30	18	0.26	0/525	0.50	0/691
30	28	0.22	0/525	0.42	0/691
31	19	0.28	0/310	0.47	0/407
31	29	0.22	0/310	0.42	0/407
32	1a	0.21	2/35795 (0.0%)	0.39	0/55864
32	2a	0.20	1/35886 (0.0%)	0.38	2/56005 (0.0%)
33	1b	0.23	0/1881	0.51	0/2542
33	2b	0.24	0/1860	0.49	0/2518
34	1c	0.22	0/1572	0.43	0/2126
34	2c	0.20	0/1566	0.42	0/2119
35	1d	0.20	0/1685	0.43	0/2262
35	2d	0.20	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.48	0/1543
36	2e	0.22	0/1149	0.47	0/1548
37	1f	0.20	0/823	0.40	0/1115
37	2f	0.21	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.21	0/1250	0.40	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.22	0/1108	0.42	0/1494
39	2h	0.18	0/1108	0.45	1/1494 (0.1%)
40	1i	0.21	0/1002	0.48	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.22	0/722	0.43	0/982
41	2j	0.22	0/727	0.46	0/988
42	1k	0.19	0/844	0.41	0/1145
42	2k	0.19	0/848	0.39	0/1149
43	1l	0.21	0/937	0.45	0/1260
43	2l	0.20	0/937	0.44	0/1260
44	1m	0.21	0/929	0.46	0/1250
44	2m	0.21	0/917	0.45	0/1234
45	1n	0.20	0/501	0.44	0/664
45	2n	0.21	0/501	0.42	0/664
46	1o	0.21	0/739	0.43	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.19	0/693	0.41	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.20	0/836	0.46	0/1117
49	1r	0.21	0/560	0.45	0/746
49	2r	0.20	0/560	0.40	0/746
50	1s	0.21	0/667	0.49	0/900
50	2s	0.21	0/661	0.45	0/893
51	1t	0.19	0/730	0.46	0/965
51	2t	0.22	0/729	0.46	0/965
52	1u	0.21	0/203	0.44	0/266
52	2u	0.20	0/203	0.48	0/266
53	1v	0.25	0/213	0.48	0/329
53	2v	0.20	0/213	0.34	0/329
54	1w	0.22	0/1963	0.42	0/2645
54	2w	0.22	0/1981	0.43	0/2668
55	1x	0.25	1/1555 (0.1%)	0.37	0/2419
55	2x	0.23	0/1555	0.36	0/2419
56	1z	0.33	0/29	0.53	0/37
56	2z	0.21	0/24	0.38	0/30
All	All	0.23	4/313618 (0.0%)	0.42	9/468557 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
21	1Z	0	2
33	1b	0	3
33	2b	0	2
56	1z	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	O3'-P	5.57	1.61	1.56
32	2a	527	G7M	O3'-P	5.28	1.61	1.56
32	1a	1498	UR3	O3'-P	5.16	1.61	1.56
32	1a	527	G7M	O3'-P	5.13	1.61	1.56

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.97	119.95	109.50
39	2h	19	VAL	N-CA-C	-6.36	106.32	112.29
1	2A	1992	G	C2'-C3'-O3'	6.34	119.00	109.50
26	14	54	GLY	CA-C-N	5.86	132.72	121.54
26	14	54	GLY	C-N-CA	5.86	132.72	121.54

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
21	1Z	146	ILE	Peptide
33	1b	122	PHE	Peptide
33	1b	9	GLU	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	579	0
1	2A	60322	0	30427	655	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	27	0
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	49	0
4	1E	1559	0	1618	25	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	45	0
6	1G	1423	0	1436	36	0
6	2G	1428	0	1438	51	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	37	0
8	1I	1097	0	1140	22	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	15	0
10	1O	933	0	996	21	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	26	0
12	1Q	1122	0	1179	13	0
12	2Q	1122	0	1179	16	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	15	0
14	1S	873	0	927	20	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	20	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	8	0
17	2V	771	0	830	12	0
18	1W	886	0	940	13	0
18	2W	886	0	940	10	0
19	1X	750	0	814	17	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	19	0
21	1Z	1240	0	1240	30	0
21	2Z	1271	0	1273	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	604	0	619	11	0
22	20	604	0	619	11	0
23	11	755	0	826	16	0
23	21	755	0	826	18	0
24	12	588	0	643	6	0
24	22	588	0	643	8	0
25	13	469	0	518	3	0
25	23	464	0	514	13	0
26	14	552	0	533	22	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	8	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	12	0
29	27	418	0	467	10	0
30	18	517	0	582	8	0
30	28	517	0	582	13	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	444	0
32	2a	32327	0	16338	453	0
33	1b	1846	0	1867	54	0
33	2b	1825	0	1828	66	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	64	0
35	1d	1655	0	1672	54	0
35	2d	1674	0	1713	48	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	43	0
37	1f	810	0	804	18	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	29	0
38	2g	1235	0	1249	32	0
39	1h	1088	0	1126	21	0
39	2h	1088	0	1126	25	0
40	1i	983	0	986	38	0
40	2i	978	0	966	50	0
41	1j	709	0	650	25	0
41	2j	714	0	672	33	0
42	1k	829	0	825	15	0
42	2k	833	0	836	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	21	0
43	2l	932	0	981	20	0
44	1m	919	0	951	34	0
44	2m	907	0	934	43	0
45	1n	492	0	529	20	0
45	2n	492	0	529	26	0
46	1o	728	0	760	16	0
46	2o	728	0	760	16	0
47	1p	681	0	697	27	0
47	2p	677	0	686	14	0
48	1q	823	0	891	8	0
48	2q	823	0	891	14	0
49	1r	555	0	618	14	0
49	2r	555	0	618	16	0
50	1s	652	0	662	27	0
50	2s	646	0	644	29	0
51	1t	728	0	798	20	0
51	2t	727	0	796	25	0
52	1u	199	0	208	6	0
52	2u	199	0	208	10	0
53	1v	191	0	97	2	0
53	2v	191	0	97	1	0
54	1w	1935	0	1920	32	0
54	2w	1953	0	1930	43	0
55	1x	1577	0	801	12	0
55	2x	1577	0	801	11	0
56	1z	30	0	32	2	0
56	2z	25	0	27	1	0
57	10	9	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	15	9	0	0	0	0
57	16	3	0	0	0	0
57	17	6	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1084	0	0	0	0
57	1B	39	0	0	0	0
57	1D	14	0	0	0	0
57	1E	13	0	0	0	0
57	1F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	5	0	0	0	0
57	1H	1	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
57	1P	3	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	5	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	12	0	0	0	0
57	1V	8	0	0	0	0
57	1W	5	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	221	0	0	0	0
57	1b	2	0	0	0	0
57	1d	1	0	0	0	0
57	1e	1	0	0	0	0
57	1f	2	0	0	0	0
57	1k	1	0	0	0	0
57	1l	1	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	2	0	0	0	0
57	1w	1	0	0	0	0
57	1x	13	0	0	0	0
57	21	2	0	0	0	0
57	23	1	0	0	0	0
57	25	4	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	3	0	0	0	0
57	2A	835	0	0	0	0
57	2B	18	0	0	0	0
57	2D	5	0	0	0	0
57	2E	10	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2O	3	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	1	0	0	0	0
57	2T	4	0	0	0	0
57	2U	4	0	0	0	0
57	2V	2	0	0	0	0
57	2W	3	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	178	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	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	2	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2x	8	0	0	0	0
58	1A	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	9	0	0	0	0
61	11	8	0	0	0	0
61	12	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	13	4	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	1	0
61	18	12	0	0	0	0
61	1A	1897	0	0	67	0
61	1B	61	0	0	2	0
61	1D	30	0	0	1	0
61	1E	27	0	0	3	0
61	1F	18	0	0	1	0
61	1G	5	0	0	3	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	8	0	0	0	0
61	1O	6	0	0	0	0
61	1P	23	0	0	0	0
61	1Q	11	0	0	1	0
61	1R	11	0	0	2	0
61	1S	1	0	0	0	0
61	1T	7	0	0	1	0
61	1U	13	0	0	0	0
61	1V	6	0	0	0	0
61	1W	12	0	0	1	0
61	1X	10	0	0	0	0
61	1Y	2	0	0	0	0
61	1a	259	0	0	18	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	2	0	0	0	0
61	1n	1	0	0	0	0
61	1q	4	0	0	0	0
61	1u	1	0	0	0	0
61	1v	3	0	0	0	0
61	1w	3	0	0	0	0
61	1x	25	0	0	3	0
61	20	2	0	0	0	0
61	21	10	0	0	1	0
61	25	3	0	0	0	0
61	27	2	0	0	0	0
61	28	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	1	0	0	0	0
61	2A	1003	0	0	73	0
61	2B	14	0	0	0	0
61	2D	25	0	0	1	0
61	2E	14	0	0	0	0
61	2F	12	0	0	0	0
61	2N	1	0	0	0	0
61	2O	3	0	0	1	0
61	2P	7	0	0	0	0
61	2Q	3	0	0	0	0
61	2R	4	0	0	1	0
61	2T	5	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	1	0	0	0	0
61	2X	2	0	0	0	0
61	2a	130	0	0	5	0
61	2e	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	4	0	0	1	0
61	2n	1	0	0	0	0
61	2q	2	0	0	0	0
61	2t	2	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	14	0	0	2	0
All	All	296656	0	197040	3915	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 3915 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)
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.03
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.24	1.02
1:1A:1082:U:C4	1:1A:1086:A:N1	2.34	0.96
41:2j:30:SER:HB3	41:2j:81:THR:HB	1.46	0.95
1:2A:784:A:OP2	61:2A:3903:HOH:O	1.83	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%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	25	56
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	56
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	25	56
5	2F	201/210 (96%)	186 (92%)	14 (7%)	1 (0%)	25	56
6	1G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	7	26
6	2G	179/182 (98%)	160 (89%)	14 (8%)	5 (3%)	4	14
7	1H	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	11	34
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	22	51
8	1I	144/148 (97%)	126 (88%)	18 (12%)	0	100	100
8	2I	144/148 (97%)	118 (82%)	21 (15%)	5 (4%)	3	10
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	44
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	19	48
12	1Q	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	9	30
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	9	30
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14	42
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	44
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	21
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	39
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	13	39
20	2Y	105/110 (96%)	91 (87%)	13 (12%)	1 (1%)	13	39
21	1Z	148/206 (72%)	130 (88%)	13 (9%)	5 (3%)	3	11
21	2Z	156/206 (76%)	138 (88%)	15 (10%)	3 (2%)	6	23
22	10	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
22	20	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	37
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	7
26	24	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	190 (83%)	32 (14%)	7 (3%)	3	12
33	2b	229/256 (90%)	193 (84%)	32 (14%)	4 (2%)	7	26
34	1c	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	6	21
34	2c	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
35	1d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	25	56
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	9	30
36	2e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5	20
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	131 (86%)	20 (13%)	2 (1%)	10	32
38	2g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	6	21
39	1h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	19	48
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	44
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	16	44
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	20
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	12	37
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	42
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	7	24
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	116/126 (92%)	106 (91%)	9 (8%)	1 (1%)	14	42
44	2m	114/126 (90%)	98 (86%)	14 (12%)	2 (2%)	7	24
45	1n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	13	39
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	64 (79%)	17 (21%)	0	100	100
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	11	34
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	20
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	20
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
54	1w	247/354 (70%)	227 (92%)	17 (7%)	3 (1%)	11	34
54	2w	251/354 (71%)	232 (92%)	17 (7%)	2 (1%)	16	44
56	1z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
56	2z	2/7 (29%)	2 (100%)	0	0	100	100
All	All	11848/12850 (92%)	10869 (92%)	880 (7%)	99 (1%)	16	44

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	96	ARG
6	1G	126	ASP
12	1Q	16	ARG
21	1Z	53	ILE

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	20	51
3	2D	215/218 (99%)	203 (94%)	12 (6%)	17	47
4	1E	164/166 (99%)	156 (95%)	8 (5%)	21	52
4	2E	164/166 (99%)	157 (96%)	7 (4%)	25	57
5	1F	160/166 (96%)	148 (92%)	12 (8%)	11	33
5	2F	159/166 (96%)	143 (90%)	16 (10%)	6	20
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3	9
6	2G	143/156 (92%)	126 (88%)	17 (12%)	4	14
7	1H	144/148 (97%)	131 (91%)	13 (9%)	8	25
7	2H	144/148 (97%)	131 (91%)	13 (9%)	8	25
8	1I	113/124 (91%)	105 (93%)	8 (7%)	12	35
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	4
9	1N	118/119 (99%)	108 (92%)	10 (8%)	8	27
9	2N	118/119 (99%)	107 (91%)	11 (9%)	7	23
10	1O	100/100 (100%)	98 (98%)	2 (2%)	50	81
10	2O	100/100 (100%)	96 (96%)	4 (4%)	27	60
11	1P	115/116 (99%)	100 (87%)	15 (13%)	3	11
11	2P	115/116 (99%)	103 (90%)	12 (10%)	5	18
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	23	55
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	12	34
13	1R	101/101 (100%)	100 (99%)	1 (1%)	73	91
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50	81
14	1S	86/88 (98%)	80 (93%)	6 (7%)	12	36
14	2S	85/88 (97%)	77 (91%)	8 (9%)	7	23
15	1T	115/127 (91%)	104 (90%)	11 (10%)	7	22
15	2T	113/127 (89%)	109 (96%)	4 (4%)	31	65
16	1U	93/94 (99%)	88 (95%)	5 (5%)	18	48
16	2U	93/94 (99%)	86 (92%)	7 (8%)	11	33
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	75
17	2V	80/82 (98%)	76 (95%)	4 (5%)	20	51
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	47
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27	61
19	2X	77/78 (99%)	73 (95%)	4 (5%)	19	50
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	16	44
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	9	29
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	3	10
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	2	7
22	10	61/67 (91%)	60 (98%)	1 (2%)	58	85
22	20	61/67 (91%)	59 (97%)	2 (3%)	33	67
23	11	80/83 (96%)	74 (92%)	6 (8%)	11	33
23	21	80/83 (96%)	77 (96%)	3 (4%)	28	62
24	12	65/67 (97%)	60 (92%)	5 (8%)	10	31
24	22	65/67 (97%)	62 (95%)	3 (5%)	23	55
25	13	51/52 (98%)	45 (88%)	6 (12%)	4	14
25	23	50/52 (96%)	45 (90%)	5 (10%)	6	20
26	14	59/63 (94%)	52 (88%)	7 (12%)	4	14
26	24	53/63 (84%)	45 (85%)	8 (15%)	2	8
27	15	50/52 (96%)	46 (92%)	4 (8%)	10	30
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	30
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	10
28	26	50/52 (96%)	48 (96%)	2 (4%)	27	60
29	17	41/42 (98%)	39 (95%)	2 (5%)	21	52
29	27	41/42 (98%)	37 (90%)	4 (10%)	6	21
30	18	54/55 (98%)	52 (96%)	2 (4%)	29	63
30	28	54/55 (98%)	52 (96%)	2 (4%)	29	63
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	8	26
33	1b	192/220 (87%)	166 (86%)	26 (14%)	3	10
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	9
34	1c	142/188 (76%)	124 (87%)	18 (13%)	3	12
34	2c	140/188 (74%)	129 (92%)	11 (8%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	1d	169/181 (93%)	160 (95%)	9 (5%)	19	49
35	2d	173/181 (96%)	153 (88%)	20 (12%)	4	15
36	1e	113/123 (92%)	100 (88%)	13 (12%)	4	15
36	2e	114/123 (93%)	103 (90%)	11 (10%)	7	22
37	1f	84/90 (93%)	78 (93%)	6 (7%)	12	35
37	2f	85/90 (94%)	79 (93%)	6 (7%)	12	35
38	1g	119/127 (94%)	109 (92%)	10 (8%)	9	28
38	2g	120/127 (94%)	109 (91%)	11 (9%)	7	24
39	1h	114/119 (96%)	102 (90%)	12 (10%)	5	18
39	2h	114/119 (96%)	103 (90%)	11 (10%)	7	22
40	1i	90/99 (91%)	78 (87%)	12 (13%)	3	10
40	2i	89/99 (90%)	77 (86%)	12 (14%)	3	10
41	1j	66/92 (72%)	56 (85%)	10 (15%)	2	7
41	2j	69/92 (75%)	65 (94%)	4 (6%)	17	45
42	1k	82/99 (83%)	70 (85%)	12 (15%)	2	8
42	2k	83/99 (84%)	74 (89%)	9 (11%)	5	17
43	1l	96/108 (89%)	87 (91%)	9 (9%)	7	23
43	2l	96/108 (89%)	88 (92%)	8 (8%)	9	28
44	1m	89/101 (88%)	70 (79%)	19 (21%)	1	3
44	2m	88/101 (87%)	81 (92%)	7 (8%)	10	30
45	1n	49/50 (98%)	40 (82%)	9 (18%)	1	4
45	2n	49/50 (98%)	45 (92%)	4 (8%)	9	29
46	1o	78/80 (98%)	71 (91%)	7 (9%)	8	25
46	2o	78/80 (98%)	69 (88%)	9 (12%)	4	15
47	1p	69/74 (93%)	56 (81%)	13 (19%)	1	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	6
48	1q	94/97 (97%)	82 (87%)	12 (13%)	3	12
48	2q	94/97 (97%)	86 (92%)	8 (8%)	8	27
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	66
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	66
50	1s	69/80 (86%)	60 (87%)	9 (13%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2s	67/80 (84%)	59 (88%)	8 (12%)	4	14
51	1t	70/82 (85%)	68 (97%)	2 (3%)	37	71
51	2t	70/82 (85%)	67 (96%)	3 (4%)	25	57
52	1u	18/22 (82%)	17 (94%)	1 (6%)	17	47
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	47
54	1w	204/299 (68%)	183 (90%)	21 (10%)	6	19
54	2w	204/299 (68%)	171 (84%)	33 (16%)	2	6
56	1z	2/3 (67%)	2 (100%)	0	100	100
56	2z	2/3 (67%)	2 (100%)	0	100	100
All	All	9699/10668 (91%)	8836 (91%)	863 (9%)	8	25

5 of 863 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	2F	190	GLU
17	2V	73	SER
47	2p	5	ARG
6	2G	135	LEU
5	2F	183	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
37	2f	100	ASN
40	2i	3	GLN
44	2m	12	ASN
35	1d	161	ASN
35	1d	160	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	449 (15%)	30 (1%)
1	2A	2791/2915 (95%)	458 (16%)	19 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	18 (15%)	0
32	1a	1497/1521 (98%)	295 (19%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2a	1501/1521 (98%)	279 (18%)	0
53	1v	8/24 (33%)	1 (12%)	0
53	2v	8/24 (33%)	1 (12%)	0
55	1x	72/74 (97%)	12 (16%)	0
55	2x	72/74 (97%)	5 (6%)	0
All	All	9050/9310 (97%)	1527 (16%)	49 (0%)

5 of 1527 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2689	U
1	2A	752	A
1	1A	2756	U
1	2A	277	C
1	2A	893	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
55	5MU	1x	54	55	19,22,23	1.37	3 (15%)	27,32,35	1.81	5 (18%)
55	8AN	2x	76	57,56,55	17,24,25	1.12	2 (11%)	13,35,38	2.86	2 (15%)
43	0TD	1l	92	43	8,9,10	4.74	2 (25%)	6,11,13	5.96	3 (50%)

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	1.02	0	26,32,35	1.68	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	5 (23%)
32	PSU	1a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.99	3 (16%)
32	5MC	2a	1400	32	19,22,23	1.48	3 (15%)	26,32,35	1.25	4 (15%)
32	M2G	2a	966	32	20,27,28	1.30	3 (15%)	19,40,43	1.07	2 (10%)
32	MA6	1a	1519	32	19,26,27	1.05	2 (10%)	18,38,41	2.02	3 (16%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	2 (7%)
1	OMU	1A	2552	57,1	19,22,23	1.25	3 (15%)	25,31,34	1.67	5 (20%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.10	3 (11%)
55	PSU	1x	55	55	18,21,22	1.30	2 (11%)	21,30,33	2.03	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.21	3 (15%)	25,31,34	1.70	5 (20%)
1	PSU	1A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.11	5 (23%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	27,32,35	2.06	5 (18%)
1	PSU	2A	1911	1	18,21,22	1.38	3 (16%)	21,30,33	2.02	4 (19%)
1	5MU	2A	1939	57,1	19,22,23	1.40	5 (26%)	27,32,35	2.22	6 (22%)
55	PSU	2x	39	55	18,21,22	1.43	3 (16%)	21,30,33	1.71	4 (19%)
55	H2U	1x	20	55	18,21,22	0.93	2 (11%)	19,30,33	1.01	1 (5%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	27,32,35	2.29	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.50	3 (15%)	26,32,35	1.24	3 (11%)
1	2MA	1A	2503	57,1	18,25,26	0.72	0	20,37,40	1.91	3 (15%)
1	5MU	2A	1915	57,1	19,22,23	1.46	6 (31%)	27,32,35	2.18	6 (22%)
55	4SU	1x	8	55	18,21,22	1.85	4 (22%)	25,30,33	1.78	4 (16%)
32	5MC	1a	967	32	19,22,23	1.57	3 (15%)	26,32,35	1.16	2 (7%)
55	8AN	1x	76	57,56,55	17,24,25	1.11	2 (11%)	13,35,38	2.84	2 (15%)
55	MIA	1x	37	55	17,24,32	1.00	1 (5%)	16,35,47	1.34	2 (12%)
1	2MA	2A	2503	57,1	18,25,26	0.70	0	20,37,40	1.93	4 (20%)
55	MIA	2x	37	55	17,24,32	0.99	1 (5%)	16,35,47	1.49	3 (18%)
55	PSU	1x	32	57,55	18,21,22	1.30	2 (11%)	21,30,33	1.94	4 (19%)
55	H2U	2x	20	55	18,21,22	0.96	2 (11%)	19,30,33	0.95	1 (5%)
1	OMG	1A	2251	57,55,1	19,26,27	0.94	1 (5%)	21,38,41	1.21	3 (14%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.18	1 (6%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.82	3 (16%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.88	0
55	PSU	1x	39	55	18,21,22	1.37	2 (11%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	1a	1402	57,32	20,23,24	0.75	0	25,32,35	0.98	2 (8%)
55	PSU	2x	32	55	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.82	0
32	5MC	1a	1407	32	19,22,23	1.53	3 (15%)	26,32,35	0.97	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.13	2 (10%)	26,32,35	1.74	5 (19%)
1	PSU	1A	2605	57,1	18,21,22	1.32	2 (11%)	21,30,33	2.02	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.52	3 (15%)	26,32,35	1.19	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	2.27	4 (19%)
32	2MG	1a	1207	57,32	18,26,27	0.90	1 (5%)	16,38,41	1.34	3 (18%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.98	4 (19%)
32	PSU	2a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	1.95	5 (23%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.19	2 (7%)
1	OMG	2A	2251	55,1	19,26,27	0.97	1 (5%)	21,38,41	1.01	2 (9%)
43	0TD	2l	92	43	8,9,10	4.52	1 (12%)	6,11,13	8.81	3 (50%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.21	3 (11%)
1	5MC	2A	1962	57,1	19,22,23	1.52	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
55	5MU	2x	54	55	19,22,23	1.40	4 (21%)	27,32,35	2.05	6 (22%)
32	G7M	2a	527	57,32	20,26,27	1.20	2 (10%)	16,39,42	0.64	0
32	4OC	2a	1402	57,32	20,23,24	0.79	0	25,32,35	0.94	1 (4%)
32	MA6	2a	1519	32	19,26,27	1.02	2 (10%)	18,38,41	1.92	3 (16%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.27	3 (11%)
55	H2U	1x	21	55	18,21,22	0.94	2 (11%)	19,30,33	0.93	1 (5%)
32	G7M	1a	527	32	20,26,27	1.16	2 (10%)	16,39,42	0.51	0
55	4SU	2x	8	55	18,21,22	1.80	4 (22%)	25,30,33	2.12	5 (20%)
55	H2U	2x	21	55	18,21,22	0.99	2 (11%)	19,30,33	0.88	1 (5%)
32	M2G	1a	966	32	20,27,28	1.38	2 (10%)	19,40,43	1.11	2 (10%)
1	5MC	1A	1962	57,1	19,22,23	1.60	3 (15%)	26,32,35	1.06	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	55	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	8AN	2x	76	57,56,55	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/3/25/26	0/3/3/3
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,56,55	-	1/3/25/26	0/3/3/3
55	MIA	1x	37	55	-	2/3/25/34	0/3/3/3
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
55	MIA	2x	37	55	-	2/3/25/34	0/3/3/3
55	PSU	1x	32	57,55	-	0/7/25/26	0/2/2/2
55	H2U	2x	20	55	-	0/7/38/39	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	57,32	-	3/9/29/30	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	57,32	-	0/5/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	57,32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	1/3/25/26	0/3/3/3
32	4OC	2a	1402	57,32	-	3/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1942	1	-	1/7/25/26	0/2/2/2
55	H2U	1x	21	55	-	4/7/38/39	0/2/2/2
32	G7M	1a	527	32	-	2/3/25/26	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	H2U	2x	21	55	-	2/7/38/39	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.57	1.69	1.82
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
32	2a	967	5MC	C5-C4	6.37	1.48	1.44
32	1a	1404	5MC	C5-C4	6.36	1.48	1.44
32	2a	1404	5MC	C5-C4	5.86	1.48	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-21.15	64.35	102.36
43	1l	92	0TD	CSB-SB-CB	-14.05	77.11	102.36
55	1x	76	8AN	C4'-O4'-C1'	-7.66	102.91	109.92
55	2x	76	8AN	C4'-O4'-C1'	-7.59	102.97	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2605	PSU	N1-C2-N3	7.00	122.55	115.17

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB

There are no ring outliers.

28 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	76	8AN	1	0
43	1l	92	0TD	1	0
32	1a	516	PSU	1	0
32	1a	1518	MA6	2	0
32	1a	1519	MA6	2	0
32	2a	1404	5MC	1	0
1	1A	2552	OMU	1	0
1	1A	1939	5MU	1	0
1	2A	1939	5MU	1	0
55	1x	20	H2U	1	0
1	1A	1915	5MU	2	0
1	1A	2503	2MA	1	0
55	1x	8	4SU	1	0
55	1x	76	8AN	4	0
32	2a	1207	2MG	2	0
32	2a	1518	MA6	4	0
1	1A	1920	OMC	1	0
32	1a	1402	4OC	2	0
32	1a	1207	2MG	2	0
55	2x	55	PSU	1	0
1	2A	2251	OMG	1	0
32	1a	1404	5MC	1	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	3	0
1	1A	1942	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	21	H2U	1	0
55	2x	8	4SU	1	0
32	1a	966	M2G	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2664 ligands modelled in this entry, 2662 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	SF4	2d	303	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	302	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	-0.32	180 (6%)	27	21	9, 24, 87, 101	0
1	2A	2789/2915 (95%)	0.09	145 (5%)	34	26	22, 43, 83, 100	0
2	1B	120/121 (99%)	-0.24	0	100	100	20, 40, 53, 78	0
2	2B	120/121 (99%)	0.64	0	100	100	45, 64, 73, 84	0
3	1D	275/276 (99%)	-0.56	1 (0%)	89	85	12, 24, 38, 68	0
3	2D	275/276 (99%)	-0.21	3 (1%)	77	71	20, 36, 48, 68	0
4	1E	204/206 (99%)	-0.56	0	100	100	10, 25, 46, 60	0
4	2E	204/206 (99%)	-0.06	1 (0%)	87	83	23, 41, 57, 68	0
5	1F	203/210 (96%)	-0.44	0	100	100	10, 27, 57, 78	0
5	2F	203/210 (96%)	0.22	2 (0%)	79	73	22, 51, 66, 78	0
6	1G	181/182 (99%)	0.51	8 (4%)	39	32	34, 51, 66, 77	0
6	2G	181/182 (99%)	1.14	23 (12%)	9	8	58, 66, 76, 84	0
7	1H	174/180 (96%)	0.01	3 (1%)	69	61	26, 39, 53, 60	0
7	2H	174/180 (96%)	1.01	17 (9%)	14	11	53, 69, 79, 85	0
8	1I	146/148 (98%)	0.52	2 (1%)	73	66	31, 58, 68, 72	0
8	2I	146/148 (98%)	0.60	4 (2%)	56	47	42, 61, 68, 75	0
9	1N	140/140 (100%)	-0.57	1 (0%)	84	79	15, 24, 45, 61	0
9	2N	140/140 (100%)	0.23	1 (0%)	84	79	30, 49, 63, 70	0
10	1O	122/122 (100%)	-0.55	0	100	100	16, 26, 43, 47	0
10	2O	122/122 (100%)	-0.15	0	100	100	30, 39, 54, 60	0
11	1P	149/150 (99%)	-0.34	0	100	100	10, 32, 53, 66	0
11	2P	149/150 (99%)	0.33	1 (0%)	84	79	29, 53, 68, 75	0
12	1Q	141/141 (100%)	-0.40	2 (1%)	73	66	16, 27, 42, 53	0
12	2Q	141/141 (100%)	0.29	3 (2%)	63	55	32, 49, 60, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.66	0 100 100	15, 22, 35, 47	0
13	2R	118/118 (100%)	-0.17	0 100 100	29, 38, 50, 59	0
14	1S	110/112 (98%)	-0.15	1 (0%) 81 75	29, 40, 52, 58	0
14	2S	110/112 (98%)	0.95	11 (10%) 14 11	48, 59, 67, 71	0
15	1T	131/146 (89%)	-0.34	2 (1%) 71 64	20, 30, 58, 65	0
15	2T	131/146 (89%)	0.07	1 (0%) 82 77	34, 43, 66, 71	0
16	1U	116/118 (98%)	-0.69	1 (0%) 81 75	11, 17, 29, 47	0
16	2U	116/118 (98%)	0.04	0 100 100	29, 46, 58, 66	0
17	1V	101/101 (100%)	-0.60	0 100 100	11, 24, 42, 59	0
17	2V	101/101 (100%)	0.25	0 100 100	30, 54, 66, 73	0
18	1W	112/113 (99%)	-0.66	1 (0%) 81 75	11, 18, 36, 68	0
18	2W	112/113 (99%)	-0.20	0 100 100	27, 37, 52, 75	0
19	1X	95/96 (98%)	-0.42	0 100 100	15, 27, 51, 64	0
19	2X	95/96 (98%)	0.28	3 (3%) 50 42	37, 47, 62, 75	0
20	1Y	107/110 (97%)	-0.12	3 (2%) 55 46	22, 35, 53, 73	0
20	2Y	107/110 (97%)	0.64	5 (4%) 37 30	45, 58, 70, 77	0
21	1Z	154/206 (74%)	0.16	3 (1%) 66 58	26, 44, 62, 66	0
21	2Z	160/206 (77%)	0.81	7 (4%) 39 32	49, 63, 73, 76	0
22	10	76/85 (89%)	-0.50	1 (1%) 74 67	18, 25, 44, 58	0
22	20	76/85 (89%)	0.49	5 (6%) 26 19	38, 49, 62, 72	0
23	11	97/98 (98%)	-0.25	1 (1%) 79 73	16, 31, 57, 63	0
23	21	97/98 (98%)	0.09	1 (1%) 79 73	28, 44, 64, 68	0
24	12	70/72 (97%)	-0.24	0 100 100	24, 36, 48, 64	0
24	22	70/72 (97%)	0.40	1 (1%) 73 66	46, 56, 67, 71	0
25	13	59/60 (98%)	-0.54	0 100 100	15, 21, 42, 59	0
25	23	59/60 (98%)	0.10	0 100 100	39, 46, 63, 66	0
26	14	69/71 (97%)	1.10	12 (17%) 5 4	44, 68, 82, 86	0
26	24	69/71 (97%)	1.55	15 (21%) 3 3	60, 74, 81, 88	0
27	15	59/60 (98%)	-0.75	0 100 100	9, 19, 37, 44	0
27	25	59/60 (98%)	-0.15	1 (1%) 69 61	22, 39, 53, 64	0
28	16	53/54 (98%)	-0.48	0 100 100	23, 29, 38, 46	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	-0.02	0	100	100	37, 46, 55, 60	0
29	17	48/49 (97%)	-0.34	2 (4%)	41	33	12, 18, 43, 52	0
29	27	48/49 (97%)	-0.03	1 (2%)	63	55	23, 31, 51, 63	0
30	18	64/65 (98%)	-0.71	0	100	100	15, 21, 28, 39	0
30	28	64/65 (98%)	0.11	0	100	100	33, 42, 49, 55	0
31	19	37/37 (100%)	-0.44	0	100	100	17, 27, 45, 45	0
31	29	37/37 (100%)	0.55	0	100	100	44, 51, 59, 61	0
32	1a	1488/1521 (97%)	0.72	127 (8%)	18	14	21, 61, 84, 99	0
32	2a	1491/1521 (98%)	0.71	129 (8%)	17	13	31, 61, 85, 98	0
33	1b	231/256 (90%)	1.16	35 (15%)	6	5	50, 67, 76, 83	0
33	2b	231/256 (90%)	1.29	48 (20%)	3	3	56, 71, 79, 86	0
34	1c	206/239 (86%)	1.25	28 (13%)	8	7	56, 69, 77, 80	0
34	2c	206/239 (86%)	1.23	31 (15%)	6	6	59, 70, 77, 84	0
35	1d	208/209 (99%)	0.94	18 (8%)	17	13	47, 61, 71, 78	0
35	2d	208/209 (99%)	0.63	8 (3%)	44	36	47, 57, 66, 71	0
36	1e	148/162 (91%)	0.36	1 (0%)	84	79	33, 54, 65, 75	0
36	2e	148/162 (91%)	0.59	7 (4%)	37	30	44, 57, 66, 76	0
37	1f	100/101 (99%)	0.48	2 (2%)	64	56	42, 56, 64, 68	0
37	2f	100/101 (99%)	0.63	4 (4%)	43	35	53, 61, 68, 71	0
38	1g	155/156 (99%)	0.89	14 (9%)	17	12	53, 64, 76, 80	0
38	2g	155/156 (99%)	1.10	18 (11%)	11	9	58, 68, 77, 82	0
39	1h	137/138 (99%)	0.48	4 (2%)	54	45	44, 55, 62, 68	0
39	2h	137/138 (99%)	0.43	0	100	100	47, 58, 65, 73	0
40	1i	127/128 (99%)	1.56	29 (22%)	2	3	51, 69, 74, 80	0
40	2i	127/128 (99%)	1.71	43 (33%)	1	1	61, 73, 77, 82	0
41	1j	97/105 (92%)	1.59	27 (27%)	2	2	56, 72, 80, 83	0
41	2j	96/105 (91%)	1.99	41 (42%)	1	1	61, 74, 81, 84	0
42	1k	114/129 (88%)	0.35	4 (3%)	47	39	28, 54, 66, 73	0
42	2k	114/129 (88%)	0.53	7 (6%)	28	21	45, 59, 70, 80	0
43	1l	121/132 (91%)	0.45	6 (4%)	35	28	35, 48, 60, 67	0
43	2l	121/132 (91%)	0.16	1 (0%)	82	77	40, 47, 57, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	1.41	25 (21%) 3 3	56, 68, 74, 78	0
44	2m	116/126 (92%)	1.58	30 (25%) 2 2	60, 71, 76, 77	0
45	1n	60/61 (98%)	1.60	14 (23%) 2 3	57, 69, 74, 76	0
45	2n	60/61 (98%)	1.75	20 (33%) 1 1	63, 72, 77, 78	0
46	1o	88/89 (98%)	0.36	2 (2%) 61 52	35, 53, 64, 68	0
46	2o	88/89 (98%)	0.69	7 (7%) 20 15	45, 58, 67, 73	0
47	1p	82/88 (93%)	1.28	17 (20%) 3 3	52, 61, 71, 79	0
47	2p	82/88 (93%)	0.68	5 (6%) 28 21	46, 56, 63, 70	0
48	1q	99/105 (94%)	0.52	2 (2%) 64 56	43, 53, 65, 68	0
48	2q	99/105 (94%)	0.26	2 (2%) 64 56	43, 54, 63, 69	0
49	1r	68/88 (77%)	0.27	0 100 100	41, 52, 67, 71	0
49	2r	68/88 (77%)	0.73	3 (4%) 39 32	52, 60, 69, 76	0
50	1s	83/93 (89%)	1.83	31 (37%) 1 1	63, 72, 79, 81	0
50	2s	83/93 (89%)	1.85	33 (39%) 1 1	67, 76, 82, 84	0
51	1t	96/106 (90%)	0.64	6 (6%) 27 21	47, 58, 67, 78	0
51	2t	96/106 (90%)	0.67	4 (4%) 41 33	44, 55, 67, 70	0
52	1u	23/27 (85%)	1.96	8 (34%) 1 1	56, 68, 71, 75	0
52	2u	23/27 (85%)	1.42	6 (26%) 2 2	64, 69, 74, 78	0
53	1v	9/24 (37%)	0.61	2 (22%) 3 3	39, 41, 73, 83	0
53	2v	9/24 (37%)	1.19	3 (33%) 1 1	49, 53, 80, 87	0
54	1w	249/354 (70%)	0.18	6 (2%) 59 51	15, 48, 66, 80	0
54	2w	253/354 (71%)	0.40	6 (2%) 59 51	32, 55, 72, 82	0
55	1x	65/74 (87%)	0.11	0 100 100	16, 50, 66, 71	0
55	2x	65/74 (87%)	0.40	0 100 100	32, 60, 73, 79	0
56	1z	5/7 (71%)	0.82	1 (20%) 3 3	16, 20, 34, 50	0
56	2z	4/7 (57%)	0.57	1 (25%) 2 2	33, 35, 36, 40	0
All	All	21074/22160 (95%)	0.30	1341 (6%) 27 20	9, 50, 77, 101	0

The worst 5 of 1341 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	9.0
1	2A	2147	G	8.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	8.7
1	2A	2145	C	8.7
1	1A	2117	A	8.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	H2U	1x	21	20/21	0.74	0.16	66,85,89,106	0
55	H2U	2x	21	20/21	0.74	0.17	76,84,91,98	0
55	H2U	2x	20	20/21	0.75	0.14	68,78,83,86	0
32	2MG	1a	1207	24/25	0.82	0.16	65,74,83,85	0
55	PSU	2x	55	20/21	0.82	0.12	62,69,77,82	0
32	2MG	2a	1207	24/25	0.84	0.15	61,71,77,79	0
55	PSU	2x	32	20/21	0.87	0.12	54,62,67,68	0
55	5MU	2x	54	21/22	0.88	0.11	62,68,75,80	0
43	0TD	1l	92	10/11	0.88	0.13	44,49,53,68	0
55	MIA	2x	37	22/30	0.89	0.11	53,62,64,66	0
32	PSU	1a	516	20/21	0.90	0.11	54,61,65,66	0
55	5MU	1x	54	21/22	0.90	0.13	51,61,69,73	0
55	H2U	1x	20	20/21	0.90	0.10	52,67,79,79	0
55	PSU	1x	55	20/21	0.90	0.11	52,59,69,71	0
32	G7M	2a	527	24/25	0.90	0.12	47,56,60,65	0
1	5MU	2A	1915	21/22	0.91	0.11	41,49,55,60	0
32	M2G	2a	966	25/26	0.91	0.13	46,56,67,71	0
32	PSU	2a	516	20/21	0.91	0.12	47,60,66,67	0
55	PSU	2x	39	20/21	0.91	0.10	43,60,64,66	0
43	0TD	2l	92	10/11	0.92	0.10	43,48,51,59	0
55	PSU	1x	32	20/21	0.92	0.11	50,54,63,66	0
32	M2G	1a	966	25/26	0.92	0.11	40,49,55,57	0
32	5MC	2a	967	21/22	0.93	0.12	52,56,65,68	0
55	MIA	1x	37	22/30	0.94	0.09	41,51,55,60	0
32	5MC	2a	1400	21/22	0.94	0.12	45,55,60,62	0
55	PSU	1x	39	20/21	0.94	0.10	35,44,51,55	0
32	5MC	1a	967	21/22	0.94	0.10	42,48,59,64	0
32	4OC	2a	1402	22/23	0.95	0.10	39,44,48,49	0
32	UR3	2a	1498	21/22	0.95	0.09	38,43,47,53	0
32	MA6	2a	1518	24/25	0.95	0.10	34,45,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MA6	2a	1519	24/25	0.95	0.11	39,43,50,51	0
1	5MU	1A	1915	21/22	0.95	0.08	36,44,48,53	0
55	4SU	2x	8	20/21	0.95	0.09	45,63,67,68	0
1	PSU	2A	1911	20/21	0.95	0.09	40,47,49,51	0
1	PSU	1A	1911	20/21	0.95	0.08	25,38,41,42	0
1	PSU	2A	1917	20/21	0.95	0.09	39,47,54,57	0
32	G7M	1a	527	24/25	0.95	0.09	35,47,52,54	0
32	5MC	2a	1404	21/22	0.96	0.09	30,36,39,43	0
32	5MC	2a	1407	21/22	0.96	0.09	29,37,42,48	0
1	5MC	2A	1942	21/22	0.96	0.08	29,37,41,44	0
32	5MC	1a	1407	21/22	0.96	0.11	20,30,37,39	0
32	MA6	1a	1519	24/25	0.96	0.09	23,29,36,40	0
1	PSU	1A	1917	20/21	0.96	0.09	31,40,44,45	0
55	4SU	1x	8	20/21	0.96	0.08	29,40,45,45	0
32	5MC	1a	1400	21/22	0.96	0.10	39,46,49,50	0
32	4OC	1a	1402	22/23	0.96	0.08	32,37,40,43	0
32	5MC	1a	1404	21/22	0.96	0.08	27,31,34,38	0
1	OMC	2A	1920	21/22	0.96	0.08	41,45,50,51	0
1	OMC	1A	1920	21/22	0.97	0.08	28,34,41,42	0
1	5MC	1A	1942	21/22	0.97	0.07	14,24,29,31	0
1	5MC	1A	1962	21/22	0.97	0.09	16,24,26,32	0
1	OMG	2A	2251	24/25	0.97	0.07	22,28,34,35	0
1	2MA	2A	2503	23/24	0.97	0.07	20,23,27,30	0
1	PSU	2A	2605	20/21	0.97	0.07	20,25,29,31	0
32	UR3	1a	1498	21/22	0.97	0.07	26,32,34,37	0
55	8AN	2x	76	22/23	0.97	0.08	27,32,34,43	0
1	5MU	1A	1939	21/22	0.98	0.06	11,16,20,22	0
1	5MC	2A	1962	21/22	0.98	0.07	26,30,36,40	0
1	OMG	1A	2251	24/25	0.98	0.07	9,12,14,19	0
1	2MA	1A	2503	23/24	0.98	0.06	8,11,13,14	0
1	OMU	2A	2552	21/22	0.98	0.08	19,25,29,31	0
1	OMU	1A	2552	21/22	0.98	0.06	11,16,19,20	0
1	PSU	1A	2605	20/21	0.98	0.07	13,15,19,22	0
32	MA6	1a	1518	24/25	0.98	0.07	21,29,31,34	0
55	8AN	1x	76	22/23	0.98	0.06	10,14,18,21	0
1	5MU	2A	1939	21/22	0.98	0.07	22,25,28,33	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	1X	105	1/1	0.52	0.26	58,58,58,58	0
57	MG	2A	3835	1/1	0.56	0.16	58,58,58,58	0
57	MG	2a	1731	1/1	0.61	0.20	57,57,57,57	0
57	MG	2A	3593	1/1	0.62	0.26	65,65,65,65	0
57	MG	1A	3524	1/1	0.63	0.24	57,57,57,57	0
57	MG	2A	3049	1/1	0.63	0.30	55,55,55,55	0
57	MG	2A	3490	1/1	0.63	0.26	54,54,54,54	0
57	MG	1A	3848	1/1	0.63	0.24	42,42,42,42	0
57	MG	1A	4032	1/1	0.63	0.43	75,75,75,75	0
57	MG	1B	233	1/1	0.63	0.22	74,74,74,74	0
57	MG	2A	3094	1/1	0.64	0.37	71,71,71,71	0
57	MG	1A	3917	1/1	0.65	0.15	20,20,20,20	0
57	MG	2B	207	1/1	0.66	0.21	64,64,64,64	0
57	MG	2A	3808	1/1	0.66	0.20	62,62,62,62	0
57	MG	1a	3675	1/1	0.67	0.34	65,65,65,65	0
57	MG	2A	3335	1/1	0.67	0.24	47,47,47,47	0
57	MG	2A	3118	1/1	0.68	0.19	65,65,65,65	0
57	MG	1A	3949	1/1	0.68	0.19	59,59,59,59	0
57	MG	1a	3681	1/1	0.69	0.31	57,57,57,57	0
57	MG	2A	3694	1/1	0.69	0.18	53,53,53,53	0
57	MG	2A	3263	1/1	0.69	0.14	51,51,51,51	0
57	MG	2a	1740	1/1	0.69	0.29	68,68,68,68	0
57	MG	2A	3083	1/1	0.70	0.18	77,77,77,77	0
57	MG	1B	236	1/1	0.70	0.27	58,58,58,58	0
57	MG	1A	4077	1/1	0.70	0.20	39,39,39,39	0
57	MG	2A	3626	1/1	0.70	0.22	66,66,66,66	0
57	MG	1a	3563	1/1	0.70	0.28	65,65,65,65	0
57	MG	2a	1747	1/1	0.70	0.27	69,69,69,69	0
57	MG	2A	3816	1/1	0.71	0.14	50,50,50,50	0
57	MG	2A	3622	1/1	0.71	0.15	55,55,55,55	0
57	MG	1a	3613	1/1	0.71	0.23	46,46,46,46	0
57	MG	1A	3496	1/1	0.71	0.11	55,55,55,55	0
57	MG	2A	3700	1/1	0.71	0.18	40,40,40,40	0
57	MG	2A	3295	1/1	0.71	0.22	55,55,55,55	0
57	MG	1A	3773	1/1	0.72	0.17	53,53,53,53	0
57	MG	1A	3970	1/1	0.72	0.22	67,67,67,67	0
57	MG	1B	219	1/1	0.72	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3383	1/1	0.73	0.12	54,54,54,54	0
57	MG	1A	3808	1/1	0.73	0.13	38,38,38,38	0
57	MG	2f	201	1/1	0.73	0.22	48,48,48,48	0
57	MG	1a	3655	1/1	0.74	0.25	62,62,62,62	0
57	MG	1A	4031	1/1	0.74	0.15	66,66,66,66	0
57	MG	1A	3969	1/1	0.74	0.28	51,51,51,51	0
57	MG	2A	3803	1/1	0.74	0.13	57,57,57,57	0
57	MG	2A	3162	1/1	0.74	0.24	57,57,57,57	0
57	MG	1A	3804	1/1	0.74	0.12	44,44,44,44	0
57	MG	2i	201	1/1	0.74	0.14	58,58,58,58	0
57	MG	2A	3334	1/1	0.75	0.19	48,48,48,48	0
57	MG	2A	3033	1/1	0.75	0.16	44,44,44,44	0
57	MG	1B	222	1/1	0.75	0.14	42,42,42,42	0
57	MG	2A	3519	1/1	0.75	0.16	46,46,46,46	0
57	MG	2A	3163	1/1	0.75	0.13	51,51,51,51	0
57	MG	2R	201	1/1	0.75	0.16	38,38,38,38	0
57	MG	2A	3246	1/1	0.75	0.26	49,49,49,49	0
57	MG	1A	3685	1/1	0.75	0.14	57,57,57,57	0
57	MG	1A	3866	1/1	0.75	0.22	52,52,52,52	0
57	MG	2a	1757	1/1	0.75	0.20	58,58,58,58	0
57	MG	2A	3326	1/1	0.75	0.28	62,62,62,62	0
57	MG	2A	3746	1/1	0.75	0.28	80,80,80,80	0
57	MG	2A	3396	1/1	0.76	0.18	57,57,57,57	0
57	MG	1A	4064	1/1	0.76	0.16	38,38,38,38	0
57	MG	2a	1732	1/1	0.76	0.28	75,75,75,75	0
57	MG	1a	3624	1/1	0.76	0.38	62,62,62,62	0
57	MG	1A	3344	1/1	0.76	0.19	63,63,63,63	0
57	MG	1A	3854	1/1	0.76	0.13	9,9,9,9	0
57	MG	1A	3464	1/1	0.76	0.21	56,56,56,56	0
57	MG	1a	3595	1/1	0.76	0.26	48,48,48,48	0
57	MG	1A	3514	1/1	0.77	0.28	50,50,50,50	0
57	MG	1A	3810	1/1	0.77	0.22	46,46,46,46	0
57	MG	2A	3499	1/1	0.77	0.19	48,48,48,48	0
57	MG	1I	201	1/1	0.77	0.15	56,56,56,56	0
57	MG	1U	212	1/1	0.77	0.55	53,53,53,53	0
57	MG	1x	108	1/1	0.77	0.15	66,66,66,66	0
57	MG	1A	3770	1/1	0.77	0.16	8,8,8,8	0
57	MG	2A	3310	1/1	0.77	0.16	56,56,56,56	0
57	MG	1A	4081	1/1	0.77	0.21	39,39,39,39	0
57	MG	1A	3430	1/1	0.77	0.20	52,52,52,52	0
57	MG	1A	3611	1/1	0.77	0.12	13,13,13,13	0
57	MG	2A	3804	1/1	0.77	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	3712	1/1	0.78	0.18	66,66,66,66	0
57	MG	1x	106	1/1	0.78	0.11	60,60,60,60	0
57	MG	2B	202	1/1	0.78	0.22	61,61,61,61	0
57	MG	2B	203	1/1	0.78	0.19	60,60,60,60	0
57	MG	1A	3999	1/1	0.78	0.11	43,43,43,43	0
57	MG	2B	210	1/1	0.78	0.23	63,63,63,63	0
57	MG	1A	3520	1/1	0.78	0.16	44,44,44,44	0
57	MG	2a	1655	1/1	0.78	0.15	56,56,56,56	0
57	MG	2A	3633	1/1	0.78	0.21	63,63,63,63	0
57	MG	1A	3244	1/1	0.78	0.13	45,45,45,45	0
57	MG	2A	3352	1/1	0.78	0.14	52,52,52,52	0
57	MG	2A	3247	1/1	0.78	0.22	49,49,49,49	0
57	MG	1A	3742	1/1	0.78	0.17	17,17,17,17	0
57	MG	2a	1759	1/1	0.78	0.15	66,66,66,66	0
57	MG	2A	3275	1/1	0.78	0.16	50,50,50,50	0
57	MG	2g	201	1/1	0.78	0.15	60,60,60,60	0
57	MG	2A	3515	1/1	0.78	0.18	43,43,43,43	0
57	MG	1B	232	1/1	0.79	0.20	58,58,58,58	0
57	MG	1A	3282	1/1	0.79	0.12	40,40,40,40	0
57	MG	1a	3676	1/1	0.79	0.21	74,74,74,74	0
57	MG	1a	3679	1/1	0.79	0.21	66,66,66,66	0
57	MG	1B	235	1/1	0.79	0.12	40,40,40,40	0
57	MG	1A	3409	1/1	0.79	0.26	59,59,59,59	0
57	MG	1A	3892	1/1	0.79	0.18	66,66,66,66	0
57	MG	2A	3348	1/1	0.79	0.11	60,60,60,60	0
57	MG	1A	4034	1/1	0.79	0.16	44,44,44,44	0
57	MG	2A	3030	1/1	0.79	0.12	56,56,56,56	0
57	MG	1A	3507	1/1	0.79	0.15	60,60,60,60	0
57	MG	2a	1610	1/1	0.79	0.17	48,48,48,48	0
57	MG	1a	3506	1/1	0.79	0.17	65,65,65,65	0
57	MG	1a	3533	1/1	0.79	0.12	59,59,59,59	0
57	MG	1a	3541	1/1	0.79	0.26	56,56,56,56	0
57	MG	1A	3630	1/1	0.79	0.14	34,34,34,34	0
57	MG	2A	3144	1/1	0.79	0.13	56,56,56,56	0
57	MG	1A	3510	1/1	0.79	0.33	50,50,50,50	0
57	MG	1A	3381	1/1	0.79	0.16	49,49,49,49	0
57	MG	2A	3646	1/1	0.79	0.09	44,44,44,44	0
57	MG	1A	3972	1/1	0.79	0.16	57,57,57,57	0
57	MG	1a	3646	1/1	0.79	0.12	59,59,59,59	0
57	MG	1A	3977	1/1	0.80	0.16	23,23,23,23	0
57	MG	1a	3564	1/1	0.80	0.16	57,57,57,57	0
57	MG	2A	3361	1/1	0.80	0.24	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	3791	1/1	0.80	0.18	42,42,42,42	0
57	MG	1a	3602	1/1	0.80	0.14	53,53,53,53	0
57	MG	1a	3719	1/1	0.80	0.20	58,58,58,58	0
57	MG	1A	4004	1/1	0.80	0.16	54,54,54,54	0
57	MG	1a	3503	1/1	0.80	0.26	74,74,74,74	0
57	MG	2A	3548	1/1	0.80	0.13	53,53,53,53	0
57	MG	1a	3630	1/1	0.80	0.12	51,51,51,51	0
57	MG	2A	3602	1/1	0.80	0.11	33,33,33,33	0
57	MG	26	101	1/1	0.80	0.14	44,44,44,44	0
57	MG	2A	3276	1/1	0.80	0.17	57,57,57,57	0
57	MG	1A	3919	1/1	0.80	0.15	52,52,52,52	0
57	MG	2a	1667	1/1	0.80	0.32	47,47,47,47	0
57	MG	2a	1690	1/1	0.80	0.15	53,53,53,53	0
57	MG	2a	1714	1/1	0.80	0.16	47,47,47,47	0
57	MG	1A	3900	1/1	0.80	0.15	18,18,18,18	0
57	MG	2A	3643	1/1	0.80	0.28	68,68,68,68	0
57	MG	1a	3659	1/1	0.80	0.16	56,56,56,56	0
57	MG	2A	3663	1/1	0.80	0.13	39,39,39,39	0
57	MG	2A	3669	1/1	0.80	0.13	59,59,59,59	0
57	MG	1E	311	1/1	0.80	0.14	50,50,50,50	0
57	MG	2A	3117	1/1	0.80	0.20	56,56,56,56	0
57	MG	2A	3703	1/1	0.80	0.21	59,59,59,59	0
57	MG	2A	3728	1/1	0.80	0.11	53,53,53,53	0
57	MG	2j	202	1/1	0.80	0.15	53,53,53,53	0
57	MG	2A	3500	1/1	0.81	0.12	26,26,26,26	0
57	MG	2A	3810	1/1	0.81	0.14	36,36,36,36	0
57	MG	1a	3664	1/1	0.81	0.37	61,61,61,61	0
57	MG	1a	3673	1/1	0.81	0.18	48,48,48,48	0
57	MG	1B	214	1/1	0.81	0.17	36,36,36,36	0
57	MG	2A	3557	1/1	0.81	0.23	57,57,57,57	0
57	MG	1A	3246	1/1	0.81	0.47	36,36,36,36	0
57	MG	2A	3594	1/1	0.81	0.14	33,33,33,33	0
57	MG	1A	3442	1/1	0.81	0.10	55,55,55,55	0
57	MG	1A	4009	1/1	0.81	0.16	39,39,39,39	0
57	MG	1a	3702	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3629	1/1	0.81	0.14	38,38,38,38	0
57	MG	1A	4027	1/1	0.81	0.09	41,41,41,41	0
57	MG	2a	1668	1/1	0.81	0.39	56,56,56,56	0
57	MG	2A	3641	1/1	0.81	0.20	61,61,61,61	0
57	MG	1A	3817	1/1	0.81	0.19	40,40,40,40	0
57	MG	1A	3446	1/1	0.81	0.17	46,46,46,46	0
57	MG	1B	237	1/1	0.81	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3613	1/1	0.81	0.18	45,45,45,45	0
57	MG	1A	3201	1/1	0.81	0.08	37,37,37,37	0
57	MG	2a	1750	1/1	0.81	0.25	63,63,63,63	0
57	MG	1A	3871	1/1	0.81	0.10	53,53,53,53	0
57	MG	2A	3075	1/1	0.81	0.29	46,46,46,46	0
57	MG	2a	1769	1/1	0.81	0.14	52,52,52,52	0
57	MG	1A	3662	1/1	0.81	0.12	10,10,10,10	0
57	MG	1a	3647	1/1	0.81	0.13	34,34,34,34	0
57	MG	1Y	202	1/1	0.81	0.08	46,46,46,46	0
57	MG	18	104	1/1	0.81	0.19	38,38,38,38	0
57	MG	2A	3715	1/1	0.82	0.13	39,39,39,39	0
57	MG	2A	3340	1/1	0.82	0.21	37,37,37,37	0
57	MG	1a	3615	1/1	0.82	0.27	59,59,59,59	0
57	MG	15	3209	1/1	0.82	0.16	45,45,45,45	0
57	MG	2A	3031	1/1	0.82	0.12	43,43,43,43	0
57	MG	2A	3385	1/1	0.82	0.30	50,50,50,50	0
57	MG	1a	3628	1/1	0.82	0.22	46,46,46,46	0
57	MG	1A	3807	1/1	0.82	0.10	22,22,22,22	0
57	MG	1a	3631	1/1	0.82	0.24	61,61,61,61	0
57	MG	1A	3450	1/1	0.82	0.18	52,52,52,52	0
57	MG	2A	3502	1/1	0.82	0.22	53,53,53,53	0
57	MG	1A	3756	1/1	0.82	0.12	70,70,70,70	0
57	MG	2A	3098	1/1	0.82	0.30	61,61,61,61	0
57	MG	1a	3518	1/1	0.82	0.12	59,59,59,59	0
57	MG	1A	3097	1/1	0.82	0.13	40,40,40,40	0
57	MG	1a	3540	1/1	0.82	0.12	50,50,50,50	0
57	MG	2a	1631	1/1	0.82	0.18	58,58,58,58	0
57	MG	2a	1635	1/1	0.82	0.24	56,56,56,56	0
57	MG	2a	1636	1/1	0.82	0.21	52,52,52,52	0
57	MG	1A	3656	1/1	0.82	0.09	30,30,30,30	0
57	MG	1A	3785	1/1	0.82	0.18	45,45,45,45	0
57	MG	2A	3621	1/1	0.82	0.16	49,49,49,49	0
57	MG	2A	3188	1/1	0.82	0.17	59,59,59,59	0
57	MG	1A	3588	1/1	0.82	0.08	6,6,6,6	0
57	MG	1a	3574	1/1	0.82	0.13	48,48,48,48	0
57	MG	1a	3579	1/1	0.82	0.25	68,68,68,68	0
57	MG	2A	3640	1/1	0.82	0.19	50,50,50,50	0
57	MG	2A	3269	1/1	0.82	0.17	54,54,54,54	0
57	MG	1a	3682	1/1	0.82	0.12	54,54,54,54	0
57	MG	2a	1751	1/1	0.82	0.22	60,60,60,60	0
57	MG	1a	3699	1/1	0.82	0.12	46,46,46,46	0
57	MG	2A	3660	1/1	0.82	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	1760	1/1	0.82	0.16	48,48,48,48	0
57	MG	1A	3793	1/1	0.82	0.12	24,24,24,24	0
57	MG	2a	1774	1/1	0.82	0.29	57,57,57,57	0
57	MG	1A	3794	1/1	0.82	0.21	32,32,32,32	0
57	MG	1a	3607	1/1	0.82	0.30	75,75,75,75	0
57	MG	1l	201	1/1	0.82	0.14	55,55,55,55	0
57	MG	1A	3087	1/1	0.82	0.15	37,37,37,37	0
57	MG	2A	3758	1/1	0.83	0.19	47,47,47,47	0
57	MG	2A	3783	1/1	0.83	0.17	29,29,29,29	0
57	MG	2A	3364	1/1	0.83	0.21	44,44,44,44	0
57	MG	1B	223	1/1	0.83	0.09	40,40,40,40	0
57	MG	2A	3093	1/1	0.83	0.27	55,55,55,55	0
57	MG	2A	3403	1/1	0.83	0.22	55,55,55,55	0
57	MG	1B	231	1/1	0.83	0.13	51,51,51,51	0
57	MG	1A	3719	1/1	0.83	0.16	52,52,52,52	0
57	MG	2A	3114	1/1	0.83	0.12	39,39,39,39	0
57	MG	1A	3350	1/1	0.83	0.14	47,47,47,47	0
57	MG	1A	3367	1/1	0.83	0.17	42,42,42,42	0
57	MG	1A	3283	1/1	0.83	0.16	35,35,35,35	0
57	MG	2D	304	1/1	0.83	0.23	40,40,40,40	0
57	MG	1a	3570	1/1	0.83	0.11	53,53,53,53	0
57	MG	2A	3549	1/1	0.83	0.15	60,60,60,60	0
57	MG	1A	3936	1/1	0.83	0.09	41,41,41,41	0
57	MG	2a	1625	1/1	0.83	0.26	51,51,51,51	0
57	MG	2a	1630	1/1	0.83	0.26	69,69,69,69	0
57	MG	2A	3585	1/1	0.83	0.23	56,56,56,56	0
57	MG	2a	1634	1/1	0.83	0.15	51,51,51,51	0
57	MG	1A	3449	1/1	0.83	0.10	50,50,50,50	0
57	MG	1a	3689	1/1	0.83	0.24	55,55,55,55	0
57	MG	1a	3696	1/1	0.83	0.26	60,60,60,60	0
57	MG	2a	1661	1/1	0.83	0.26	51,51,51,51	0
57	MG	1F	310	1/1	0.83	0.10	44,44,44,44	0
57	MG	2A	3266	1/1	0.83	0.14	48,48,48,48	0
57	MG	2a	1677	1/1	0.83	0.25	61,61,61,61	0
57	MG	2a	1688	1/1	0.83	0.31	54,54,54,54	0
57	MG	1A	3832	1/1	0.83	0.14	43,43,43,43	0
57	MG	2a	1710	1/1	0.83	0.27	64,64,64,64	0
57	MG	2A	3273	1/1	0.83	0.28	60,60,60,60	0
57	MG	1S	203	1/1	0.83	0.11	56,56,56,56	0
57	MG	1A	4075	1/1	0.83	0.15	49,49,49,49	0
57	MG	1A	4076	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3301	1/1	0.83	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3315	1/1	0.83	0.14	35,35,35,35	0
57	MG	1a	3625	1/1	0.83	0.18	57,57,57,57	0
57	MG	2A	3331	1/1	0.83	0.14	58,58,58,58	0
57	MG	1x	111	1/1	0.83	0.18	52,52,52,52	0
57	MG	13	102	1/1	0.83	0.17	40,40,40,40	0
57	MG	1A	3119	1/1	0.83	0.27	45,45,45,45	0
57	MG	1A	3568	1/1	0.83	0.27	55,55,55,55	0
57	MG	1A	3690	1/1	0.83	0.11	49,49,49,49	0
57	MG	2A	3357	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	4002	1/1	0.83	0.14	69,69,69,69	0
57	MG	2A	3748	1/1	0.83	0.09	41,41,41,41	0
57	MG	2A	3628	1/1	0.84	0.11	30,30,30,30	0
57	MG	1A	3503	1/1	0.84	0.14	34,34,34,34	0
57	MG	2A	3387	1/1	0.84	0.24	38,38,38,38	0
57	MG	1B	227	1/1	0.84	0.20	65,65,65,65	0
57	MG	1a	3668	1/1	0.84	0.23	64,64,64,64	0
57	MG	2A	3421	1/1	0.84	0.29	61,61,61,61	0
57	MG	2A	3440	1/1	0.84	0.11	54,54,54,54	0
57	MG	2A	3458	1/1	0.84	0.13	52,52,52,52	0
57	MG	2A	3476	1/1	0.84	0.20	46,46,46,46	0
57	MG	1v	101	1/1	0.84	0.27	77,77,77,77	0
57	MG	2A	3681	1/1	0.84	0.23	47,47,47,47	0
57	MG	1A	3907	1/1	0.84	0.17	59,59,59,59	0
57	MG	2A	3122	1/1	0.84	0.13	42,42,42,42	0
57	MG	1A	3393	1/1	0.84	0.18	47,47,47,47	0
57	MG	1a	3559	1/1	0.84	0.19	70,70,70,70	0
57	MG	2a	1683	1/1	0.84	0.22	55,55,55,55	0
57	MG	1A	3593	1/1	0.84	0.12	26,26,26,26	0
57	MG	2A	3729	1/1	0.84	0.18	53,53,53,53	0
57	MG	2A	3177	1/1	0.84	0.17	60,60,60,60	0
57	MG	1A	3788	1/1	0.84	0.11	46,46,46,46	0
57	MG	2A	3757	1/1	0.84	0.17	51,51,51,51	0
57	MG	2A	3343	1/1	0.84	0.33	64,64,64,64	0
57	MG	2A	3581	1/1	0.84	0.22	41,41,41,41	0
57	MG	2a	1743	1/1	0.84	0.20	52,52,52,52	0
57	MG	2A	3584	1/1	0.84	0.12	46,46,46,46	0
57	MG	2A	3347	1/1	0.84	0.14	51,51,51,51	0
57	MG	1A	3941	1/1	0.84	0.12	21,21,21,21	0
57	MG	2a	1753	1/1	0.84	0.23	51,51,51,51	0
57	MG	1A	3439	1/1	0.84	0.20	58,58,58,58	0
57	MG	2A	3355	1/1	0.84	0.15	53,53,53,53	0
57	MG	2A	3830	1/1	0.84	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3606	1/1	0.84	0.16	19,19,19,19	0
57	MG	2a	1772	1/1	0.84	0.17	59,59,59,59	0
57	MG	2A	3610	1/1	0.84	0.17	64,64,64,64	0
57	MG	1a	3577	1/1	0.84	0.29	51,51,51,51	0
57	MG	1A	3889	1/1	0.84	0.18	39,39,39,39	0
57	MG	1A	3669	1/1	0.84	0.14	18,18,18,18	0
57	MG	2j	201	1/1	0.84	0.10	55,55,55,55	0
57	MG	2B	215	1/1	0.84	0.17	63,63,63,63	0
57	MG	2A	3590	1/1	0.85	0.14	41,41,41,41	0
57	MG	1A	3780	1/1	0.85	0.17	42,42,42,42	0
57	MG	1F	311	1/1	0.85	0.10	44,44,44,44	0
57	MG	1A	3698	1/1	0.85	0.14	55,55,55,55	0
57	MG	2B	211	1/1	0.85	0.11	49,49,49,49	0
57	MG	1A	3605	1/1	0.85	0.11	47,47,47,47	0
57	MG	1A	3061	1/1	0.85	0.28	49,49,49,49	0
57	MG	2D	305	1/1	0.85	0.12	45,45,45,45	0
57	MG	2G	201	1/1	0.85	0.22	53,53,53,53	0
57	MG	2A	3349	1/1	0.85	0.18	47,47,47,47	0
57	MG	1A	3479	1/1	0.85	0.16	45,45,45,45	0
57	MG	1A	3918	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	3692	1/1	0.85	0.18	50,50,50,50	0
57	MG	10	101	1/1	0.85	0.13	41,41,41,41	0
57	MG	1A	3345	1/1	0.85	0.26	45,45,45,45	0
57	MG	2A	3174	1/1	0.85	0.18	47,47,47,47	0
57	MG	1B	224	1/1	0.85	0.17	54,54,54,54	0
57	MG	1A	3797	1/1	0.85	0.09	28,28,28,28	0
57	MG	1a	3716	1/1	0.85	0.17	51,51,51,51	0
57	MG	2A	3405	1/1	0.85	0.23	49,49,49,49	0
57	MG	2A	3416	1/1	0.85	0.11	50,50,50,50	0
57	MG	2A	3668	1/1	0.85	0.18	57,57,57,57	0
57	MG	1A	3798	1/1	0.85	0.10	42,42,42,42	0
57	MG	2A	3436	1/1	0.85	0.13	47,47,47,47	0
57	MG	2A	3693	1/1	0.85	0.23	52,52,52,52	0
57	MG	2A	3254	1/1	0.85	0.10	55,55,55,55	0
57	MG	2a	1692	1/1	0.85	0.23	67,67,67,67	0
57	MG	2a	1695	1/1	0.85	0.30	54,54,54,54	0
57	MG	1b	302	1/1	0.85	0.15	75,75,75,75	0
57	MG	2A	3464	1/1	0.85	0.24	66,66,66,66	0
57	MG	2a	1719	1/1	0.85	0.12	41,41,41,41	0
57	MG	2a	1724	1/1	0.85	0.12	50,50,50,50	0
57	MG	2A	3704	1/1	0.85	0.22	59,59,59,59	0
57	MG	2A	3709	1/1	0.85	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3467	1/1	0.85	0.26	49,49,49,49	0
57	MG	1A	3942	1/1	0.85	0.10	26,26,26,26	0
57	MG	2A	3484	1/1	0.85	0.19	36,36,36,36	0
57	MG	2A	3734	1/1	0.85	0.14	67,67,67,67	0
57	MG	1A	3947	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3272	1/1	0.85	0.20	56,56,56,56	0
57	MG	1a	3520	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	3638	1/1	0.85	0.16	39,39,39,39	0
57	MG	1a	3523	1/1	0.85	0.11	51,51,51,51	0
57	MG	2a	1762	1/1	0.85	0.26	58,58,58,58	0
57	MG	1A	3654	1/1	0.85	0.10	55,55,55,55	0
57	MG	1A	4055	1/1	0.85	0.11	30,30,30,30	0
57	MG	2A	3806	1/1	0.85	0.11	50,50,50,50	0
57	MG	2a	1777	1/1	0.85	0.29	53,53,53,53	0
57	MG	1A	3951	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3321	1/1	0.85	0.23	48,48,48,48	0
57	MG	1A	3958	1/1	0.85	0.11	63,63,63,63	0
57	MG	1F	304	1/1	0.85	0.11	19,19,19,19	0
57	MG	1a	3672	1/1	0.85	0.11	51,51,51,51	0
57	MG	2A	3209	1/1	0.86	0.13	46,46,46,46	0
57	MG	1a	3606	1/1	0.86	0.25	49,49,49,49	0
57	MG	1A	3538	1/1	0.86	0.12	38,38,38,38	0
57	MG	1A	3314	1/1	0.86	0.17	29,29,29,29	0
57	MG	2A	3824	1/1	0.86	0.12	20,20,20,20	0
57	MG	1F	305	1/1	0.86	0.11	44,44,44,44	0
57	MG	1a	3507	1/1	0.86	0.12	52,52,52,52	0
57	MG	1a	3511	1/1	0.86	0.16	54,54,54,54	0
57	MG	1a	3515	1/1	0.86	0.13	58,58,58,58	0
57	MG	1v	102	1/1	0.86	0.12	41,41,41,41	0
57	MG	1x	101	1/1	0.86	0.22	52,52,52,52	0
57	MG	1x	105	1/1	0.86	0.18	45,45,45,45	0
57	MG	2A	3282	1/1	0.86	0.18	48,48,48,48	0
57	MG	1A	3586	1/1	0.86	0.11	22,22,22,22	0
57	MG	2A	3298	1/1	0.86	0.19	54,54,54,54	0
57	MG	2E	301	1/1	0.86	0.19	58,58,58,58	0
57	MG	2E	304	1/1	0.86	0.12	55,55,55,55	0
57	MG	1A	3635	1/1	0.86	0.13	34,34,34,34	0
57	MG	2Q	203	1/1	0.86	0.12	50,50,50,50	0
57	MG	2Q	204	1/1	0.86	0.19	43,43,43,43	0
57	MG	1A	4036	1/1	0.86	0.12	30,30,30,30	0
57	MG	2U	201	1/1	0.86	0.23	49,49,49,49	0
57	MG	2W	201	1/1	0.86	0.39	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3314	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	1602	1/1	0.86	0.11	63,63,63,63	0
57	MG	2a	1607	1/1	0.86	0.25	45,45,45,45	0
57	MG	2A	3316	1/1	0.86	0.08	52,52,52,52	0
57	MG	2a	1617	1/1	0.86	0.13	45,45,45,45	0
57	MG	1A	4038	1/1	0.86	0.15	23,23,23,23	0
57	MG	2A	3324	1/1	0.86	0.09	52,52,52,52	0
57	MG	2A	3325	1/1	0.86	0.11	45,45,45,45	0
57	MG	2A	3624	1/1	0.86	0.13	46,46,46,46	0
57	MG	1T	202	1/1	0.86	0.14	47,47,47,47	0
57	MG	1U	202	1/1	0.86	0.29	36,36,36,36	0
57	MG	2A	3039	1/1	0.86	0.19	51,51,51,51	0
57	MG	1a	3657	1/1	0.86	0.16	55,55,55,55	0
57	MG	2A	3056	1/1	0.86	0.13	49,49,49,49	0
57	MG	1a	3550	1/1	0.86	0.19	44,44,44,44	0
57	MG	1a	3551	1/1	0.86	0.24	64,64,64,64	0
57	MG	2a	1681	1/1	0.86	0.20	45,45,45,45	0
57	MG	2A	3090	1/1	0.86	0.21	58,58,58,58	0
57	MG	2A	3653	1/1	0.86	0.29	46,46,46,46	0
57	MG	2a	1689	1/1	0.86	0.32	54,54,54,54	0
57	MG	1a	3557	1/1	0.86	0.19	59,59,59,59	0
57	MG	1U	204	1/1	0.86	0.13	41,41,41,41	0
57	MG	1A	3382	1/1	0.86	0.26	61,61,61,61	0
57	MG	2A	3109	1/1	0.86	0.33	51,51,51,51	0
57	MG	2a	1711	1/1	0.86	0.12	54,54,54,54	0
57	MG	2A	3110	1/1	0.86	0.15	46,46,46,46	0
57	MG	2A	3692	1/1	0.86	0.18	48,48,48,48	0
57	MG	1A	3592	1/1	0.86	0.09	34,34,34,34	0
57	MG	2a	1730	1/1	0.86	0.12	46,46,46,46	0
57	MG	1A	3759	1/1	0.86	0.11	38,38,38,38	0
57	MG	1A	3763	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	1736	1/1	0.86	0.12	35,35,35,35	0
57	MG	2A	3392	1/1	0.86	0.20	45,45,45,45	0
57	MG	10	107	1/1	0.86	0.17	49,49,49,49	0
57	MG	2A	3142	1/1	0.86	0.25	48,48,48,48	0
57	MG	11	102	1/1	0.86	0.10	26,26,26,26	0
57	MG	2A	3723	1/1	0.86	0.14	40,40,40,40	0
57	MG	2A	3412	1/1	0.86	0.22	42,42,42,42	0
57	MG	2A	3160	1/1	0.86	0.08	60,60,60,60	0
57	MG	2A	3733	1/1	0.86	0.13	37,37,37,37	0
57	MG	1a	3590	1/1	0.86	0.18	52,52,52,52	0
57	MG	2a	1761	1/1	0.86	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3740	1/1	0.86	0.13	50,50,50,50	0
57	MG	1a	3591	1/1	0.86	0.23	61,61,61,61	0
57	MG	2A	3168	1/1	0.86	0.18	55,55,55,55	0
57	MG	2A	3453	1/1	0.86	0.16	53,53,53,53	0
57	MG	1a	3693	1/1	0.86	0.21	46,46,46,46	0
57	MG	2A	3766	1/1	0.86	0.15	55,55,55,55	0
57	MG	2A	3776	1/1	0.86	0.14	50,50,50,50	0
57	MG	1A	3088	1/1	0.86	0.24	39,39,39,39	0
57	MG	1A	3207	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3199	1/1	0.86	0.16	41,41,41,41	0
57	MG	2x	108	1/1	0.86	0.27	50,50,50,50	0
57	MG	1a	3555	1/1	0.87	0.22	55,55,55,55	0
57	MG	1A	3356	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3864	1/1	0.87	0.09	18,18,18,18	0
57	MG	1a	3695	1/1	0.87	0.25	48,48,48,48	0
57	MG	2A	3201	1/1	0.87	0.18	54,54,54,54	0
57	MG	2A	3488	1/1	0.87	0.23	44,44,44,44	0
57	MG	1A	4010	1/1	0.87	0.10	30,30,30,30	0
57	MG	2A	3820	1/1	0.87	0.11	48,48,48,48	0
57	MG	2A	3235	1/1	0.87	0.19	50,50,50,50	0
57	MG	2A	3238	1/1	0.87	0.35	57,57,57,57	0
57	MG	2A	3831	1/1	0.87	0.07	38,38,38,38	0
57	MG	1A	3251	1/1	0.87	0.09	49,49,49,49	0
57	MG	2A	3508	1/1	0.87	0.15	34,34,34,34	0
57	MG	1a	3701	1/1	0.87	0.22	60,60,60,60	0
57	MG	1A	3470	1/1	0.87	0.42	37,37,37,37	0
57	MG	2A	3525	1/1	0.87	0.16	25,25,25,25	0
57	MG	2A	3528	1/1	0.87	0.19	37,37,37,37	0
57	MG	2A	3546	1/1	0.87	0.17	38,38,38,38	0
57	MG	1a	3705	1/1	0.87	0.09	53,53,53,53	0
57	MG	1a	3707	1/1	0.87	0.14	57,57,57,57	0
57	MG	2A	3268	1/1	0.87	0.17	48,48,48,48	0
57	MG	2A	3571	1/1	0.87	0.14	48,48,48,48	0
57	MG	2F	304	1/1	0.87	0.13	41,41,41,41	0
57	MG	2A	3573	1/1	0.87	0.31	48,48,48,48	0
57	MG	2A	3574	1/1	0.87	0.12	57,57,57,57	0
57	MG	1P	203	1/1	0.87	0.23	36,36,36,36	0
57	MG	1A	3765	1/1	0.87	0.18	48,48,48,48	0
57	MG	1A	3600	1/1	0.87	0.10	19,19,19,19	0
57	MG	1T	203	1/1	0.87	0.16	43,43,43,43	0
57	MG	2A	3591	1/1	0.87	0.24	47,47,47,47	0
57	MG	1A	3473	1/1	0.87	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1603	1/1	0.87	0.16	55,55,55,55	0
57	MG	1A	4037	1/1	0.87	0.18	52,52,52,52	0
57	MG	1a	3598	1/1	0.87	0.21	44,44,44,44	0
57	MG	1A	3610	1/1	0.87	0.18	34,34,34,34	0
57	MG	1V	203	1/1	0.87	0.32	25,25,25,25	0
57	MG	1A	4040	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	4052	1/1	0.87	0.11	32,32,32,32	0
57	MG	1A	3167	1/1	0.87	0.27	47,47,47,47	0
57	MG	2A	3004	1/1	0.87	0.30	56,56,56,56	0
57	MG	2A	3019	1/1	0.87	0.20	50,50,50,50	0
57	MG	1A	3787	1/1	0.87	0.13	25,25,25,25	0
57	MG	2A	3630	1/1	0.87	0.12	50,50,50,50	0
57	MG	2a	1662	1/1	0.87	0.16	35,35,35,35	0
57	MG	2a	1663	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3632	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3178	1/1	0.87	0.14	28,28,28,28	0
57	MG	2A	3635	1/1	0.87	0.14	49,49,49,49	0
57	MG	1a	3627	1/1	0.87	0.14	47,47,47,47	0
57	MG	12	101	1/1	0.87	0.10	43,43,43,43	0
57	MG	1A	3923	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3644	1/1	0.87	0.27	57,57,57,57	0
57	MG	1A	3928	1/1	0.87	0.20	53,53,53,53	0
57	MG	1a	3636	1/1	0.87	0.20	56,56,56,56	0
57	MG	2A	3346	1/1	0.87	0.24	44,44,44,44	0
57	MG	2a	1700	1/1	0.87	0.14	56,56,56,56	0
57	MG	2A	3076	1/1	0.87	0.16	33,33,33,33	0
57	MG	17	103	1/1	0.87	0.11	33,33,33,33	0
57	MG	1A	3931	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3676	1/1	0.87	0.23	44,44,44,44	0
57	MG	2A	3677	1/1	0.87	0.17	46,46,46,46	0
57	MG	2A	3091	1/1	0.87	0.15	33,33,33,33	0
57	MG	1A	3614	1/1	0.87	0.13	47,47,47,47	0
57	MG	1A	3499	1/1	0.87	0.16	42,42,42,42	0
57	MG	1A	3500	1/1	0.87	0.10	38,38,38,38	0
57	MG	2A	3362	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3284	1/1	0.87	0.20	48,48,48,48	0
57	MG	1A	3187	1/1	0.87	0.20	40,40,40,40	0
57	MG	1A	3137	1/1	0.87	0.09	35,35,35,35	0
57	MG	2A	3711	1/1	0.87	0.14	43,43,43,43	0
57	MG	2A	3714	1/1	0.87	0.24	37,37,37,37	0
57	MG	1A	3317	1/1	0.87	0.14	39,39,39,39	0
57	MG	1A	3146	1/1	0.87	0.28	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3153	1/1	0.87	0.07	26,26,26,26	0
57	MG	2A	3123	1/1	0.87	0.20	62,62,62,62	0
57	MG	2A	3408	1/1	0.87	0.24	55,55,55,55	0
57	MG	1A	3445	1/1	0.87	0.18	52,52,52,52	0
57	MG	2a	1770	1/1	0.87	0.12	52,52,52,52	0
57	MG	1a	3677	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3418	1/1	0.87	0.10	45,45,45,45	0
57	MG	1A	3822	1/1	0.87	0.25	37,37,37,37	0
57	MG	2A	3754	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3155	1/1	0.87	0.10	18,18,18,18	0
57	MG	1A	3352	1/1	0.87	0.16	44,44,44,44	0
57	MG	2A	3445	1/1	0.87	0.28	57,57,57,57	0
57	MG	1a	3684	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3778	1/1	0.87	0.11	35,35,35,35	0
57	MG	1A	3890	1/1	0.88	0.23	48,48,48,48	0
57	MG	2A	3304	1/1	0.88	0.14	46,46,46,46	0
57	MG	2A	3084	1/1	0.88	0.20	52,52,52,52	0
57	MG	2A	3833	1/1	0.88	0.11	58,58,58,58	0
57	MG	2A	3086	1/1	0.88	0.11	46,46,46,46	0
57	MG	2A	3089	1/1	0.88	0.18	47,47,47,47	0
57	MG	2A	3319	1/1	0.88	0.13	47,47,47,47	0
57	MG	2B	206	1/1	0.88	0.20	47,47,47,47	0
57	MG	1A	3891	1/1	0.88	0.11	25,25,25,25	0
57	MG	1A	3743	1/1	0.88	0.11	8,8,8,8	0
57	MG	10	109	1/1	0.88	0.14	46,46,46,46	0
57	MG	1a	3685	1/1	0.88	0.16	59,59,59,59	0
57	MG	1A	3899	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3108	1/1	0.88	0.35	51,51,51,51	0
57	MG	1a	3596	1/1	0.88	0.37	47,47,47,47	0
57	MG	2A	3615	1/1	0.88	0.11	35,35,35,35	0
57	MG	2E	305	1/1	0.88	0.12	62,62,62,62	0
57	MG	2E	308	1/1	0.88	0.09	18,18,18,18	0
57	MG	2A	3619	1/1	0.88	0.10	54,54,54,54	0
57	MG	1A	3651	1/1	0.88	0.18	46,46,46,46	0
57	MG	2O	201	1/1	0.88	0.16	53,53,53,53	0
57	MG	1A	3800	1/1	0.88	0.16	35,35,35,35	0
57	MG	2A	3623	1/1	0.88	0.18	50,50,50,50	0
57	MG	1A	3596	1/1	0.88	0.13	39,39,39,39	0
57	MG	1A	4020	1/1	0.88	0.29	47,47,47,47	0
57	MG	2A	3627	1/1	0.88	0.16	56,56,56,56	0
57	MG	1a	3609	1/1	0.88	0.23	49,49,49,49	0
57	MG	28	101	1/1	0.88	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3080	1/1	0.88	0.27	26,26,26,26	0
57	MG	2A	3351	1/1	0.88	0.15	49,49,49,49	0
57	MG	2A	3131	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3136	1/1	0.88	0.19	49,49,49,49	0
57	MG	2a	1614	1/1	0.88	0.25	43,43,43,43	0
57	MG	1A	3414	1/1	0.88	0.10	33,33,33,33	0
57	MG	1a	3618	1/1	0.88	0.19	63,63,63,63	0
57	MG	1a	3710	1/1	0.88	0.11	42,42,42,42	0
57	MG	1A	3668	1/1	0.88	0.14	22,22,22,22	0
57	MG	2A	3370	1/1	0.88	0.19	27,27,27,27	0
57	MG	1a	3715	1/1	0.88	0.12	44,44,44,44	0
57	MG	1D	311	1/1	0.88	0.09	27,27,27,27	0
57	MG	2A	3388	1/1	0.88	0.21	35,35,35,35	0
57	MG	2A	3390	1/1	0.88	0.12	40,40,40,40	0
57	MG	2A	3169	1/1	0.88	0.15	51,51,51,51	0
57	MG	2A	3171	1/1	0.88	0.12	42,42,42,42	0
57	MG	1E	306	1/1	0.88	0.21	32,32,32,32	0
57	MG	1A	3269	1/1	0.88	0.11	31,31,31,31	0
57	MG	2a	1669	1/1	0.88	0.19	54,54,54,54	0
57	MG	2a	1671	1/1	0.88	0.22	58,58,58,58	0
57	MG	2A	3180	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3690	1/1	0.88	0.17	42,42,42,42	0
57	MG	1f	201	1/1	0.88	0.22	40,40,40,40	0
57	MG	1A	3819	1/1	0.88	0.08	44,44,44,44	0
57	MG	1A	3779	1/1	0.88	0.34	17,17,17,17	0
57	MG	1a	3632	1/1	0.88	0.31	54,54,54,54	0
57	MG	2a	1691	1/1	0.88	0.19	54,54,54,54	0
57	MG	2A	3210	1/1	0.88	0.20	58,58,58,58	0
57	MG	2A	3212	1/1	0.88	0.24	56,56,56,56	0
57	MG	2A	3705	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3451	1/1	0.88	0.17	42,42,42,42	0
57	MG	2A	3236	1/1	0.88	0.11	49,49,49,49	0
57	MG	1A	3325	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3459	1/1	0.88	0.08	34,34,34,34	0
57	MG	2a	1723	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3239	1/1	0.88	0.13	50,50,50,50	0
57	MG	1G	203	1/1	0.88	0.06	54,54,54,54	0
57	MG	1A	3944	1/1	0.88	0.21	52,52,52,52	0
57	MG	1a	3649	1/1	0.88	0.20	66,66,66,66	0
57	MG	2A	3255	1/1	0.88	0.10	55,55,55,55	0
57	MG	1A	3384	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3265	1/1	0.88	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3747	1/1	0.88	0.12	59,59,59,59	0
57	MG	1A	3377	1/1	0.88	0.25	40,40,40,40	0
57	MG	2A	3752	1/1	0.88	0.21	57,57,57,57	0
57	MG	1A	3733	1/1	0.88	0.12	12,12,12,12	0
57	MG	1A	3954	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3509	1/1	0.88	0.14	48,48,48,48	0
57	MG	1A	3739	1/1	0.88	0.10	26,26,26,26	0
57	MG	1A	3874	1/1	0.88	0.17	30,30,30,30	0
57	MG	1A	4084	1/1	0.88	0.14	53,53,53,53	0
57	MG	2A	3052	1/1	0.88	0.11	48,48,48,48	0
57	MG	2A	3789	1/1	0.88	0.14	49,49,49,49	0
57	MG	2A	3802	1/1	0.88	0.14	69,69,69,69	0
57	MG	2a	1773	1/1	0.88	0.24	56,56,56,56	0
57	MG	2A	3530	1/1	0.88	0.14	42,42,42,42	0
57	MG	2A	3533	1/1	0.88	0.15	29,29,29,29	0
57	MG	2a	1778	1/1	0.88	0.18	55,55,55,55	0
57	MG	2A	3535	1/1	0.88	0.13	23,23,23,23	0
57	MG	1a	3569	1/1	0.88	0.22	42,42,42,42	0
57	MG	2A	3292	1/1	0.88	0.18	51,51,51,51	0
57	MG	2A	3813	1/1	0.88	0.16	57,57,57,57	0
57	MG	1B	208	1/1	0.88	0.17	44,44,44,44	0
57	MG	2l	202	1/1	0.88	0.07	47,47,47,47	0
57	MG	2r	101	1/1	0.88	0.28	62,62,62,62	0
57	MG	2v	101	1/1	0.88	0.35	46,46,46,46	0
57	MG	2x	104	1/1	0.88	0.26	59,59,59,59	0
57	MG	1A	3477	1/1	0.88	0.19	46,46,46,46	0
58	K	1A	3537	1/1	0.88	0.18	65,65,65,65	0
57	MG	1a	3717	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3821	1/1	0.89	0.16	58,58,58,58	0
57	MG	1a	3720	1/1	0.89	0.19	58,58,58,58	0
57	MG	1A	3229	1/1	0.89	0.23	49,49,49,49	0
57	MG	2A	3369	1/1	0.89	0.26	31,31,31,31	0
57	MG	2F	301	1/1	0.89	0.12	30,30,30,30	0
57	MG	2F	302	1/1	0.89	0.11	41,41,41,41	0
57	MG	2A	3631	1/1	0.89	0.19	51,51,51,51	0
57	MG	1B	201	1/1	0.89	0.10	42,42,42,42	0
57	MG	2A	3178	1/1	0.89	0.13	45,45,45,45	0
57	MG	1f	202	1/1	0.89	0.28	54,54,54,54	0
57	MG	2A	3638	1/1	0.89	0.26	33,33,33,33	0
57	MG	1B	207	1/1	0.89	0.24	40,40,40,40	0
57	MG	1A	3518	1/1	0.89	0.17	52,52,52,52	0
57	MG	1B	209	1/1	0.89	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2Z	301	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3205	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3142	1/1	0.89	0.11	28,28,28,28	0
57	MG	2A	3651	1/1	0.89	0.20	45,45,45,45	0
57	MG	1A	3194	1/1	0.89	0.10	43,43,43,43	0
57	MG	2A	3654	1/1	0.89	0.10	69,69,69,69	0
57	MG	1A	3858	1/1	0.89	0.11	37,37,37,37	0
57	MG	2a	1611	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3410	1/1	0.89	0.12	37,37,37,37	0
57	MG	2A	3228	1/1	0.89	0.13	46,46,46,46	0
57	MG	1A	3386	1/1	0.89	0.20	42,42,42,42	0
57	MG	1A	3769	1/1	0.89	0.13	14,14,14,14	0
57	MG	2A	3002	1/1	0.89	0.29	35,35,35,35	0
57	MG	1A	3973	1/1	0.89	0.15	48,48,48,48	0
57	MG	2A	3682	1/1	0.89	0.10	50,50,50,50	0
57	MG	2A	3685	1/1	0.89	0.19	61,61,61,61	0
57	MG	2a	1649	1/1	0.89	0.17	50,50,50,50	0
57	MG	2A	3687	1/1	0.89	0.13	49,49,49,49	0
57	MG	2a	1656	1/1	0.89	0.21	72,72,72,72	0
57	MG	1A	3565	1/1	0.89	0.08	45,45,45,45	0
57	MG	1A	3979	1/1	0.89	0.22	30,30,30,30	0
57	MG	2A	3249	1/1	0.89	0.13	42,42,42,42	0
57	MG	1A	3636	1/1	0.89	0.10	32,32,32,32	0
57	MG	1A	3480	1/1	0.89	0.10	33,33,33,33	0
57	MG	1a	3528	1/1	0.89	0.19	46,46,46,46	0
57	MG	2a	1670	1/1	0.89	0.23	50,50,50,50	0
57	MG	1A	3570	1/1	0.89	0.28	55,55,55,55	0
57	MG	1A	4007	1/1	0.89	0.10	19,19,19,19	0
57	MG	1A	3573	1/1	0.89	0.20	44,44,44,44	0
57	MG	1a	3542	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3575	1/1	0.89	0.09	24,24,24,24	0
57	MG	1A	4019	1/1	0.89	0.08	21,21,21,21	0
57	MG	2A	3718	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3492	1/1	0.89	0.18	50,50,50,50	0
57	MG	1A	4021	1/1	0.89	0.08	25,25,25,25	0
57	MG	2A	3277	1/1	0.89	0.21	39,39,39,39	0
57	MG	2A	3730	1/1	0.89	0.11	46,46,46,46	0
57	MG	2a	1706	1/1	0.89	0.22	59,59,59,59	0
57	MG	1A	3247	1/1	0.89	0.08	51,51,51,51	0
57	MG	2A	3290	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3672	1/1	0.89	0.12	37,37,37,37	0
57	MG	2a	1716	1/1	0.89	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3916	1/1	0.89	0.22	18,18,18,18	0
57	MG	1a	3567	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3299	1/1	0.89	0.17	49,49,49,49	0
57	MG	2a	1728	1/1	0.89	0.29	61,61,61,61	0
57	MG	1A	3590	1/1	0.89	0.10	24,24,24,24	0
57	MG	1A	3591	1/1	0.89	0.10	34,34,34,34	0
57	MG	2A	3541	1/1	0.89	0.14	51,51,51,51	0
57	MG	2A	3102	1/1	0.89	0.20	50,50,50,50	0
57	MG	1A	3086	1/1	0.89	0.10	35,35,35,35	0
57	MG	1A	3705	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3551	1/1	0.89	0.12	45,45,45,45	0
57	MG	2A	3554	1/1	0.89	0.14	42,42,42,42	0
57	MG	1A	3706	1/1	0.89	0.10	39,39,39,39	0
57	MG	2a	1752	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3566	1/1	0.89	0.17	49,49,49,49	0
57	MG	2a	1754	1/1	0.89	0.17	40,40,40,40	0
57	MG	1a	3580	1/1	0.89	0.11	38,38,38,38	0
57	MG	1a	3584	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3206	1/1	0.89	0.17	48,48,48,48	0
57	MG	1A	3933	1/1	0.89	0.08	20,20,20,20	0
57	MG	1a	3592	1/1	0.89	0.11	55,55,55,55	0
57	MG	2a	1768	1/1	0.89	0.27	65,65,65,65	0
57	MG	2A	3332	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3127	1/1	0.89	0.17	46,46,46,46	0
57	MG	2A	3817	1/1	0.89	0.14	33,33,33,33	0
57	MG	1a	3593	1/1	0.89	0.19	51,51,51,51	0
57	MG	2A	3339	1/1	0.89	0.29	47,47,47,47	0
57	MG	2a	1775	1/1	0.89	0.08	57,57,57,57	0
57	MG	2A	3829	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3723	1/1	0.89	0.11	39,39,39,39	0
57	MG	2A	3137	1/1	0.89	0.23	43,43,43,43	0
57	MG	2A	3345	1/1	0.89	0.10	40,40,40,40	0
57	MG	2A	3607	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3141	1/1	0.89	0.15	36,36,36,36	0
57	MG	2A	3611	1/1	0.89	0.14	37,37,37,37	0
57	MG	1A	4067	1/1	0.89	0.15	42,42,42,42	0
57	MG	2A	3143	1/1	0.89	0.18	56,56,56,56	0
57	MG	1A	3458	1/1	0.89	0.12	43,43,43,43	0
57	MG	2x	103	1/1	0.89	0.15	31,31,31,31	0
57	MG	1A	3460	1/1	0.89	0.15	34,34,34,34	0
57	MG	1a	3604	1/1	0.89	0.29	58,58,58,58	0
57	MG	1A	3060	1/1	0.89	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3146	1/1	0.90	0.18	50,50,50,50	0
57	MG	2A	3153	1/1	0.90	0.09	42,42,42,42	0
57	MG	2A	3158	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3159	1/1	0.90	0.10	53,53,53,53	0
57	MG	2E	302	1/1	0.90	0.16	52,52,52,52	0
57	MG	1A	3368	1/1	0.90	0.10	33,33,33,33	0
57	MG	1a	3594	1/1	0.90	0.25	35,35,35,35	0
57	MG	1A	3343	1/1	0.90	0.16	44,44,44,44	0
57	MG	1Z	302	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3432	1/1	0.90	0.21	44,44,44,44	0
57	MG	10	106	1/1	0.90	0.09	44,44,44,44	0
57	MG	2F	305	1/1	0.90	0.13	45,45,45,45	0
57	MG	1a	3721	1/1	0.90	0.10	55,55,55,55	0
57	MG	1A	3952	1/1	0.90	0.07	43,43,43,43	0
57	MG	2A	3383	1/1	0.90	0.23	50,50,50,50	0
57	MG	1A	3784	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3434	1/1	0.90	0.11	45,45,45,45	0
57	MG	1A	3961	1/1	0.90	0.10	15,15,15,15	0
57	MG	2V	202	1/1	0.90	0.08	38,38,38,38	0
57	MG	2A	3642	1/1	0.90	0.14	45,45,45,45	0
57	MG	2Y	201	1/1	0.90	0.08	52,52,52,52	0
57	MG	1A	3868	1/1	0.90	0.14	38,38,38,38	0
57	MG	25	103	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3686	1/1	0.90	0.17	37,37,37,37	0
57	MG	16	102	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3649	1/1	0.90	0.13	55,55,55,55	0
57	MG	1B	210	1/1	0.90	0.09	44,44,44,44	0
57	MG	1A	3519	1/1	0.90	0.17	43,43,43,43	0
57	MG	1x	107	1/1	0.90	0.17	56,56,56,56	0
57	MG	2A	3655	1/1	0.90	0.10	22,22,22,22	0
57	MG	2A	3656	1/1	0.90	0.10	47,47,47,47	0
57	MG	2A	3217	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3223	1/1	0.90	0.30	50,50,50,50	0
57	MG	2a	1628	1/1	0.90	0.13	36,36,36,36	0
57	MG	19	101	1/1	0.90	0.12	36,36,36,36	0
57	MG	1A	3879	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3419	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3886	1/1	0.90	0.10	10,10,10,10	0
57	MG	2A	3679	1/1	0.90	0.13	52,52,52,52	0
57	MG	2a	1641	1/1	0.90	0.24	34,34,34,34	0
57	MG	2A	3430	1/1	0.90	0.15	45,45,45,45	0
57	MG	2a	1651	1/1	0.90	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3433	1/1	0.90	0.23	52,52,52,52	0
57	MG	1A	3307	1/1	0.90	0.09	31,31,31,31	0
57	MG	2A	3005	1/1	0.90	0.24	54,54,54,54	0
57	MG	2A	3441	1/1	0.90	0.09	43,43,43,43	0
57	MG	2A	3444	1/1	0.90	0.14	43,43,43,43	0
57	MG	2a	1665	1/1	0.90	0.20	46,46,46,46	0
57	MG	2A	3012	1/1	0.90	0.13	31,31,31,31	0
57	MG	1A	3981	1/1	0.90	0.10	26,26,26,26	0
57	MG	1A	3987	1/1	0.90	0.11	26,26,26,26	0
57	MG	2A	3253	1/1	0.90	0.11	51,51,51,51	0
57	MG	1A	3249	1/1	0.90	0.15	44,44,44,44	0
57	MG	1A	3607	1/1	0.90	0.08	15,15,15,15	0
57	MG	2a	1678	1/1	0.90	0.24	46,46,46,46	0
57	MG	2A	3469	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3475	1/1	0.90	0.16	44,44,44,44	0
57	MG	1A	3795	1/1	0.90	0.14	28,28,28,28	0
57	MG	2A	3264	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3046	1/1	0.90	0.21	47,47,47,47	0
57	MG	2A	3719	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3527	1/1	0.90	0.38	42,42,42,42	0
57	MG	2a	1694	1/1	0.90	0.27	52,52,52,52	0
57	MG	2A	3493	1/1	0.90	0.12	27,27,27,27	0
57	MG	1a	3653	1/1	0.90	0.19	56,56,56,56	0
57	MG	1a	3654	1/1	0.90	0.11	61,61,61,61	0
57	MG	1a	3531	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3507	1/1	0.90	0.11	36,36,36,36	0
57	MG	2a	1712	1/1	0.90	0.20	43,43,43,43	0
57	MG	2A	3739	1/1	0.90	0.17	71,71,71,71	0
57	MG	1A	3039	1/1	0.90	0.10	20,20,20,20	0
57	MG	2a	1717	1/1	0.90	0.11	39,39,39,39	0
57	MG	2A	3742	1/1	0.90	0.07	53,53,53,53	0
57	MG	2A	3743	1/1	0.90	0.07	30,30,30,30	0
57	MG	1a	3538	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3562	1/1	0.90	0.07	32,32,32,32	0
57	MG	1B	238	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3278	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3280	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3529	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	4018	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3761	1/1	0.90	0.27	72,72,72,72	0
57	MG	1A	3915	1/1	0.90	0.13	44,44,44,44	0
57	MG	1A	3217	1/1	0.90	0.17	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	2A	3294	1/1	0.90	0.19	46,46,46,46	0
57	MG	1A	3447	1/1	0.90	0.25	32,32,32,32	0
57	MG	2A	3296	1/1	0.90	0.29	39,39,39,39	0
57	MG	1A	4022	1/1	0.90	0.12	34,34,34,34	0
57	MG	2a	1755	1/1	0.90	0.23	54,54,54,54	0
57	MG	1A	3631	1/1	0.90	0.08	17,17,17,17	0
57	MG	1a	3680	1/1	0.90	0.22	48,48,48,48	0
57	MG	2A	3805	1/1	0.90	0.19	47,47,47,47	0
57	MG	1a	3560	1/1	0.90	0.19	62,62,62,62	0
57	MG	1A	3355	1/1	0.90	0.08	31,31,31,31	0
57	MG	2a	1763	1/1	0.90	0.21	60,60,60,60	0
57	MG	2a	1764	1/1	0.90	0.16	53,53,53,53	0
57	MG	2a	1767	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3311	1/1	0.90	0.13	57,57,57,57	0
57	MG	1F	312	1/1	0.90	0.22	41,41,41,41	0
57	MG	1A	3498	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3291	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3819	1/1	0.90	0.18	49,49,49,49	0
57	MG	1a	3691	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3821	1/1	0.90	0.14	62,62,62,62	0
57	MG	1N	201	1/1	0.90	0.21	47,47,47,47	0
57	MG	2A	3827	1/1	0.90	0.20	56,56,56,56	0
57	MG	2A	3828	1/1	0.90	0.20	38,38,38,38	0
57	MG	2f	202	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3580	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3335	1/1	0.90	0.18	43,43,43,43	0
57	MG	1a	3578	1/1	0.90	0.15	69,69,69,69	0
57	MG	1A	3934	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3825	1/1	0.90	0.09	51,51,51,51	0
57	MG	2A	3139	1/1	0.90	0.14	28,28,28,28	0
57	MG	2A	3140	1/1	0.90	0.12	54,54,54,54	0
57	MG	2x	101	1/1	0.90	0.25	51,51,51,51	0
57	MG	1A	3829	1/1	0.90	0.16	31,31,31,31	0
57	MG	1A	3456	1/1	0.90	0.09	41,41,41,41	0
57	MG	1A	3844	1/1	0.90	0.17	26,26,26,26	0
57	MG	1A	3946	1/1	0.90	0.14	46,46,46,46	0
57	MG	1A	4043	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	3295	1/1	0.91	0.24	43,43,43,43	0
57	MG	1V	208	1/1	0.91	0.07	48,48,48,48	0
57	MG	2A	3243	1/1	0.91	0.20	42,42,42,42	0
57	MG	2A	3245	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3503	1/1	0.91	0.12	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	3599	1/1	0.91	0.22	33,33,33,33	0
57	MG	1a	3601	1/1	0.91	0.27	47,47,47,47	0
57	MG	2A	3823	1/1	0.91	0.13	33,33,33,33	0
57	MG	1A	4053	1/1	0.91	0.08	28,28,28,28	0
57	MG	2A	3511	1/1	0.91	0.10	20,20,20,20	0
57	MG	2A	3514	1/1	0.91	0.09	24,24,24,24	0
57	MG	1A	3692	1/1	0.91	0.16	36,36,36,36	0
57	MG	1a	3605	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3361	1/1	0.91	0.28	36,36,36,36	0
57	MG	2A	3256	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3834	1/1	0.91	0.09	38,38,38,38	0
57	MG	2A	3259	1/1	0.91	0.09	46,46,46,46	0
57	MG	1A	3306	1/1	0.91	0.12	40,40,40,40	0
57	MG	1a	3608	1/1	0.91	0.15	41,41,41,41	0
57	MG	1A	4069	1/1	0.91	0.10	33,33,33,33	0
57	MG	2A	3536	1/1	0.91	0.15	38,38,38,38	0
57	MG	2B	208	1/1	0.91	0.20	47,47,47,47	0
57	MG	2A	3014	1/1	0.91	0.13	41,41,41,41	0
57	MG	2A	3015	1/1	0.91	0.16	53,53,53,53	0
57	MG	2B	212	1/1	0.91	0.16	58,58,58,58	0
57	MG	1A	3818	1/1	0.91	0.14	41,41,41,41	0
57	MG	2B	216	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3022	1/1	0.91	0.26	54,54,54,54	0
57	MG	2A	3024	1/1	0.91	0.28	42,42,42,42	0
57	MG	1A	3110	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3555	1/1	0.91	0.14	29,29,29,29	0
57	MG	2E	303	1/1	0.91	0.23	47,47,47,47	0
57	MG	1A	3371	1/1	0.91	0.08	35,35,35,35	0
57	MG	2A	3565	1/1	0.91	0.09	39,39,39,39	0
57	MG	1a	3623	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3568	1/1	0.91	0.11	28,28,28,28	0
57	MG	2A	3570	1/1	0.91	0.22	46,46,46,46	0
57	MG	1A	3721	1/1	0.91	0.15	29,29,29,29	0
57	MG	2A	3279	1/1	0.91	0.10	39,39,39,39	0
57	MG	1A	3028	1/1	0.91	0.15	17,17,17,17	0
57	MG	2A	3577	1/1	0.91	0.15	47,47,47,47	0
57	MG	2A	3281	1/1	0.91	0.12	34,34,34,34	0
57	MG	1A	3728	1/1	0.91	0.11	36,36,36,36	0
57	MG	2A	3288	1/1	0.91	0.08	45,45,45,45	0
57	MG	2T	201	1/1	0.91	0.08	39,39,39,39	0
57	MG	2A	3587	1/1	0.91	0.21	43,43,43,43	0
57	MG	2U	204	1/1	0.91	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1B	203	1/1	0.91	0.23	39,39,39,39	0
57	MG	1A	3511	1/1	0.91	0.14	30,30,30,30	0
57	MG	2A	3057	1/1	0.91	0.13	45,45,45,45	0
57	MG	2A	3069	1/1	0.91	0.15	29,29,29,29	0
57	MG	1A	3836	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3837	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3955	1/1	0.91	0.18	41,41,41,41	0
57	MG	2A	3608	1/1	0.91	0.16	50,50,50,50	0
57	MG	2A	3609	1/1	0.91	0.16	38,38,38,38	0
57	MG	1A	3838	1/1	0.91	0.10	13,13,13,13	0
57	MG	2A	3303	1/1	0.91	0.09	51,51,51,51	0
57	MG	1a	3640	1/1	0.91	0.08	40,40,40,40	0
57	MG	1a	3642	1/1	0.91	0.09	41,41,41,41	0
57	MG	1A	3960	1/1	0.91	0.15	14,14,14,14	0
57	MG	2a	1618	1/1	0.91	0.10	46,46,46,46	0
57	MG	2a	1623	1/1	0.91	0.24	41,41,41,41	0
57	MG	1A	3204	1/1	0.91	0.12	44,44,44,44	0
57	MG	1A	3845	1/1	0.91	0.17	23,23,23,23	0
57	MG	1a	3517	1/1	0.91	0.23	44,44,44,44	0
57	MG	2A	3095	1/1	0.91	0.22	53,53,53,53	0
57	MG	2a	1633	1/1	0.91	0.20	49,49,49,49	0
57	MG	2A	3322	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3454	1/1	0.91	0.14	38,38,38,38	0
57	MG	2A	3099	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3165	1/1	0.91	0.07	18,18,18,18	0
57	MG	2a	1645	1/1	0.91	0.13	51,51,51,51	0
57	MG	2a	1648	1/1	0.91	0.15	43,43,43,43	0
57	MG	2A	3107	1/1	0.91	0.29	45,45,45,45	0
57	MG	1a	3521	1/1	0.91	0.18	46,46,46,46	0
57	MG	1B	230	1/1	0.91	0.07	49,49,49,49	0
57	MG	1a	3660	1/1	0.91	0.20	40,40,40,40	0
57	MG	2a	1659	1/1	0.91	0.37	54,54,54,54	0
57	MG	2A	3336	1/1	0.91	0.17	52,52,52,52	0
57	MG	2A	3337	1/1	0.91	0.13	41,41,41,41	0
57	MG	2A	3338	1/1	0.91	0.23	36,36,36,36	0
57	MG	2a	1664	1/1	0.91	0.27	59,59,59,59	0
57	MG	1A	3322	1/1	0.91	0.22	41,41,41,41	0
57	MG	1A	3523	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3261	1/1	0.91	0.09	31,31,31,31	0
57	MG	1a	3536	1/1	0.91	0.16	66,66,66,66	0
57	MG	2A	3647	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3623	1/1	0.91	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1672	1/1	0.91	0.38	49,49,49,49	0
57	MG	2a	1673	1/1	0.91	0.24	59,59,59,59	0
57	MG	1A	3869	1/1	0.91	0.12	38,38,38,38	0
57	MG	1A	3333	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3535	1/1	0.91	0.18	41,41,41,41	0
57	MG	2A	3350	1/1	0.91	0.14	49,49,49,49	0
57	MG	1a	3543	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3658	1/1	0.91	0.20	47,47,47,47	0
57	MG	1a	3548	1/1	0.91	0.32	47,47,47,47	0
57	MG	2A	3353	1/1	0.91	0.10	54,54,54,54	0
57	MG	1B	239	1/1	0.91	0.07	25,25,25,25	0
57	MG	2a	1693	1/1	0.91	0.26	53,53,53,53	0
57	MG	1A	3632	1/1	0.91	0.11	25,25,25,25	0
57	MG	2A	3670	1/1	0.91	0.19	34,34,34,34	0
57	MG	2A	3675	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3360	1/1	0.91	0.10	45,45,45,45	0
57	MG	1a	3553	1/1	0.91	0.15	34,34,34,34	0
57	MG	1A	3038	1/1	0.91	0.16	45,45,45,45	0
57	MG	1A	3888	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3367	1/1	0.91	0.19	35,35,35,35	0
57	MG	2A	3683	1/1	0.91	0.14	42,42,42,42	0
57	MG	2A	3145	1/1	0.91	0.10	39,39,39,39	0
57	MG	1A	3547	1/1	0.91	0.24	30,30,30,30	0
57	MG	2a	1721	1/1	0.91	0.14	37,37,37,37	0
57	MG	2A	3373	1/1	0.91	0.20	41,41,41,41	0
57	MG	2A	3150	1/1	0.91	0.09	50,50,50,50	0
57	MG	2a	1726	1/1	0.91	0.18	38,38,38,38	0
57	MG	1A	3638	1/1	0.91	0.09	16,16,16,16	0
57	MG	2A	3386	1/1	0.91	0.22	52,52,52,52	0
57	MG	1A	3646	1/1	0.91	0.07	9,9,9,9	0
57	MG	1A	3275	1/1	0.91	0.39	32,32,32,32	0
57	MG	1a	3565	1/1	0.91	0.13	62,62,62,62	0
57	MG	1a	3566	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3707	1/1	0.91	0.12	53,53,53,53	0
57	MG	2a	1745	1/1	0.91	0.08	48,48,48,48	0
57	MG	2A	3395	1/1	0.91	0.25	44,44,44,44	0
57	MG	1A	3072	1/1	0.91	0.21	50,50,50,50	0
57	MG	2A	3164	1/1	0.91	0.19	53,53,53,53	0
57	MG	1F	313	1/1	0.91	0.22	26,26,26,26	0
57	MG	2A	3407	1/1	0.91	0.42	65,65,65,65	0
57	MG	1A	3566	1/1	0.91	0.15	50,50,50,50	0
57	MG	1a	3708	1/1	0.91	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3792	1/1	0.91	0.07	11,11,11,11	0
57	MG	1A	3222	1/1	0.91	0.10	32,32,32,32	0
57	MG	1O	204	1/1	0.91	0.06	41,41,41,41	0
57	MG	2A	3732	1/1	0.91	0.19	44,44,44,44	0
57	MG	1A	3182	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3420	1/1	0.91	0.17	58,58,58,58	0
57	MG	2A	3182	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3187	1/1	0.91	0.15	49,49,49,49	0
57	MG	1Q	206	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3191	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3194	1/1	0.91	0.07	47,47,47,47	0
57	MG	1a	3718	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3442	1/1	0.91	0.17	49,49,49,49	0
57	MG	1S	202	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3204	1/1	0.91	0.16	40,40,40,40	0
57	MG	2a	1776	1/1	0.91	0.13	54,54,54,54	0
57	MG	1a	3589	1/1	0.91	0.26	39,39,39,39	0
57	MG	2A	3208	1/1	0.91	0.13	34,34,34,34	0
57	MG	2A	3759	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3484	1/1	0.91	0.11	42,42,42,42	0
57	MG	2A	3463	1/1	0.91	0.33	42,42,42,42	0
57	MG	1b	301	1/1	0.91	0.09	68,68,68,68	0
57	MG	1A	3002	1/1	0.91	0.09	29,29,29,29	0
57	MG	2A	3215	1/1	0.91	0.17	52,52,52,52	0
57	MG	1e	201	1/1	0.91	0.14	39,39,39,39	0
57	MG	2A	3793	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3794	1/1	0.91	0.10	30,30,30,30	0
57	MG	1A	3494	1/1	0.91	0.15	42,42,42,42	0
57	MG	2A	3477	1/1	0.91	0.11	23,23,23,23	0
57	MG	2A	3482	1/1	0.91	0.10	13,13,13,13	0
57	MG	1A	3292	1/1	0.91	0.08	36,36,36,36	0
57	MG	1A	3688	1/1	0.91	0.17	48,48,48,48	0
59	ZN	24	501	1/1	0.91	0.10	120,120,120,120	0
57	MG	1A	3553	1/1	0.92	0.21	59,59,59,59	0
57	MG	2A	3797	1/1	0.92	0.09	35,35,35,35	0
57	MG	2A	3800	1/1	0.92	0.33	57,57,57,57	0
57	MG	1a	3549	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3665	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3266	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3471	1/1	0.92	0.18	47,47,47,47	0
57	MG	2A	3213	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3331	1/1	0.92	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3943	1/1	0.92	0.21	40,40,40,40	0
57	MG	2A	3812	1/1	0.92	0.10	28,28,28,28	0
57	MG	2A	3218	1/1	0.92	0.19	36,36,36,36	0
57	MG	2A	3220	1/1	0.92	0.14	69,69,69,69	0
57	MG	2A	3487	1/1	0.92	0.07	44,44,44,44	0
57	MG	1A	3801	1/1	0.92	0.18	33,33,33,33	0
57	MG	1A	3093	1/1	0.92	0.08	25,25,25,25	0
57	MG	2A	3231	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3497	1/1	0.92	0.11	23,23,23,23	0
57	MG	2A	3232	1/1	0.92	0.10	42,42,42,42	0
57	MG	1A	3673	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3677	1/1	0.92	0.08	16,16,16,16	0
57	MG	1A	3027	1/1	0.92	0.09	31,31,31,31	0
57	MG	2A	3504	1/1	0.92	0.15	37,37,37,37	0
57	MG	2A	3506	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3813	1/1	0.92	0.21	49,49,49,49	0
57	MG	1A	3815	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3478	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3401	1/1	0.92	0.09	44,44,44,44	0
57	MG	1k	201	1/1	0.92	0.10	44,44,44,44	0
57	MG	1D	314	1/1	0.92	0.19	26,26,26,26	0
57	MG	1a	3573	1/1	0.92	0.22	53,53,53,53	0
57	MG	1E	305	1/1	0.92	0.23	28,28,28,28	0
57	MG	1a	3575	1/1	0.92	0.21	55,55,55,55	0
57	MG	1x	103	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3258	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3405	1/1	0.92	0.17	29,29,29,29	0
57	MG	2A	3260	1/1	0.92	0.24	43,43,43,43	0
57	MG	2B	218	1/1	0.92	0.07	48,48,48,48	0
57	MG	1A	3483	1/1	0.92	0.30	46,46,46,46	0
57	MG	2A	3539	1/1	0.92	0.17	48,48,48,48	0
57	MG	1A	3693	1/1	0.92	0.08	35,35,35,35	0
57	MG	2A	3544	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3583	1/1	0.92	0.08	22,22,22,22	0
57	MG	1x	110	1/1	0.92	0.14	36,36,36,36	0
57	MG	2A	3267	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3827	1/1	0.92	0.13	8,8,8,8	0
57	MG	2E	309	1/1	0.92	0.09	49,49,49,49	0
57	MG	2E	310	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3552	1/1	0.92	0.24	47,47,47,47	0
57	MG	1a	3585	1/1	0.92	0.28	52,52,52,52	0
57	MG	1A	3408	1/1	0.92	0.13	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	3485	1/1	0.92	0.22	49,49,49,49	0
57	MG	2F	306	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3707	1/1	0.92	0.08	35,35,35,35	0
57	MG	1A	3710	1/1	0.92	0.10	31,31,31,31	0
57	MG	2A	3567	1/1	0.92	0.15	43,43,43,43	0
57	MG	1A	3711	1/1	0.92	0.11	32,32,32,32	0
57	MG	1A	3988	1/1	0.92	0.09	17,17,17,17	0
57	MG	1N	203	1/1	0.92	0.10	30,30,30,30	0
57	MG	2T	202	1/1	0.92	0.14	57,57,57,57	0
57	MG	2A	3023	1/1	0.92	0.18	49,49,49,49	0
57	MG	1O	201	1/1	0.92	0.06	54,54,54,54	0
57	MG	1A	3841	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3283	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3285	1/1	0.92	0.07	47,47,47,47	0
57	MG	2A	3286	1/1	0.92	0.19	42,42,42,42	0
57	MG	25	102	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3287	1/1	0.92	0.16	49,49,49,49	0
57	MG	1A	3488	1/1	0.92	0.32	45,45,45,45	0
57	MG	27	102	1/1	0.92	0.15	44,44,44,44	0
57	MG	27	103	1/1	0.92	0.13	39,39,39,39	0
57	MG	1a	3600	1/1	0.92	0.23	29,29,29,29	0
57	MG	2A	3291	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3037	1/1	0.92	0.08	38,38,38,38	0
57	MG	2A	3596	1/1	0.92	0.16	22,22,22,22	0
57	MG	2A	3599	1/1	0.92	0.10	25,25,25,25	0
57	MG	2A	3601	1/1	0.92	0.11	29,29,29,29	0
57	MG	1A	3336	1/1	0.92	0.12	33,33,33,33	0
57	MG	2a	1615	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	4006	1/1	0.92	0.13	41,41,41,41	0
57	MG	2A	3047	1/1	0.92	0.20	33,33,33,33	0
57	MG	1a	3603	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3493	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3300	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3853	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3276	1/1	0.92	0.24	26,26,26,26	0
57	MG	2A	3064	1/1	0.92	0.21	28,28,28,28	0
57	MG	2A	3065	1/1	0.92	0.21	33,33,33,33	0
57	MG	1A	4014	1/1	0.92	0.07	37,37,37,37	0
57	MG	2A	3312	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3428	1/1	0.92	0.19	41,41,41,41	0
57	MG	1A	3738	1/1	0.92	0.10	14,14,14,14	0
57	MG	2a	1647	1/1	0.92	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3317	1/1	0.92	0.31	56,56,56,56	0
57	MG	2A	3080	1/1	0.92	0.22	46,46,46,46	0
57	MG	1A	3865	1/1	0.92	0.14	14,14,14,14	0
57	MG	1a	3614	1/1	0.92	0.28	61,61,61,61	0
57	MG	1V	207	1/1	0.92	0.14	47,47,47,47	0
57	MG	2a	1658	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3088	1/1	0.92	0.12	35,35,35,35	0
57	MG	1a	3616	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3634	1/1	0.92	0.12	34,34,34,34	0
57	MG	2A	3330	1/1	0.92	0.10	38,38,38,38	0
57	MG	1a	3617	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3597	1/1	0.92	0.10	27,27,27,27	0
57	MG	2a	1666	1/1	0.92	0.17	43,43,43,43	0
57	MG	2A	3333	1/1	0.92	0.11	47,47,47,47	0
57	MG	1a	3621	1/1	0.92	0.19	48,48,48,48	0
57	MG	1a	3622	1/1	0.92	0.10	59,59,59,59	0
57	MG	1A	3098	1/1	0.92	0.07	33,33,33,33	0
57	MG	1Y	201	1/1	0.92	0.13	35,35,35,35	0
57	MG	1A	4025	1/1	0.92	0.10	11,11,11,11	0
57	MG	1A	3209	1/1	0.92	0.18	26,26,26,26	0
57	MG	2A	3103	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3105	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3870	1/1	0.92	0.12	18,18,18,18	0
57	MG	10	102	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3752	1/1	0.92	0.15	22,22,22,22	0
57	MG	1A	3872	1/1	0.92	0.11	42,42,42,42	0
57	MG	1a	3635	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3661	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3115	1/1	0.92	0.22	40,40,40,40	0
57	MG	1A	3213	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3875	1/1	0.92	0.12	41,41,41,41	0
57	MG	2A	3119	1/1	0.92	0.10	42,42,42,42	0
57	MG	2a	1696	1/1	0.92	0.26	49,49,49,49	0
57	MG	2A	3354	1/1	0.92	0.07	51,51,51,51	0
57	MG	1A	3290	1/1	0.92	0.08	42,42,42,42	0
57	MG	1A	3883	1/1	0.92	0.33	29,29,29,29	0
57	MG	2A	3678	1/1	0.92	0.20	43,43,43,43	0
57	MG	15	3202	1/1	0.92	0.17	31,31,31,31	0
57	MG	1A	3440	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	4048	1/1	0.92	0.12	33,33,33,33	0
57	MG	1A	4050	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3612	1/1	0.92	0.18	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3074	1/1	0.92	0.06	19,19,19,19	0
57	MG	1A	3112	1/1	0.92	0.23	29,29,29,29	0
57	MG	2A	3371	1/1	0.92	0.17	37,37,37,37	0
57	MG	1a	3504	1/1	0.92	0.13	47,47,47,47	0
57	MG	2A	3380	1/1	0.92	0.20	31,31,31,31	0
57	MG	2A	3696	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3698	1/1	0.92	0.12	30,30,30,30	0
57	MG	2A	3381	1/1	0.92	0.30	44,44,44,44	0
57	MG	2a	1733	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3359	1/1	0.92	0.07	41,41,41,41	0
57	MG	1A	3775	1/1	0.92	0.11	40,40,40,40	0
57	MG	1a	3508	1/1	0.92	0.27	59,59,59,59	0
57	MG	1a	3670	1/1	0.92	0.09	59,59,59,59	0
57	MG	1a	3671	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3389	1/1	0.92	0.18	35,35,35,35	0
57	MG	1a	3510	1/1	0.92	0.22	44,44,44,44	0
57	MG	1A	3113	1/1	0.92	0.26	37,37,37,37	0
57	MG	1a	3513	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	4073	1/1	0.92	0.10	32,32,32,32	0
57	MG	1A	4074	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3116	1/1	0.92	0.16	30,30,30,30	0
57	MG	1A	3901	1/1	0.92	0.09	27,27,27,27	0
57	MG	1A	3783	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3052	1/1	0.92	0.08	36,36,36,36	0
57	MG	1a	3525	1/1	0.92	0.21	39,39,39,39	0
57	MG	1a	3527	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3176	1/1	0.92	0.14	44,44,44,44	0
57	MG	2a	1765	1/1	0.92	0.19	55,55,55,55	0
57	MG	1A	3129	1/1	0.92	0.14	26,26,26,26	0
57	MG	1a	3690	1/1	0.92	0.08	31,31,31,31	0
57	MG	1a	3529	1/1	0.92	0.15	41,41,41,41	0
57	MG	1A	3786	1/1	0.92	0.15	45,45,45,45	0
57	MG	2a	1771	1/1	0.92	0.13	40,40,40,40	0
57	MG	2A	3432	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3453	1/1	0.92	0.18	38,38,38,38	0
57	MG	2A	3750	1/1	0.92	0.13	47,47,47,47	0
57	MG	1A	3525	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3089	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3755	1/1	0.92	0.12	32,32,32,32	0
57	MG	2A	3193	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3924	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3196	1/1	0.92	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3380	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3764	1/1	0.92	0.10	42,42,42,42	0
57	MG	2A	3450	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3768	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3770	1/1	0.92	0.16	59,59,59,59	0
57	MG	2q	201	1/1	0.92	0.07	55,55,55,55	0
57	MG	2A	3771	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3774	1/1	0.92	0.10	30,30,30,30	0
57	MG	2A	3452	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3200	1/1	0.92	0.11	26,26,26,26	0
57	MG	1A	3141	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	3544	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3792	1/1	0.92	0.15	31,31,31,31	0
57	MG	2A	3460	1/1	0.92	0.15	36,36,36,36	0
57	MG	1A	3351	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3779	1/1	0.93	0.11	30,30,30,30	0
57	MG	2A	3781	1/1	0.93	0.15	51,51,51,51	0
57	MG	2A	3782	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3812	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3784	1/1	0.93	0.12	22,22,22,22	0
57	MG	1A	3268	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3192	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3353	1/1	0.93	0.19	44,44,44,44	0
57	MG	2A	3455	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3354	1/1	0.93	0.16	47,47,47,47	0
57	MG	2A	3798	1/1	0.93	0.10	38,38,38,38	0
57	MG	1a	3688	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3198	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3461	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3463	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3166	1/1	0.93	0.28	32,32,32,32	0
57	MG	2A	3202	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3270	1/1	0.93	0.19	46,46,46,46	0
57	MG	1A	3629	1/1	0.93	0.10	33,33,33,33	0
57	MG	2A	3474	1/1	0.93	0.16	38,38,38,38	0
57	MG	2A	3206	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3077	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3826	1/1	0.93	0.07	36,36,36,36	0
57	MG	2A	3479	1/1	0.93	0.07	50,50,50,50	0
57	MG	2A	3481	1/1	0.93	0.11	41,41,41,41	0
57	MG	1A	3475	1/1	0.93	0.07	41,41,41,41	0
57	MG	1a	3698	1/1	0.93	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3476	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3830	1/1	0.93	0.13	41,41,41,41	0
57	MG	2A	3489	1/1	0.93	0.14	34,34,34,34	0
57	MG	1A	3831	1/1	0.93	0.31	21,21,21,21	0
57	MG	2A	3491	1/1	0.93	0.08	34,34,34,34	0
57	MG	1a	3524	1/1	0.93	0.14	47,47,47,47	0
57	MG	1A	3360	1/1	0.93	0.09	31,31,31,31	0
57	MG	2A	3498	1/1	0.93	0.18	48,48,48,48	0
57	MG	2A	3221	1/1	0.93	0.15	41,41,41,41	0
57	MG	2B	201	1/1	0.93	0.08	58,58,58,58	0
57	MG	1a	3526	1/1	0.93	0.16	35,35,35,35	0
57	MG	2A	3226	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3835	1/1	0.93	0.10	33,33,33,33	0
57	MG	1a	3711	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3174	1/1	0.93	0.09	25,25,25,25	0
57	MG	2B	209	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3363	1/1	0.93	0.18	42,42,42,42	0
57	MG	1A	3364	1/1	0.93	0.09	30,30,30,30	0
57	MG	2A	3237	1/1	0.93	0.13	47,47,47,47	0
57	MG	2B	213	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3840	1/1	0.93	0.05	23,23,23,23	0
57	MG	1A	3482	1/1	0.93	0.13	37,37,37,37	0
57	MG	1A	4058	1/1	0.93	0.12	13,13,13,13	0
57	MG	1a	3539	1/1	0.93	0.36	54,54,54,54	0
57	MG	1A	3210	1/1	0.93	0.26	24,24,24,24	0
57	MG	1A	3212	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	4068	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3049	1/1	0.93	0.12	14,14,14,14	0
57	MG	1A	4071	1/1	0.93	0.21	46,46,46,46	0
57	MG	1A	3852	1/1	0.93	0.07	30,30,30,30	0
57	MG	2E	307	1/1	0.93	0.12	36,36,36,36	0
57	MG	1A	3215	1/1	0.93	0.26	29,29,29,29	0
57	MG	1A	3181	1/1	0.93	0.06	43,43,43,43	0
57	MG	1n	101	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3542	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3221	1/1	0.93	0.20	45,45,45,45	0
57	MG	1A	3671	1/1	0.93	0.15	15,15,15,15	0
57	MG	1A	3047	1/1	0.93	0.13	22,22,22,22	0
57	MG	1A	3296	1/1	0.93	0.23	21,21,21,21	0
57	MG	2F	307	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3497	1/1	0.93	0.07	48,48,48,48	0
57	MG	1A	3298	1/1	0.93	0.07	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	3561	1/1	0.93	0.10	50,50,50,50	0
57	MG	1B	205	1/1	0.93	0.28	50,50,50,50	0
57	MG	1A	3227	1/1	0.93	0.24	21,21,21,21	0
57	MG	1A	3389	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3274	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3183	1/1	0.93	0.08	23,23,23,23	0
57	MG	2U	203	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3394	1/1	0.93	0.12	46,46,46,46	0
57	MG	2V	201	1/1	0.93	0.27	42,42,42,42	0
57	MG	1A	3509	1/1	0.93	0.16	31,31,31,31	0
57	MG	2A	3006	1/1	0.93	0.14	45,45,45,45	0
57	MG	2W	202	1/1	0.93	0.16	43,43,43,43	0
57	MG	2W	203	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3397	1/1	0.93	0.16	37,37,37,37	0
57	MG	1A	3700	1/1	0.93	0.10	41,41,41,41	0
57	MG	1A	3702	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3398	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3311	1/1	0.93	0.18	42,42,42,42	0
57	MG	1A	3517	1/1	0.93	0.17	25,25,25,25	0
57	MG	1A	3402	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3588	1/1	0.93	0.11	17,17,17,17	0
57	MG	28	102	1/1	0.93	0.19	39,39,39,39	0
57	MG	2a	1601	1/1	0.93	0.21	45,45,45,45	0
57	MG	2A	3028	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3231	1/1	0.93	0.28	43,43,43,43	0
57	MG	2a	1605	1/1	0.93	0.16	49,49,49,49	0
57	MG	1A	3714	1/1	0.93	0.13	31,31,31,31	0
57	MG	1A	3406	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3235	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3243	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3041	1/1	0.93	0.21	36,36,36,36	0
57	MG	1A	3727	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3410	1/1	0.93	0.25	46,46,46,46	0
57	MG	2a	1622	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3729	1/1	0.93	0.10	30,30,30,30	0
57	MG	2a	1624	1/1	0.93	0.15	50,50,50,50	0
57	MG	1D	313	1/1	0.93	0.20	36,36,36,36	0
57	MG	2A	3053	1/1	0.93	0.08	36,36,36,36	0
57	MG	2A	3302	1/1	0.93	0.22	47,47,47,47	0
57	MG	2A	3054	1/1	0.93	0.13	38,38,38,38	0
57	MG	2A	3613	1/1	0.93	0.21	46,46,46,46	0
57	MG	2A	3055	1/1	0.93	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	3308	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3731	1/1	0.93	0.09	32,32,32,32	0
57	MG	1A	3411	1/1	0.93	0.15	29,29,29,29	0
57	MG	2A	3062	1/1	0.93	0.24	38,38,38,38	0
57	MG	1A	3529	1/1	0.93	0.10	42,42,42,42	0
57	MG	1E	307	1/1	0.93	0.09	36,36,36,36	0
57	MG	1A	3530	1/1	0.93	0.28	27,27,27,27	0
57	MG	2a	1650	1/1	0.93	0.16	57,57,57,57	0
57	MG	2A	3072	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3073	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3074	1/1	0.93	0.16	40,40,40,40	0
57	MG	1E	313	1/1	0.93	0.13	46,46,46,46	0
57	MG	1F	303	1/1	0.93	0.17	14,14,14,14	0
57	MG	2a	1660	1/1	0.93	0.34	50,50,50,50	0
57	MG	1A	3532	1/1	0.93	0.09	18,18,18,18	0
57	MG	2A	3328	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3413	1/1	0.93	0.09	21,21,21,21	0
57	MG	1F	309	1/1	0.93	0.04	15,15,15,15	0
57	MG	1A	3745	1/1	0.93	0.10	11,11,11,11	0
57	MG	1A	3186	1/1	0.93	0.06	41,41,41,41	0
57	MG	1A	3540	1/1	0.93	0.30	27,27,27,27	0
57	MG	1A	3940	1/1	0.93	0.14	39,39,39,39	0
57	MG	1a	3610	1/1	0.93	0.23	43,43,43,43	0
57	MG	2A	3092	1/1	0.93	0.20	48,48,48,48	0
57	MG	1a	3611	1/1	0.93	0.09	41,41,41,41	0
57	MG	1F	314	1/1	0.93	0.09	33,33,33,33	0
57	MG	1A	3415	1/1	0.93	0.29	43,43,43,43	0
57	MG	2a	1676	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3342	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3096	1/1	0.93	0.15	20,20,20,20	0
57	MG	1G	204	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3417	1/1	0.93	0.08	58,58,58,58	0
57	MG	2a	1686	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3558	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3559	1/1	0.93	0.25	28,28,28,28	0
57	MG	1A	3424	1/1	0.93	0.10	20,20,20,20	0
57	MG	2A	3662	1/1	0.93	0.12	65,65,65,65	0
57	MG	2A	3106	1/1	0.93	0.28	52,52,52,52	0
57	MG	1A	3150	1/1	0.93	0.09	30,30,30,30	0
57	MG	1A	3948	1/1	0.93	0.16	42,42,42,42	0
57	MG	1A	3099	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3674	1/1	0.93	0.09	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	2a	1699	1/1	0.93	0.21	37,37,37,37	0
57	MG	1R	205	1/1	0.93	0.13	22,22,22,22	0
57	MG	2A	3113	1/1	0.93	0.12	46,46,46,46	0
57	MG	1a	3626	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3359	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3950	1/1	0.93	0.16	32,32,32,32	0
57	MG	1A	3567	1/1	0.93	0.10	26,26,26,26	0
57	MG	1a	3629	1/1	0.93	0.13	45,45,45,45	0
57	MG	1A	3332	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3684	1/1	0.93	0.11	24,24,24,24	0
57	MG	2a	1720	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3569	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3196	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3126	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	1725	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3691	1/1	0.93	0.20	59,59,59,59	0
57	MG	1a	3634	1/1	0.93	0.33	38,38,38,38	0
57	MG	1A	3436	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3377	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3695	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3378	1/1	0.93	0.27	46,46,46,46	0
57	MG	2a	1734	1/1	0.93	0.22	46,46,46,46	0
57	MG	2a	1735	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3959	1/1	0.93	0.07	43,43,43,43	0
57	MG	2a	1737	1/1	0.93	0.18	38,38,38,38	0
57	MG	2a	1739	1/1	0.93	0.15	43,43,43,43	0
57	MG	1a	3637	1/1	0.93	0.14	44,44,44,44	0
57	MG	2a	1742	1/1	0.93	0.17	48,48,48,48	0
57	MG	2A	3702	1/1	0.93	0.10	28,28,28,28	0
57	MG	2a	1744	1/1	0.93	0.29	45,45,45,45	0
57	MG	1V	202	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3384	1/1	0.93	0.21	41,41,41,41	0
57	MG	1a	3639	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3438	1/1	0.93	0.11	32,32,32,32	0
57	MG	1A	3579	1/1	0.93	0.10	14,14,14,14	0
57	MG	1A	3963	1/1	0.93	0.08	9,9,9,9	0
57	MG	1A	3965	1/1	0.93	0.09	20,20,20,20	0
57	MG	1a	3648	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3966	1/1	0.93	0.06	73,73,73,73	0
57	MG	2A	3394	1/1	0.93	0.20	41,41,41,41	0
57	MG	2A	3720	1/1	0.93	0.07	41,41,41,41	0
57	MG	2A	3721	1/1	0.93	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3334	1/1	0.93	0.08	22,22,22,22	0
57	MG	1A	3789	1/1	0.93	0.51	22,22,22,22	0
57	MG	2A	3398	1/1	0.93	0.07	33,33,33,33	0
57	MG	2A	3154	1/1	0.93	0.16	42,42,42,42	0
57	MG	2A	3404	1/1	0.93	0.20	41,41,41,41	0
57	MG	1A	3581	1/1	0.93	0.13	16,16,16,16	0
57	MG	2A	3406	1/1	0.93	0.18	40,40,40,40	0
57	MG	2A	3736	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3092	1/1	0.93	0.15	45,45,45,45	0
57	MG	1a	3658	1/1	0.93	0.14	46,46,46,46	0
57	MG	2A	3741	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3409	1/1	0.93	0.12	45,45,45,45	0
57	MG	10	105	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3744	1/1	0.93	0.08	33,33,33,33	0
57	MG	2A	3411	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3253	1/1	0.93	0.07	24,24,24,24	0
57	MG	2d	301	1/1	0.93	0.25	45,45,45,45	0
57	MG	2A	3415	1/1	0.93	0.15	44,44,44,44	0
57	MG	1A	3444	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3340	1/1	0.93	0.19	33,33,33,33	0
57	MG	1A	3254	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3259	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3448	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3426	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3160	1/1	0.93	0.27	16,16,16,16	0
57	MG	1A	3346	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3805	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3434	1/1	0.93	0.13	49,49,49,49	0
57	MG	1A	3347	1/1	0.93	0.12	27,27,27,27	0
57	MG	1A	3111	1/1	0.93	0.06	24,24,24,24	0
57	MG	2A	3183	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3186	1/1	0.93	0.19	50,50,50,50	0
57	MG	2A	3443	1/1	0.93	0.29	52,52,52,52	0
57	MG	17	105	1/1	0.94	0.06	41,41,41,41	0
57	MG	18	101	1/1	0.94	0.24	47,47,47,47	0
57	MG	18	102	1/1	0.94	0.11	27,27,27,27	0
57	MG	2A	3087	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3013	1/1	0.94	0.12	17,17,17,17	0
57	MG	1a	3643	1/1	0.94	0.11	26,26,26,26	0
57	MG	1A	4057	1/1	0.94	0.09	28,28,28,28	0
57	MG	2A	3543	1/1	0.94	0.09	24,24,24,24	0
57	MG	1A	3617	1/1	0.94	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	4060	1/1	0.94	0.08	38,38,38,38	0
57	MG	2B	204	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3547	1/1	0.94	0.16	44,44,44,44	0
57	MG	1a	3505	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	4062	1/1	0.94	0.11	36,36,36,36	0
57	MG	1A	3776	1/1	0.94	0.08	10,10,10,10	0
57	MG	1A	3094	1/1	0.94	0.08	31,31,31,31	0
57	MG	1A	3893	1/1	0.94	0.15	47,47,47,47	0
57	MG	1A	3898	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3556	1/1	0.94	0.11	22,22,22,22	0
57	MG	2B	214	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3100	1/1	0.94	0.11	44,44,44,44	0
57	MG	2A	3563	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3625	1/1	0.94	0.09	46,46,46,46	0
57	MG	2D	301	1/1	0.94	0.14	35,35,35,35	0
57	MG	2A	3306	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3781	1/1	0.94	0.10	29,29,29,29	0
57	MG	1a	3663	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3188	1/1	0.94	0.37	23,23,23,23	0
57	MG	1A	3190	1/1	0.94	0.09	29,29,29,29	0
57	MG	2A	3572	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3313	1/1	0.94	0.17	42,42,42,42	0
57	MG	1a	3669	1/1	0.94	0.19	50,50,50,50	0
57	MG	1a	3519	1/1	0.94	0.06	37,37,37,37	0
57	MG	2A	3580	1/1	0.94	0.13	22,22,22,22	0
57	MG	1A	3909	1/1	0.94	0.12	26,26,26,26	0
57	MG	2A	3318	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3111	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3320	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3913	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3118	1/1	0.94	0.31	36,36,36,36	0
57	MG	1a	3674	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	3156	1/1	0.94	0.17	32,32,32,32	0
57	MG	1A	3521	1/1	0.94	0.15	30,30,30,30	0
57	MG	1A	3388	1/1	0.94	0.30	32,32,32,32	0
57	MG	2A	3329	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3280	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3642	1/1	0.94	0.09	29,29,29,29	0
57	MG	2A	3605	1/1	0.94	0.17	48,48,48,48	0
57	MG	2T	204	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3124	1/1	0.94	0.15	37,37,37,37	0
57	MG	1A	3390	1/1	0.94	0.06	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	3926	1/1	0.94	0.06	48,48,48,48	0
57	MG	2A	3130	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3391	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3133	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3135	1/1	0.94	0.23	48,48,48,48	0
57	MG	1A	3342	1/1	0.94	0.14	43,43,43,43	0
57	MG	1a	3687	1/1	0.94	0.15	34,34,34,34	0
57	MG	2A	3620	1/1	0.94	0.28	48,48,48,48	0
57	MG	2A	3138	1/1	0.94	0.16	26,26,26,26	0
57	MG	1A	3932	1/1	0.94	0.05	24,24,24,24	0
57	MG	1A	3232	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3395	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3625	1/1	0.94	0.20	37,37,37,37	0
57	MG	1A	3663	1/1	0.94	0.12	6,6,6,6	0
57	MG	1A	3533	1/1	0.94	0.26	29,29,29,29	0
57	MG	1A	3534	1/1	0.94	0.18	21,21,21,21	0
57	MG	1A	3802	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3396	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3149	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3021	1/1	0.94	0.17	31,31,31,31	0
57	MG	2a	1608	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3462	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3064	1/1	0.94	0.10	37,37,37,37	0
57	MG	2a	1612	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3356	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3156	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3358	1/1	0.94	0.19	59,59,59,59	0
57	MG	1A	3552	1/1	0.94	0.13	26,26,26,26	0
57	MG	2a	1621	1/1	0.94	0.07	36,36,36,36	0
57	MG	1a	3554	1/1	0.94	0.13	55,55,55,55	0
57	MG	1a	3706	1/1	0.94	0.06	60,60,60,60	0
57	MG	1A	3678	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3679	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	1626	1/1	0.94	0.13	45,45,45,45	0
57	MG	1a	3709	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3167	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3650	1/1	0.94	0.13	41,41,41,41	0
57	MG	1a	3558	1/1	0.94	0.32	62,62,62,62	0
57	MG	2A	3652	1/1	0.94	0.06	37,37,37,37	0
57	MG	1D	301	1/1	0.94	0.18	24,24,24,24	0
57	MG	1D	302	1/1	0.94	0.08	25,25,25,25	0
57	MG	2a	1637	1/1	0.94	0.34	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1640	1/1	0.94	0.26	39,39,39,39	0
57	MG	2A	3375	1/1	0.94	0.19	24,24,24,24	0
57	MG	2a	1644	1/1	0.94	0.29	40,40,40,40	0
57	MG	1D	305	1/1	0.94	0.15	30,30,30,30	0
57	MG	2A	3175	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3379	1/1	0.94	0.24	35,35,35,35	0
57	MG	1D	309	1/1	0.94	0.13	28,28,28,28	0
57	MG	1A	3682	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3285	1/1	0.94	0.10	33,33,33,33	0
57	MG	2a	1652	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3179	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3469	1/1	0.94	0.13	28,28,28,28	0
57	MG	2a	1657	1/1	0.94	0.20	33,33,33,33	0
57	MG	1A	3289	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3561	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3471	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3404	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3694	1/1	0.94	0.06	10,10,10,10	0
57	MG	2A	3190	1/1	0.94	0.12	39,39,39,39	0
57	MG	2A	3393	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3348	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3135	1/1	0.94	0.35	26,26,26,26	0
57	MG	1A	3044	1/1	0.94	0.07	19,19,19,19	0
57	MG	2A	3397	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3169	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3401	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3195	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3140	1/1	0.94	0.10	35,35,35,35	0
57	MG	1p	101	1/1	0.94	0.14	44,44,44,44	0
57	MG	2a	1674	1/1	0.94	0.24	55,55,55,55	0
57	MG	2a	1675	1/1	0.94	0.18	57,57,57,57	0
57	MG	1A	3055	1/1	0.94	0.20	35,35,35,35	0
57	MG	2A	3200	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3412	1/1	0.94	0.08	30,30,30,30	0
57	MG	2a	1679	1/1	0.94	0.12	45,45,45,45	0
57	MG	1a	3588	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3975	1/1	0.94	0.06	38,38,38,38	0
57	MG	1A	3578	1/1	0.94	0.10	36,36,36,36	0
57	MG	2a	1687	1/1	0.94	0.29	43,43,43,43	0
57	MG	1A	3252	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3091	1/1	0.94	0.12	37,37,37,37	0
57	MG	1A	3984	1/1	0.94	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1x	109	1/1	0.94	0.16	39,39,39,39	0
57	MG	2A	3706	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3211	1/1	0.94	0.29	38,38,38,38	0
57	MG	1A	3358	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3710	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3842	1/1	0.94	0.16	31,31,31,31	0
57	MG	2a	1697	1/1	0.94	0.26	55,55,55,55	0
57	MG	1x	113	1/1	0.94	0.16	38,38,38,38	0
57	MG	2A	3428	1/1	0.94	0.15	35,35,35,35	0
57	MG	2a	1704	1/1	0.94	0.16	51,51,51,51	0
57	MG	1N	206	1/1	0.94	0.09	32,32,32,32	0
57	MG	2a	1709	1/1	0.94	0.22	44,44,44,44	0
57	MG	2A	3003	1/1	0.94	0.25	38,38,38,38	0
57	MG	2A	3219	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3992	1/1	0.94	0.12	25,25,25,25	0
57	MG	1A	3994	1/1	0.94	0.05	29,29,29,29	0
57	MG	2A	3725	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3727	1/1	0.94	0.17	25,25,25,25	0
57	MG	2A	3437	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3438	1/1	0.94	0.34	43,43,43,43	0
57	MG	2A	3439	1/1	0.94	0.15	48,48,48,48	0
57	MG	2A	3731	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3222	1/1	0.94	0.12	29,29,29,29	0
57	MG	1P	202	1/1	0.94	0.51	21,21,21,21	0
57	MG	1A	3995	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3997	1/1	0.94	0.12	50,50,50,50	0
57	MG	2a	1729	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3229	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3843	1/1	0.94	0.08	26,26,26,26	0
57	MG	1A	3145	1/1	0.94	0.11	25,25,25,25	0
57	MG	2A	3233	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3418	1/1	0.94	0.15	27,27,27,27	0
57	MG	1A	3420	1/1	0.94	0.10	29,29,29,29	0
57	MG	2A	3456	1/1	0.94	0.27	46,46,46,46	0
57	MG	1A	3849	1/1	0.94	0.15	11,11,11,11	0
57	MG	1A	3851	1/1	0.94	0.11	19,19,19,19	0
57	MG	1A	3309	1/1	0.94	0.14	39,39,39,39	0
57	MG	2A	3751	1/1	0.94	0.23	63,63,63,63	0
57	MG	2A	3240	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3495	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3426	1/1	0.94	0.14	35,35,35,35	0
57	MG	2a	1746	1/1	0.94	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3036	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3737	1/1	0.94	0.09	9,9,9,9	0
57	MG	2A	3248	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3473	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3762	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3861	1/1	0.94	0.11	12,12,12,12	0
57	MG	2A	3765	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3040	1/1	0.94	0.17	44,44,44,44	0
57	MG	2a	1758	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	3255	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3042	1/1	0.94	0.23	56,56,56,56	0
57	MG	2A	3045	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3257	1/1	0.94	0.21	45,45,45,45	0
57	MG	1W	204	1/1	0.94	0.17	28,28,28,28	0
57	MG	1A	3595	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3485	1/1	0.94	0.11	29,29,29,29	0
57	MG	1A	4023	1/1	0.94	0.12	16,16,16,16	0
57	MG	2A	3261	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3050	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3740	1/1	0.94	0.10	21,21,21,21	0
57	MG	1A	3256	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3258	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3433	1/1	0.94	0.26	54,54,54,54	0
57	MG	10	103	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3601	1/1	0.94	0.07	29,29,29,29	0
57	MG	2A	3270	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3271	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3058	1/1	0.94	0.12	32,32,32,32	0
57	MG	1A	3873	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3505	1/1	0.94	0.21	25,25,25,25	0
57	MG	1A	3506	1/1	0.94	0.27	30,30,30,30	0
57	MG	1A	4041	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	3877	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3809	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3319	1/1	0.94	0.13	32,32,32,32	0
57	MG	1A	3216	1/1	0.94	0.11	30,30,30,30	0
57	MG	1A	3263	1/1	0.94	0.21	37,37,37,37	0
57	MG	2A	3516	1/1	0.94	0.11	31,31,31,31	0
57	MG	2A	3517	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3771	1/1	0.94	0.08	22,22,22,22	0
57	MG	2A	3520	1/1	0.94	0.07	25,25,25,25	0
57	MG	2A	3081	1/1	0.94	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3526	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3082	1/1	0.94	0.05	42,42,42,42	0
57	MG	2A	3284	1/1	0.94	0.12	41,41,41,41	0
57	MG	18	105	1/1	0.95	0.09	30,30,30,30	0
57	MG	2A	3462	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3154	1/1	0.95	0.21	22,22,22,22	0
57	MG	1a	3713	1/1	0.95	0.06	42,42,42,42	0
57	MG	2A	3465	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3067	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3105	1/1	0.95	0.18	23,23,23,23	0
57	MG	1A	4024	1/1	0.95	0.08	19,19,19,19	0
57	MG	2A	3224	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3225	1/1	0.95	0.04	45,45,45,45	0
57	MG	1A	3681	1/1	0.95	0.14	42,42,42,42	0
57	MG	2A	3227	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	4026	1/1	0.95	0.10	28,28,28,28	0
57	MG	2A	3478	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3441	1/1	0.95	0.13	22,22,22,22	0
57	MG	2A	3230	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	4028	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3683	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3814	1/1	0.95	0.06	37,37,37,37	0
57	MG	1a	3512	1/1	0.95	0.13	12,12,12,12	0
57	MG	2A	3486	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3818	1/1	0.95	0.15	31,31,31,31	0
57	MG	1A	3684	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	3286	1/1	0.95	0.20	47,47,47,47	0
57	MG	1a	3516	1/1	0.95	0.08	67,67,67,67	0
57	MG	1A	4035	1/1	0.95	0.06	36,36,36,36	0
57	MG	1A	3846	1/1	0.95	0.19	24,24,24,24	0
57	MG	2A	3825	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3287	1/1	0.95	0.17	21,21,21,21	0
57	MG	2A	3241	1/1	0.95	0.13	30,30,30,30	0
57	MG	2A	3242	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3106	1/1	0.95	0.15	13,13,13,13	0
57	MG	2A	3244	1/1	0.95	0.11	52,52,52,52	0
57	MG	1t	201	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3161	1/1	0.95	0.09	43,43,43,43	0
57	MG	1a	3522	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3366	1/1	0.95	0.09	29,29,29,29	0
57	MG	1A	3548	1/1	0.95	0.09	26,26,26,26	0
57	MG	2A	3250	1/1	0.95	0.16	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	2A	3251	1/1	0.95	0.16	41,41,41,41	0
57	MG	2B	205	1/1	0.95	0.12	55,55,55,55	0
57	MG	1x	104	1/1	0.95	0.30	38,38,38,38	0
57	MG	1A	4045	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	4046	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3162	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3695	1/1	0.95	0.18	46,46,46,46	0
57	MG	1A	4051	1/1	0.95	0.12	12,12,12,12	0
57	MG	1A	3163	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3522	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3555	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3556	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3370	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3293	1/1	0.95	0.09	24,24,24,24	0
57	MG	1A	3452	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3532	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3373	1/1	0.95	0.05	37,37,37,37	0
57	MG	2A	3534	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3375	1/1	0.95	0.21	12,12,12,12	0
57	MG	2A	3009	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3455	1/1	0.95	0.09	22,22,22,22	0
57	MG	1A	3715	1/1	0.95	0.08	8,8,8,8	0
57	MG	2E	306	1/1	0.95	0.12	24,24,24,24	0
57	MG	1a	3545	1/1	0.95	0.13	58,58,58,58	0
57	MG	1a	3546	1/1	0.95	0.24	39,39,39,39	0
57	MG	1a	3547	1/1	0.95	0.17	58,58,58,58	0
57	MG	2A	3545	1/1	0.95	0.16	28,28,28,28	0
57	MG	1A	3716	1/1	0.95	0.10	17,17,17,17	0
57	MG	1A	4070	1/1	0.95	0.16	45,45,45,45	0
57	MG	2A	3027	1/1	0.95	0.20	34,34,34,34	0
57	MG	1A	3718	1/1	0.95	0.05	11,11,11,11	0
57	MG	2A	3550	1/1	0.95	0.08	13,13,13,13	0
57	MG	2A	3029	1/1	0.95	0.19	31,31,31,31	0
57	MG	1A	3223	1/1	0.95	0.23	28,28,28,28	0
57	MG	1A	3457	1/1	0.95	0.17	29,29,29,29	0
57	MG	2Q	202	1/1	0.95	0.17	37,37,37,37	0
57	MG	2A	3032	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3880	1/1	0.95	0.15	27,27,27,27	0
57	MG	1A	3224	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3226	1/1	0.95	0.14	24,24,24,24	0
57	MG	1A	4078	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	4079	1/1	0.95	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3887	1/1	0.95	0.13	21,21,21,21	0
57	MG	1A	3300	1/1	0.95	0.15	34,34,34,34	0
57	MG	2A	3569	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3289	1/1	0.95	0.23	49,49,49,49	0
57	MG	2A	3043	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3044	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3301	1/1	0.95	0.22	40,40,40,40	0
57	MG	2A	3293	1/1	0.95	0.08	34,34,34,34	0
57	MG	1B	202	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3730	1/1	0.95	0.08	9,9,9,9	0
57	MG	2I	102	1/1	0.95	0.12	39,39,39,39	0
57	MG	23	101	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3576	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3577	1/1	0.95	0.10	18,18,18,18	0
57	MG	1A	3304	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3895	1/1	0.95	0.16	26,26,26,26	0
57	MG	1a	3571	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3897	1/1	0.95	0.08	43,43,43,43	0
57	MG	1B	211	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3592	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3040	1/1	0.95	0.18	20,20,20,20	0
57	MG	1B	216	1/1	0.95	0.07	29,29,29,29	0
57	MG	2a	1604	1/1	0.95	0.18	44,44,44,44	0
57	MG	2A	3307	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3598	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3387	1/1	0.95	0.08	29,29,29,29	0
57	MG	2A	3600	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3309	1/1	0.95	0.17	40,40,40,40	0
57	MG	1B	220	1/1	0.95	0.09	27,27,27,27	0
57	MG	2a	1613	1/1	0.95	0.21	44,44,44,44	0
57	MG	1B	221	1/1	0.95	0.08	23,23,23,23	0
57	MG	1a	3582	1/1	0.95	0.21	36,36,36,36	0
57	MG	2a	1616	1/1	0.95	0.09	45,45,45,45	0
57	MG	1a	3583	1/1	0.95	0.10	33,33,33,33	0
57	MG	1A	3043	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3582	1/1	0.95	0.08	37,37,37,37	0
57	MG	1a	3586	1/1	0.95	0.14	59,59,59,59	0
57	MG	2A	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	1a	3587	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3614	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3902	1/1	0.95	0.10	27,27,27,27	0
57	MG	2A	3617	1/1	0.95	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1629	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3618	1/1	0.95	0.20	46,46,46,46	0
57	MG	1B	225	1/1	0.95	0.15	50,50,50,50	0
57	MG	1B	226	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3323	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3308	1/1	0.95	0.13	27,27,27,27	0
57	MG	1A	3474	1/1	0.95	0.23	34,34,34,34	0
57	MG	1A	3750	1/1	0.95	0.08	10,10,10,10	0
57	MG	2a	1638	1/1	0.95	0.22	37,37,37,37	0
57	MG	2A	3327	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3015	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3755	1/1	0.95	0.05	11,11,11,11	0
57	MG	1B	234	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3310	1/1	0.95	0.05	28,28,28,28	0
57	MG	1A	3168	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3046	1/1	0.95	0.11	27,27,27,27	0
57	MG	1A	3920	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3922	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3764	1/1	0.95	0.09	38,38,38,38	0
57	MG	2a	1654	1/1	0.95	0.28	31,31,31,31	0
57	MG	1A	3114	1/1	0.95	0.20	24,24,24,24	0
57	MG	2A	3636	1/1	0.95	0.10	50,50,50,50	0
57	MG	1D	303	1/1	0.95	0.22	31,31,31,31	0
57	MG	1A	3766	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3594	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3929	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3085	1/1	0.95	0.20	26,26,26,26	0
57	MG	2A	3344	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3318	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3245	1/1	0.95	0.21	32,32,32,32	0
57	MG	1A	3774	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3935	1/1	0.95	0.09	16,16,16,16	0
57	MG	1A	3179	1/1	0.95	0.17	29,29,29,29	0
57	MG	1A	3937	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3324	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3602	1/1	0.95	0.08	9,9,9,9	0
57	MG	1A	3403	1/1	0.95	0.13	48,48,48,48	0
57	MG	1F	307	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3490	1/1	0.95	0.16	32,32,32,32	0
57	MG	2A	3659	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3782	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3608	1/1	0.95	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3609	1/1	0.95	0.09	21,21,21,21	0
57	MG	1A	3180	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3664	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	1680	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3666	1/1	0.95	0.14	44,44,44,44	0
57	MG	2a	1682	1/1	0.95	0.27	46,46,46,46	0
57	MG	2A	3667	1/1	0.95	0.11	19,19,19,19	0
57	MG	2a	1684	1/1	0.95	0.25	48,48,48,48	0
57	MG	1A	3327	1/1	0.95	0.22	40,40,40,40	0
57	MG	1G	201	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3129	1/1	0.95	0.09	37,37,37,37	0
57	MG	1G	202	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3117	1/1	0.95	0.16	28,28,28,28	0
57	MG	2A	3368	1/1	0.95	0.26	37,37,37,37	0
57	MG	1A	3407	1/1	0.95	0.12	46,46,46,46	0
57	MG	1a	3633	1/1	0.95	0.24	36,36,36,36	0
57	MG	1G	205	1/1	0.95	0.10	40,40,40,40	0
57	MG	1H	201	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3374	1/1	0.95	0.15	33,33,33,33	0
57	MG	1A	3016	1/1	0.95	0.24	32,32,32,32	0
57	MG	2a	1698	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3376	1/1	0.95	0.07	29,29,29,29	0
57	MG	1A	3615	1/1	0.95	0.12	14,14,14,14	0
57	MG	2a	1701	1/1	0.95	0.18	46,46,46,46	0
57	MG	1N	202	1/1	0.95	0.14	29,29,29,29	0
57	MG	2a	1705	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3616	1/1	0.95	0.07	18,18,18,18	0
57	MG	2a	1707	1/1	0.95	0.15	27,27,27,27	0
57	MG	2a	1708	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3019	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3618	1/1	0.95	0.07	14,14,14,14	0
57	MG	2A	3382	1/1	0.95	0.11	46,46,46,46	0
57	MG	1O	203	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3185	1/1	0.95	0.16	23,23,23,23	0
57	MG	1A	3796	1/1	0.95	0.08	27,27,27,27	0
57	MG	2A	3148	1/1	0.95	0.29	49,49,49,49	0
57	MG	2a	1718	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3699	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3127	1/1	0.95	0.13	46,46,46,46	0
57	MG	2A	3701	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3051	1/1	0.95	0.10	32,32,32,32	0
57	MG	1R	201	1/1	0.95	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1R	202	1/1	0.95	0.13	22,22,22,22	0
57	MG	1A	3799	1/1	0.95	0.07	38,38,38,38	0
57	MG	2a	1727	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3132	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3004	1/1	0.95	0.08	11,11,11,11	0
57	MG	1T	201	1/1	0.95	0.19	38,38,38,38	0
57	MG	1A	3971	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3023	1/1	0.95	0.13	36,36,36,36	0
57	MG	2A	3712	1/1	0.95	0.08	20,20,20,20	0
57	MG	1A	3633	1/1	0.95	0.08	9,9,9,9	0
57	MG	2A	3165	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3717	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3402	1/1	0.95	0.17	29,29,29,29	0
57	MG	2a	1738	1/1	0.95	0.14	37,37,37,37	0
57	MG	1a	3665	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3974	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3634	1/1	0.95	0.07	14,14,14,14	0
57	MG	2A	3722	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3195	1/1	0.95	0.10	28,28,28,28	0
57	MG	1A	3262	1/1	0.95	0.13	35,35,35,35	0
57	MG	1A	3980	1/1	0.95	0.08	14,14,14,14	0
57	MG	1A	3419	1/1	0.95	0.19	28,28,28,28	0
57	MG	2a	1748	1/1	0.95	0.18	43,43,43,43	0
57	MG	2a	1749	1/1	0.95	0.13	61,61,61,61	0
57	MG	1W	201	1/1	0.95	0.13	24,24,24,24	0
57	MG	1A	3983	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3009	1/1	0.95	0.05	12,12,12,12	0
57	MG	2A	3413	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3643	1/1	0.95	0.08	24,24,24,24	0
57	MG	1a	3678	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3012	1/1	0.95	0.11	18,18,18,18	0
57	MG	2A	3738	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	3647	1/1	0.95	0.12	10,10,10,10	0
57	MG	1A	3516	1/1	0.95	0.09	11,11,11,11	0
57	MG	1A	3001	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3202	1/1	0.95	0.08	11,11,11,11	0
57	MG	2A	3427	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3661	1/1	0.95	0.10	16,16,16,16	0
57	MG	1A	3429	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3431	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3095	1/1	0.95	0.15	11,11,11,11	0
57	MG	10	108	1/1	0.95	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	4005	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3431	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3666	1/1	0.95	0.07	10,10,10,10	0
57	MG	1A	4008	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3756	1/1	0.95	0.12	45,45,45,45	0
57	MG	1a	3694	1/1	0.95	0.12	36,36,36,36	0
57	MG	13	103	1/1	0.95	0.07	32,32,32,32	0
57	MG	13	104	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3760	1/1	0.95	0.10	39,39,39,39	0
57	MG	1A	3096	1/1	0.95	0.09	26,26,26,26	0
57	MG	2d	302	1/1	0.95	0.13	48,48,48,48	0
57	MG	15	3208	1/1	0.95	0.11	20,20,20,20	0
57	MG	2A	3763	1/1	0.95	0.10	45,45,45,45	0
57	MG	1a	3700	1/1	0.95	0.13	28,28,28,28	0
57	MG	1A	3147	1/1	0.95	0.13	18,18,18,18	0
57	MG	2A	3447	1/1	0.95	0.20	40,40,40,40	0
57	MG	2A	3449	1/1	0.95	0.11	37,37,37,37	0
57	MG	2k	201	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	4011	1/1	0.95	0.08	17,17,17,17	0
57	MG	2A	3451	1/1	0.95	0.16	46,46,46,46	0
57	MG	16	103	1/1	0.95	0.12	39,39,39,39	0
57	MG	2t	201	1/1	0.95	0.27	48,48,48,48	0
57	MG	2A	3775	1/1	0.95	0.10	23,23,23,23	0
57	MG	1A	3014	1/1	0.95	0.06	17,17,17,17	0
57	MG	1A	4017	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3834	1/1	0.95	0.07	33,33,33,33	0
57	MG	2x	107	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3066	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3216	1/1	0.95	0.23	39,39,39,39	0
57	MG	1A	3528	1/1	0.95	0.08	28,28,28,28	0
57	MG	2A	3170	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3329	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3203	1/1	0.96	0.06	18,18,18,18	0
57	MG	2A	3363	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3385	1/1	0.96	0.16	17,17,17,17	0
57	MG	1a	3537	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3032	1/1	0.96	0.18	22,22,22,22	0
57	MG	1A	3712	1/1	0.96	0.05	35,35,35,35	0
57	MG	1a	3714	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3288	1/1	0.96	0.08	30,30,30,30	0
57	MG	2A	3372	1/1	0.96	0.27	32,32,32,32	0
57	MG	1A	3968	1/1	0.96	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3512	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3185	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3143	1/1	0.96	0.33	22,22,22,22	0
57	MG	1A	3717	1/1	0.96	0.09	16,16,16,16	0
57	MG	1A	3839	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3603	1/1	0.96	0.09	18,18,18,18	0
57	MG	2O	203	1/1	0.96	0.08	44,44,44,44	0
57	MG	2P	201	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3053	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3041	1/1	0.96	0.17	19,19,19,19	0
57	MG	1A	3337	1/1	0.96	0.16	33,33,33,33	0
57	MG	1D	310	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3057	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3341	1/1	0.96	0.29	33,33,33,33	0
57	MG	2T	203	1/1	0.96	0.12	24,24,24,24	0
57	MG	1A	3120	1/1	0.96	0.14	28,28,28,28	0
57	MG	1E	304	1/1	0.96	0.13	14,14,14,14	0
57	MG	2U	202	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3294	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3121	1/1	0.96	0.35	23,23,23,23	0
57	MG	1A	3122	1/1	0.96	0.28	23,23,23,23	0
57	MG	2A	3391	1/1	0.96	0.26	40,40,40,40	0
57	MG	1E	310	1/1	0.96	0.12	11,11,11,11	0
57	MG	1A	3736	1/1	0.96	0.09	25,25,25,25	0
57	MG	1x	102	1/1	0.96	0.05	37,37,37,37	0
57	MG	2A	3207	1/1	0.96	0.24	45,45,45,45	0
57	MG	2A	3639	1/1	0.96	0.06	34,34,34,34	0
57	MG	2I	101	1/1	0.96	0.41	38,38,38,38	0
57	MG	1A	3990	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3991	1/1	0.96	0.09	20,20,20,20	0
57	MG	25	101	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3526	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3993	1/1	0.96	0.09	29,29,29,29	0
57	MG	1F	306	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3399	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3214	1/1	0.96	0.09	28,28,28,28	0
57	MG	1F	308	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3855	1/1	0.96	0.04	11,11,11,11	0
57	MG	28	103	1/1	0.96	0.09	26,26,26,26	0
57	MG	1a	3572	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3124	1/1	0.96	0.34	28,28,28,28	0
57	MG	1A	3299	1/1	0.96	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3862	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	4003	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3620	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3621	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3744	1/1	0.96	0.07	44,44,44,44	0
57	MG	1a	3581	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3417	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3013	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3257	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3531	1/1	0.96	0.18	23,23,23,23	0
57	MG	2A	3665	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3751	1/1	0.96	0.06	10,10,10,10	0
57	MG	2A	3422	1/1	0.96	0.11	35,35,35,35	0
57	MG	2a	1620	1/1	0.96	0.20	47,47,47,47	0
57	MG	1A	3627	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	3753	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	4013	1/1	0.96	0.04	32,32,32,32	0
57	MG	2A	3671	1/1	0.96	0.08	37,37,37,37	0
57	MG	2A	3026	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3234	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3628	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	4016	1/1	0.96	0.10	44,44,44,44	0
57	MG	1N	204	1/1	0.96	0.05	29,29,29,29	0
57	MG	1N	205	1/1	0.96	0.15	25,25,25,25	0
57	MG	2a	1632	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3349	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3461	1/1	0.96	0.27	27,27,27,27	0
57	MG	1O	202	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3876	1/1	0.96	0.23	36,36,36,36	0
57	MG	1A	3761	1/1	0.96	0.07	33,33,33,33	0
57	MG	1P	201	1/1	0.96	0.21	14,14,14,14	0
57	MG	2a	1639	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3126	1/1	0.96	0.11	24,24,24,24	0
57	MG	1A	3302	1/1	0.96	0.04	23,23,23,23	0
57	MG	2a	1642	1/1	0.96	0.15	63,63,63,63	0
57	MG	2a	1643	1/1	0.96	0.13	43,43,43,43	0
57	MG	1Q	202	1/1	0.96	0.11	28,28,28,28	0
57	MG	1Q	203	1/1	0.96	0.08	38,38,38,38	0
57	MG	2a	1646	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3448	1/1	0.96	0.17	39,39,39,39	0
57	MG	1Q	204	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3881	1/1	0.96	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3882	1/1	0.96	0.20	21,21,21,21	0
57	MG	1A	3303	1/1	0.96	0.09	30,30,30,30	0
57	MG	2A	3048	1/1	0.96	0.11	22,22,22,22	0
57	MG	2A	3454	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3539	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3466	1/1	0.96	0.16	26,26,26,26	0
57	MG	1A	3544	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3467	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3639	1/1	0.96	0.05	13,13,13,13	0
57	MG	1A	3640	1/1	0.96	0.06	9,9,9,9	0
57	MG	1A	3158	1/1	0.96	0.19	12,12,12,12	0
57	MG	2A	3262	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3549	1/1	0.96	0.07	23,23,23,23	0
57	MG	2A	3060	1/1	0.96	0.14	40,40,40,40	0
57	MG	2A	3713	1/1	0.96	0.15	32,32,32,32	0
57	MG	2A	3061	1/1	0.96	0.18	41,41,41,41	0
57	MG	1U	205	1/1	0.96	0.24	26,26,26,26	0
57	MG	2A	3716	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3470	1/1	0.96	0.05	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3472	1/1	0.96	0.18	49,49,49,49	0
57	MG	1U	210	1/1	0.96	0.14	17,17,17,17	0
57	MG	2A	3067	1/1	0.96	0.07	39,39,39,39	0
57	MG	1a	3619	1/1	0.96	0.20	37,37,37,37	0
57	MG	1A	3551	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3896	1/1	0.96	0.11	40,40,40,40	0
57	MG	2A	3726	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	4039	1/1	0.96	0.12	30,30,30,30	0
57	MG	1V	204	1/1	0.96	0.16	21,21,21,21	0
57	MG	2A	3480	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3048	1/1	0.96	0.09	25,25,25,25	0
57	MG	2A	3077	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3649	1/1	0.96	0.07	9,9,9,9	0
57	MG	1A	3107	1/1	0.96	0.07	18,18,18,18	0
57	MG	1A	4044	1/1	0.96	0.06	26,26,26,26	0
57	MG	1W	205	1/1	0.96	0.09	12,12,12,12	0
57	MG	1X	103	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3554	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3085	1/1	0.96	0.28	31,31,31,31	0
57	MG	1A	3193	1/1	0.96	0.23	29,29,29,29	0
57	MG	2A	3492	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3658	1/1	0.96	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3495	1/1	0.96	0.14	31,31,31,31	0
57	MG	2A	3745	1/1	0.96	0.17	43,43,43,43	0
57	MG	2A	3496	1/1	0.96	0.09	29,29,29,29	0
57	MG	1Y	203	1/1	0.96	0.29	35,35,35,35	0
57	MG	1A	3904	1/1	0.96	0.06	27,27,27,27	0
57	MG	2A	3749	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3265	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3557	1/1	0.96	0.05	27,27,27,27	0
57	MG	2a	1702	1/1	0.96	0.18	35,35,35,35	0
57	MG	2A	3501	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3753	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3911	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3076	1/1	0.96	0.11	18,18,18,18	0
57	MG	1A	3010	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3505	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3312	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3362	1/1	0.96	0.13	43,43,43,43	0
57	MG	1a	3644	1/1	0.96	0.15	24,24,24,24	0
57	MG	1A	4061	1/1	0.96	0.08	53,53,53,53	0
57	MG	2a	1715	1/1	0.96	0.20	45,45,45,45	0
57	MG	2A	3510	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3313	1/1	0.96	0.13	16,16,16,16	0
57	MG	2A	3513	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	4063	1/1	0.96	0.07	37,37,37,37	0
57	MG	13	101	1/1	0.96	0.15	25,25,25,25	0
57	MG	2A	3767	1/1	0.96	0.11	33,33,33,33	0
57	MG	2a	1722	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3136	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	4065	1/1	0.96	0.06	25,25,25,25	0
57	MG	1A	4066	1/1	0.96	0.14	28,28,28,28	0
57	MG	1a	3656	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3305	1/1	0.96	0.21	53,53,53,53	0
57	MG	1A	3481	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3777	1/1	0.96	0.13	28,28,28,28	0
57	MG	15	3204	1/1	0.96	0.13	30,30,30,30	0
57	MG	15	3205	1/1	0.96	0.15	27,27,27,27	0
57	MG	2A	3112	1/1	0.96	0.16	20,20,20,20	0
57	MG	1A	3921	1/1	0.96	0.08	35,35,35,35	0
57	MG	1a	3661	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3230	1/1	0.96	0.07	29,29,29,29	0
57	MG	2A	3786	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3787	1/1	0.96	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	16	101	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3791	1/1	0.96	0.05	38,38,38,38	0
57	MG	1A	3674	1/1	0.96	0.05	10,10,10,10	0
57	MG	2A	3315	1/1	0.96	0.18	31,31,31,31	0
57	MG	2A	3538	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3795	1/1	0.96	0.11	22,22,22,22	0
57	MG	2A	3796	1/1	0.96	0.07	26,26,26,26	0
57	MG	1a	3666	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3540	1/1	0.96	0.07	31,31,31,31	0
57	MG	2A	3121	1/1	0.96	0.07	34,34,34,34	0
57	MG	1a	3667	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3421	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3422	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3927	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3572	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3680	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3197	1/1	0.96	0.04	25,25,25,25	0
57	MG	1A	3487	1/1	0.96	0.15	18,18,18,18	0
57	MG	2A	3132	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3425	1/1	0.96	0.06	40,40,40,40	0
57	MG	1a	3502	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3806	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3198	1/1	0.96	0.19	8,8,8,8	0
57	MG	1A	4085	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3427	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3559	1/1	0.96	0.09	38,38,38,38	0
57	MG	2a	1766	1/1	0.96	0.13	38,38,38,38	0
57	MG	2A	3561	1/1	0.96	0.11	18,18,18,18	0
57	MG	1A	3809	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3233	1/1	0.96	0.17	17,17,17,17	0
57	MG	1A	3320	1/1	0.96	0.08	29,29,29,29	0
57	MG	2A	3826	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3372	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3814	1/1	0.96	0.08	23,23,23,23	0
57	MG	1A	3079	1/1	0.96	0.24	25,25,25,25	0
57	MG	1A	3945	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3241	1/1	0.96	0.08	27,27,27,27	0
57	MG	1B	212	1/1	0.96	0.09	33,33,33,33	0
57	MG	1B	213	1/1	0.96	0.14	23,23,23,23	0
57	MG	2A	3152	1/1	0.96	0.35	51,51,51,51	0
57	MG	2A	3576	1/1	0.96	0.09	38,38,38,38	0
57	MG	2e	201	1/1	0.96	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3025	1/1	0.96	0.25	53,53,53,53	0
57	MG	2A	3578	1/1	0.96	0.21	39,39,39,39	0
57	MG	2A	3579	1/1	0.96	0.07	12,12,12,12	0
57	MG	1A	3326	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3155	1/1	0.96	0.31	53,53,53,53	0
57	MG	2A	3583	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3820	1/1	0.96	0.08	30,30,30,30	0
57	MG	2l	201	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3062	1/1	0.96	0.20	29,29,29,29	0
57	MG	1A	3502	1/1	0.96	0.13	47,47,47,47	0
57	MG	2q	202	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3823	1/1	0.96	0.07	9,9,9,9	0
57	MG	1A	3953	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3701	1/1	0.96	0.11	18,18,18,18	0
57	MG	2v	102	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3437	1/1	0.96	0.14	24,24,24,24	0
57	MG	2x	102	1/1	0.96	0.15	44,44,44,44	0
57	MG	1a	3703	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3166	1/1	0.96	0.13	24,24,24,24	0
57	MG	2x	106	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3956	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3597	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3328	1/1	0.96	0.19	27,27,27,27	0
57	MG	1a	3530	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3762	1/1	0.97	0.08	7,7,7,7	0
57	MG	1A	3102	1/1	0.97	0.18	29,29,29,29	0
57	MG	2A	3197	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3641	1/1	0.97	0.07	16,16,16,16	0
57	MG	2O	202	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3472	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3103	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3767	1/1	0.97	0.07	9,9,9,9	0
57	MG	2A	3399	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3236	1/1	0.97	0.09	18,18,18,18	0
57	MG	2A	3203	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3237	1/1	0.97	0.09	19,19,19,19	0
57	MG	1A	3104	1/1	0.97	0.35	29,29,29,29	0
57	MG	1A	3297	1/1	0.97	0.16	32,32,32,32	0
57	MG	1x	112	1/1	0.97	0.09	31,31,31,31	0
57	MG	1A	3652	1/1	0.97	0.05	36,36,36,36	0
57	MG	1a	3576	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	4029	1/1	0.97	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	4030	1/1	0.97	0.08	10,10,10,10	0
57	MG	1A	3242	1/1	0.97	0.05	26,26,26,26	0
57	MG	1O	205	1/1	0.97	0.04	29,29,29,29	0
57	MG	2A	3007	1/1	0.97	0.07	31,31,31,31	0
57	MG	2A	3645	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3655	1/1	0.97	0.06	11,11,11,11	0
57	MG	2A	3010	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	4033	1/1	0.97	0.10	11,11,11,11	0
57	MG	1A	3037	1/1	0.97	0.24	22,22,22,22	0
57	MG	1Q	201	1/1	0.97	0.14	19,19,19,19	0
57	MG	1A	3005	1/1	0.97	0.08	29,29,29,29	0
57	MG	2A	3017	1/1	0.97	0.21	48,48,48,48	0
57	MG	2A	3018	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3424	1/1	0.97	0.06	40,40,40,40	0
57	MG	25	104	1/1	0.97	0.05	43,43,43,43	0
57	MG	2A	3425	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3657	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3416	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3021	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3563	1/1	0.97	0.08	13,13,13,13	0
57	MG	2A	3429	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3192	1/1	0.97	0.29	14,14,14,14	0
57	MG	1A	3664	1/1	0.97	0.07	12,12,12,12	0
57	MG	2A	3025	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3144	1/1	0.97	0.14	17,17,17,17	0
57	MG	1A	3024	1/1	0.97	0.27	28,28,28,28	0
57	MG	2a	1606	1/1	0.97	0.11	23,23,23,23	0
57	MG	2A	3435	1/1	0.97	0.06	31,31,31,31	0
57	MG	1S	201	1/1	0.97	0.06	34,34,34,34	0
57	MG	2a	1609	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3905	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3108	1/1	0.97	0.11	18,18,18,18	0
57	MG	1A	3305	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3250	1/1	0.97	0.10	44,44,44,44	0
57	MG	1A	4047	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3034	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3035	1/1	0.97	0.25	34,34,34,34	0
57	MG	1A	3790	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3489	1/1	0.97	0.16	23,23,23,23	0
57	MG	2a	1619	1/1	0.97	0.12	36,36,36,36	0
57	MG	2A	3446	1/1	0.97	0.09	45,45,45,45	0
57	MG	2A	3038	1/1	0.97	0.25	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3423	1/1	0.97	0.16	25,25,25,25	0
57	MG	1A	3109	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3675	1/1	0.97	0.11	6,6,6,6	0
57	MG	1A	3676	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3688	1/1	0.97	0.10	39,39,39,39	0
57	MG	2a	1627	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3148	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	3365	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3149	1/1	0.97	0.10	32,32,32,32	0
57	MG	1V	206	1/1	0.97	0.12	24,24,24,24	0
57	MG	1A	3054	1/1	0.97	0.12	19,19,19,19	0
57	MG	2A	3457	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3006	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3925	1/1	0.97	0.15	34,34,34,34	0
57	MG	1a	3612	1/1	0.97	0.15	47,47,47,47	0
57	MG	1W	202	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3369	1/1	0.97	0.20	16,16,16,16	0
57	MG	1A	3083	1/1	0.97	0.11	13,13,13,13	0
57	MG	1A	3084	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3585	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3930	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3058	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3059	1/1	0.97	0.15	32,32,32,32	0
57	MG	2A	3708	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3501	1/1	0.97	0.14	44,44,44,44	0
57	MG	1a	3620	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3587	1/1	0.97	0.07	19,19,19,19	0
57	MG	2A	3063	1/1	0.97	0.10	26,26,26,26	0
57	MG	1Z	301	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3689	1/1	0.97	0.10	19,19,19,19	0
57	MG	2A	3066	1/1	0.97	0.04	36,36,36,36	0
57	MG	1Z	303	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3068	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3026	1/1	0.97	0.09	11,11,11,11	0
57	MG	2A	3070	1/1	0.97	0.04	25,25,25,25	0
57	MG	2A	3071	1/1	0.97	0.09	19,19,19,19	0
57	MG	1A	3205	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3435	1/1	0.97	0.11	31,31,31,31	0
57	MG	10	104	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3011	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3938	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3939	1/1	0.97	0.07	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3078	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3376	1/1	0.97	0.14	14,14,14,14	0
57	MG	1A	4080	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3696	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3494	1/1	0.97	0.11	42,42,42,42	0
57	MG	1I	103	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3816	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3735	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3697	1/1	0.97	0.15	37,37,37,37	0
57	MG	2A	3737	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3508	1/1	0.97	0.23	34,34,34,34	0
57	MG	1A	3699	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3059	1/1	0.97	0.08	25,25,25,25	0
57	MG	15	3201	1/1	0.97	0.37	27,27,27,27	0
57	MG	1B	204	1/1	0.97	0.09	33,33,33,33	0
57	MG	15	3203	1/1	0.97	0.35	17,17,17,17	0
57	MG	1A	3378	1/1	0.97	0.42	29,29,29,29	0
57	MG	1B	206	1/1	0.97	0.06	34,34,34,34	0
57	MG	15	3206	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3297	1/1	0.97	0.10	63,63,63,63	0
57	MG	2a	1685	1/1	0.97	0.12	42,42,42,42	0
57	MG	15	3207	1/1	0.97	0.17	24,24,24,24	0
57	MG	1a	3650	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3379	1/1	0.97	0.22	27,27,27,27	0
57	MG	2A	3097	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3007	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3824	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3513	1/1	0.97	0.12	34,34,34,34	0
57	MG	1A	3264	1/1	0.97	0.09	26,26,26,26	0
57	MG	17	102	1/1	0.97	0.06	20,20,20,20	0
57	MG	2A	3518	1/1	0.97	0.11	18,18,18,18	0
57	MG	2A	3104	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3708	1/1	0.97	0.07	18,18,18,18	0
57	MG	2A	3521	1/1	0.97	0.08	22,22,22,22	0
57	MG	17	104	1/1	0.97	0.12	25,25,25,25	0
57	MG	2A	3523	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3828	1/1	0.97	0.11	12,12,12,12	0
57	MG	1a	3662	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3045	1/1	0.97	0.10	21,21,21,21	0
57	MG	1B	215	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3323	1/1	0.97	0.12	26,26,26,26	0
57	MG	2A	3531	1/1	0.97	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3606	1/1	0.97	0.07	16,16,16,16	0
57	MG	18	106	1/1	0.97	0.10	52,52,52,52	0
57	MG	2A	3772	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3773	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3713	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	3501	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3116	1/1	0.97	0.10	41,41,41,41	0
57	MG	2A	3537	1/1	0.97	0.09	22,22,22,22	0
57	MG	1A	3833	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3211	1/1	0.97	0.16	29,29,29,29	0
57	MG	2A	3780	1/1	0.97	0.08	18,18,18,18	0
57	MG	1A	3962	1/1	0.97	0.07	17,17,17,17	0
57	MG	2A	3120	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3267	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3030	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3008	1/1	0.97	0.05	6,6,6,6	0
57	MG	1A	3065	1/1	0.97	0.10	15,15,15,15	0
57	MG	1a	3509	1/1	0.97	0.07	55,55,55,55	0
57	MG	2A	3790	1/1	0.97	0.10	31,31,31,31	0
57	MG	1B	228	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3033	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3330	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3125	1/1	0.97	0.07	47,47,47,47	0
57	MG	1a	3514	1/1	0.97	0.17	48,48,48,48	0
57	MG	1a	3683	1/1	0.97	0.05	61,61,61,61	0
57	MG	2A	3553	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3725	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3392	1/1	0.97	0.17	31,31,31,31	0
57	MG	1a	3686	1/1	0.97	0.18	61,61,61,61	0
57	MG	1A	3279	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3035	1/1	0.97	0.07	8,8,8,8	0
57	MG	1A	3281	1/1	0.97	0.12	30,30,30,30	0
57	MG	2a	1741	1/1	0.97	0.31	46,46,46,46	0
57	MG	2A	3562	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3341	1/1	0.97	0.04	34,34,34,34	0
57	MG	2A	3564	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3847	1/1	0.97	0.26	19,19,19,19	0
57	MG	1A	3170	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3732	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	3850	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3172	1/1	0.97	0.26	25,25,25,25	0
57	MG	1A	3986	1/1	0.97	0.06	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3147	1/1	0.97	0.12	32,32,32,32	0
57	MG	1D	307	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3735	1/1	0.97	0.06	11,11,11,11	0
57	MG	1A	3622	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3822	1/1	0.97	0.12	41,41,41,41	0
57	MG	2a	1756	1/1	0.97	0.21	39,39,39,39	0
57	MG	2A	3575	1/1	0.97	0.12	29,29,29,29	0
57	MG	1A	3068	1/1	0.97	0.14	10,10,10,10	0
57	MG	1D	312	1/1	0.97	0.12	16,16,16,16	0
57	MG	1A	3624	1/1	0.97	0.09	46,46,46,46	0
57	MG	1a	3532	1/1	0.97	0.29	42,42,42,42	0
57	MG	1a	3704	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3857	1/1	0.97	0.11	11,11,11,11	0
57	MG	2A	3582	1/1	0.97	0.06	29,29,29,29	0
57	MG	1a	3534	1/1	0.97	0.12	17,17,17,17	0
57	MG	2A	3832	1/1	0.97	0.06	47,47,47,47	0
57	MG	1a	3535	1/1	0.97	0.13	42,42,42,42	0
57	MG	1E	302	1/1	0.97	0.11	23,23,23,23	0
57	MG	1A	3225	1/1	0.97	0.13	17,17,17,17	0
57	MG	1A	3860	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3589	1/1	0.97	0.05	19,19,19,19	0
57	MG	1A	3626	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3741	1/1	0.97	0.07	19,19,19,19	0
57	MG	2A	3366	1/1	0.97	0.17	30,30,30,30	0
57	MG	1E	309	1/1	0.97	0.03	28,28,28,28	0
57	MG	1A	3998	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3595	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3069	1/1	0.97	0.05	5,5,5,5	0
57	MG	1A	4000	1/1	0.97	0.05	37,37,37,37	0
57	MG	1F	302	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	4001	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3536	1/1	0.97	0.18	27,27,27,27	0
57	MG	1A	3130	1/1	0.97	0.28	18,18,18,18	0
57	MG	1A	3465	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3603	1/1	0.97	0.12	30,30,30,30	0
57	MG	2A	3604	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3070	1/1	0.97	0.15	23,23,23,23	0
57	MG	2D	302	1/1	0.97	0.12	17,17,17,17	0
57	MG	1A	3543	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3134	1/1	0.97	0.07	23,23,23,23	0
57	MG	2A	3181	1/1	0.97	0.21	41,41,41,41	0
57	MG	1A	3545	1/1	0.97	0.23	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	1A	3754	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3184	1/1	0.97	0.05	33,33,33,33	0
57	MG	2A	3612	1/1	0.97	0.08	40,40,40,40	0
57	MG	1a	3556	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3468	1/1	0.97	0.05	35,35,35,35	0
57	MG	1m	3001	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3050	1/1	0.97	0.14	12,12,12,12	0
57	MG	1A	3758	1/1	0.97	0.05	17,17,17,17	0
57	MG	2x	105	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3100	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3878	1/1	0.97	0.10	19,19,19,19	0
57	MG	2F	303	1/1	0.97	0.10	39,39,39,39	0
57	MG	1a	3562	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3550	1/1	0.97	0.10	22,22,22,22	0
59	ZN	2n	501	1/1	0.97	0.04	89,89,89,89	0
60	SF4	1d	302	8/8	0.97	0.05	56,62,66,68	0
57	MG	1E	303	1/1	0.98	0.08	17,17,17,17	0
57	MG	1A	3274	1/1	0.98	0.12	16,16,16,16	0
57	MG	2A	3151	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3486	1/1	0.98	0.28	11,11,11,11	0
57	MG	1A	3746	1/1	0.98	0.08	10,10,10,10	0
57	MG	2A	3011	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3748	1/1	0.98	0.05	41,41,41,41	0
57	MG	1E	308	1/1	0.98	0.11	11,11,11,11	0
57	MG	2A	3157	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3667	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3240	1/1	0.98	0.23	23,23,23,23	0
57	MG	2A	3016	1/1	0.98	0.13	25,25,25,25	0
57	MG	2A	3616	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3785	1/1	0.98	0.09	42,42,42,42	0
57	MG	2A	3161	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3598	1/1	0.98	0.10	9,9,9,9	0
57	MG	2A	3788	1/1	0.98	0.10	27,27,27,27	0
57	MG	1E	312	1/1	0.98	0.27	32,32,32,32	0
57	MG	1A	3670	1/1	0.98	0.07	11,11,11,11	0
57	MG	1F	301	1/1	0.98	0.13	30,30,30,30	0
57	MG	2a	1653	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3599	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3208	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3277	1/1	0.98	0.19	19,19,19,19	0
57	MG	2A	3466	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3443	1/1	0.98	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3468	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3491	1/1	0.98	0.15	24,24,24,24	0
57	MG	1A	4042	1/1	0.98	0.04	7,7,7,7	0
57	MG	2A	3801	1/1	0.98	0.09	43,43,43,43	0
57	MG	2A	3173	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3760	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3604	1/1	0.98	0.06	8,8,8,8	0
57	MG	1A	3278	1/1	0.98	0.29	19,19,19,19	0
57	MG	1A	3546	1/1	0.98	0.11	22,22,22,22	0
57	MG	2A	3807	1/1	0.98	0.05	24,24,24,24	0
57	MG	1a	3641	1/1	0.98	0.10	54,54,54,54	0
57	MG	1A	3400	1/1	0.98	0.06	41,41,41,41	0
57	MG	2A	3637	1/1	0.98	0.10	54,54,54,54	0
57	MG	2A	3811	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3357	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	4049	1/1	0.98	0.08	14,14,14,14	0
57	MG	1a	3645	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3815	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3316	1/1	0.98	0.11	17,17,17,17	0
57	MG	1A	3131	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3483	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3164	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3101	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	4054	1/1	0.98	0.08	32,32,32,32	0
57	MG	1a	3652	1/1	0.98	0.08	22,22,22,22	0
57	MG	2A	3648	1/1	0.98	0.09	27,27,27,27	0
57	MG	2A	3189	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3036	1/1	0.98	0.16	22,22,22,22	0
57	MG	1A	3772	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3859	1/1	0.98	0.11	35,35,35,35	0
57	MG	1A	4059	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3321	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3687	1/1	0.98	0.07	6,6,6,6	0
57	MG	1A	3189	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3957	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3051	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3075	1/1	0.98	0.11	16,16,16,16	0
57	MG	1A	3248	1/1	0.98	0.19	42,42,42,42	0
57	MG	1A	3691	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3867	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3504	1/1	0.98	0.21	23,23,23,23	0
57	MG	1A	3619	1/1	0.98	0.04	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3191	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3560	1/1	0.98	0.04	21,21,21,21	0
57	MG	2a	1703	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	4072	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3967	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3123	1/1	0.98	0.26	21,21,21,21	0
57	MG	1A	3152	1/1	0.98	0.17	30,30,30,30	0
57	MG	1Q	205	1/1	0.98	0.06	19,19,19,19	0
57	MG	2A	3672	1/1	0.98	0.08	37,37,37,37	0
57	MG	1A	3063	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3564	1/1	0.98	0.11	20,20,20,20	0
57	MG	1A	3171	1/1	0.98	0.08	26,26,26,26	0
57	MG	2a	1713	1/1	0.98	0.20	42,42,42,42	0
57	MG	1R	203	1/1	0.98	0.15	20,20,20,20	0
57	MG	2B	217	1/1	0.98	0.22	47,47,47,47	0
57	MG	1R	204	1/1	0.98	0.14	21,21,21,21	0
57	MG	1A	3138	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3173	1/1	0.98	0.15	19,19,19,19	0
57	MG	2D	303	1/1	0.98	0.29	32,32,32,32	0
57	MG	2A	3365	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3374	1/1	0.98	0.24	18,18,18,18	0
57	MG	1A	4082	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	4083	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3686	1/1	0.98	0.05	26,26,26,26	0
57	MG	1a	3552	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3524	1/1	0.98	0.09	19,19,19,19	0
57	MG	1A	3976	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3018	1/1	0.98	0.17	32,32,32,32	0
57	MG	2A	3527	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3199	1/1	0.98	0.09	17,17,17,17	0
57	MG	1A	3571	1/1	0.98	0.14	7,7,7,7	0
57	MG	1A	3709	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3982	1/1	0.98	0.06	56,56,56,56	0
57	MG	1U	207	1/1	0.98	0.16	23,23,23,23	0
57	MG	1U	208	1/1	0.98	0.29	28,28,28,28	0
57	MG	1U	209	1/1	0.98	0.13	21,21,21,21	0
57	MG	1A	3884	1/1	0.98	0.09	14,14,14,14	0
57	MG	1A	3515	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3985	1/1	0.98	0.08	8,8,8,8	0
57	MG	1a	3697	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3228	1/1	0.98	0.21	34,34,34,34	0
57	MG	1A	3574	1/1	0.98	0.07	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1V	205	1/1	0.98	0.22	20,20,20,20	0
57	MG	2Q	201	1/1	0.98	0.12	37,37,37,37	0
57	MG	1a	3568	1/1	0.98	0.14	39,39,39,39	0
57	MG	1A	3177	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3260	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3078	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3803	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3338	1/1	0.98	0.19	15,15,15,15	0
57	MG	1W	203	1/1	0.98	0.20	20,20,20,20	0
57	MG	1A	3339	1/1	0.98	0.25	17,17,17,17	0
57	MG	1A	3522	1/1	0.98	0.07	29,29,29,29	0
57	MG	2A	3101	1/1	0.98	0.08	39,39,39,39	0
57	MG	1X	101	1/1	0.98	0.29	24,24,24,24	0
57	MG	1B	217	1/1	0.98	0.06	37,37,37,37	0
57	MG	1X	104	1/1	0.98	0.10	42,42,42,42	0
57	MG	2A	3252	1/1	0.98	0.06	46,46,46,46	0
57	MG	2A	3400	1/1	0.98	0.29	41,41,41,41	0
57	MG	1A	3996	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3724	1/1	0.98	0.06	54,54,54,54	0
57	MG	2A	3558	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3157	1/1	0.98	0.17	19,19,19,19	0
57	MG	2A	3560	1/1	0.98	0.20	39,39,39,39	0
57	MG	1A	3720	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3645	1/1	0.98	0.09	10,10,10,10	0
57	MG	1A	3722	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3029	1/1	0.98	0.19	18,18,18,18	0
57	MG	1A	3724	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3903	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3128	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3726	1/1	0.98	0.10	11,11,11,11	0
57	MG	1B	229	1/1	0.98	0.10	30,30,30,30	0
57	MG	1d	301	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3906	1/1	0.98	0.04	6,6,6,6	0
57	MG	1A	3648	1/1	0.98	0.05	9,9,9,9	0
57	MG	1A	3584	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3910	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3650	1/1	0.98	0.04	15,15,15,15	0
57	MG	1l	101	1/1	0.98	0.26	27,27,27,27	0
57	MG	1a	3597	1/1	0.98	0.22	33,33,33,33	0
57	MG	1A	3912	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3125	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3423	1/1	0.98	0.11	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	4012	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3234	1/1	0.98	0.08	10,10,10,10	0
57	MG	12	102	1/1	0.98	0.16	35,35,35,35	0
57	MG	1A	3914	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3020	1/1	0.98	0.04	17,17,17,17	0
57	MG	2A	3586	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3653	1/1	0.98	0.07	10,10,10,10	0
57	MG	1A	3073	1/1	0.98	0.08	17,17,17,17	0
57	MG	2A	3134	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3734	1/1	0.98	0.08	32,32,32,32	0
57	MG	1D	304	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3184	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3589	1/1	0.98	0.08	19,19,19,19	0
57	MG	1A	3657	1/1	0.98	0.05	10,10,10,10	0
57	MG	1A	3238	1/1	0.98	0.38	21,21,21,21	0
57	MG	1A	3659	1/1	0.98	0.04	19,19,19,19	0
57	MG	1A	3239	1/1	0.98	0.14	17,17,17,17	0
57	MG	1A	3271	1/1	0.98	0.10	24,24,24,24	0
57	MG	2A	3001	1/1	0.98	0.26	33,33,33,33	0
57	MG	1A	3272	1/1	0.98	0.15	18,18,18,18	0
57	MG	1E	301	1/1	0.98	0.29	21,21,21,21	0
59	ZN	14	501	1/1	0.98	0.06	98,98,98,98	0
59	ZN	1n	102	1/1	0.98	0.04	72,72,72,72	0
59	ZN	2Y	202	1/1	0.98	0.04	75,75,75,75	0
57	MG	2A	3769	1/1	0.98	0.07	41,41,41,41	0
59	ZN	29	501	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3273	1/1	0.98	0.15	18,18,18,18	0
57	MG	17	101	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3017	1/1	0.99	0.07	11,11,11,11	0
57	MG	1A	3031	1/1	0.99	0.14	18,18,18,18	0
57	MG	1A	3459	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3042	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3218	1/1	0.99	0.12	28,28,28,28	0
57	MG	1w	401	1/1	0.99	0.10	23,23,23,23	0
57	MG	1A	3811	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3964	1/1	0.99	0.07	10,10,10,10	0
57	MG	1A	3777	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3885	1/1	0.99	0.04	17,17,17,17	0
57	MG	2A	3414	1/1	0.99	0.23	29,29,29,29	0
57	MG	2A	3799	1/1	0.99	0.09	18,18,18,18	0
57	MG	1A	3778	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3219	1/1	0.99	0.04	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3172	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3660	1/1	0.99	0.06	10,10,10,10	0
57	MG	1A	3747	1/1	0.99	0.02	11,11,11,11	0
57	MG	1B	218	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3220	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	4015	1/1	0.99	0.05	27,27,27,27	0
57	MG	1A	3749	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3133	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3022	1/1	0.99	0.11	6,6,6,6	0
57	MG	1A	3894	1/1	0.99	0.07	39,39,39,39	0
57	MG	1U	201	1/1	0.99	0.17	17,17,17,17	0
57	MG	2A	3680	1/1	0.99	0.08	33,33,33,33	0
57	MG	1A	3856	1/1	0.99	0.08	16,16,16,16	0
57	MG	1U	203	1/1	0.99	0.20	16,16,16,16	0
57	MG	1A	3056	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3978	1/1	0.99	0.07	11,11,11,11	0
57	MG	2A	3008	1/1	0.99	0.05	26,26,26,26	0
57	MG	1A	3637	1/1	0.99	0.05	23,23,23,23	0
57	MG	2A	3128	1/1	0.99	0.35	34,34,34,34	0
57	MG	1A	3071	1/1	0.99	0.19	6,6,6,6	0
57	MG	2A	3689	1/1	0.99	0.02	34,34,34,34	0
57	MG	1A	3151	1/1	0.99	0.06	15,15,15,15	0
57	MG	1A	3090	1/1	0.99	0.15	12,12,12,12	0
57	MG	1A	3757	1/1	0.99	0.04	17,17,17,17	0
57	MG	1U	211	1/1	0.99	0.13	19,19,19,19	0
57	MG	1A	3863	1/1	0.99	0.10	10,10,10,10	0
57	MG	1a	3651	1/1	0.99	0.02	27,27,27,27	0
57	MG	1V	201	1/1	0.99	0.12	15,15,15,15	0
57	MG	2A	3697	1/1	0.99	0.09	30,30,30,30	0
57	MG	1A	3003	1/1	0.99	0.04	11,11,11,11	0
57	MG	1A	3541	1/1	0.99	0.08	11,11,11,11	0
57	MG	2A	3020	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3542	1/1	0.99	0.17	18,18,18,18	0
57	MG	1A	3644	1/1	0.99	0.06	12,12,12,12	0
57	MG	1A	3989	1/1	0.99	0.03	22,22,22,22	0
57	MG	1A	3139	1/1	0.99	0.06	9,9,9,9	0
57	MG	2A	3512	1/1	0.99	0.04	29,29,29,29	0
57	MG	17	106	1/1	0.99	0.05	26,26,26,26	0
57	MG	1A	3908	1/1	0.99	0.05	15,15,15,15	0
57	MG	1A	3081	1/1	0.99	0.08	24,24,24,24	0
57	MG	27	101	1/1	0.99	0.09	38,38,38,38	0
57	MG	18	103	1/1	0.99	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3115	1/1	0.99	0.26	24,24,24,24	0
57	MG	1A	3082	1/1	0.99	0.08	23,23,23,23	0
57	MG	1A	3034	1/1	0.99	0.11	25,25,25,25	0
57	MG	1D	306	1/1	0.99	0.03	10,10,10,10	0
57	MG	1A	3175	1/1	0.99	0.10	17,17,17,17	0
59	ZN	1Y	204	1/1	0.99	0.03	54,54,54,54	0
57	MG	1X	102	1/1	0.99	0.09	33,33,33,33	0
59	ZN	15	3210	1/1	0.99	0.07	43,43,43,43	0
59	ZN	16	104	1/1	0.99	0.03	31,31,31,31	0
57	MG	1D	308	1/1	0.99	0.11	19,19,19,19	0
57	MG	1A	3768	1/1	0.99	0.03	8,8,8,8	0
57	MG	1A	3176	1/1	0.99	0.08	15,15,15,15	0
59	ZN	25	105	1/1	0.99	0.04	46,46,46,46	0
59	ZN	26	102	1/1	0.99	0.03	47,47,47,47	0
57	MG	1X	106	1/1	0.99	0.10	16,16,16,16	0
57	MG	1A	3159	1/1	0.99	0.17	19,19,19,19	0
57	MG	1A	3214	1/1	0.99	0.23	23,23,23,23	0
60	SF4	2d	303	8/8	0.99	0.04	51,58,65,70	0
59	ZN	19	102	1/1	1.00	0.03	30,30,30,30	0
57	MG	1A	3703	1/1	1.00	0.06	5,5,5,5	0
57	MG	2A	3673	1/1	1.00	0.01	19,19,19,19	0
57	MG	1A	4056	1/1	1.00	0.03	17,17,17,17	0
57	MG	1A	3704	1/1	1.00	0.02	6,6,6,6	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.