



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 06:42 AM EDT

PDB ID : 8CVL / pdb_00008cvl
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNA^{phe}, peptidyl P-site fMTTHSMRC-NH-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.30Å resolution
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Deposited on : 2022-05-18
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

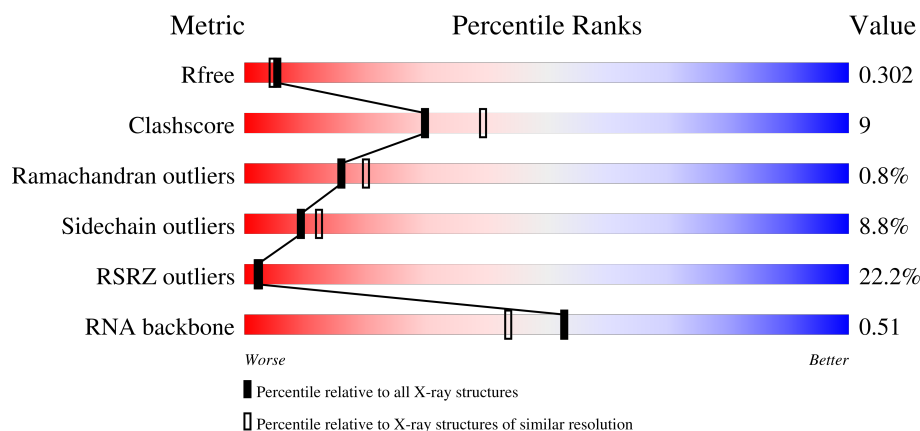
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
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	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1z	7	
56	2z	7	
57	1y	76	
57	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3442	-	-	-	X
58	MG	1a	1742	-	-	-	X
58	MG	2A	3156	-	-	-	X
58	MG	2n	101	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Phe-NH-tRNA_{Phe}.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA_{met} RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA_{met} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			
56	2z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			

- Molecule 57 is a RNA chain called E-site Deacylated tRNA_{Phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1101	Total Mg 1101 1101	0	0
58	1B	38	Total Mg 38 38	0	0
58	1D	13	Total Mg 13 13	0	0
58	1E	12	Total Mg 12 12	0	0
58	1F	12	Total Mg 12 12	0	0
58	1G	5	Total Mg 5 5	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	5	Total Mg 5 5	0	0
58	1O	5	Total Mg 5 5	0	0
58	1P	7	Total Mg 7 7	0	0
58	1Q	8	Total Mg 8 8	0	0
58	1R	4	Total Mg 4 4	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	2	Total Mg 2 2	0	0
58	1U	10	Total Mg 10 10	0	0
58	1V	7	Total Mg 7 7	0	0
58	1W	4	Total Mg 4 4	0	0
58	1X	4	Total Mg 4 4	0	0
58	1Y	4	Total Mg 4 4	0	0
58	1Z	4	Total Mg 4 4	0	0
58	10	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	6	Total 6	Mg 6	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	4	Total 4	Mg 4	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	7	Total 7	Mg 7	0	0
58	16	1	Total 1	Mg 1	0	0
58	17	5	Total 5	Mg 5	0	0
58	18	7	Total 7	Mg 7	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	210	Total 210	Mg 210	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1w	7	Total 7	Mg 7	0	0
58	1x	12	Total 12	Mg 12	0	0
58	2A	851	Total 851	Mg 851	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2B	20	Total 20	Mg 20	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	10	Total 10	Mg 10	0	0
58	2F	6	Total 6	Mg 6	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	0	0
58	2P	2	Total 2	Mg 2	0	0
58	2Q	4	Total 4	Mg 4	0	0
58	2R	4	Total 4	Mg 4	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	1	Total 1	Mg 1	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	2	Total 2	Mg 2	0	0
58	21	1	Total 1	Mg 1	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	2	Total 2	Mg 2	0	0
58	28	4	Total 4	Mg 4	0	0
58	29	1	Total 1	Mg 1	0	0
58	2a	220	Total 220	Mg 220	0	0
58	2d	3	Total 3	Mg 3	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2i	1	Total 1	Mg 1	0	0
58	2j	2	Total 2	Mg 2	0	0
58	2k	1	Total 1	Mg 1	0	0
58	2l	3	Total 3	Mg 3	0	0
58	2n	1	Total 1	Mg 1	0	0
58	2q	3	Total 3	Mg 3	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	2	Total 2	Mg 2	0	0
58	2v	4	Total 4	Mg 4	0	0
58	2w	4	Total 4	Mg 4	0	0
58	2x	6	Total 6	Mg 6	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1	Total 1	K 1	0	0

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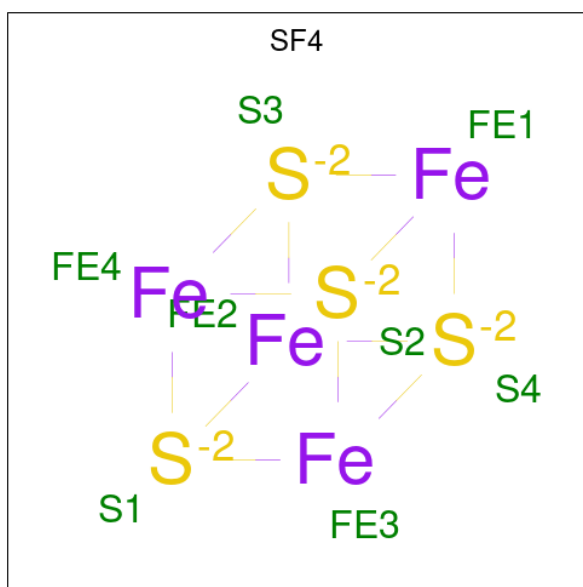
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2A	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1949	Total	O	0	0
			1949	1949		
62	1B	58	Total	O	0	0
			58	58		
62	1D	26	Total	O	0	0
			26	26		
62	1E	28	Total	O	0	0
			28	28		
62	1F	18	Total	O	0	0
			18	18		
62	1G	3	Total	O	0	0
			3	3		
62	1H	2	Total	O	0	0
			2	2		
62	1N	6	Total	O	0	0
			6	6		
62	1O	6	Total	O	0	0
			6	6		
62	1P	19	Total	O	0	0
			19	19		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1Q	7	Total 7	O 7	0	0
62	1R	10	Total 10	O 10	0	0
62	1S	4	Total 4	O 4	0	0
62	1T	7	Total 7	O 7	0	0
62	1U	13	Total 13	O 13	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	7	Total 7	O 7	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	13	Total 13	O 13	0	0
62	11	7	Total 7	O 7	0	0
62	12	3	Total 3	O 3	0	0
62	13	6	Total 6	O 6	0	0
62	15	8	Total 8	O 8	0	0
62	16	2	Total 2	O 2	0	0
62	17	8	Total 8	O 8	0	0
62	18	12	Total 12	O 12	0	0
62	1a	301	Total 301	O 301	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	5	Total 5	O 5	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	2	Total 2	O 2	0	0
62	1q	2	Total 2	O 2	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	7	Total 7	O 7	0	0
62	1z	3	Total 3	O 3	0	0
62	2A	1047	Total 1047	O 1047	0	0
62	2B	20	Total 20	O 20	0	0
62	2D	26	Total 26	O 26	0	0
62	2E	15	Total 15	O 15	0	0
62	2F	14	Total 14	O 14	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	2	Total 2	O 2	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	6	Total 6	O 6	0	0

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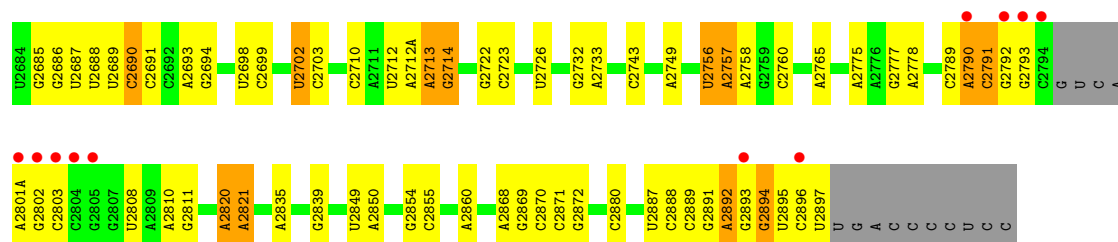
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2U	1	Total 1	O 1	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	5	Total 5	O 5	0	0
62	20	2	Total 2	O 2	0	0
62	21	7	Total 7	O 7	0	0
62	22	1	Total 1	O 1	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	27	5	Total 5	O 5	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	196	Total 196	O 196	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0
62	2e	2	Total 2	O 2	0	0
62	2g	1	Total 1	O 1	0	0
62	2i	1	Total 1	O 1	0	0
62	2j	2	Total 2	O 2	0	0
62	2l	5	Total 5	O 5	0	0
62	2r	1	Total 1	O 1	0	0

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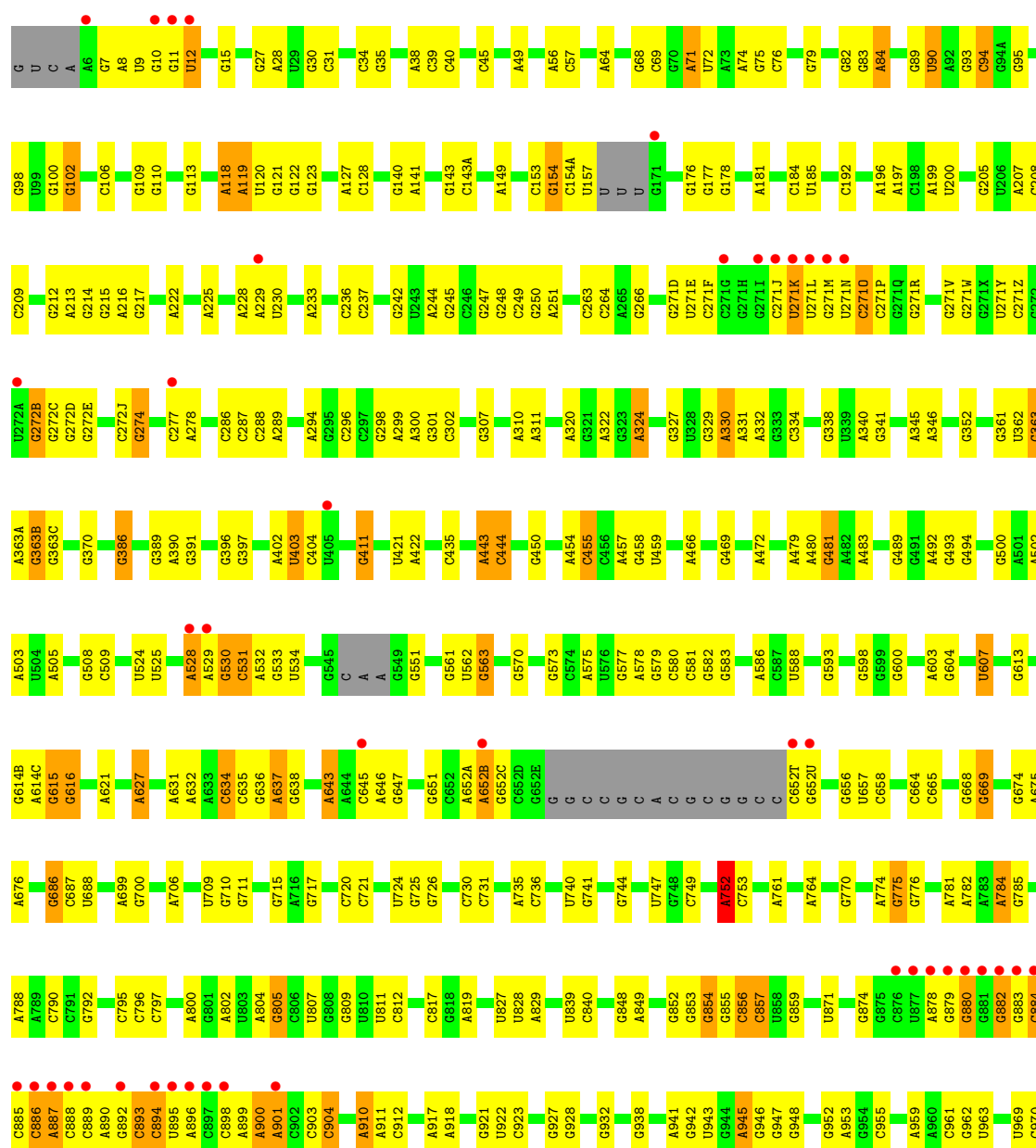
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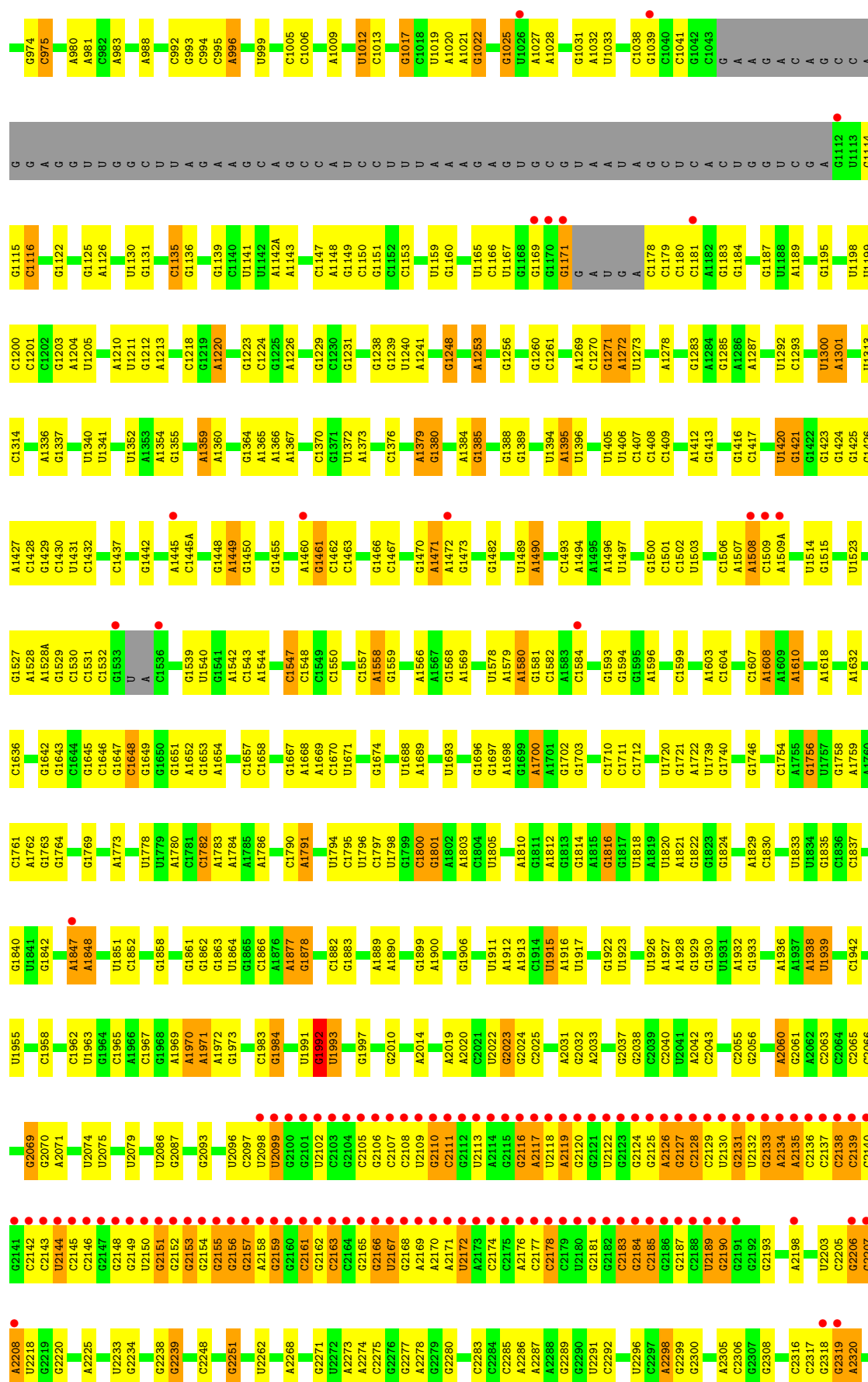
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2t	1	Total	O	0	0
			1	1		
62	2v	2	Total	O	0	0
			2	2		
62	2w	6	Total	O	0	0
			6	6		
62	2x	4	Total	O	0	0
			4	4		
62	2z	1	Total	O	0	0
			1	1		

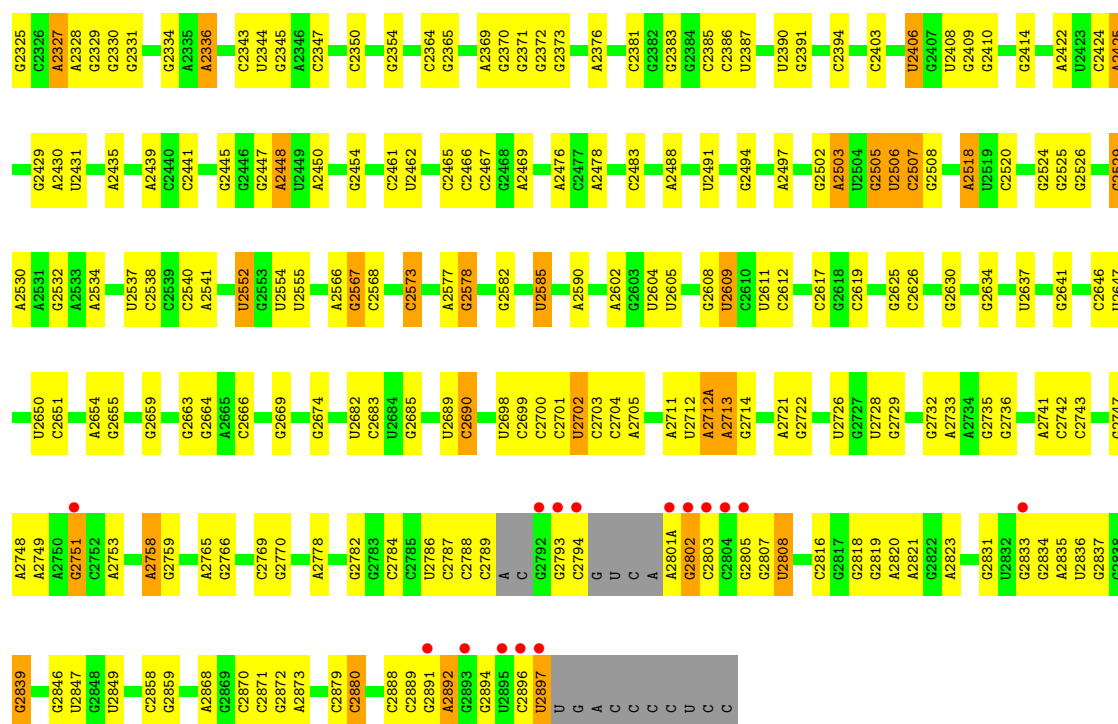
U2555	A2425	U2312	G2192	U2132	C2040	U1917	A1786	G1647	A1509A	A1384	G1248	U1113	A1054
C2556	A2426	C2313	G2193	G2133	U2041	A1918	A1791	C1648	A1509B	G1385	G1249	G1114	G1055
G2557	G2427	G2314	G2194	A2134	A2042	A1919			U1512	A1395	G1252	G1115	G1056
	G2428	G2315		A2135	C2043	C1920		A1654	C1513	U1396	A1253	C1116	G1057
U2562	G2429	G2319	A2198	C2137	A2051	G1929	U1794	A1569	U1518	G1400	G1256	G1117	G1058
U2563	A2430	A2320	C2203	C2138	C2055	G1930	U1796	C1670	G1519	G1401		G1118	G1059
A2564	U2431	G2321	C2205	C2139	G2056	C1934	U1797	G1674	G1526				U1060
A2565	A2435	A2322	G2207	C2140			U1798		G1527			G1125	G1062
G2567			G2208	G2141	A2059	A1937	G1799	G1675	U1526	U1405	A1265	C1135	G1063
	A2439	G2325	G2209	C2142	A2060	A1938	C1800	A1676	G1527	U1406	U1267	C1136	G1064
C2573	C2440	G2326	U2218	U2143	A2061	A1939	G1801	A1677	G1530	C1407	U1268	G1137	U1065
G2574	C2441	A2327	G2219	U2144		U1939	A1802		C1531	C1408	A1269	G1138	U1066
C2575	A2328			C2145			A1803	U1680	G1532	C1409	G1270	G1139	U1067
G2576	G2329	G2222		G2146	G2069	C1942			C1532		G1271	C1140	U1068
A2577				C2147			A1810	C1683	G1533	G1416	A1272	U1141	U1069
G2578	G2330	A2225		U2148	U2074	A1952	G1811	C1684	U	G1417	U1273	U1142	A1070
	G2331			G2149	U2075	A1953	A1812	C1685	A	A1418	A1274	A1142A	G1071
G2583	G2334	U2233	U2233	U2150		G1954	G1813	C1686	C	A1419	A1275		C1072
U2584	A2335	G2234		G2151	G2080	U1955	G1814	U1687	G1537	U1420	A1276	G1149	U1073
U2585	G2336		G2238	G2152	U2086	C1962	A1815	U1688	G1538	G1427	A1277	A1155	G1074
	G2337			G2153	G2087	U1963	G1816		G1539	A1428	A1278	A1156	C1075
C2591	U2344			G2154			G1817	U1693		G1429			U1076
G2592	U2345	U2096	U2096	G2155		C1967	U1818	G1696	A1542	C1430	C1293	G1164	U1077
	U2444	C2097	C2097	G2156			A1825					U1185	U1078
A2602	C2347	U2098	U2098	G2157		A1970		A1700	C1546	U1300		U1186	C1079
G2603	U2348	G2251	G2251	A2158	U2099	A1971	G1828	C1648	C1547	A1301	U1167	C1166	C1080
U2604	G2349	G2252	G2252	G2159	G2100	A1972	A1829	G1703		A1302		U1167	U1081
U2605	C2350			G2160	C2101	G1973			C1550	G1303		G1170	U1082
		A2268	A2268	G2161	U2102	C1974	C1837	U1720	A1445			G1171	U1083
G2482	G2354	A2269	A2269	G2162	C2103			G1721	C1445A			G1172	A1084
C2483				C2163		U1991	A1847	A1722	C1446			G1173	A1085
G2484	A2361	G2277	G2277	C2164	G2104	G1992		U1739				A1174	A1086
				G2165	C2105	G1993	A1859	G1740	A1568			G1175	G1087
U2491	G2365	C2283	C2283	G2166	G2106	U1993		A1741	A1566			G1176	U1088
C2499		G2284	G2284	U2167	C2107		U1864	G1742				C1177	G1089
A2377	A2377	C2285	C2285	G2168	U2109	G1997	G1865	C1743	A1569			C1178	U1090
A2378	G2378	A2286	A2286	G2169	G2110	G2002	C1866		A1570			C1179	G1091
G2379	G2379	A2287	A2287	A2170	C2111		A1876	G1746	A1571			C1180	U1092
				G2171	U2011		G1877					C1181	G1093
G2382	G2382	G2289	G2289	U2172	G2112	G2012	A1878	G1750	U1578			G1183	U1094
G2383	G2383	G2290	G2290	A2173	A2113	A2013	G1882		A1579			G1187	A1095
G2384	G2384	U2291	U2291	C2174	A2114	A2014	G1883	G1753	A1580				U1096
G2385	G2385	C2292	C2292	G2175	G2115			G1756	G1581			G1190	A1097
				A2176	G2116							G1191	G1098
		U2296	U2296	C2177	A2117	U2017	A1889	G1766	C1584			G1192	U1101
		C2297	C2297	G2178	U2118	A2020	A1890		A1586			C1201	C1102
		A2298	A2298	C2179	G2119	C2021		G1762	A1587			G1219	A1103
		G2299	G2299	U2180	G2120	U2022	C1588	G1764	C1589			G1220	U1105
				G2181	G2121	G2023	C1589					A1220	G1106
		G2302	G2302	G2182	U2122			G1769				G1229	G1107
		G2303	G2303	C2183	G2123		A1603					G1236	U1108
		G2304	G2304	G2184	G2124	U2028	A1494					A1237	C1109
		A2305	A2305	G2185	G2125	G1907	A1495					G1244	G1110
		G2306	G2306	G2186	A2126	C1908	A1496						U1109
		G2307	G2307	G2187	A2127	A2030	U1497						U1108
				C2188	G2128	U1911	A1608						C1109
		G2308	G2308	U2189	C2129	G1781	A1609						G1110
		A2309	A2309	G2190	U2130	C1782	A1610						A1111
		U2423	U2423	A2310		A1783							G1112
		C2424	C2424	G2191	C2039		A1632						



● Molecule 1: 23S Ribosomal RNA



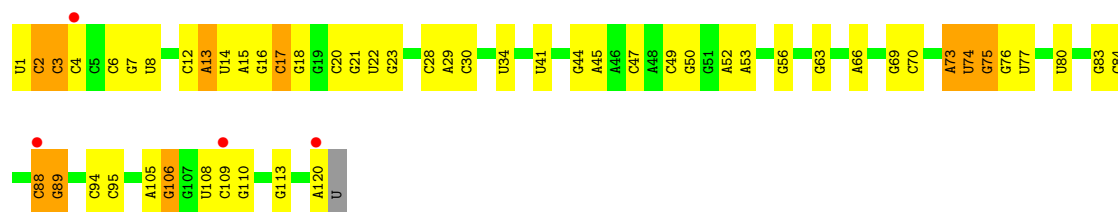




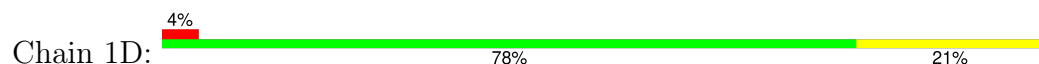
• Molecule 2: 5S Ribosomal RNA



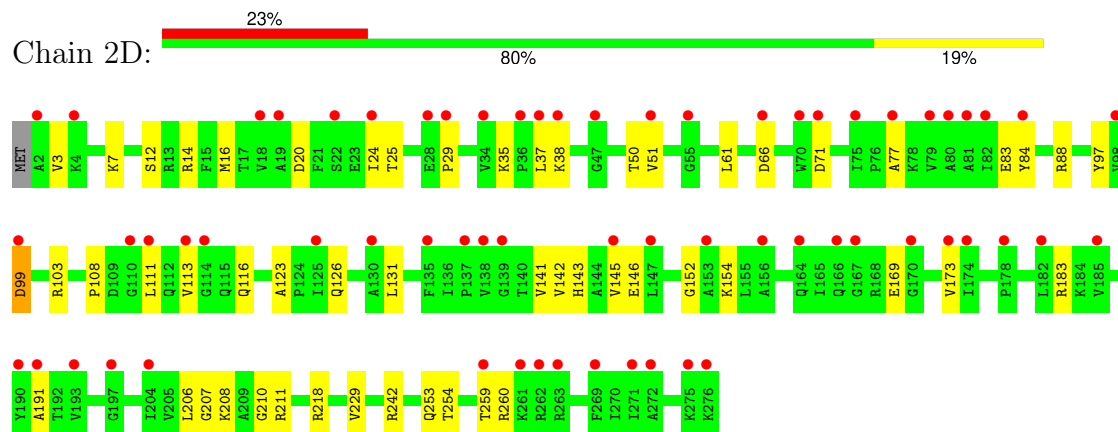
• Molecule 2: 5S Ribosomal RNA



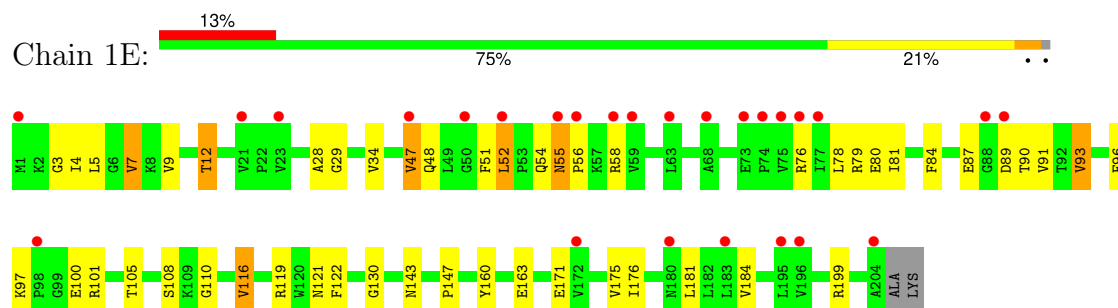
• Molecule 3: 50S ribosomal protein L2



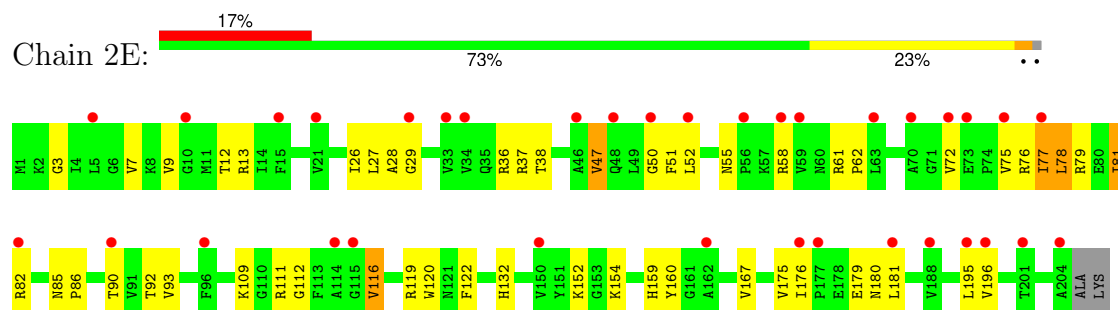
- Molecule 3: 50S ribosomal protein L2



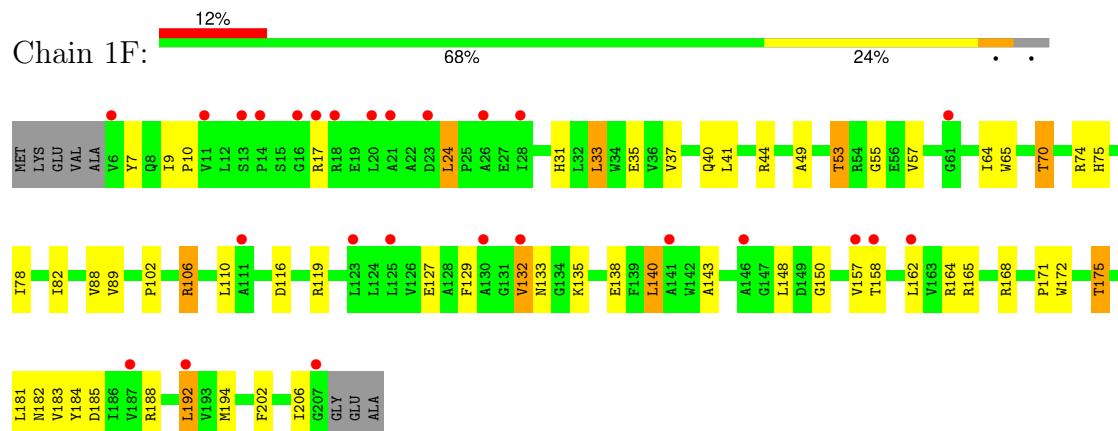
- Molecule 4: 50S ribosomal protein L3



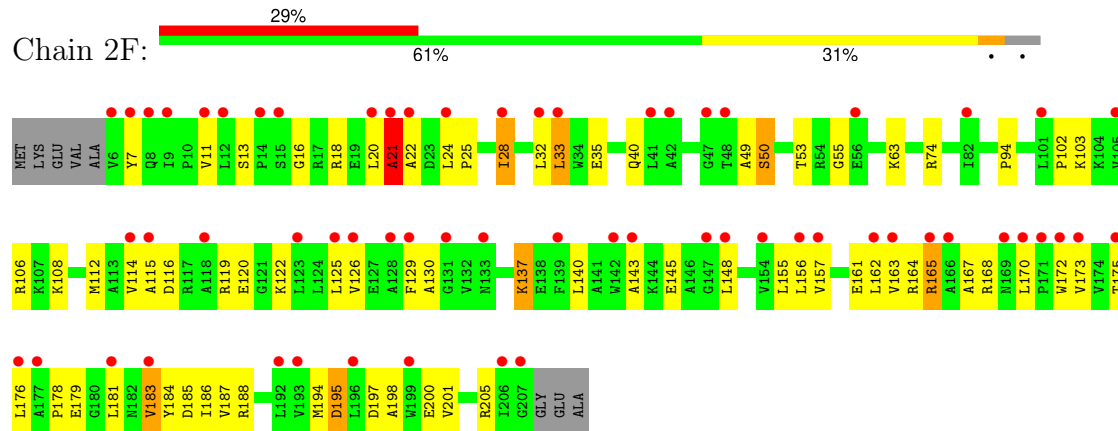
- Molecule 4: 50S ribosomal protein L3



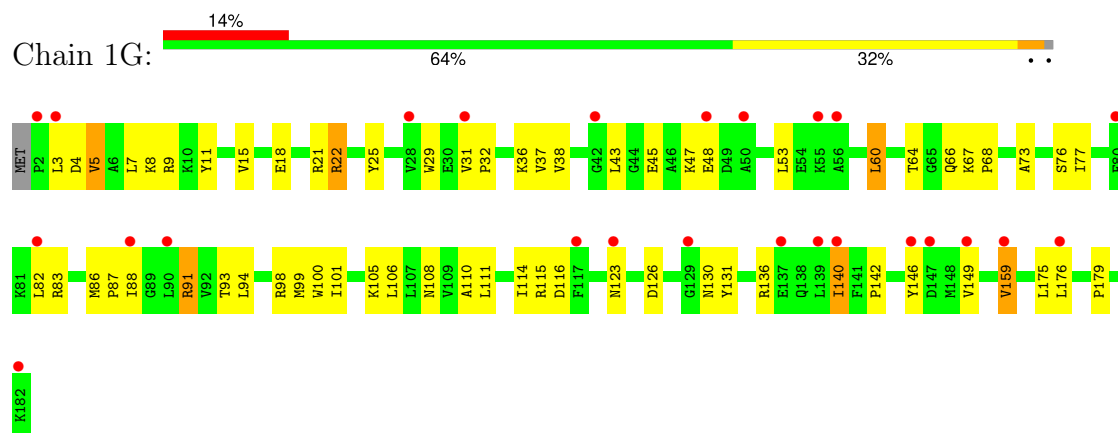
- Molecule 5: 50S ribosomal protein L4



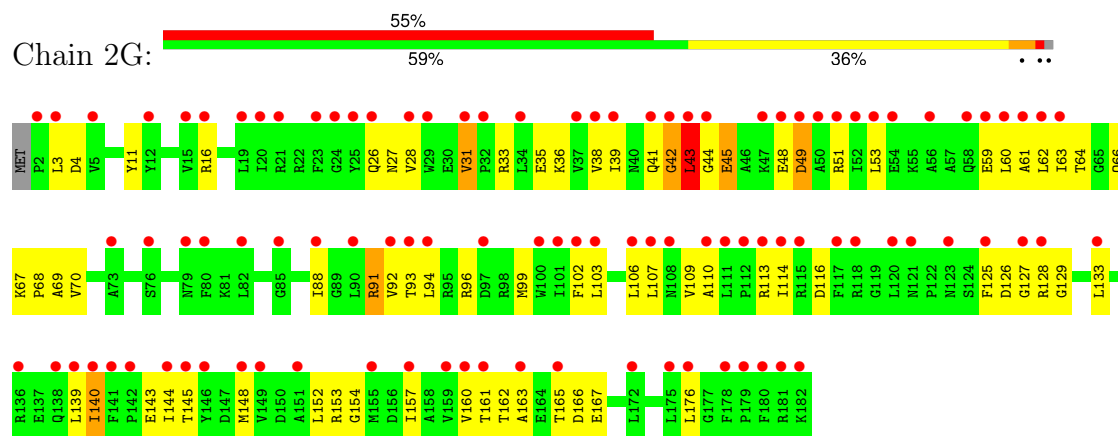
- Molecule 5: 50S ribosomal protein L4



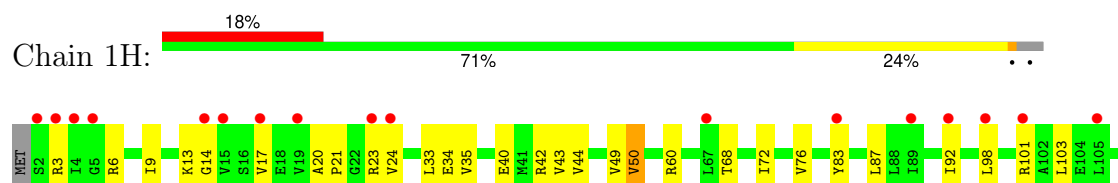
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

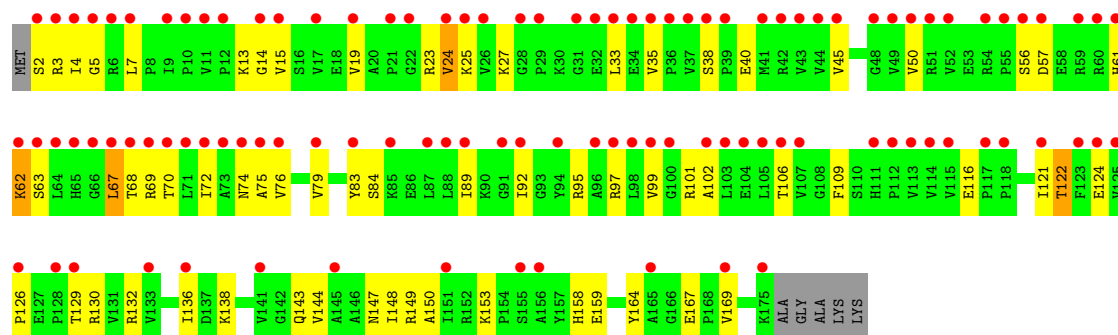


- Molecule 7: 50S ribosomal protein L6

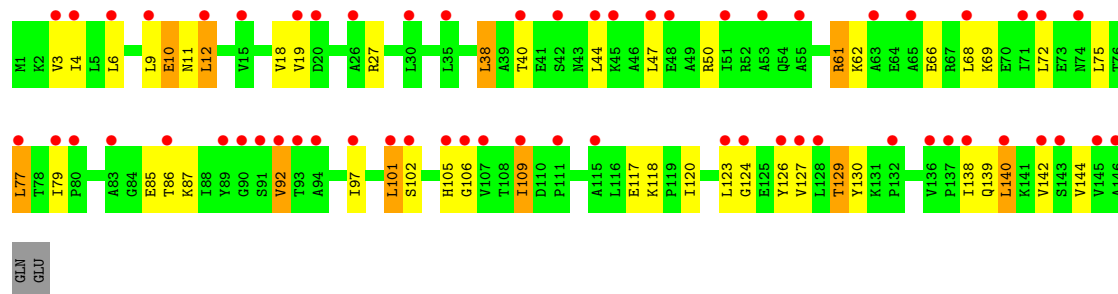
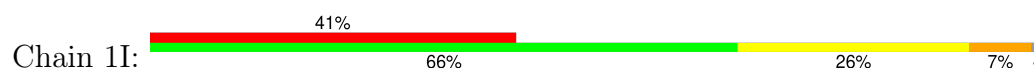




• Molecule 7: 50S ribosomal protein L6



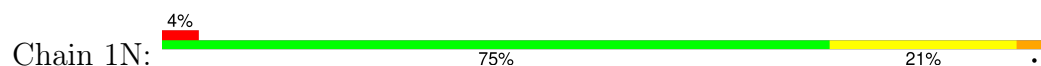
• Molecule 8: 50S ribosomal protein L9

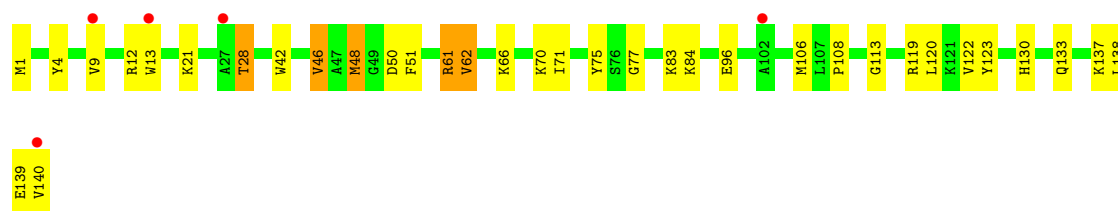


• Molecule 8: 50S ribosomal protein L9

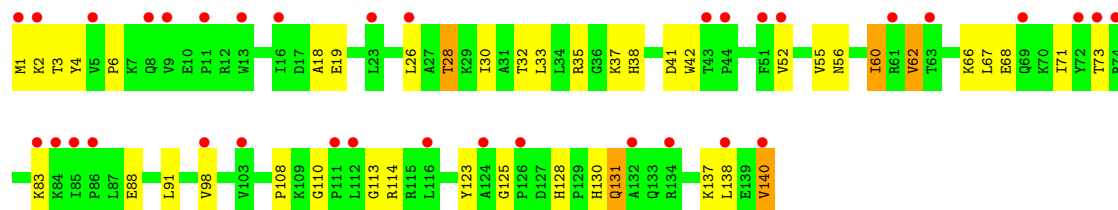


• Molecule 9: 50S ribosomal protein L13

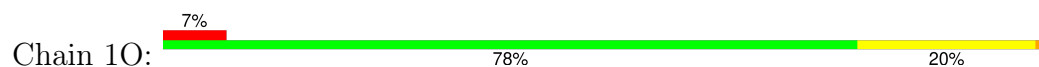




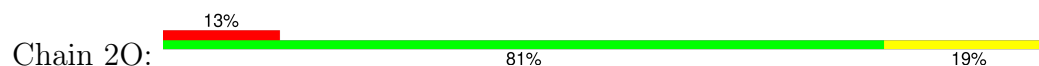
- Molecule 9: 50S ribosomal protein L13



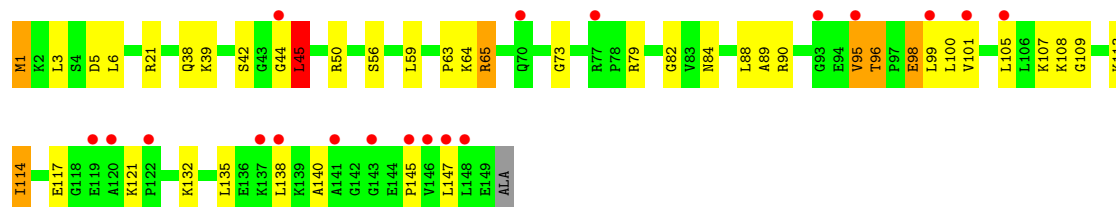
- Molecule 10: 50S ribosomal protein L14



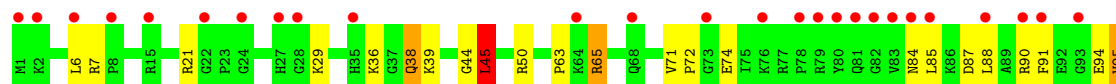
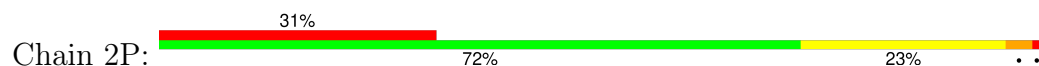
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

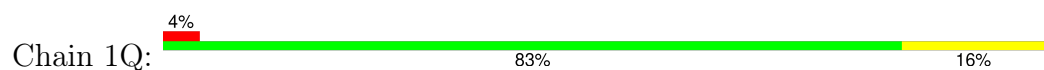


- Molecule 11: 50S ribosomal protein L15

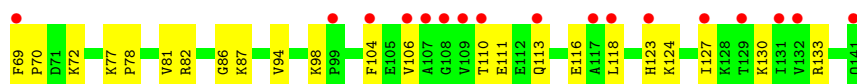
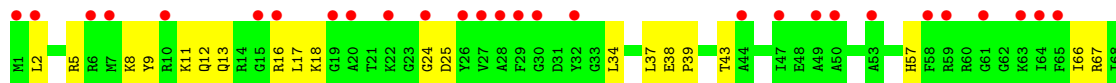
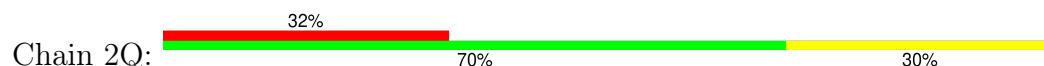




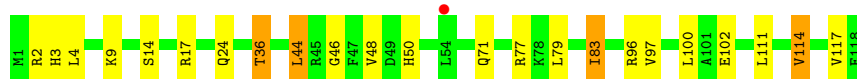
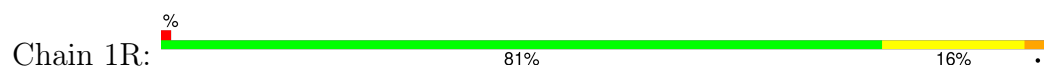
- Molecule 12: 50S ribosomal protein L16



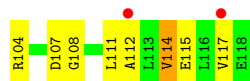
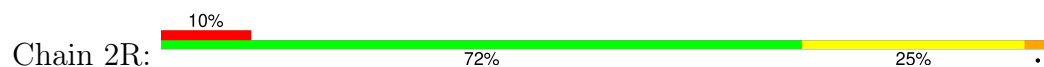
- Molecule 12: 50S ribosomal protein L16



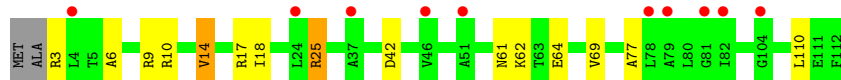
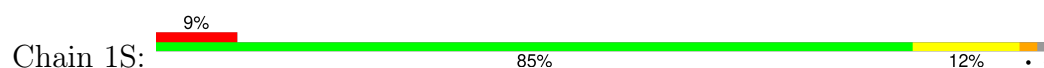
- Molecule 13: 50S ribosomal protein L17



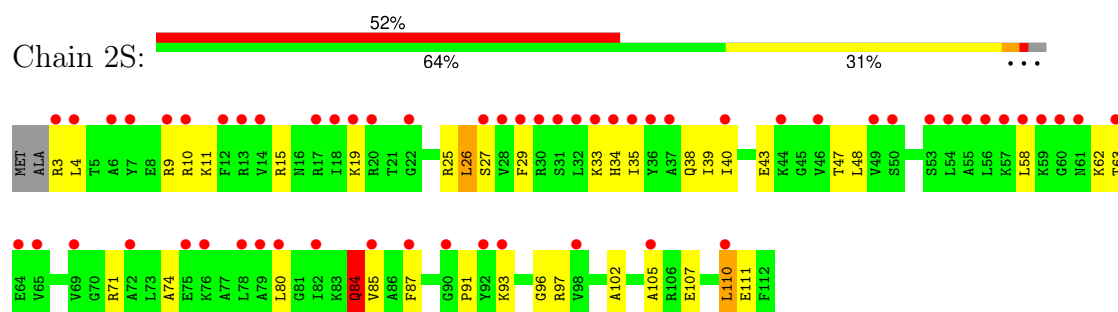
- Molecule 13: 50S ribosomal protein L17



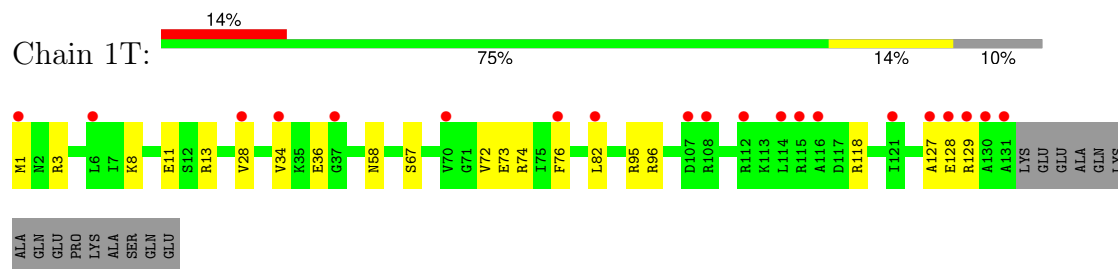
- Molecule 14: 50S ribosomal protein L18



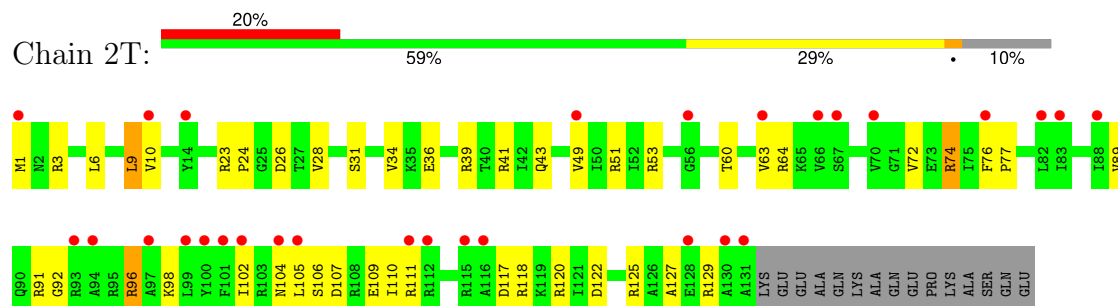
- Molecule 14: 50S ribosomal protein L18



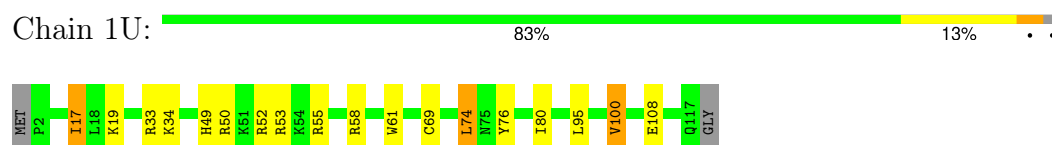
- Molecule 15: 50S ribosomal protein L19



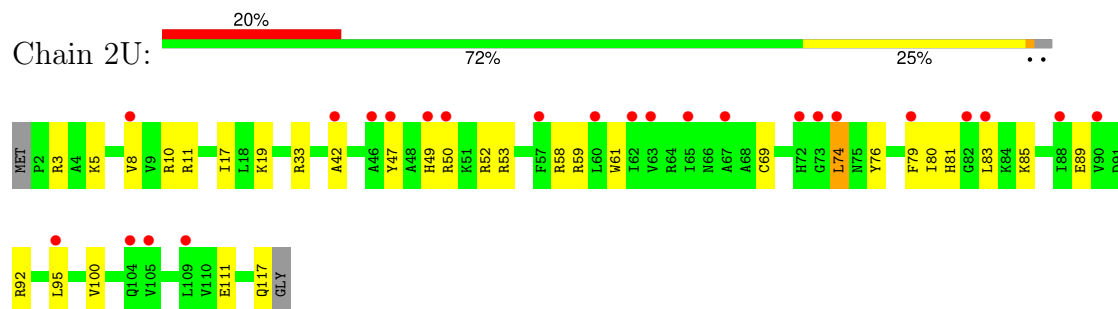
- Molecule 15: 50S ribosomal protein L19



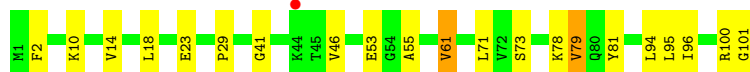
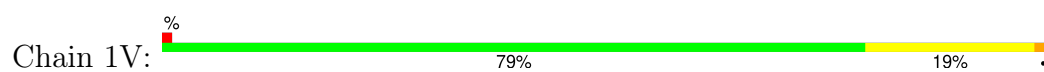
- Molecule 16: 50S ribosomal protein L20



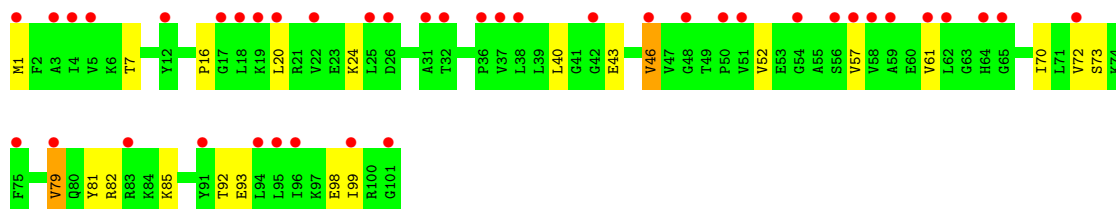
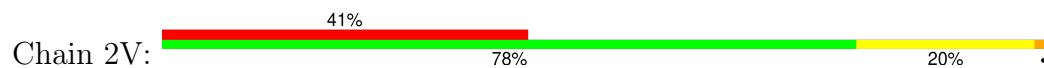
- Molecule 16: 50S ribosomal protein L20



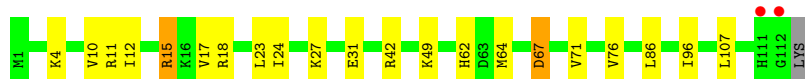
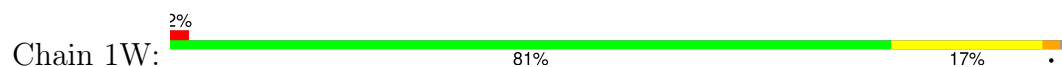
- Molecule 17: 50S ribosomal protein L21



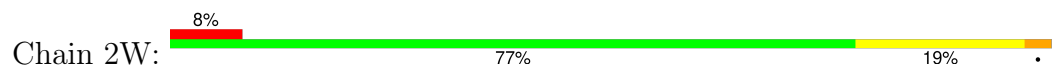
- Molecule 17: 50S ribosomal protein L21



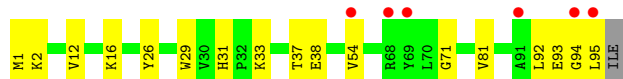
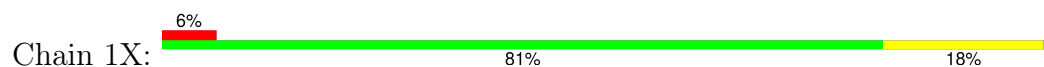
- Molecule 18: 50S ribosomal protein L22



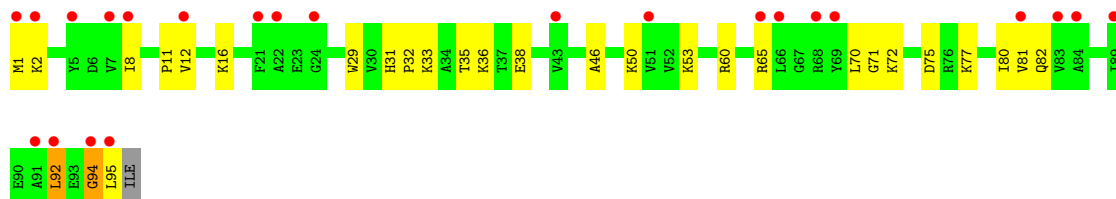
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

- Molecule 22: 50S ribosomal protein L27

Chain 10: 

MET A2 R11 R14 A18 R19 R20 T43 F60 Q70 D71 R72 L76 H80 V81 R82 P83 L84 ALA

- Molecule 22: 50S ribosomal protein L27

Chain 20: 

MET A2 H3 K4 S16 Q17 A18 R19 R20 R21 Q22 V23 T26 V30 R41 G42 T43 R44 F45 K49 R55 L59 F60 A61 L62 V63 D64 V67 E68 F69 Q70 D71 R74 L75 G76 R77 Y78 V79 R82 P83 L84 ALA

- Molecule 23: 50S ribosomal protein L28

Chain 11: 

MET S2 K3 R11 L18 K23 G29 T35 G36 I37 R50 V51 R52 G55 I58 T59 F60 R61 S65 H66 E75 R76 A77 V78 K79 L80 K81 L82 L85 K91 L94 L97 L98

- Molecule 23: 50S ribosomal protein L28

Chain 21: 

MET S2 K3 V4 I7 R11 A15 R21 G22 K23 R26 G29 V30 G31 K32 T34 S38 K39 R40 R41 K48 V49 R50 V51 R52 V53 A54 Q55 Q56 E57 T58 F59 F60 R61 V62 I67 P68 K69 V70 Y71 E72 L73 V74 E75 E76 A77 K78 G79 L80 K81 L82 E83 G84 L85 S86 E89 L94 L98

- Molecule 24: 50S ribosomal protein L29

Chain 12: 

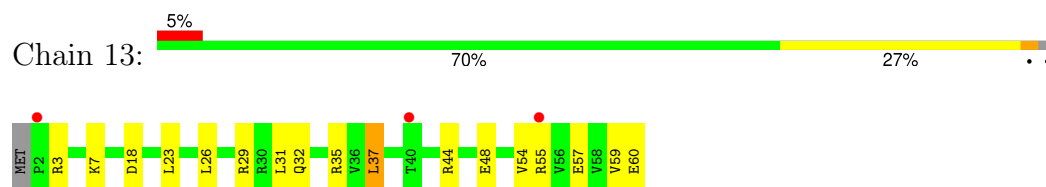
M1 R14 R15 S4 V6 S17 P18 V19 E20 L24 V25 E27 K28 F37 I41 R51 D52 L53 K54 R55 K67 R68 R69 Q70 ASN ALA

- Molecule 24: 50S ribosomal protein L29

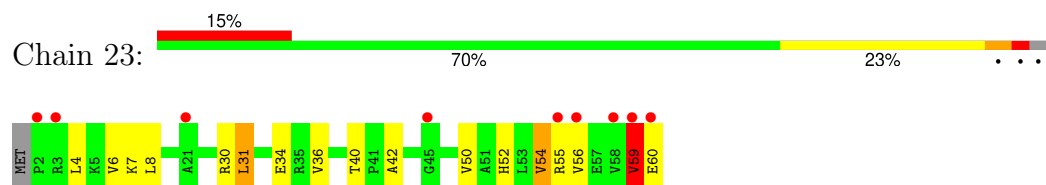
Chain 22: 

M1 K2 L3 S4 V6 R7 L10 E11 E12 A13 L16 S17 P18 L21 E22 R23 L24 V25 R26 K29 L32 M33 E34 L35 R36 Q43 L44 S45 K49 I50 R51 D52 L53 K54 R55 Q56 I57 A58 R59 L60 L61 T62 V63 V64 N65 E66 E67 R68 R69 Q70 ASN ALA

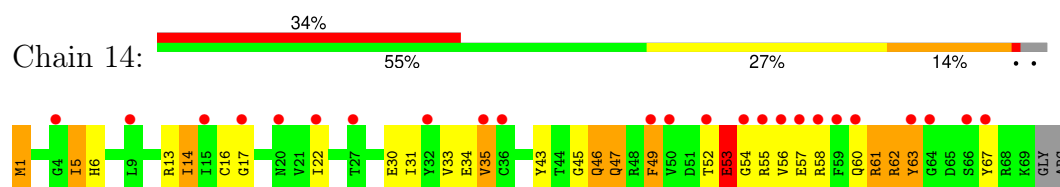
• Molecule 25: 50S ribosomal protein L30



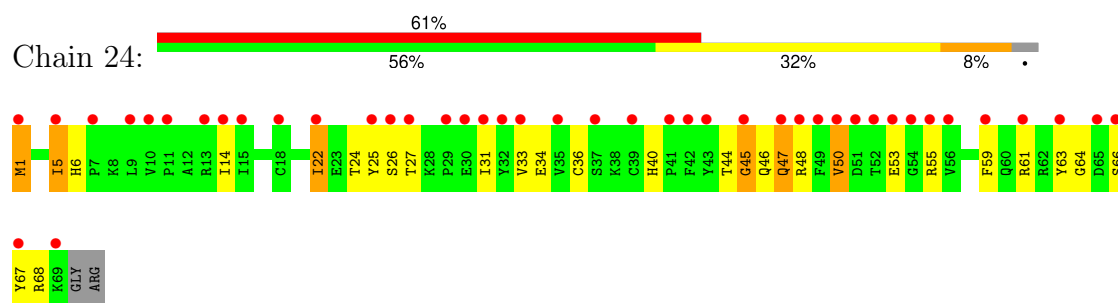
• Molecule 25: 50S ribosomal protein L30



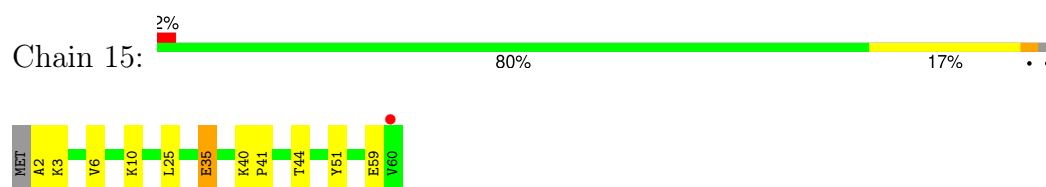
• Molecule 26: 50S ribosomal protein L31



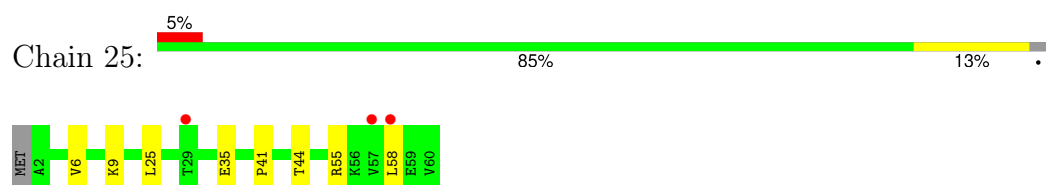
• Molecule 26: 50S ribosomal protein L31



• Molecule 27: 50S ribosomal protein L32



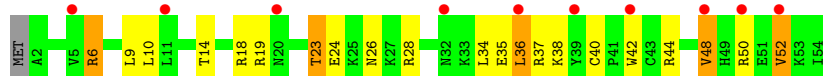
• Molecule 27: 50S ribosomal protein L32



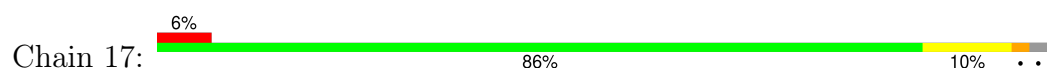
• Molecule 28: 50S ribosomal protein L33



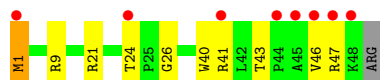
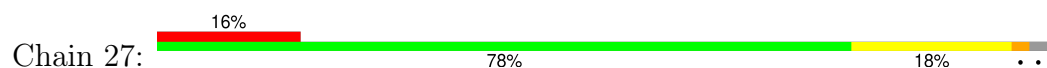
- Molecule 28: 50S ribosomal protein L33



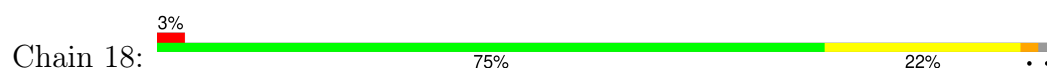
- Molecule 29: 50S ribosomal protein L34



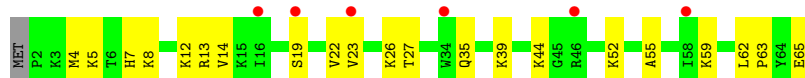
- Molecule 29: 50S ribosomal protein L34



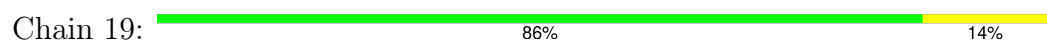
- Molecule 30: 50S ribosomal protein L35



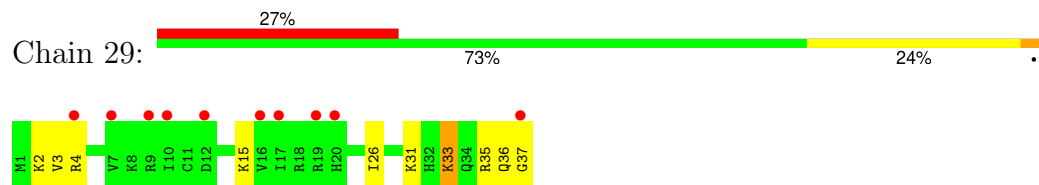
- Molecule 30: 50S ribosomal protein L35



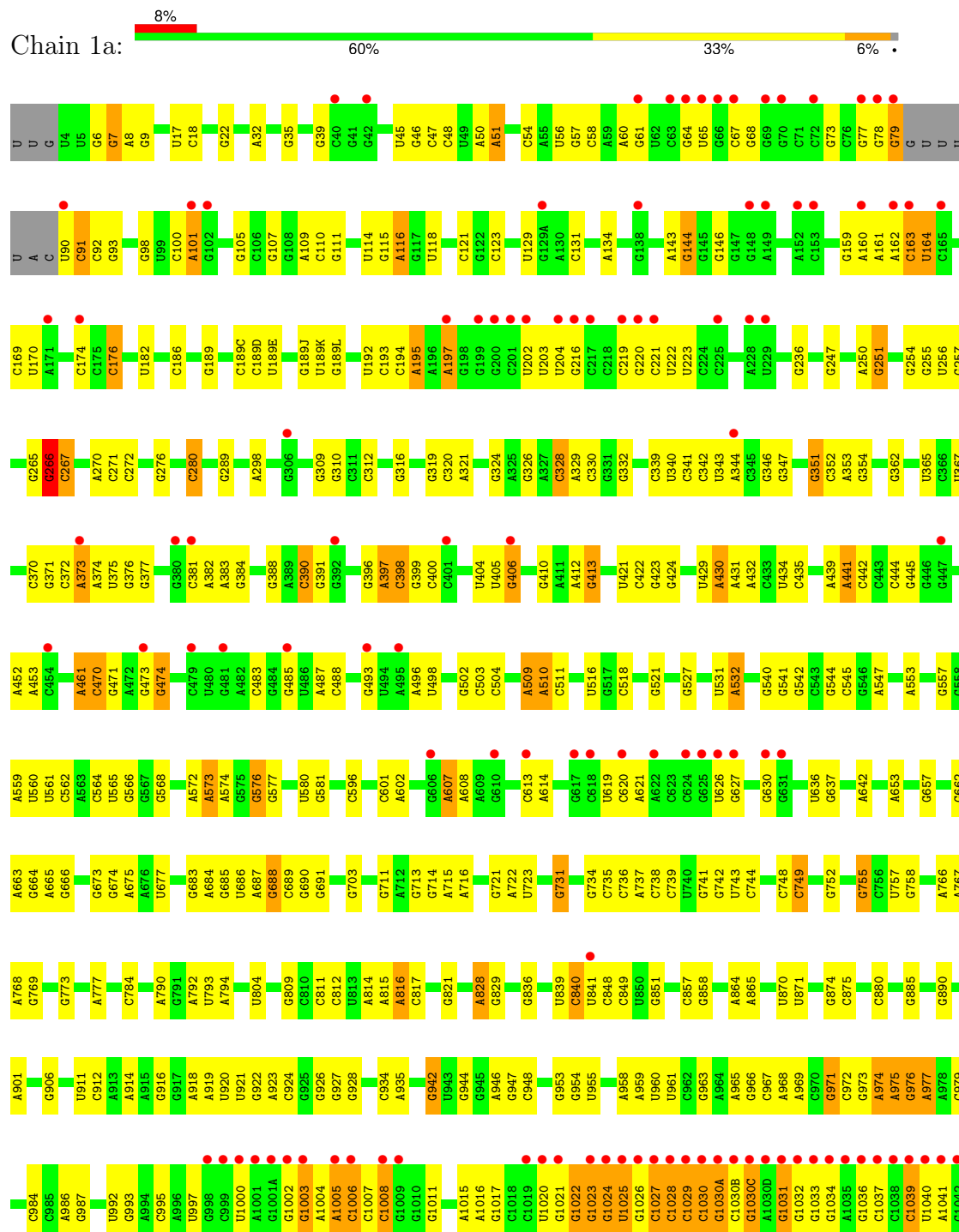
- Molecule 31: 50S ribosomal protein L36

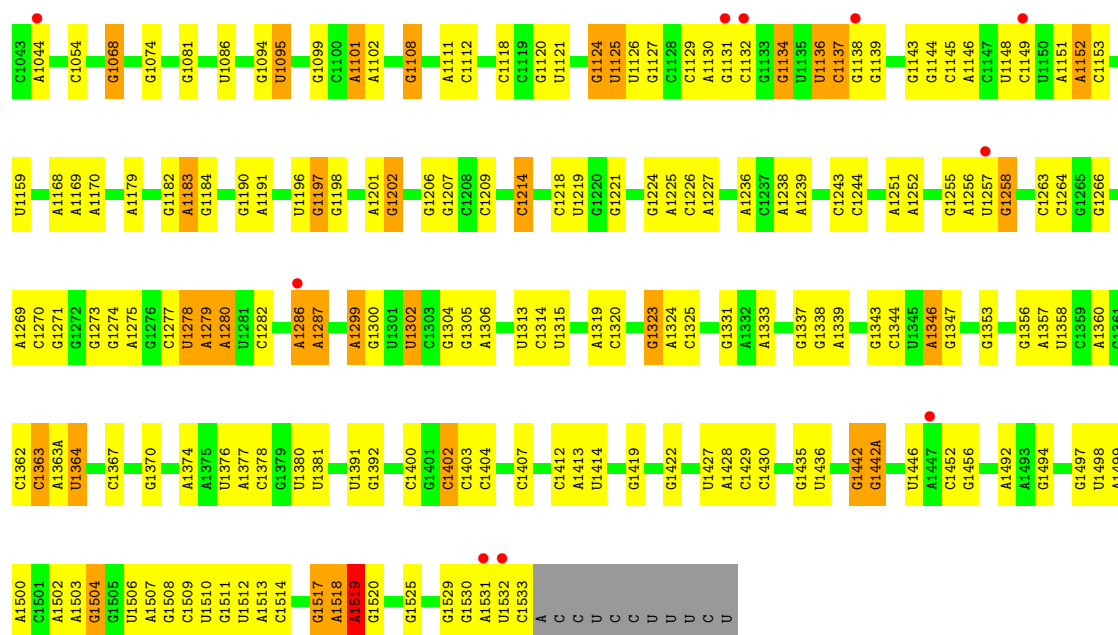


- Molecule 31: 50S ribosomal protein L36

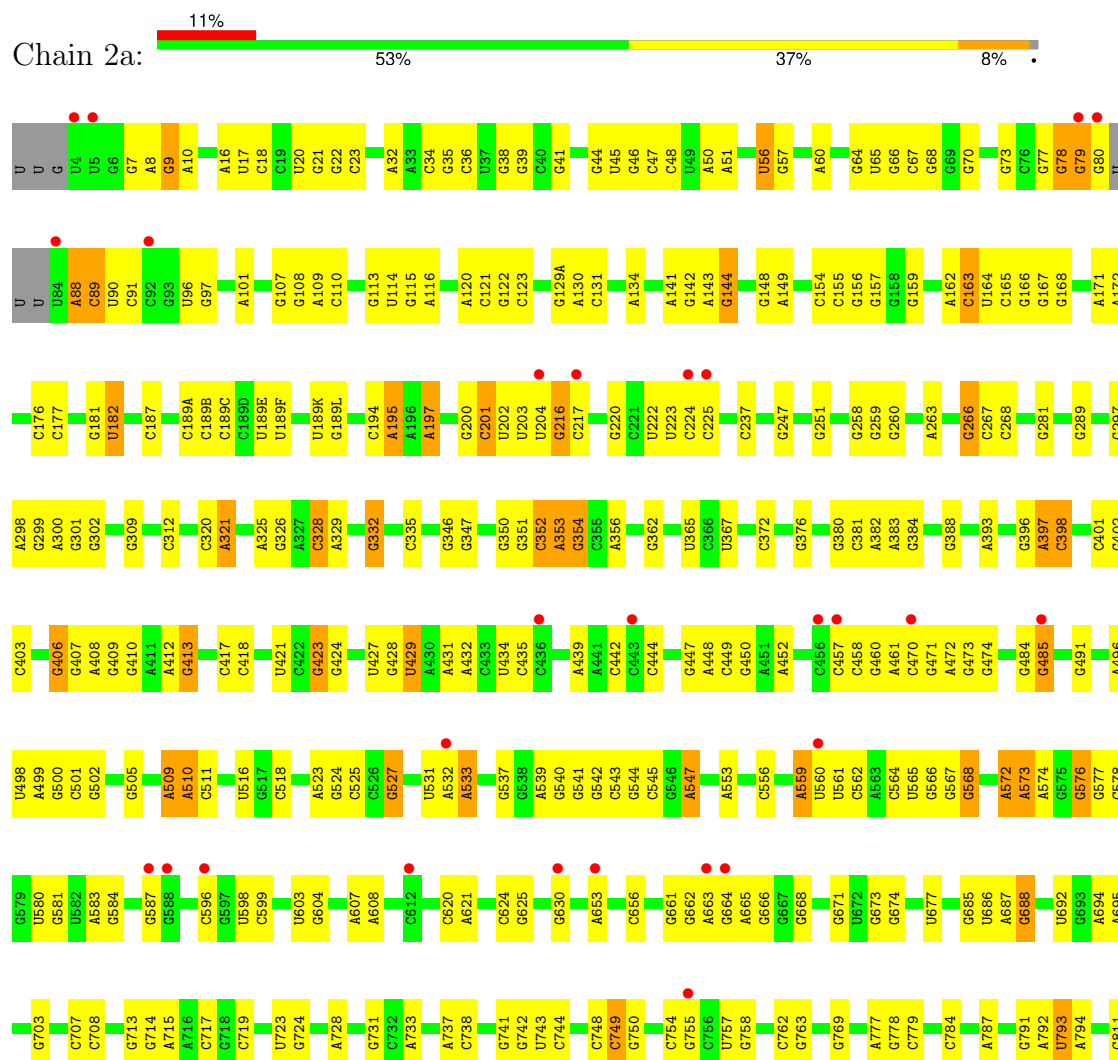


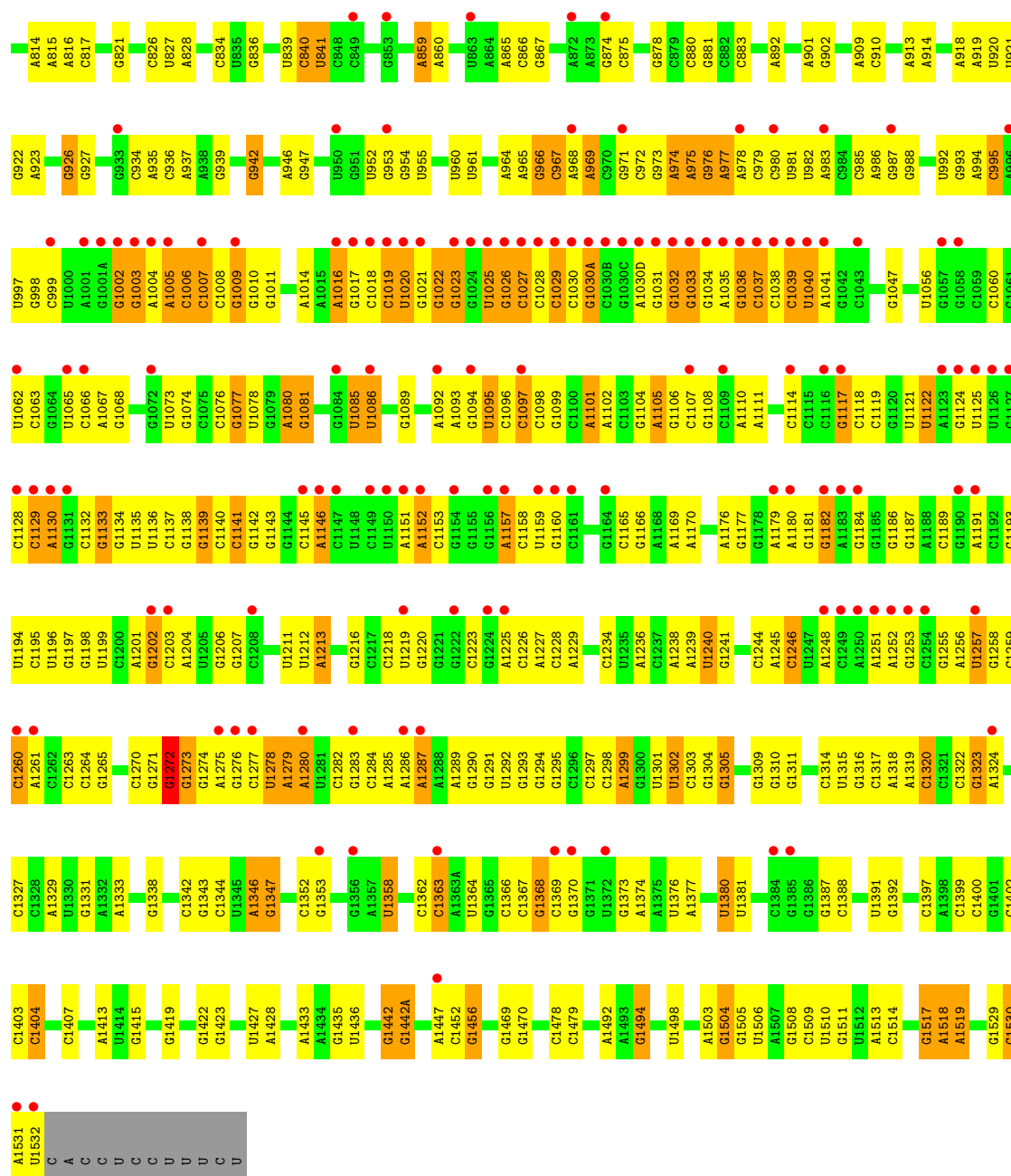
- Molecule 32: 16S Ribosomal RNA





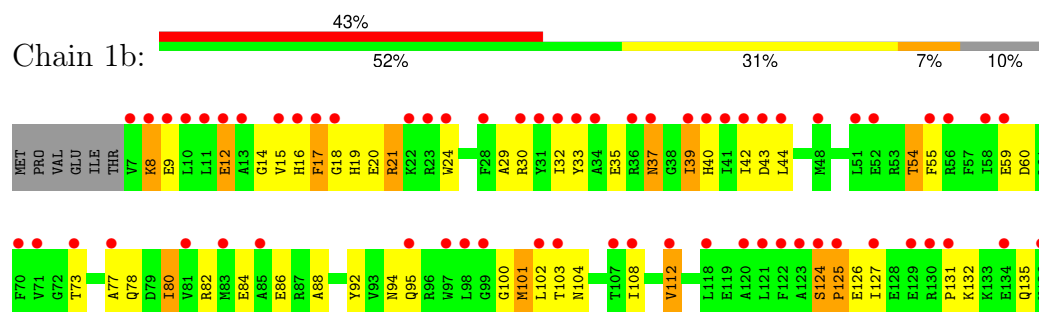
• Molecule 32: 16S Ribosomal RNA

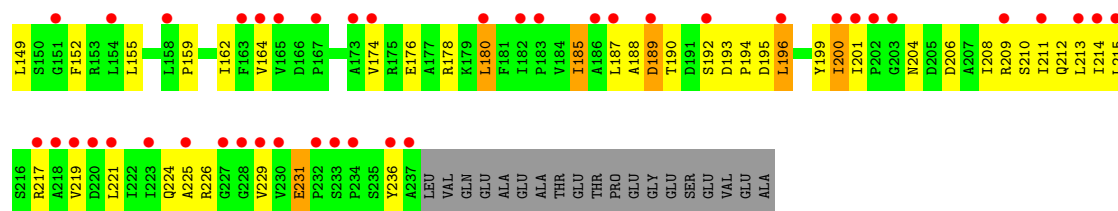




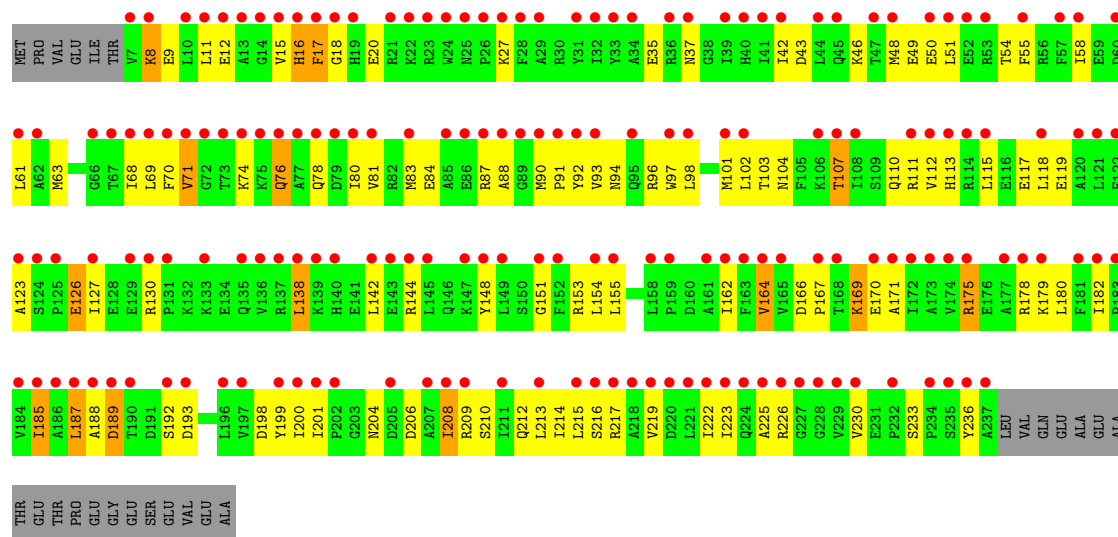
• Molecule 33: 30S ribosomal protein S2

Chain 1b:





• Molecule 33: 30S ribosomal protein S2

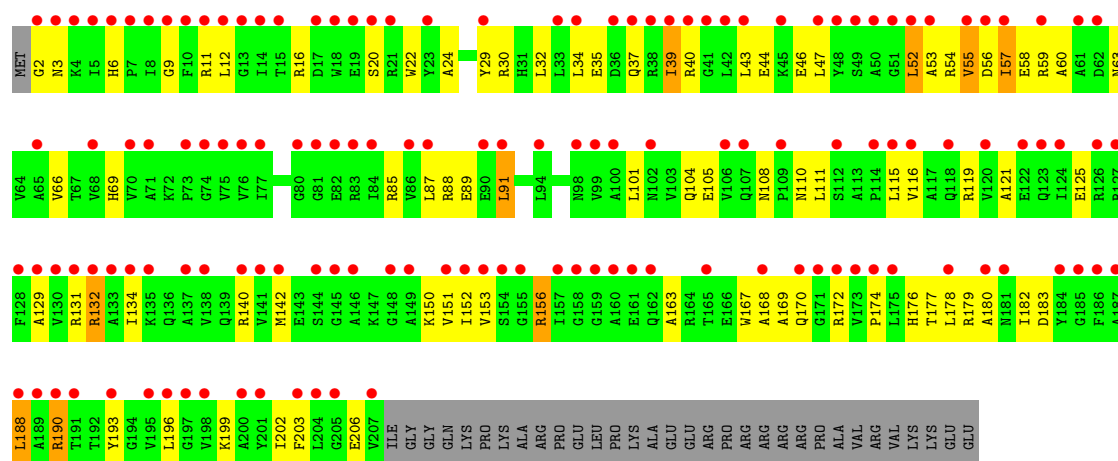


• Molecule 34: 30S ribosomal protein S3



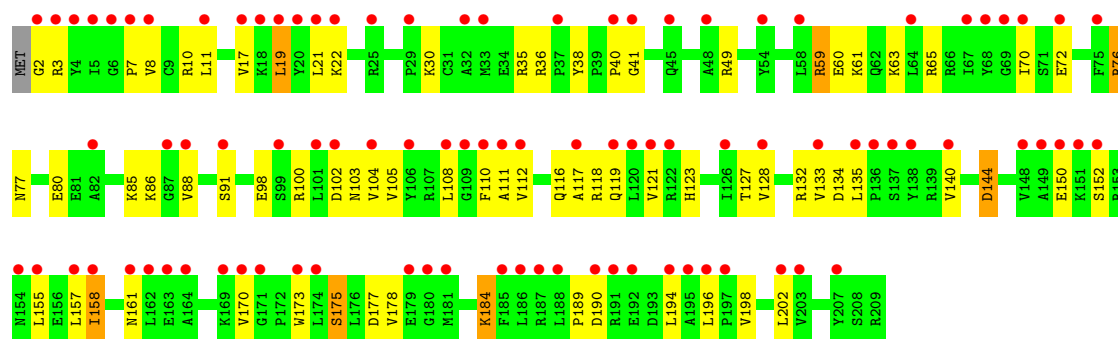
• Molecule 34: 30S ribosomal protein S3

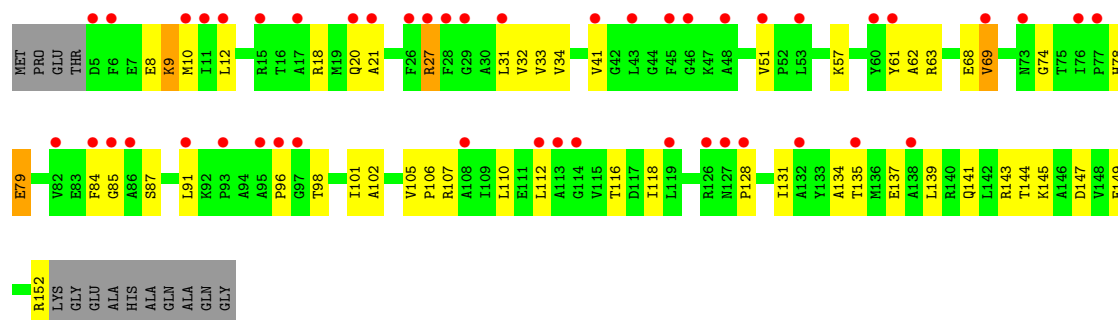




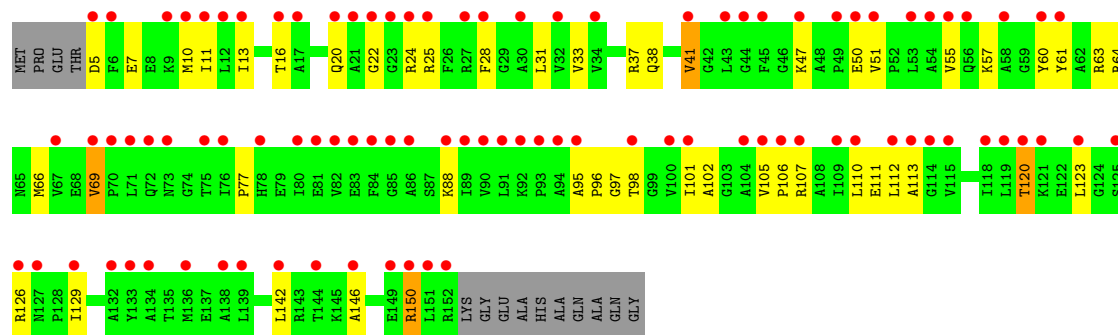
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 45% 65% 32%

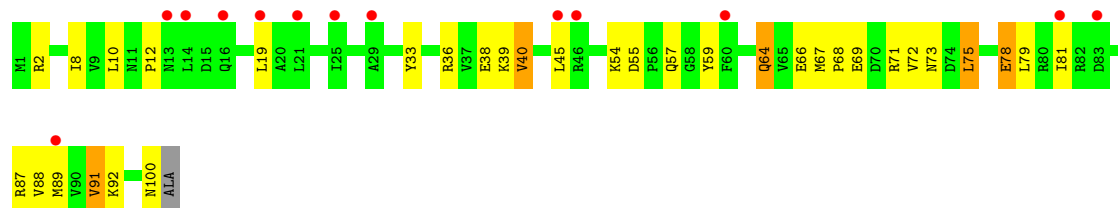




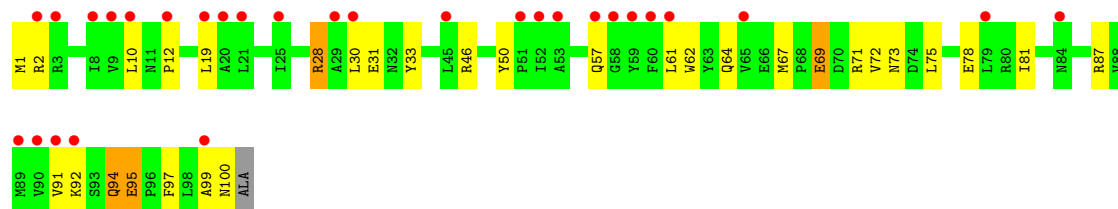
• Molecule 36: 30S ribosomal protein S5



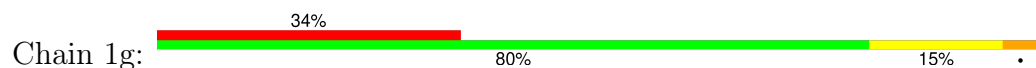
• Molecule 37: 30S ribosomal protein S6

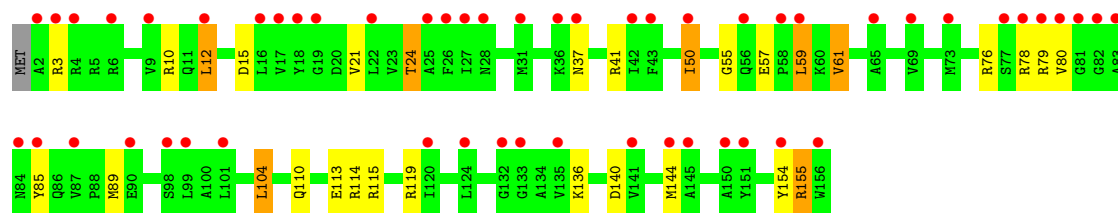


• Molecule 37: 30S ribosomal protein S6

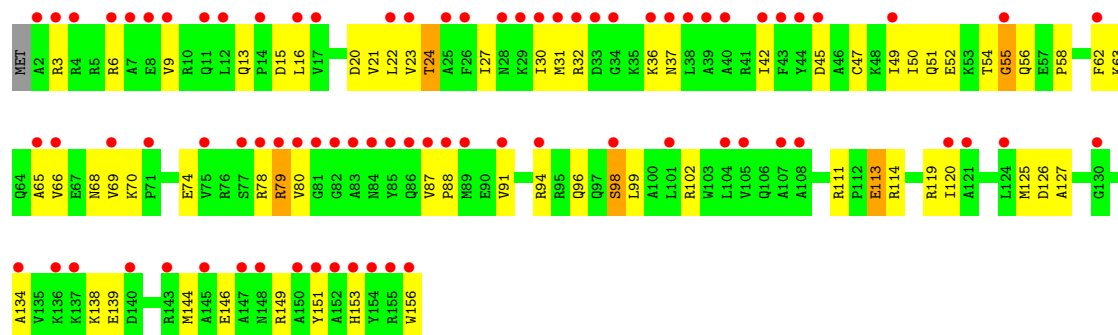


• Molecule 38: 30S ribosomal protein S7

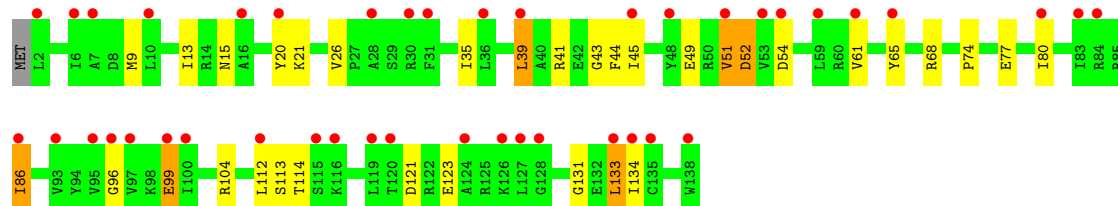
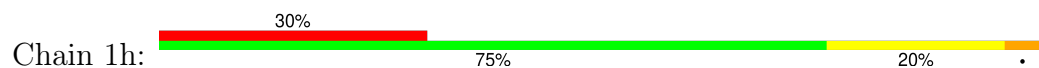




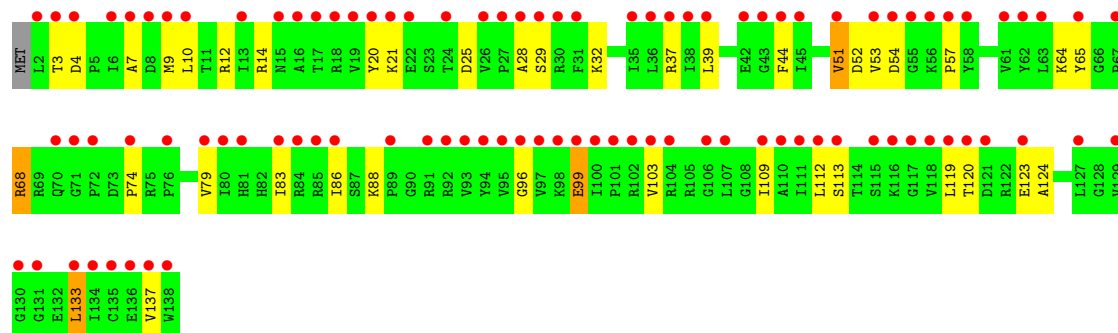
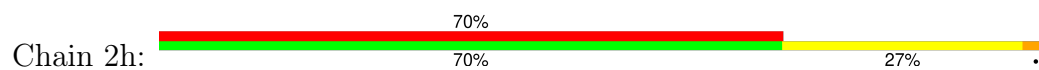
• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8

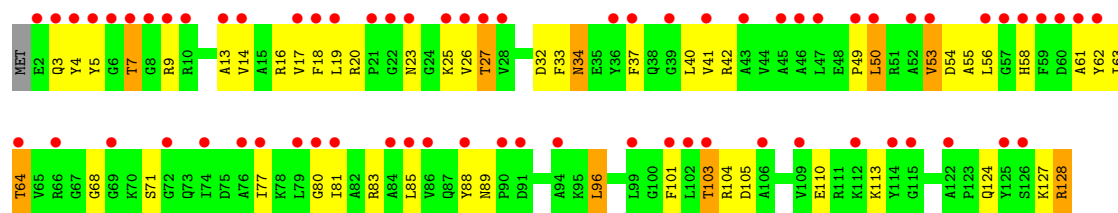


• Molecule 39: 30S ribosomal protein S8

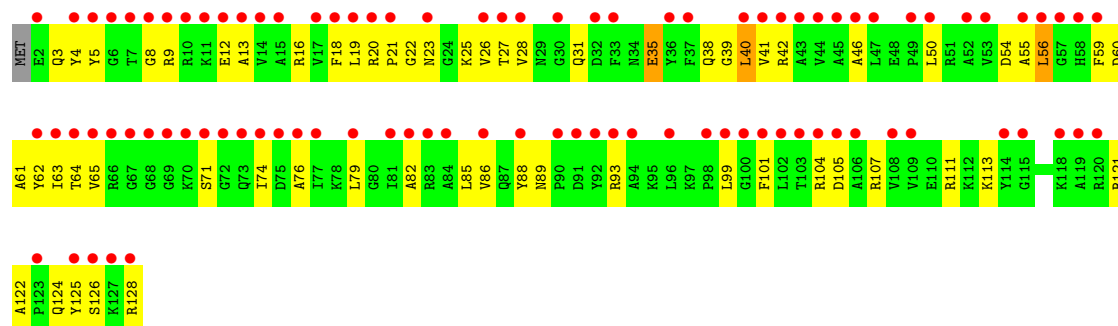
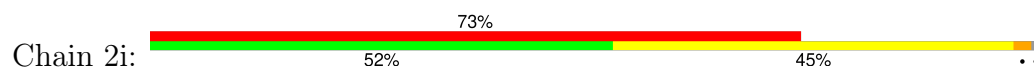


• Molecule 40: 30S ribosomal protein S9

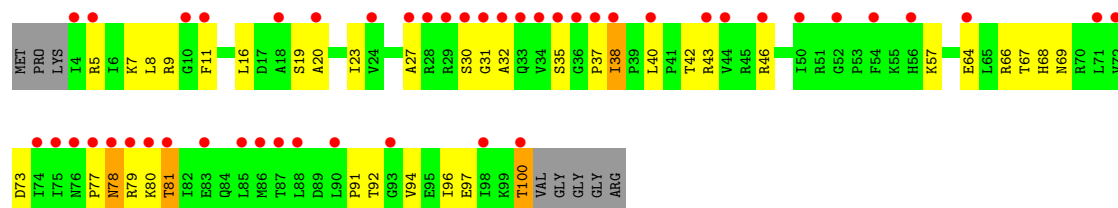




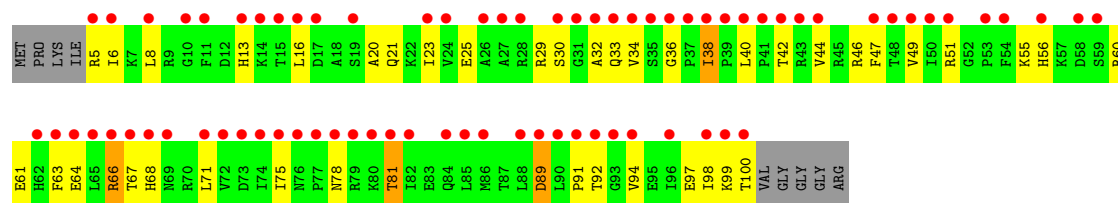
• Molecule 40: 30S ribosomal protein S9



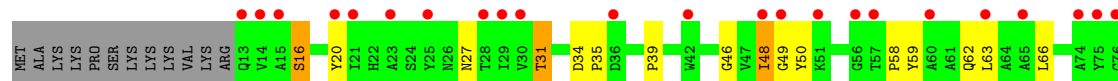
• Molecule 41: 30S ribosomal protein S10

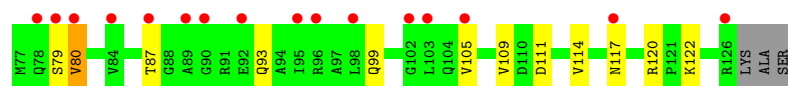


• Molecule 41: 30S ribosomal protein S10

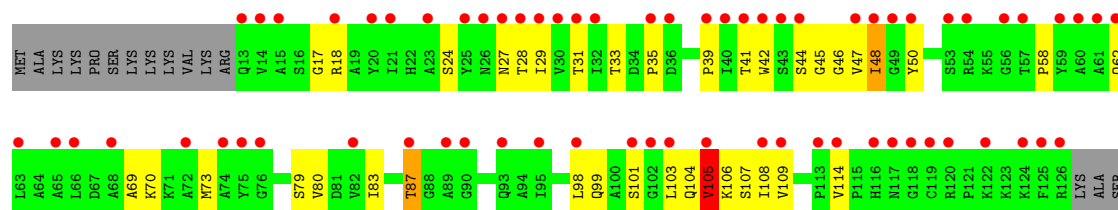


• Molecule 42: 30S ribosomal protein S11

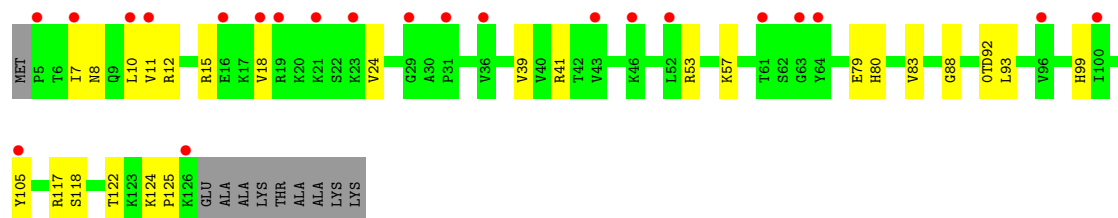
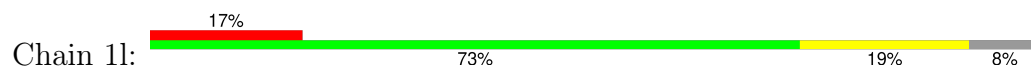




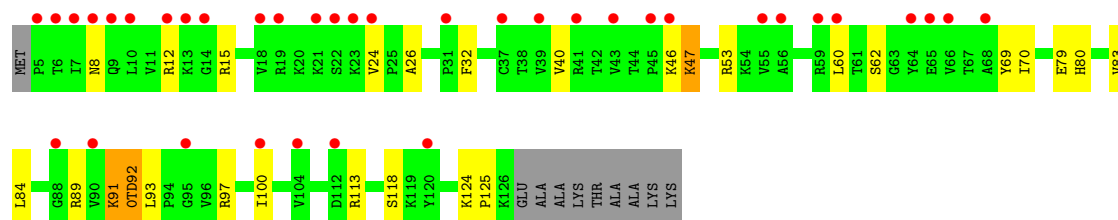
- Molecule 42: 30S ribosomal protein S11



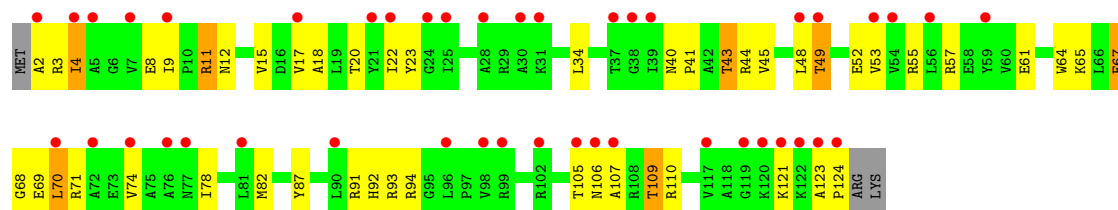
- Molecule 43: 30S ribosomal protein S12



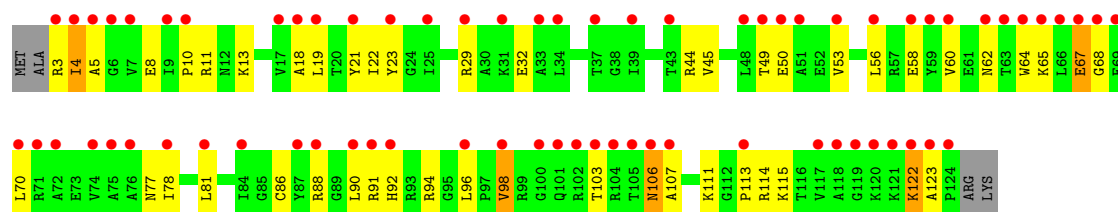
- Molecule 43: 30S ribosomal protein S12



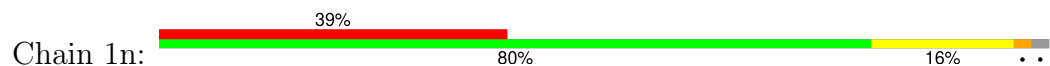
- Molecule 44: 30S ribosomal protein S13



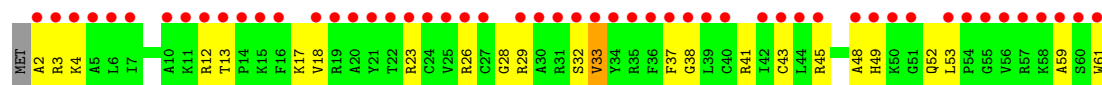
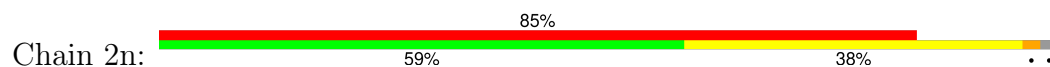
- Molecule 44: 30S ribosomal protein S13



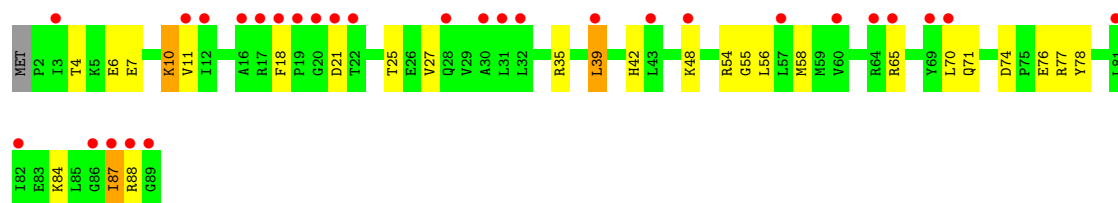
- Molecule 45: 30S ribosomal protein S14 type Z



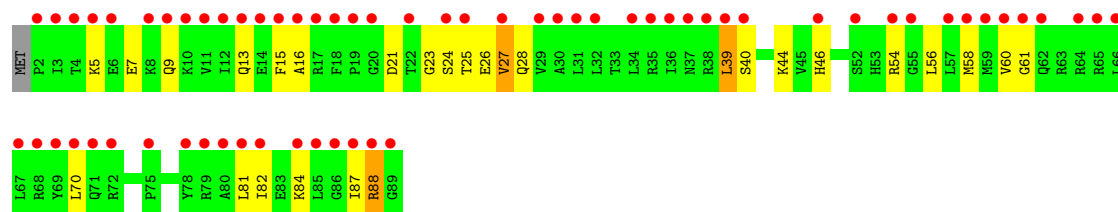
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

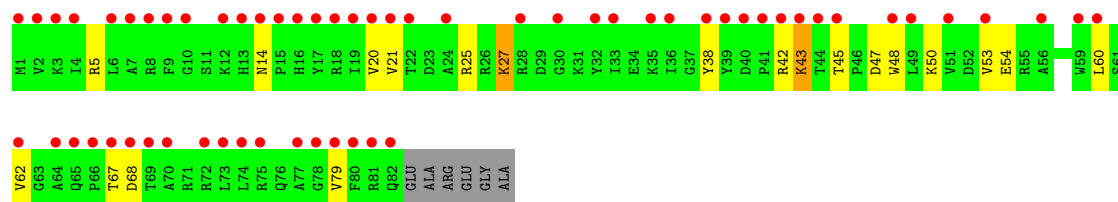


- Molecule 46: 30S ribosomal protein S15

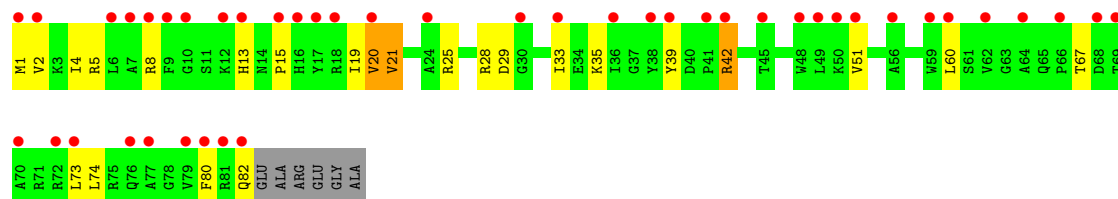


- Molecule 47: 30S ribosomal protein S16

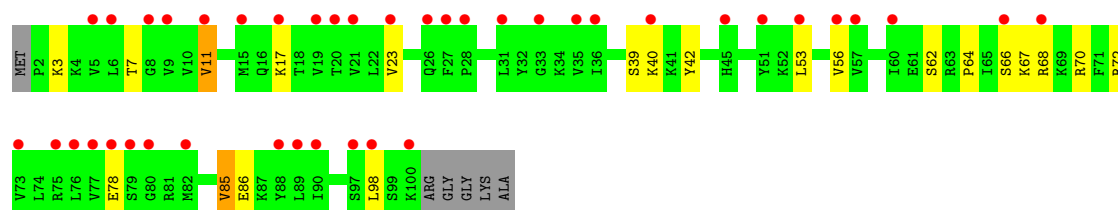
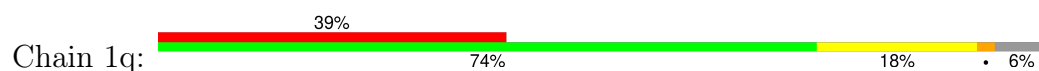




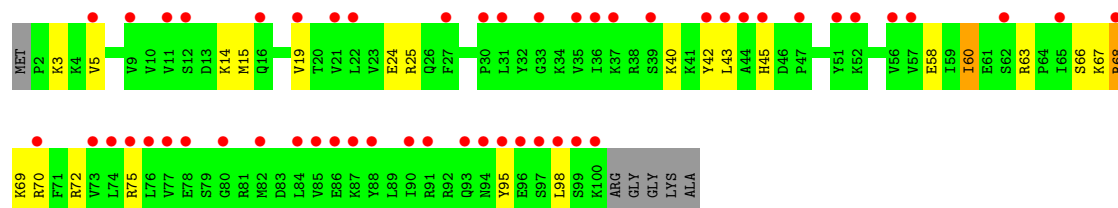
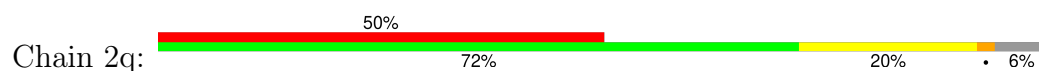
• Molecule 47: 30S ribosomal protein S16



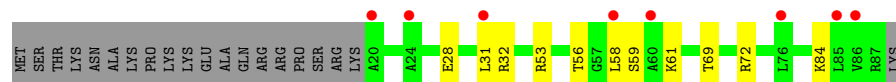
• Molecule 48: 30S ribosomal protein S17



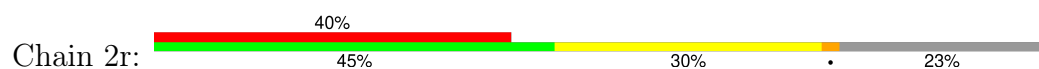
• Molecule 48: 30S ribosomal protein S17

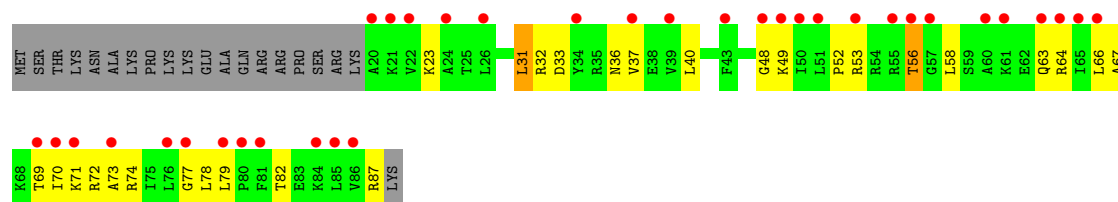


• Molecule 49: 30S ribosomal protein S18

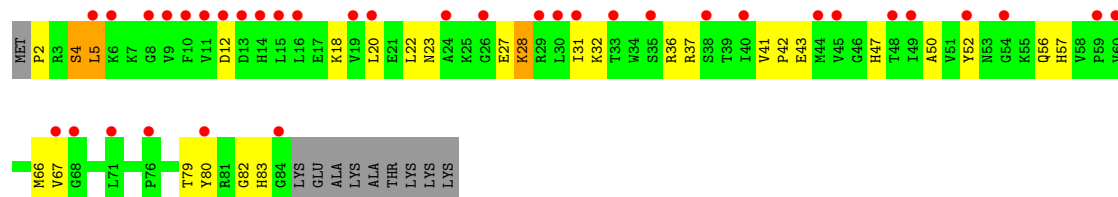
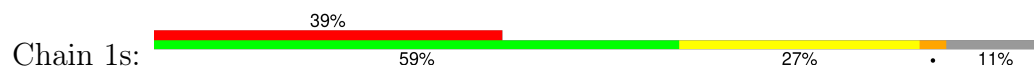


• Molecule 49: 30S ribosomal protein S18

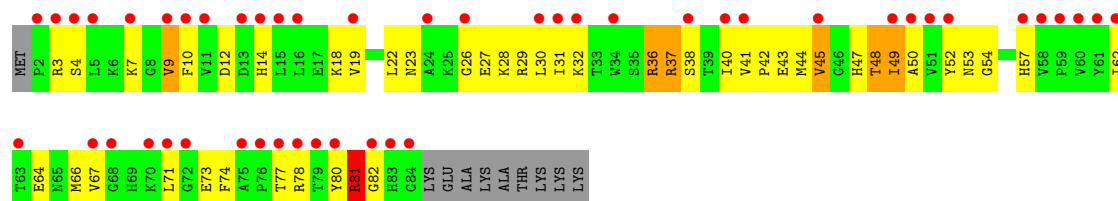




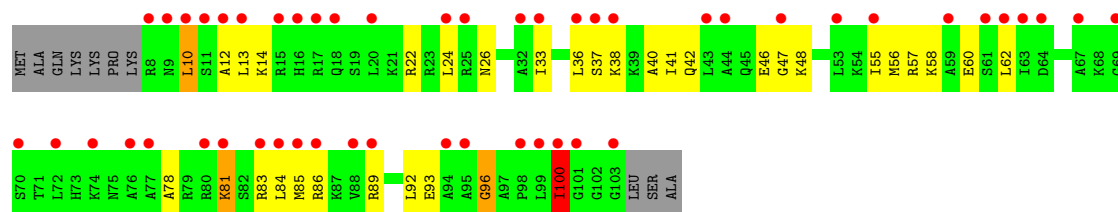
• Molecule 50: 30S ribosomal protein S19



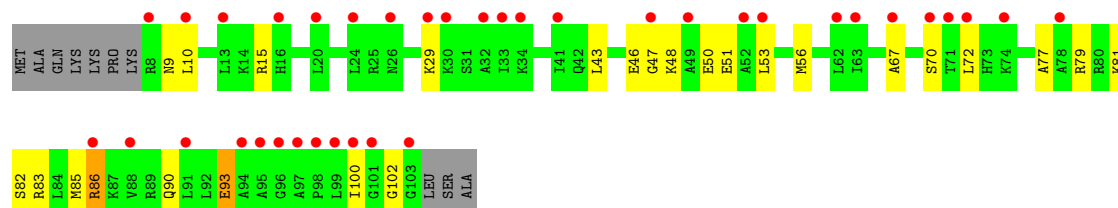
• Molecule 50: 30S ribosomal protein S19



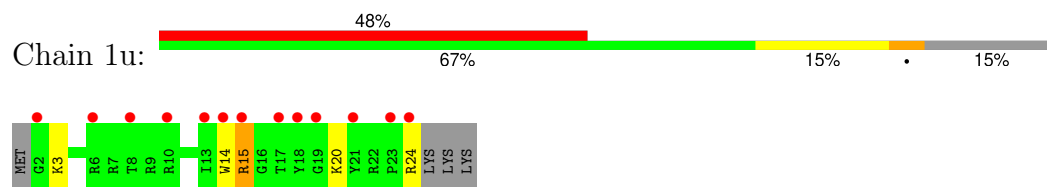
• Molecule 51: 30S ribosomal protein S20



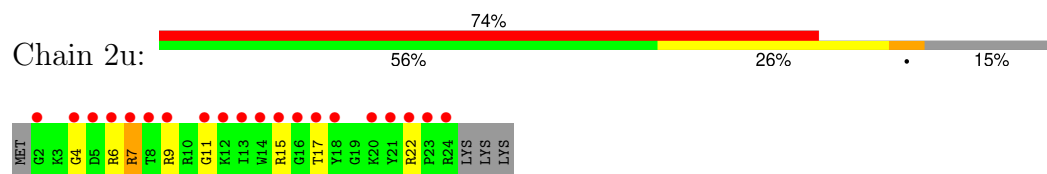
• Molecule 51: 30S ribosomal protein S20



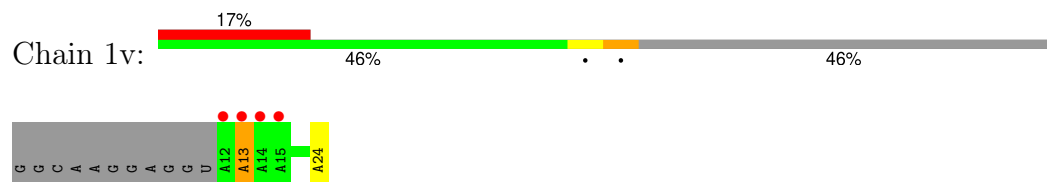
- Molecule 52: 30S ribosomal protein Thx



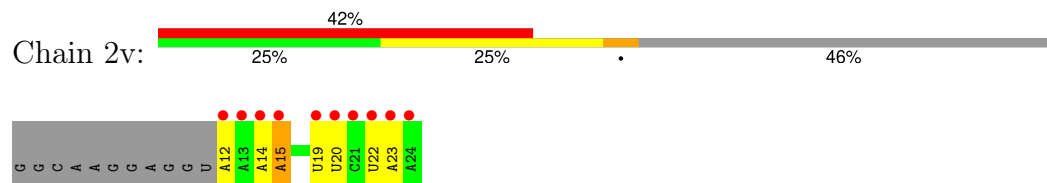
- Molecule 52: 30S ribosomal protein Thx



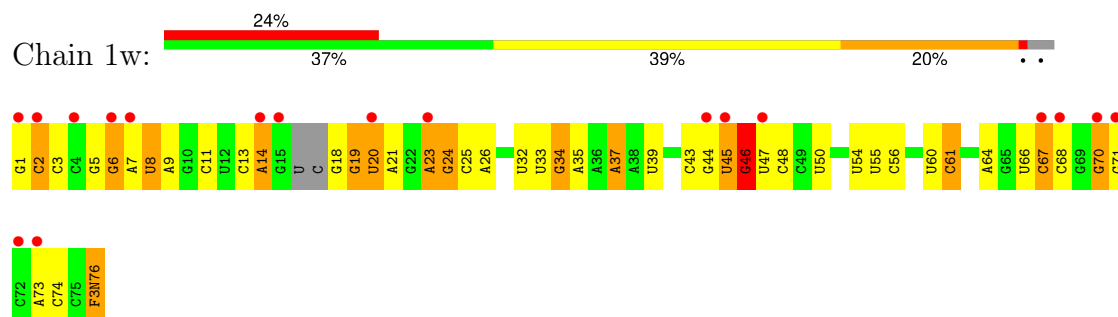
- Molecule 53: MF-mRNA



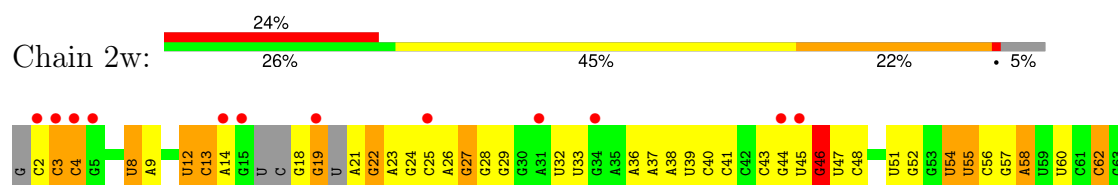
- Molecule 53: MF-mRNA

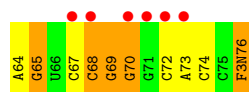


- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe

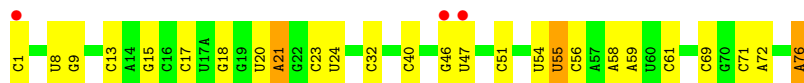




- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} RNA-part



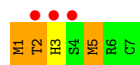
- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} RNA-part



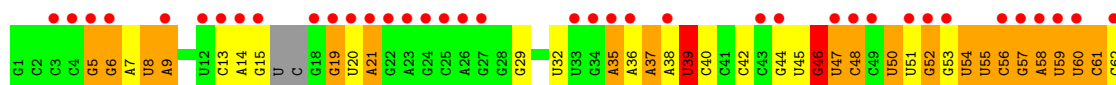
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} Peptide-part



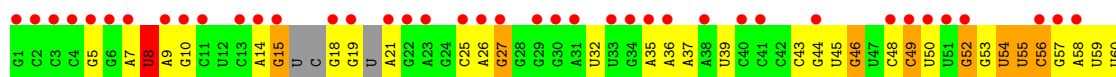
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} Peptide-part



- Molecule 57: E-site Deacylated tRNA^{phe}



- Molecule 57: E-site Deacylated tRNA^{phe}



C61	C62	G63	A64	G65	U66	C67	C68	G69	G70	G71	C72	A73	C74	C75	A76
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 447.70Å 618.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.53 – 2.30 121.53 – 2.47	Depositor EDS
% Data completeness (in resolution range)	97.5 (121.53-2.30) 98.6 (121.53-2.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.237 , 0.281 0.271 , 0.302	Depositor DCC
R_{free} test set	101013 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	299898	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, MG, 4OC, FME, K, F3N, G7M, ZN, OMC, PSU, OMU, MIA, 0TD, 2MA, 4SU, M2G, 5MU, UR3, OMG, 5MC, MA6, 2MG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	1/69011 (0.0%)	0.48	2/107720 (0.0%)
1	2A	0.22	0/67295	0.41	2/105042 (0.0%)
2	1B	0.22	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.22	0/2186	0.44	0/2944
4	1E	0.28	0/1592	0.53	0/2149
4	2E	0.21	0/1592	0.44	0/2149
5	1F	0.26	0/1618	0.49	0/2191
5	2F	0.20	0/1614	0.45	2/2186 (0.1%)
6	1G	0.21	0/1448	0.44	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.44	0/1834
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.19	0/1112	0.43	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.49	0/1269
10	2O	0.22	0/943	0.44	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.20	0/1152	0.48	0/1533
12	1Q	0.25	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.22	0/1105	0.46	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.41	0/1301
17	1V	0.25	0/782	0.50	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.22	0/897	0.43	0/1205
19	1X	0.25	0/764	0.51	0/1025
19	2X	0.20	0/764	0.51	2/1025 (0.2%)
20	1Y	0.21	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.42	0/1095
21	1Z	0.22	0/1267	0.48	0/1717
21	2Z	0.21	0/1299	0.44	0/1763
22	10	0.24	0/662	0.46	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.43	0/1014
23	21	0.21	0/762	0.42	0/1014
24	12	0.21	0/590	0.43	0/781
24	22	0.19	0/590	0.42	0/781
25	13	0.24	0/474	0.46	0/635
25	23	0.18	0/469	0.42	0/630
26	14	0.23	0/565	0.53	0/761
26	24	0.24	0/545	0.56	1/737 (0.1%)
27	15	0.25	0/469	0.48	0/635
27	25	0.23	0/469	0.48	0/635
28	16	0.25	0/460	0.48	0/613
28	26	0.20	0/456	0.41	0/608
29	17	0.29	0/426	0.55	0/561
29	27	0.23	0/426	0.50	0/561
30	18	0.27	0/525	0.46	0/691
30	28	0.21	0/525	0.39	0/691
31	19	0.27	0/310	0.52	0/407
31	29	0.21	0/310	0.44	0/407
32	1a	0.20	0/35795	0.40	1/55864 (0.0%)
32	2a	0.19	0/35886	0.38	1/56005 (0.0%)
33	1b	0.20	0/1881	0.46	0/2542
33	2b	0.21	0/1860	0.48	0/2518
34	1c	0.18	0/1572	0.41	0/2126
34	2c	0.19	0/1566	0.41	0/2119
35	1d	0.19	0/1685	0.45	0/2262
35	2d	0.19	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.20	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.40	0/1679
38	2g	0.19	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.39	0/1494
39	2h	0.18	0/1108	0.39	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.21	0/997	0.52	0/1343
41	1j	0.20	0/722	0.47	0/982
41	2j	0.21	0/727	0.43	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.22	0/937	0.43	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.20	0/969	0.51	0/1302
44	2m	0.18	0/961	0.45	0/1291
45	1n	0.21	0/501	0.47	0/664
45	2n	0.20	0/501	0.44	0/664
46	1o	0.18	0/739	0.35	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.17	0/836	0.43	0/1117
49	1r	0.21	0/560	0.41	0/746
49	2r	0.17	0/560	0.41	0/746
50	1s	0.25	0/667	0.48	0/900
50	2s	0.23	0/661	0.55	0/893
51	1t	0.20	0/730	0.47	0/965
51	2t	0.19	0/729	0.44	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.21	0/203	0.45	0/266
53	1v	0.22	0/310	0.33	0/480
53	2v	0.27	0/310	0.47	0/480
54	1w	0.30	1/1581 (0.1%)	0.43	0/2458
54	2w	0.29	1/1531 (0.1%)	0.42	0/2379
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	0/1723	0.40	0/2684
56	1z	0.45	0/48	0.58	0/62
56	2z	0.33	0/48	0.55	0/62
57	1y	0.31	2/1606 (0.1%)	0.41	0/2497
57	2y	0.32	2/1583 (0.1%)	0.42	0/2459
All	All	0.23	7/316730 (0.0%)	0.43	11/474161 (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
12	1Q	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	46	G7M	O3'-P	5.60	1.61	1.56
54	1w	46	G7M	O3'-P	5.43	1.61	1.56
54	2w	46	G7M	O3'-P	5.36	1.61	1.56
1	1A	2552	OMU	O3'-P	5.20	1.61	1.56
57	1y	8	4SU	O3'-P	5.12	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.85	119.77	109.50
26	24	5	ILE	N-CA-C	-6.11	107.91	113.71
1	2A	1992	G	C2'-C3'-O3'	5.76	118.14	109.50
19	2X	94	GLY	CA-C-N	5.67	131.91	121.70
19	2X	94	GLY	C-N-CA	5.67	131.91	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	15	GLY	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	31196	627	0
1	2A	60322	0	30425	699	0
2	1B	2577	0	1305	18	0
2	2B	2575	0	1303	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	40	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	33	0
5	1F	1583	0	1625	38	0
5	2F	1579	0	1619	53	0
6	1G	1423	0	1436	44	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	36	0
8	1I	1097	0	1140	32	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	21	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	35	0
11	2P	1135	0	1212	27	0
12	1Q	1122	0	1179	15	0
12	2Q	1122	0	1179	31	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	19	0
14	1S	873	0	927	14	0
14	2S	870	0	923	26	0
15	1T	1091	0	1151	17	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	10	0
17	2V	771	0	830	8	0
18	1W	886	0	940	12	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	814	28	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	26	0
21	1Z	1240	0	1240	25	0
21	2Z	1271	0	1273	44	0
22	10	653	0	674	8	0
22	20	653	0	674	12	0
23	11	755	0	826	14	0
23	21	755	0	826	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	4	0
24	22	588	0	643	17	0
25	13	469	0	518	10	0
25	23	464	0	514	12	0
26	14	552	0	533	28	0
26	24	532	0	503	18	0
27	15	455	0	465	6	0
27	25	455	0	464	3	0
28	16	453	0	473	10	0
28	26	449	0	469	14	0
29	17	418	0	467	3	0
29	27	418	0	467	10	0
30	18	517	0	582	13	0
30	28	517	0	582	15	0
31	19	307	0	335	3	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	362	0
32	2a	32327	0	16338	486	0
33	1b	1846	0	1867	63	0
33	2b	1825	0	1828	70	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	60	0
35	1d	1655	0	1672	40	0
35	2d	1674	0	1714	52	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	34	0
37	1f	810	0	804	17	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	17	0
38	2g	1235	0	1249	39	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	19	0
40	1i	983	0	986	38	0
40	2i	978	0	966	40	0
41	1j	709	0	650	26	0
41	2j	714	0	672	29	0
42	1k	829	0	825	17	0
42	2k	833	0	835	19	0
43	1l	932	0	981	13	0
43	2l	932	0	980	20	0
44	1m	958	0	1002	29	0
44	2m	950	0	988	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	7	0
45	2n	492	0	529	27	0
46	1o	728	0	760	14	0
46	2o	728	0	760	19	0
47	1p	681	0	697	12	0
47	2p	677	0	686	17	0
48	1q	823	0	891	15	0
48	2q	823	0	891	12	0
49	1r	555	0	618	8	0
49	2r	555	0	618	24	0
50	1s	652	0	662	21	0
50	2s	646	0	644	34	0
51	1t	728	0	798	21	0
51	2t	727	0	796	18	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1v	277	0	140	2	0
53	2v	277	0	140	8	0
54	1w	1603	0	828	22	0
54	2w	1555	0	797	37	0
55	1x	1646	0	838	15	0
55	2x	1646	0	838	12	0
56	1z	58	0	56	3	0
56	2z	58	0	56	3	0
57	1y	1585	0	803	40	0
57	2y	1565	0	793	34	0
58	10	9	0	0	0	0
58	11	6	0	0	0	0
58	12	2	0	0	0	0
58	13	4	0	0	0	0
58	14	1	0	0	0	0
58	15	7	0	0	0	0
58	16	1	0	0	0	0
58	17	5	0	0	0	0
58	18	7	0	0	0	0
58	19	1	0	0	0	0
58	1A	1101	0	0	0	0
58	1B	38	0	0	0	0
58	1D	13	0	0	0	0
58	1E	12	0	0	0	0
58	1F	12	0	0	0	0
58	1G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	7	0	0	0	0
58	1Q	8	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	10	0	0	0	0
58	1V	7	0	0	0	0
58	1W	4	0	0	0	0
58	1X	4	0	0	0	0
58	1Y	4	0	0	0	0
58	1Z	4	0	0	0	0
58	1a	210	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1t	1	0	0	0	0
58	1w	7	0	0	0	0
58	1x	12	0	0	0	0
58	20	2	0	0	0	0
58	21	1	0	0	0	0
58	23	3	0	0	0	0
58	25	3	0	0	0	0
58	27	2	0	0	0	0
58	28	4	0	0	0	0
58	29	1	0	0	0	0
58	2A	851	0	0	0	0
58	2B	20	0	0	0	0
58	2D	7	0	0	0	0
58	2E	10	0	0	0	0
58	2F	6	0	0	0	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	2	0	0	0	0
58	2P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2Q	4	0	0	0	0
58	2R	4	0	0	0	0
58	2T	4	0	0	0	0
58	2U	1	0	0	0	0
58	2V	2	0	0	0	0
58	2W	1	0	0	0	0
58	2X	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	220	0	0	0	0
58	2d	3	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2i	1	0	0	0	0
58	2j	2	0	0	0	0
58	2k	1	0	0	0	0
58	2l	3	0	0	0	0
58	2n	1	0	0	0	0
58	2q	3	0	0	0	0
58	2r	1	0	0	0	0
58	2t	2	0	0	0	0
58	2v	4	0	0	0	0
58	2w	4	0	0	0	0
58	2x	6	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	13	0	0	0	0
62	11	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	12	3	0	0	0	0
62	13	6	0	0	0	0
62	15	8	0	0	0	0
62	16	2	0	0	0	0
62	17	8	0	0	0	0
62	18	12	0	0	0	0
62	1A	1949	0	0	79	0
62	1B	58	0	0	3	0
62	1D	26	0	0	0	0
62	1E	28	0	0	3	0
62	1F	18	0	0	2	0
62	1G	3	0	0	1	0
62	1H	2	0	0	0	0
62	1N	6	0	0	0	0
62	1O	6	0	0	0	0
62	1P	19	0	0	2	0
62	1Q	7	0	0	0	0
62	1R	10	0	0	4	0
62	1S	4	0	0	0	0
62	1T	7	0	0	0	0
62	1U	13	0	0	0	0
62	1V	9	0	0	0	0
62	1W	7	0	0	0	0
62	1X	5	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	301	0	0	21	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	5	0	0	0	0
62	1m	1	0	0	0	0
62	1o	2	0	0	0	0
62	1q	2	0	0	0	0
62	1v	5	0	0	0	0
62	1w	9	0	0	0	0
62	1x	7	0	0	2	0
62	1z	3	0	0	0	0
62	20	2	0	0	0	0
62	21	7	0	0	1	0
62	22	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	23	2	0	0	0	0
62	25	2	0	0	0	0
62	27	5	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1047	0	0	73	0
62	2B	20	0	0	1	0
62	2D	26	0	0	0	0
62	2E	15	0	0	1	0
62	2F	14	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	2	0	0	0	0
62	2R	3	0	0	0	0
62	2T	6	0	0	0	0
62	2U	1	0	0	1	0
62	2V	1	0	0	0	0
62	2W	3	0	0	0	0
62	2X	5	0	0	1	0
62	2a	196	0	0	8	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2e	2	0	0	0	0
62	2g	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	2	0	0	0	0
62	2l	5	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	2	0	0	0	0
62	2w	6	0	0	1	0
62	2x	4	0	0	0	0
62	2z	1	0	0	0	0
All	All	299898	0	196836	4043	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 9.

The worst 5 of 4043 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.23	1.36
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.02
1:1A:1054:A:N6	1:1A:1105:U:H3	1.57	1.01
54:2w:4:C:N4	54:2w:69:G:H1	1.59	1.01
1:1A:2499:C:OP1	62:1A:4204:HOH:O	1.80	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	31
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	31
5	1F	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
5	2F	200/210 (95%)	187 (94%)	10 (5%)	3 (2%)	8	8
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
6	2G	179/182 (98%)	158 (88%)	19 (11%)	2 (1%)	11	13
7	1H	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	21	27
7	2H	172/180 (96%)	146 (85%)	24 (14%)	2 (1%)	10	12
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	18	23
8	2I	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	9	9
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	23
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	20
10	2O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	23
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	2
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	6	5
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	15
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	15
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	13
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	18	23
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	3	2
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	13
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	8	8
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	6
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	51 (76%)	14 (21%)	2 (3%)	3	2
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	196 (86%)	27 (12%)	6 (3%)	4	3
33	2b	229/256 (90%)	196 (86%)	29 (13%)	4 (2%)	7	7
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	12	15
35	1d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	9
36	2e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	4	3
37	1f	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	15
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	18	23
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	6	5
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	20
40	2i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	20
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	2
41	2j	94/105 (90%)	77 (82%)	15 (16%)	2 (2%)	5	4
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	17
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	20
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	20
44	1m	121/126 (96%)	102 (84%)	17 (14%)	2 (2%)	7	7
44	2m	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	7	7
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	12
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	15
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	4	3
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5	4
51	2t	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	11	13
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	1z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
56	2z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
All	All	11378/12142 (94%)	10471 (92%)	817 (7%)	90 (1%)	16	20

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
33	1b	124	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	21	32
3	2D	215/218 (99%)	202 (94%)	13 (6%)	17	25
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	21
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	21
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	8
5	2F	159/166 (96%)	147 (92%)	12 (8%)	12	17
6	1G	143/156 (92%)	132 (92%)	11 (8%)	12	16
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	6
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	28
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	12
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	1
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	16
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	8
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	53
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	10
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	7
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	18
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	70	84
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	15
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	20
14	1S	86/88 (98%)	83 (96%)	3 (4%)	32	48
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	6
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	59
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	29
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	17
17	1V	80/82 (98%)	73 (91%)	7 (9%)	9	12
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3	3
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	21
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	12
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	77
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	59
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	19
20	2Y	85/91 (93%)	70 (82%)	15 (18%)	2	2
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	10
21	2Z	137/179 (76%)	115 (84%)	22 (16%)	2	2
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	75
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	77
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	23
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	7
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	24
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	26
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	25
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	1
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	4
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	15
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	15
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	6
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	18
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	10
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	28
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	192/220 (87%)	164 (85%)	28 (15%)	3	3
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	2
34	1c	142/188 (76%)	131 (92%)	11 (8%)	12	16
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	4
35	1d	169/181 (93%)	140 (83%)	29 (17%)	2	2
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	11
36	1e	113/123 (92%)	107 (95%)	6 (5%)	20	30
36	2e	114/123 (93%)	107 (94%)	7 (6%)	17	24
37	1f	84/90 (93%)	73 (87%)	11 (13%)	4	4
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	8
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	6
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	7
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	15
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	5
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	3
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	9
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	8
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	4
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	7
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	52
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	40
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	6
44	2m	92/101 (91%)	83 (90%)	9 (10%)	7	10
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	14
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	41
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	12
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	32
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	4
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	30
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	30
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	32
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	12
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	6
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	13
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	27
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	2
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	28
56	1z	6/6 (100%)	5 (83%)	1 (17%)	2	2
56	2z	6/6 (100%)	5 (83%)	1 (17%)	2	2
All	All	9315/10076 (92%)	8491 (91%)	824 (9%)	9	12

5 of 824 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	2I	44	LEU
20	2Y	70	SER
47	2p	42	ARG
8	2I	140	LEU
8	2I	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	13	GLN
39	2h	82	HIS
44	2m	12	ASN
38	1g	28	ASN
38	1g	13	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	30 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2791/2915 (95%)	439 (15%)	21 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	233 (15%)	0
32	2a	1501/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	9 (12%)	0
57	1y	72/76 (94%)	29 (40%)	0
57	2y	70/76 (92%)	19 (27%)	0
All	All	9345/9620 (97%)	1520 (16%)	51 (0%)

5 of 1520 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2689	U
1	2A	528	A
1	2A	2439	A
1	1A	2756	U
1	2A	266	G

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

90 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$
1	PSU	1A	1917	1	18,21,22	1.43	3 (16%)	21,30,33	1.98	4 (19%)
54	5MU	1w	54	54	19,22,23	1.32	5 (26%)	27,32,35	1.99	6 (22%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.85	6 (18%)
1	OMG	1A	2251	55,1,58	23,26,27	1.23	3 (13%)	32,38,41	1.97	6 (18%)
1	OMG	2A	2251	55,1,58	23,26,27	1.20	2 (8%)	32,38,41	2.00	8 (25%)
32	5MC	2a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.08	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.04	2 (8%)
32	G7M	1a	527	32	23,26,27	1.49	4 (17%)	34,39,42	1.65	5 (14%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.14	7 (21%)
57	4SU	2y	8	57	18,21,22	1.72	4 (22%)	25,30,33	2.16	5 (20%)
54	4SU	2w	8	54	18,21,22	1.77	4 (22%)	25,30,33	2.42	5 (20%)
1	5MU	1A	1939	1,58	19,22,23	1.37	4 (21%)	27,32,35	2.40	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.19	3 (11%)
55	8AN	2x	76	55,56,58	21,24,25	1.41	3 (14%)	26,35,38	2.30	11 (42%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.07	9 (27%)
1	OMU	2A	2552	1,58	19,22,23	1.19	2 (10%)	25,31,34	1.89	6 (24%)
1	2MA	1A	2503	1,58	22,25,26	1.50	5 (22%)	32,37,40	2.40	9 (28%)
54	4SU	1w	8	54,58	18,21,22	1.87	5 (27%)	25,30,33	1.90	5 (20%)
57	PSU	1y	55	57	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
32	UR3	1a	1498	32	19,22,23	0.96	0	26,32,35	1.75	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.14	2 (7%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.85	5 (15%)
55	4SU	2x	8	55,58	18,21,22	2.13	4 (22%)	25,30,33	1.49	5 (20%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.71	2 (10%)	26,32,35	1.11	2 (7%)
54	MIA	1w	37	54	28,31,32	2.20	6 (21%)	38,44,47	2.95	12 (31%)
54	PSU	2w	32	54	18,21,22	1.33	2 (11%)	21,30,33	1.95	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.33	4 (22%)	21,30,33	2.00	4 (19%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	2.18	6 (22%)
1	5MC	1A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.19	3 (11%)
54	F3N	2w	76	54,1	33,36,37	1.45	4 (12%)	41,51,54	1.78	10 (24%)
32	5MC	1a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.06	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1A	2552	1,58	19,22,23	1.23	2 (10%)	25,31,34	1.91	5 (20%)
55	5MU	1x	54	55	19,22,23	1.41	4 (21%)	27,32,35	2.00	6 (22%)
57	PSU	1y	32	57	18,21,22	1.38	2 (11%)	21,30,33	1.96	4 (19%)
32	G7M	2a	527	32,58	23,26,27	1.48	3 (13%)	34,39,42	1.65	5 (14%)
55	PSU	1x	55	55	18,21,22	1.42	2 (11%)	21,30,33	2.05	3 (14%)
1	5MC	2A	1962	1,58	19,22,23	1.75	3 (15%)	26,32,35	1.11	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.73	4 (15%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.15	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.13	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.36	5 (26%)	27,32,35	2.17	7 (25%)
57	4SU	1y	8	57	18,21,22	1.75	4 (22%)	25,30,33	1.96	5 (20%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
55	5MC	2x	32	55	19,22,23	1.80	3 (15%)	26,32,35	1.20	4 (15%)
57	5MU	1y	54	57	19,22,23	1.43	5 (26%)	27,32,35	1.73	6 (22%)
54	G7M	2w	46	54	23,26,27	1.44	3 (13%)	34,39,42	1.72	5 (14%)
54	PSU	1w	32	54,58	18,21,22	1.30	2 (11%)	21,30,33	2.03	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.93	0
56	FME	1z	1	56	8,9,10	0.96	0	8,9,11	1.14	1 (12%)
54	G7M	1w	46	54	23,26,27	1.54	3 (13%)	34,39,42	1.67	4 (11%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	1.99	4 (19%)
55	5MC	1x	32	55	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
57	5MU	2y	54	57	19,22,23	1.53	4 (21%)	27,32,35	2.21	6 (22%)
57	PSU	2y	55	57	18,21,22	1.36	2 (11%)	21,30,33	2.00	4 (19%)
57	G7M	1y	46	57	23,26,27	1.53	4 (17%)	34,39,42	1.74	5 (14%)
43	0TD	1l	92	43	8,9,10	4.68	1 (12%)	6,11,13	7.87	3 (50%)
54	MIA	2w	37	54	24,27,32	2.04	5 (20%)	32,39,47	2.52	11 (34%)
1	PSU	1A	2605	1,58	18,21,22	1.38	2 (11%)	21,30,33	2.26	5 (23%)
56	FME	2z	1	56	8,9,10	0.99	0	8,9,11	1.25	1 (12%)
32	2MG	1a	1207	32	23,26,27	1.31	3 (13%)	33,38,41	2.04	5 (15%)
1	2MA	2A	2503	1,58	22,25,26	1.48	4 (18%)	32,37,40	2.36	8 (25%)
54	5MU	2w	54	54	19,22,23	1.32	4 (21%)	27,32,35	1.86	6 (22%)
32	5MC	1a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.28	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.14	6 (22%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.82	3 (14%)
57	G7M	2y	46	57	23,26,27	1.66	3 (13%)	34,39,42	2.01	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
1	5MU	2A	1939	1,58	19,22,23	1.36	5 (26%)	27,32,35	2.34	8 (29%)
57	MIA	1y	37	57	21,24,32	1.61	4 (19%)	30,35,47	2.06	7 (23%)
55	8AN	1x	76	55,56,58	21,24,25	1.45	3 (14%)	26,35,38	2.68	11 (42%)
43	0TD	2l	92	43	8,9,10	4.55	1 (12%)	6,11,13	4.56	3 (50%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	2.03	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.73	0	25,32,35	1.10	2 (8%)
57	MIA	2y	37	57	21,24,32	1.61	3 (14%)	30,35,47	2.02	9 (30%)
57	PSU	1y	39	57	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.13	8 (24%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.04	4 (19%)
32	5MC	1a	967	32	19,22,23	1.56	3 (15%)	26,32,35	1.15	3 (11%)
57	PSU	2y	39	57,42	18,21,22	1.30	2 (11%)	21,30,33	2.23	4 (19%)
1	5MC	1A	1962	1,58	19,22,23	1.81	3 (15%)	26,32,35	1.17	3 (11%)
57	PSU	2y	32	57	18,21,22	1.39	2 (11%)	21,30,33	1.87	4 (19%)
54	F3N	1w	76	54,1	33,36,37	1.50	4 (12%)	41,51,54	1.77	9 (21%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.00	1 (4%)
55	4SU	1x	8	55	18,21,22	2.25	5 (27%)	25,30,33	1.74	7 (28%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.12	9 (27%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	1A	2251	55,1,58	-	1/9/27/28	0/3/3/3
1	OMG	2A	2251	55,1,58	-	0/9/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
57	4SU	2y	8	57	-	1/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,56,58	-	3/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
1	2MA	1A	2503	1,58	-	1/7/25/26	0/3/3/3
54	4SU	1w	8	54,58	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	4SU	2x	8	55,58	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	3/19/37/38	0/4/4/4
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
57	PSU	1y	32	57	-	1/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	3/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	32	54,58	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
56	FME	1z	1	56	-	4/7/9/11	-
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	2/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	3/7/9/11	-
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	2MA	2A	2503	1,58	-	0/7/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	4/7/25/26	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	1/7/25/34	0/3/3/3
55	8AN	1x	76	55,56,58	-	3/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
57	MIA	2y	37	57	-	1/7/25/34	0/3/3/3
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57,42	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2

The worst 5 of 246 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.82	1.69	1.82
43	2l	92	0TD	CB-SB	-12.40	1.69	1.82
1	1A	1962	5MC	C5-C4	6.89	1.49	1.44
55	2x	32	5MC	C5-C4	6.75	1.49	1.44
54	1w	37	MIA	C13-C14	6.67	1.52	1.32

The worst 5 of 443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-18.80	68.58	102.36
43	2l	92	0TD	CSB-SB-CB	-10.40	83.67	102.36
54	1w	37	MIA	C12-C13-C14	-10.31	108.50	127.01
54	2w	37	MIA	C5-C4-N3	-8.24	118.50	127.18
54	1w	37	MIA	C5-C4-N3	-7.98	118.77	127.18

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P
57	2y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

40 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1917	PSU	1	0
1	1A	2251	OMG	1	0
1	2A	2251	OMG	1	0
32	2a	967	5MC	1	0
57	2y	8	4SU	1	0
1	1A	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	76	8AN	1	0
32	1a	1519	MA6	2	0
1	2A	2552	OMU	1	0
57	1y	55	PSU	2	0
54	2w	55	PSU	1	0
32	2a	966	M2G	1	0
54	1w	37	MIA	1	0
54	2w	76	F3N	3	0
1	1A	2552	OMU	1	0
57	1y	8	4SU	3	0
57	1y	54	5MU	2	0
54	2w	46	G7M	1	0
56	1z	1	FME	2	0
54	1w	46	G7M	1	0
57	2y	55	PSU	5	0
57	1y	46	G7M	1	0
56	2z	1	FME	1	0
1	2A	2503	2MA	1	0
54	2w	54	5MU	1	0
1	2A	1915	5MU	1	0
57	2y	46	G7M	2	0
1	2A	1939	5MU	1	0
57	1y	37	MIA	2	0
55	1x	76	8AN	1	0
43	2l	92	0TD	1	0
32	2a	1404	5MC	2	0
32	1a	1402	4OC	2	0
57	1y	39	PSU	1	0
32	1a	1518	MA6	2	0
32	2a	1519	MA6	1	0
54	1w	76	F3N	1	0
55	1x	8	4SU	1	0
32	2a	1518	MA6	1	0
55	2x	55	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2739 ligands modelled in this entry, 2737 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	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	304	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	304	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	0.21	193 (6%)	24	26	19, 35, 83, 91	0
1	2A	2789/2915 (95%)	0.65	175 (6%)	26	28	31, 52, 81, 93	0
2	1B	120/121 (99%)	0.24	0	100	100	31, 47, 59, 77	0
2	2B	120/121 (99%)	1.01	4 (3%)	49	51	55, 66, 73, 80	0
3	1D	275/276 (99%)	0.74	11 (4%)	42	44	20, 36, 49, 69	0
3	2D	275/276 (99%)	1.40	64 (23%)	2	2	30, 46, 59, 69	0
4	1E	204/206 (99%)	1.01	26 (12%)	8	8	19, 39, 57, 67	0
4	2E	204/206 (99%)	1.26	35 (17%)	4	4	32, 53, 64, 73	0
5	1F	202/210 (96%)	0.96	26 (12%)	7	8	20, 40, 61, 73	0
5	2F	202/210 (96%)	1.59	61 (30%)	1	1	32, 61, 71, 76	0
6	1G	181/182 (99%)	1.29	25 (13%)	6	7	42, 54, 67, 78	0
6	2G	181/182 (99%)	2.12	101 (55%)	0	0	57, 68, 75, 81	0
7	1H	174/180 (96%)	1.43	32 (18%)	3	4	36, 52, 61, 66	0
7	2H	174/180 (96%)	2.39	106 (60%)	0	0	62, 71, 77, 80	0
8	1I	146/148 (98%)	1.88	60 (41%)	0	0	45, 66, 73, 77	0
8	2I	146/148 (98%)	2.66	103 (70%)	0	0	54, 70, 79, 83	0
9	1N	140/140 (100%)	0.81	5 (3%)	46	48	24, 38, 56, 70	0
9	2N	140/140 (100%)	1.52	35 (25%)	2	2	42, 57, 69, 71	0
10	1O	122/122 (100%)	0.91	8 (6%)	24	26	26, 38, 53, 58	0
10	2O	122/122 (100%)	1.32	16 (13%)	7	8	40, 52, 63, 71	0
11	1P	149/150 (99%)	0.91	19 (12%)	7	8	20, 43, 62, 67	0
11	2P	149/150 (99%)	1.61	46 (30%)	1	1	36, 60, 71, 75	0
12	1Q	141/141 (100%)	0.75	6 (4%)	40	41	23, 39, 53, 65	0
12	2Q	141/141 (100%)	1.56	45 (31%)	1	1	38, 57, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.61	1 (0%) 82 83	25, 35, 44, 54	0
13	2R	118/118 (100%)	1.01	12 (10%) 12 13	38, 49, 57, 61	0
14	1S	110/112 (98%)	1.07	10 (9%) 15 16	36, 47, 59, 62	0
14	2S	110/112 (98%)	1.99	58 (52%) 0 0	54, 63, 70, 73	0
15	1T	131/146 (89%)	1.10	20 (15%) 5 6	31, 42, 63, 73	0
15	2T	131/146 (89%)	1.48	29 (22%) 2 2	47, 55, 67, 73	0
16	1U	116/118 (98%)	0.33	0 100 100	19, 29, 46, 57	0
16	2U	116/118 (98%)	1.36	24 (20%) 2 3	41, 54, 64, 67	0
17	1V	101/101 (100%)	0.61	1 (0%) 79 80	22, 38, 51, 60	0
17	2V	101/101 (100%)	1.75	41 (40%) 0 0	40, 61, 69, 74	0
18	1W	112/113 (99%)	0.61	2 (1%) 67 69	23, 32, 47, 75	0
18	2W	112/113 (99%)	0.94	9 (8%) 18 20	36, 46, 59, 77	0
19	1X	95/96 (98%)	0.78	6 (6%) 26 28	25, 36, 54, 73	0
19	2X	95/96 (98%)	1.61	23 (24%) 2 2	42, 54, 66, 70	0
20	1Y	107/110 (97%)	1.15	12 (11%) 10 11	34, 46, 60, 70	0
20	2Y	107/110 (97%)	1.87	36 (33%) 1 1	52, 64, 71, 77	0
21	1Z	154/206 (74%)	1.62	46 (29%) 1 1	38, 59, 73, 79	0
21	2Z	160/206 (77%)	2.39	105 (65%) 0 0	55, 71, 79, 83	0
22	10	83/85 (97%)	0.64	4 (4%) 35 37	27, 36, 47, 60	0
22	20	83/85 (97%)	1.44	19 (22%) 2 2	40, 54, 61, 71	0
23	11	97/98 (98%)	1.06	10 (10%) 12 13	28, 45, 65, 69	0
23	21	97/98 (98%)	1.79	31 (31%) 1 1	40, 55, 67, 73	0
24	12	70/72 (97%)	0.88	5 (7%) 22 24	35, 44, 57, 67	0
24	22	70/72 (97%)	1.77	26 (37%) 1 1	54, 62, 69, 71	0
25	13	59/60 (98%)	0.55	3 (5%) 33 35	25, 35, 52, 63	0
25	23	59/60 (98%)	1.46	9 (15%) 5 6	48, 55, 69, 72	0
26	14	69/71 (97%)	1.87	24 (34%) 1 1	47, 68, 77, 80	0
26	24	69/71 (97%)	2.44	43 (62%) 0 0	66, 73, 79, 82	0
27	15	59/60 (98%)	0.55	1 (1%) 69 70	21, 33, 51, 64	0
27	25	59/60 (98%)	0.89	3 (5%) 33 35	33, 46, 61, 71	0
28	16	53/54 (98%)	0.74	1 (1%) 66 68	31, 39, 53, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	1.41	10 (18%) 3 4	44, 54, 62, 65	0
29	17	48/49 (97%)	0.43	3 (6%) 26 28	18, 27, 51, 57	0
29	27	48/49 (97%)	1.07	8 (16%) 4 5	33, 41, 60, 68	0
30	18	64/65 (98%)	0.56	2 (3%) 51 53	27, 33, 39, 55	0
30	28	64/65 (98%)	1.24	6 (9%) 14 15	40, 50, 54, 59	0
31	19	37/37 (100%)	0.52	0 100 100	28, 36, 49, 51	0
31	29	37/37 (100%)	1.60	10 (27%) 1 1	51, 58, 67, 69	0
32	1a	1488/1521 (97%)	1.06	121 (8%) 18 19	33, 58, 80, 90	0
32	2a	1491/1521 (98%)	1.28	163 (10%) 10 12	45, 67, 81, 91	0
33	1b	231/256 (90%)	2.07	109 (47%) 0 0	57, 68, 75, 81	0
33	2b	231/256 (90%)	2.71	176 (76%) 0 0	63, 72, 77, 83	0
34	1c	206/239 (86%)	1.91	85 (41%) 0 0	47, 61, 69, 75	0
34	2c	206/239 (86%)	2.50	141 (68%) 0 0	63, 71, 76, 81	0
35	1d	208/209 (99%)	1.94	94 (45%) 0 0	48, 59, 67, 72	0
35	2d	208/209 (99%)	2.02	105 (50%) 0 0	53, 65, 72, 79	0
36	1e	148/162 (91%)	1.76	47 (31%) 1 1	45, 56, 64, 70	0
36	2e	148/162 (91%)	2.38	94 (63%) 0 0	57, 66, 72, 78	0
37	1f	100/101 (99%)	1.40	13 (13%) 7 8	49, 58, 66, 68	0
37	2f	100/101 (99%)	1.67	29 (29%) 1 1	51, 61, 66, 69	0
38	1g	155/156 (99%)	1.79	53 (34%) 1 1	54, 62, 73, 78	0
38	2g	155/156 (99%)	2.28	80 (51%) 0 0	64, 70, 77, 80	0
39	1h	137/138 (99%)	1.71	42 (30%) 1 1	48, 59, 65, 69	0
39	2h	137/138 (99%)	2.43	97 (70%) 0 0	57, 67, 71, 75	0
40	1i	127/128 (99%)	2.06	69 (54%) 0 0	47, 66, 72, 76	0
40	2i	127/128 (99%)	2.73	94 (74%) 0 0	62, 72, 77, 79	0
41	1j	97/105 (92%)	2.08	47 (48%) 0 0	49, 65, 73, 79	0
41	2j	96/105 (91%)	2.82	75 (78%) 0 0	63, 73, 77, 79	0
42	1k	114/129 (88%)	1.80	39 (34%) 1 1	44, 61, 70, 75	0
42	2k	114/129 (88%)	2.30	67 (58%) 0 0	51, 65, 70, 74	0
43	1l	121/132 (91%)	1.29	22 (18%) 3 4	37, 47, 59, 62	0
43	2l	121/132 (91%)	1.77	37 (30%) 1 1	50, 58, 66, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
44	1m	123/126 (97%)	1.77	43 (34%)	1 1	49, 61, 69, 78	0
44	2m	122/126 (96%)	2.31	70 (57%)	0 0	61, 70, 74, 77	0
45	1n	60/61 (98%)	1.92	24 (40%)	1 0	47, 56, 63, 65	0
45	2n	60/61 (98%)	2.98	52 (86%)	0 0	66, 71, 74, 76	0
46	1o	88/89 (98%)	1.74	29 (32%)	1 1	44, 55, 65, 71	0
46	2o	88/89 (98%)	2.51	64 (72%)	0 0	53, 63, 70, 72	0
47	1p	82/88 (93%)	2.63	60 (73%)	0 0	50, 61, 66, 69	0
47	2p	82/88 (93%)	2.07	44 (53%)	0 0	56, 63, 70, 74	0
48	1q	99/105 (94%)	1.95	41 (41%)	0 0	50, 60, 67, 70	0
48	2q	99/105 (94%)	2.09	52 (52%)	0 0	56, 64, 70, 72	0
49	1r	68/88 (77%)	1.28	8 (11%)	9 10	50, 58, 66, 68	0
49	2r	68/88 (77%)	2.05	35 (51%)	0 0	56, 62, 70, 75	0
50	1s	83/93 (89%)	1.96	36 (43%)	0 0	55, 63, 71, 74	0
50	2s	83/93 (89%)	2.25	48 (57%)	0 0	67, 72, 77, 79	0
51	1t	96/106 (90%)	2.19	50 (52%)	0 0	56, 62, 70, 74	0
51	2t	96/106 (90%)	1.78	37 (38%)	1 0	54, 63, 72, 76	0
52	1u	23/27 (85%)	2.18	13 (56%)	0 0	55, 59, 62, 66	0
52	2u	23/27 (85%)	2.75	20 (86%)	0 0	68, 70, 73, 74	0
53	1v	13/24 (54%)	1.39	4 (30%)	1 1	40, 47, 82, 85	0
53	2v	13/24 (54%)	3.34	10 (76%)	0 0	60, 80, 87, 89	0
54	1w	66/76 (86%)	1.57	18 (27%)	1 1	25, 74, 83, 87	0
54	2w	64/76 (84%)	1.68	18 (28%)	1 1	42, 79, 86, 88	0
55	1x	72/77 (93%)	0.81	4 (5%)	30 32	24, 57, 71, 81	0
55	2x	72/77 (93%)	1.03	3 (4%)	40 42	37, 67, 77, 82	0
56	1z	6/7 (85%)	2.82	3 (50%)	0 0	25, 35, 44, 63	0
56	2z	6/7 (85%)	3.72	3 (50%)	0 0	37, 40, 54, 67	0
57	1y	67/76 (88%)	2.33	47 (70%)	0 0	58, 85, 88, 89	0
57	2y	66/76 (86%)	2.48	50 (75%)	0 0	68, 88, 91, 92	0
All	All	20883/21762 (95%)	1.23	4640 (22%)	2 2	18, 57, 77, 93	0

The worst 5 of 4640 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	8.9
38	1g	81	GLY	7.8
40	2i	14	VAL	7.6
45	1n	2	ALA	7.5
23	11	2	SER	7.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	4SU	2y	8	20/21	0.32	0.22	87,92,105,113	0
57	5MU	2y	54	21/22	0.50	0.21	74,87,96,109	0
57	MIA	2y	37	22/30	0.56	0.21	79,86,93,107	0
57	G7M	1y	46	24/25	0.56	0.20	78,83,88,95	0
57	4SU	1y	8	20/21	0.57	0.19	81,87,95,100	0
57	G7M	2y	46	24/25	0.61	0.17	83,86,90,104	0
57	PSU	1y	55	20/21	0.61	0.18	77,83,88,96	0
57	PSU	1y	32	20/21	0.64	0.20	75,80,91,93	0
54	G7M	2w	46	24/25	0.64	0.18	72,80,92,108	0
57	PSU	2y	55	20/21	0.65	0.18	82,86,91,100	0
57	MIA	1y	37	22/30	0.65	0.21	73,81,92,101	0
57	PSU	1y	39	20/21	0.66	0.20	75,83,86,93	0
57	PSU	2y	39	20/21	0.69	0.18	77,82,90,94	0
57	PSU	2y	32	20/21	0.70	0.19	78,85,93,95	0
57	5MU	1y	54	21/22	0.71	0.17	77,81,87,99	0
54	G7M	1w	46	24/25	0.73	0.17	65,73,89,111	0
56	FME	1z	1	10/11	0.76	0.24	51,62,66,67	0
54	4SU	1w	8	20/21	0.84	0.15	71,75,83,85	0
54	4SU	2w	8	20/21	0.85	0.14	74,79,91,92	0
54	PSU	2w	32	20/21	0.85	0.16	60,71,78,79	0
54	MIA	2w	37	25/30	0.85	0.18	61,67,79,99	0
32	M2G	2a	966	25/26	0.86	0.18	52,60,71,77	0
32	2MG	2a	1207	24/25	0.87	0.14	64,72,75,76	0
56	FME	2z	1	10/11	0.87	0.24	59,67,73,76	0
54	PSU	1w	32	20/21	0.88	0.16	49,57,68,70	0
54	PSU	1w	55	20/21	0.88	0.13	50,66,71,73	0
43	0TD	2l	92	10/11	0.89	0.14	48,53,61,66	0
55	4SU	2x	8	20/21	0.89	0.13	60,67,72,76	0
55	5MU	2x	54	21/22	0.89	0.14	67,72,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2w	55	20/21	0.89	0.11	70,74,77,82	0
55	5MU	1x	54	21/22	0.89	0.15	58,63,71,76	0
32	2MG	1a	1207	24/25	0.89	0.14	50,55,58,69	0
1	5MU	2A	1915	21/22	0.90	0.13	51,60,63,66	0
32	5MC	2a	967	21/22	0.90	0.15	58,61,66,69	0
55	PSU	1x	55	20/21	0.91	0.13	51,58,69,74	0
32	5MC	2a	1400	21/22	0.91	0.15	54,59,65,69	0
54	5MU	2w	54	21/22	0.91	0.12	64,70,73,78	0
55	PSU	2x	55	20/21	0.91	0.12	61,66,72,80	0
32	4OC	2a	1402	22/23	0.91	0.13	48,52,56,57	0
54	MIA	1w	37	29/30	0.91	0.17	38,46,64,78	0
1	PSU	2A	1917	20/21	0.91	0.11	51,56,66,70	0
32	UR3	2a	1498	21/22	0.92	0.14	48,51,55,58	0
43	0TD	1l	92	10/11	0.92	0.12	40,46,48,56	0
55	4SU	1x	8	20/21	0.92	0.12	53,59,66,67	0
32	PSU	2a	516	20/21	0.92	0.12	57,63,67,73	0
55	5MC	1x	32	21/22	0.92	0.15	41,46,52,60	0
32	5MC	2a	1404	21/22	0.92	0.13	45,52,55,57	0
54	PSU	2w	39	20/21	0.92	0.11	62,70,75,76	0
1	PSU	2A	1911	20/21	0.93	0.11	50,57,60,64	0
32	MA6	2a	1518	24/25	0.93	0.13	46,55,60,62	0
32	G7M	2a	527	24/25	0.93	0.12	49,56,62,71	0
32	PSU	1a	516	20/21	0.93	0.12	44,48,52,53	0
55	5MC	2x	32	21/22	0.93	0.13	57,60,66,72	0
1	5MU	1A	1915	21/22	0.93	0.11	33,44,48,50	0
32	5MC	2a	1407	21/22	0.93	0.12	40,47,51,60	0
32	MA6	2a	1519	24/25	0.94	0.14	41,55,60,61	0
54	PSU	1w	39	20/21	0.94	0.12	41,57,62,65	0
32	4OC	1a	1402	22/23	0.94	0.11	33,40,44,46	0
32	5MC	1a	1407	21/22	0.94	0.12	29,36,42,44	0
32	MA6	1a	1519	24/25	0.94	0.13	35,39,45,53	0
54	5MU	1w	54	21/22	0.94	0.11	50,57,62,66	0
1	PSU	1A	1911	20/21	0.94	0.10	37,43,47,49	0
1	5MC	2A	1962	21/22	0.94	0.12	36,43,49,58	0
32	M2G	1a	966	25/26	0.94	0.12	41,48,51,52	0
1	5MC	1A	1942	21/22	0.94	0.11	28,37,47,51	0
32	5MC	1a	1400	21/22	0.94	0.12	37,40,44,46	0
32	MA6	1a	1518	24/25	0.95	0.11	31,40,43,44	0
1	PSU	1A	1917	20/21	0.95	0.10	36,42,48,52	0
1	OMC	2A	1920	21/22	0.95	0.10	44,53,56,57	0
1	5MC	2A	1942	21/22	0.95	0.11	40,51,54,57	0
32	5MC	1a	967	21/22	0.95	0.11	43,51,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMU	2A	2552	21/22	0.95	0.11	31,41,45,49	0
55	8AN	2x	76	22/23	0.95	0.11	29,37,40,47	0
1	PSU	2A	2605	20/21	0.95	0.10	30,36,40,45	0
32	5MC	1a	1404	21/22	0.95	0.12	32,38,41,45	0
32	G7M	1a	527	24/25	0.95	0.10	35,41,47,54	0
55	8AN	1x	76	22/23	0.96	0.10	22,26,32,39	0
32	UR3	1a	1498	21/22	0.96	0.09	32,39,40,44	0
1	5MU	1A	1939	21/22	0.96	0.08	21,25,29,30	0
1	OMC	1A	1920	21/22	0.96	0.09	33,40,45,49	0
54	F3N	2w	76	33/34	0.96	0.10	23,37,41,41	0
1	OMG	2A	2251	24/25	0.96	0.11	34,38,41,43	0
1	OMU	1A	2552	21/22	0.96	0.09	20,25,30,30	0
1	2MA	2A	2503	23/24	0.97	0.09	25,33,39,41	0
1	5MU	2A	1939	21/22	0.97	0.09	30,36,39,42	0
54	F3N	1w	76	33/34	0.97	0.09	16,23,26,28	0
1	PSU	1A	2605	20/21	0.97	0.08	19,26,30,32	0
1	2MA	1A	2503	23/24	0.97	0.08	16,21,27,27	0
1	5MC	1A	1962	21/22	0.97	0.09	25,31,37,40	0
1	OMG	1A	2251	24/25	0.98	0.07	18,25,29,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3409	1/1	0.36	0.32	73,73,73,73	0
58	MG	2a	1805	1/1	0.43	0.27	70,70,70,70	0
58	MG	2A	3160	1/1	0.50	0.27	66,66,66,66	0
58	MG	2A	3787	1/1	0.52	0.22	57,57,57,57	0
58	MG	2v	103	1/1	0.53	0.36	79,79,79,79	0
58	MG	20	101	1/1	0.54	0.37	69,69,69,69	0
58	MG	2w	103	1/1	0.55	0.21	74,74,74,74	0
58	MG	2a	1672	1/1	0.56	0.27	69,69,69,69	0
58	MG	2a	1712	1/1	0.57	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3469	1/1	0.57	0.29	75,75,75,75	0
58	MG	1a	1742	1/1	0.58	0.47	80,80,80,80	0
58	MG	2a	1634	1/1	0.59	0.32	58,58,58,58	0
58	MG	1A	3976	1/1	0.59	0.17	65,65,65,65	0
58	MG	1Y	203	1/1	0.60	0.19	67,67,67,67	0
58	MG	1A	3439	1/1	0.60	0.20	66,66,66,66	0
58	MG	1A	4026	1/1	0.61	0.22	58,58,58,58	0
58	MG	2a	1784	1/1	0.61	0.23	67,67,67,67	0
58	MG	2A	3253	1/1	0.61	0.25	74,74,74,74	0
58	MG	2A	3307	1/1	0.61	0.27	65,65,65,65	0
58	MG	1O	201	1/1	0.61	0.33	65,65,65,65	0
58	MG	1A	3295	1/1	0.62	0.20	67,67,67,67	0
58	MG	2D	307	1/1	0.62	0.26	67,67,67,67	0
58	MG	2a	1702	1/1	0.62	0.21	68,68,68,68	0
58	MG	2A	3670	1/1	0.62	0.22	66,66,66,66	0
58	MG	1A	3721	1/1	0.63	0.32	66,66,66,66	0
58	MG	1A	3325	1/1	0.63	0.28	50,50,50,50	0
58	MG	1A	3559	1/1	0.63	0.27	72,72,72,72	0
58	MG	2a	1724	1/1	0.63	0.33	75,75,75,75	0
58	MG	2B	215	1/1	0.64	0.30	68,68,68,68	0
58	MG	1A	3568	1/1	0.64	0.21	59,59,59,59	0
58	MG	2n	101	1/1	0.64	0.44	77,77,77,77	0
58	MG	2a	1635	1/1	0.64	0.20	64,64,64,64	0
58	MG	2a	1640	1/1	0.64	0.37	74,74,74,74	0
58	MG	2a	1661	1/1	0.65	0.26	65,65,65,65	0
58	MG	2A	3750	1/1	0.65	0.23	60,60,60,60	0
58	MG	1A	3740	1/1	0.65	0.12	51,51,51,51	0
58	MG	1A	3705	1/1	0.65	0.33	66,66,66,66	0
58	MG	2A	3289	1/1	0.65	0.25	58,58,58,58	0
58	MG	1a	1694	1/1	0.65	0.29	71,71,71,71	0
58	MG	2A	3374	1/1	0.65	0.18	66,66,66,66	0
58	MG	1a	1717	1/1	0.65	0.28	59,59,59,59	0
58	MG	2a	1637	1/1	0.65	0.24	78,78,78,78	0
58	MG	1A	3537	1/1	0.65	0.33	64,64,64,64	0
58	MG	2A	3837	1/1	0.66	0.27	72,72,72,72	0
58	MG	1A	3453	1/1	0.66	0.19	67,67,67,67	0
58	MG	1A	4035	1/1	0.66	0.20	53,53,53,53	0
58	MG	1A	3603	1/1	0.66	0.28	66,66,66,66	0
58	MG	2A	3432	1/1	0.66	0.27	70,70,70,70	0
58	MG	1w	103	1/1	0.66	0.28	72,72,72,72	0
58	MG	2A	3156	1/1	0.66	0.43	70,70,70,70	0
58	MG	1A	3519	1/1	0.66	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1615	1/1	0.66	0.23	58,58,58,58	0
58	MG	2A	3193	1/1	0.67	0.23	64,64,64,64	0
58	MG	1a	1642	1/1	0.67	0.24	55,55,55,55	0
58	MG	2A	3777	1/1	0.67	0.23	61,61,61,61	0
58	MG	2A	3272	1/1	0.67	0.28	70,70,70,70	0
58	MG	1a	1803	1/1	0.67	0.17	72,72,72,72	0
58	MG	1A	3728	1/1	0.67	0.28	70,70,70,70	0
58	MG	1a	1704	1/1	0.67	0.24	66,66,66,66	0
58	MG	1a	1639	1/1	0.67	0.24	65,65,65,65	0
58	MG	2A	3458	1/1	0.67	0.21	69,69,69,69	0
58	MG	2A	3179	1/1	0.67	0.22	62,62,62,62	0
58	MG	2A	3481	1/1	0.67	0.28	66,66,66,66	0
58	MG	2A	3144	1/1	0.68	0.19	66,66,66,66	0
58	MG	2A	3407	1/1	0.68	0.16	51,51,51,51	0
58	MG	1B	228	1/1	0.68	0.22	63,63,63,63	0
58	MG	1A	3852	1/1	0.68	0.18	46,46,46,46	0
58	MG	2a	1820	1/1	0.68	0.25	68,68,68,68	0
58	MG	2A	3274	1/1	0.68	0.16	62,62,62,62	0
58	MG	2A	3165	1/1	0.68	0.30	60,60,60,60	0
58	MG	2A	3096	1/1	0.68	0.28	66,66,66,66	0
58	MG	2A	3321	1/1	0.69	0.19	70,70,70,70	0
58	MG	1a	1690	1/1	0.69	0.25	60,60,60,60	0
58	MG	1A	3482	1/1	0.69	0.24	74,74,74,74	0
58	MG	2A	3781	1/1	0.69	0.23	51,51,51,51	0
58	MG	1A	3687	1/1	0.69	0.15	66,66,66,66	0
58	MG	2A	3280	1/1	0.69	0.22	58,58,58,58	0
58	MG	1a	1708	1/1	0.69	0.32	63,63,63,63	0
58	MG	1A	4066	1/1	0.69	0.18	59,59,59,59	0
58	MG	2A	3197	1/1	0.70	0.23	67,67,67,67	0
58	MG	1a	1737	1/1	0.70	0.19	71,71,71,71	0
58	MG	1A	3102	1/1	0.70	0.20	63,63,63,63	0
58	MG	1B	236	1/1	0.70	0.21	73,73,73,73	0
58	MG	1A	3946	1/1	0.70	0.13	71,71,71,71	0
58	MG	2A	3801	1/1	0.70	0.20	49,49,49,49	0
58	MG	2A	3047	1/1	0.70	0.20	66,66,66,66	0
58	MG	1B	224	1/1	0.70	0.26	61,61,61,61	0
58	MG	2a	1696	1/1	0.70	0.26	69,69,69,69	0
58	MG	1A	3264	1/1	0.71	0.14	53,53,53,53	0
58	MG	2A	3695	1/1	0.71	0.21	63,63,63,63	0
58	MG	2A	3720	1/1	0.71	0.29	67,67,67,67	0
58	MG	2a	1644	1/1	0.71	0.34	67,67,67,67	0
58	MG	2A	3327	1/1	0.71	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3345	1/1	0.71	0.20	57,57,57,57	0
58	MG	2A	3258	1/1	0.71	0.26	61,61,61,61	0
58	MG	2A	3389	1/1	0.71	0.18	69,69,69,69	0
58	MG	1A	3369	1/1	0.71	0.23	49,49,49,49	0
58	MG	1x	108	1/1	0.71	0.18	30,30,30,30	0
58	MG	1a	1621	1/1	0.71	0.23	58,58,58,58	0
58	MG	2a	1804	1/1	0.71	0.22	64,64,64,64	0
58	MG	2A	3214	1/1	0.71	0.28	57,57,57,57	0
58	MG	2A	3238	1/1	0.71	0.25	60,60,60,60	0
58	MG	2a	1605	1/1	0.71	0.21	69,69,69,69	0
58	MG	2a	1630	1/1	0.71	0.28	71,71,71,71	0
58	MG	2A	3610	1/1	0.71	0.21	62,62,62,62	0
58	MG	2a	1700	1/1	0.72	0.29	80,80,80,80	0
58	MG	1A	3956	1/1	0.72	0.26	45,45,45,45	0
58	MG	1A	3207	1/1	0.72	0.18	69,69,69,69	0
58	MG	2B	216	1/1	0.72	0.19	65,65,65,65	0
58	MG	2a	1638	1/1	0.72	0.36	68,68,68,68	0
58	MG	1F	304	1/1	0.72	0.27	63,63,63,63	0
58	MG	2a	1642	1/1	0.72	0.20	62,62,62,62	0
58	MG	2V	202	1/1	0.72	0.25	68,68,68,68	0
58	MG	2A	3293	1/1	0.72	0.23	68,68,68,68	0
58	MG	1a	1626	1/1	0.72	0.29	64,64,64,64	0
58	MG	1A	3406	1/1	0.72	0.24	44,44,44,44	0
58	MG	1A	3695	1/1	0.73	0.16	35,35,35,35	0
58	MG	1A	4019	1/1	0.73	0.21	64,64,64,64	0
58	MG	2A	3733	1/1	0.73	0.28	72,72,72,72	0
58	MG	1A	3771	1/1	0.73	0.18	40,40,40,40	0
58	MG	2A	3388	1/1	0.73	0.24	64,64,64,64	0
58	MG	1A	3335	1/1	0.73	0.24	57,57,57,57	0
58	MG	1A	3542	1/1	0.73	0.16	60,60,60,60	0
58	MG	2A	3418	1/1	0.73	0.32	67,67,67,67	0
58	MG	2A	3826	1/1	0.73	0.24	61,61,61,61	0
58	MG	2A	3178	1/1	0.73	0.21	60,60,60,60	0
58	MG	1x	105	1/1	0.73	0.17	62,62,62,62	0
58	MG	2a	1704	1/1	0.73	0.27	59,59,59,59	0
58	MG	2a	1709	1/1	0.73	0.20	69,69,69,69	0
58	MG	1A	4087	1/1	0.73	0.23	78,78,78,78	0
58	MG	2A	3296	1/1	0.73	0.38	40,40,40,40	0
58	MG	2a	1725	1/1	0.73	0.24	66,66,66,66	0
58	MG	2a	1782	1/1	0.73	0.28	68,68,68,68	0
58	MG	2E	301	1/1	0.73	0.17	56,56,56,56	0
58	MG	2a	1795	1/1	0.73	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2F	301	1/1	0.73	0.19	65,65,65,65	0
58	MG	2A	3037	1/1	0.73	0.26	62,62,62,62	0
58	MG	2a	1807	1/1	0.73	0.20	70,70,70,70	0
58	MG	2A	3648	1/1	0.73	0.13	68,68,68,68	0
58	MG	2A	3657	1/1	0.73	0.21	61,61,61,61	0
58	MG	1A	3535	1/1	0.73	0.15	52,52,52,52	0
58	MG	2A	3690	1/1	0.73	0.20	75,75,75,75	0
58	MG	2A	3153	1/1	0.74	0.18	57,57,57,57	0
58	MG	2a	1649	1/1	0.74	0.35	74,74,74,74	0
58	MG	1A	4015	1/1	0.74	0.17	71,71,71,71	0
58	MG	1A	4075	1/1	0.74	0.23	53,53,53,53	0
58	MG	2a	1681	1/1	0.74	0.26	67,67,67,67	0
58	MG	2B	211	1/1	0.74	0.22	69,69,69,69	0
58	MG	1A	3719	1/1	0.74	0.25	64,64,64,64	0
58	MG	2A	3175	1/1	0.74	0.26	59,59,59,59	0
58	MG	2A	3596	1/1	0.74	0.14	39,39,39,39	0
58	MG	1a	1808	1/1	0.74	0.33	78,78,78,78	0
58	MG	18	106	1/1	0.74	0.23	55,55,55,55	0
58	MG	2Q	202	1/1	0.74	0.18	58,58,58,58	0
58	MG	2R	203	1/1	0.74	0.23	65,65,65,65	0
58	MG	2a	1748	1/1	0.74	0.23	63,63,63,63	0
58	MG	1a	1697	1/1	0.74	0.23	66,66,66,66	0
58	MG	1A	3333	1/1	0.74	0.17	45,45,45,45	0
58	MG	2A	3335	1/1	0.74	0.31	73,73,73,73	0
58	MG	2A	3203	1/1	0.74	0.27	70,70,70,70	0
58	MG	2A	3352	1/1	0.74	0.17	65,65,65,65	0
58	MG	2A	3355	1/1	0.74	0.19	62,62,62,62	0
58	MG	2a	1808	1/1	0.74	0.20	70,70,70,70	0
58	MG	1A	3204	1/1	0.74	0.21	58,58,58,58	0
58	MG	1a	1712	1/1	0.74	0.22	61,61,61,61	0
58	MG	1A	4061	1/1	0.74	0.16	48,48,48,48	0
58	MG	1a	1734	1/1	0.74	0.22	69,69,69,69	0
58	MG	2a	1749	1/1	0.75	0.22	77,77,77,77	0
58	MG	2a	1750	1/1	0.75	0.12	83,83,83,83	0
58	MG	2E	302	1/1	0.75	0.29	71,71,71,71	0
58	MG	2a	1695	1/1	0.75	0.14	51,51,51,51	0
58	MG	1a	1788	1/1	0.75	0.18	76,76,76,76	0
58	MG	2a	1803	1/1	0.75	0.14	52,52,52,52	0
58	MG	1A	3270	1/1	0.75	0.22	64,64,64,64	0
58	MG	1a	1681	1/1	0.75	0.20	53,53,53,53	0
58	MG	2A	3640	1/1	0.75	0.35	59,59,59,59	0
58	MG	2A	3783	1/1	0.75	0.22	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2B	220	1/1	0.75	0.21	69,69,69,69	0
58	MG	2d	303	1/1	0.75	0.30	68,68,68,68	0
58	MG	2a	1650	1/1	0.75	0.22	63,63,63,63	0
58	MG	2A	3116	1/1	0.75	0.21	53,53,53,53	0
58	MG	2A	3730	1/1	0.75	0.19	70,70,70,70	0
58	MG	1a	1628	1/1	0.76	0.23	59,59,59,59	0
58	MG	1A	3128	1/1	0.76	0.14	53,53,53,53	0
58	MG	2a	1698	1/1	0.76	0.32	70,70,70,70	0
58	MG	2A	3189	1/1	0.76	0.26	64,64,64,64	0
58	MG	2A	3334	1/1	0.76	0.23	67,67,67,67	0
58	MG	2A	3678	1/1	0.76	0.23	57,57,57,57	0
58	MG	1x	109	1/1	0.76	0.17	60,60,60,60	0
58	MG	1x	110	1/1	0.76	0.20	62,62,62,62	0
58	MG	2a	1721	1/1	0.76	0.17	70,70,70,70	0
58	MG	1A	3410	1/1	0.76	0.19	64,64,64,64	0
58	MG	2A	3211	1/1	0.76	0.17	58,58,58,58	0
58	MG	1A	3669	1/1	0.76	0.14	47,47,47,47	0
58	MG	2a	1611	1/1	0.76	0.21	66,66,66,66	0
58	MG	1A	3347	1/1	0.76	0.23	58,58,58,58	0
58	MG	2A	3759	1/1	0.76	0.19	68,68,68,68	0
58	MG	1a	1757	1/1	0.76	0.24	60,60,60,60	0
58	MG	2a	1793	1/1	0.76	0.21	75,75,75,75	0
58	MG	1a	1607	1/1	0.76	0.16	62,62,62,62	0
58	MG	1A	3190	1/1	0.76	0.13	43,43,43,43	0
58	MG	1A	3284	1/1	0.76	0.18	52,52,52,52	0
58	MG	2A	3788	1/1	0.76	0.19	60,60,60,60	0
58	MG	2A	3278	1/1	0.76	0.18	66,66,66,66	0
58	MG	1n	101	1/1	0.76	0.27	57,57,57,57	0
58	MG	2a	1810	1/1	0.76	0.30	79,79,79,79	0
58	MG	2a	1811	1/1	0.76	0.17	57,57,57,57	0
58	MG	2A	3475	1/1	0.76	0.22	52,52,52,52	0
58	MG	1w	101	1/1	0.76	0.32	66,66,66,66	0
58	MG	2a	1665	1/1	0.76	0.28	63,63,63,63	0
58	MG	2A	3166	1/1	0.76	0.25	60,60,60,60	0
58	MG	1A	3869	1/1	0.76	0.19	63,63,63,63	0
58	MG	1A	3342	1/1	0.77	0.22	57,57,57,57	0
58	MG	2A	3683	1/1	0.77	0.17	68,68,68,68	0
58	MG	1a	1623	1/1	0.77	0.19	56,56,56,56	0
58	MG	1a	1711	1/1	0.77	0.20	50,50,50,50	0
58	MG	2A	3377	1/1	0.77	0.28	70,70,70,70	0
58	MG	1A	3488	1/1	0.77	0.20	62,62,62,62	0
58	MG	2a	1720	1/1	0.77	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4090	1/1	0.77	0.18	59,59,59,59	0
58	MG	1Z	302	1/1	0.77	0.18	57,57,57,57	0
58	MG	2a	1602	1/1	0.77	0.23	67,67,67,67	0
58	MG	2A	3754	1/1	0.77	0.24	48,48,48,48	0
58	MG	1Z	303	1/1	0.77	0.15	58,58,58,58	0
58	MG	2a	1617	1/1	0.77	0.15	60,60,60,60	0
58	MG	2a	1774	1/1	0.77	0.15	49,49,49,49	0
58	MG	2a	1779	1/1	0.77	0.23	59,59,59,59	0
58	MG	1a	1680	1/1	0.77	0.22	65,65,65,65	0
58	MG	10	107	1/1	0.77	0.26	67,67,67,67	0
58	MG	2A	3298	1/1	0.77	0.22	62,62,62,62	0
58	MG	2A	3784	1/1	0.77	0.18	61,61,61,61	0
58	MG	1a	1758	1/1	0.77	0.14	67,67,67,67	0
58	MG	2A	3115	1/1	0.77	0.27	69,69,69,69	0
58	MG	2A	3554	1/1	0.77	0.20	44,44,44,44	0
58	MG	2A	3803	1/1	0.77	0.17	56,56,56,56	0
58	MG	2A	3324	1/1	0.77	0.17	60,60,60,60	0
58	MG	2A	3325	1/1	0.77	0.18	67,67,67,67	0
58	MG	2B	203	1/1	0.77	0.18	72,72,72,72	0
58	MG	1A	3442	1/1	0.77	0.42	54,54,54,54	0
58	MG	1A	3989	1/1	0.77	0.12	38,38,38,38	0
58	MG	1A	3353	1/1	0.77	0.17	56,56,56,56	0
58	MG	2A	3242	1/1	0.77	0.20	57,57,57,57	0
58	MG	2D	302	1/1	0.77	0.21	56,56,56,56	0
58	MG	1a	1665	1/1	0.78	0.26	60,60,60,60	0
58	MG	1A	3139	1/1	0.78	0.22	53,53,53,53	0
58	MG	2A	3128	1/1	0.78	0.14	51,51,51,51	0
58	MG	2A	3672	1/1	0.78	0.23	64,64,64,64	0
58	MG	1A	3871	1/1	0.78	0.18	52,52,52,52	0
58	MG	1a	1688	1/1	0.78	0.23	61,61,61,61	0
58	MG	1A	3887	1/1	0.78	0.23	57,57,57,57	0
58	MG	2A	3262	1/1	0.78	0.32	60,60,60,60	0
58	MG	2F	306	1/1	0.78	0.26	59,59,59,59	0
58	MG	1A	3245	1/1	0.78	0.28	56,56,56,56	0
58	MG	1A	3560	1/1	0.78	0.28	63,63,63,63	0
58	MG	2T	201	1/1	0.78	0.17	55,55,55,55	0
58	MG	2T	203	1/1	0.78	0.15	62,62,62,62	0
58	MG	2a	1731	1/1	0.78	0.35	64,64,64,64	0
58	MG	1A	4099	1/1	0.78	0.22	50,50,50,50	0
58	MG	2A	3735	1/1	0.78	0.24	62,62,62,62	0
58	MG	2a	1601	1/1	0.78	0.15	69,69,69,69	0
58	MG	2A	3174	1/1	0.78	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1604	1/1	0.78	0.30	71,71,71,71	0
58	MG	2A	3286	1/1	0.78	0.23	65,65,65,65	0
58	MG	1A	3494	1/1	0.78	0.30	57,57,57,57	0
58	MG	1A	3263	1/1	0.78	0.22	57,57,57,57	0
58	MG	2A	3778	1/1	0.78	0.22	58,58,58,58	0
58	MG	2A	3439	1/1	0.78	0.31	74,74,74,74	0
58	MG	1A	3668	1/1	0.78	0.15	56,56,56,56	0
58	MG	1A	3124	1/1	0.78	0.20	40,40,40,40	0
58	MG	2A	3300	1/1	0.78	0.24	69,69,69,69	0
58	MG	1a	1630	1/1	0.78	0.21	59,59,59,59	0
58	MG	2A	3500	1/1	0.78	0.24	68,68,68,68	0
58	MG	2A	3531	1/1	0.78	0.19	65,65,65,65	0
58	MG	2A	3813	1/1	0.78	0.17	45,45,45,45	0
58	MG	2A	3308	1/1	0.78	0.19	45,45,45,45	0
58	MG	2j	201	1/1	0.78	0.20	59,59,59,59	0
58	MG	2A	3309	1/1	0.78	0.15	52,52,52,52	0
58	MG	1A	3846	1/1	0.78	0.38	71,71,71,71	0
58	MG	1A	3074	1/1	0.78	0.21	59,59,59,59	0
58	MG	2x	105	1/1	0.78	0.28	63,63,63,63	0
58	MG	2A	3747	1/1	0.79	0.17	68,68,68,68	0
58	MG	2A	3198	1/1	0.79	0.15	51,51,51,51	0
58	MG	2R	204	1/1	0.79	0.22	65,65,65,65	0
58	MG	1a	1775	1/1	0.79	0.16	70,70,70,70	0
58	MG	2A	3453	1/1	0.79	0.30	70,70,70,70	0
58	MG	2a	1719	1/1	0.79	0.21	68,68,68,68	0
58	MG	1A	3942	1/1	0.79	0.14	67,67,67,67	0
58	MG	1A	3344	1/1	0.79	0.28	64,64,64,64	0
58	MG	2A	3310	1/1	0.79	0.14	60,60,60,60	0
58	MG	2A	3782	1/1	0.79	0.17	62,62,62,62	0
58	MG	2A	3318	1/1	0.79	0.17	66,66,66,66	0
58	MG	1A	3250	1/1	0.79	0.12	57,57,57,57	0
58	MG	2a	1608	1/1	0.79	0.24	67,67,67,67	0
58	MG	2A	3322	1/1	0.79	0.21	73,73,73,73	0
58	MG	1A	3314	1/1	0.79	0.18	52,52,52,52	0
58	MG	2a	1776	1/1	0.79	0.29	67,67,67,67	0
58	MG	1A	3423	1/1	0.79	0.16	59,59,59,59	0
58	MG	1a	1660	1/1	0.79	0.16	52,52,52,52	0
58	MG	2A	3329	1/1	0.79	0.18	59,59,59,59	0
58	MG	2A	3332	1/1	0.79	0.22	56,56,56,56	0
58	MG	2A	3655	1/1	0.79	0.13	65,65,65,65	0
58	MG	2A	3259	1/1	0.79	0.32	68,68,68,68	0
58	MG	2B	206	1/1	0.79	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3996	1/1	0.79	0.15	47,47,47,47	0
58	MG	1a	1671	1/1	0.79	0.37	73,73,73,73	0
58	MG	1A	3356	1/1	0.79	0.23	59,59,59,59	0
58	MG	2a	1651	1/1	0.79	0.16	71,71,71,71	0
58	MG	2a	1652	1/1	0.79	0.16	72,72,72,72	0
58	MG	1A	3709	1/1	0.79	0.24	54,54,54,54	0
58	MG	2A	3021	1/1	0.79	0.24	69,69,69,69	0
58	MG	2A	3029	1/1	0.79	0.15	53,53,53,53	0
58	MG	1A	3595	1/1	0.79	0.27	63,63,63,63	0
58	MG	2A	3041	1/1	0.79	0.26	54,54,54,54	0
58	MG	1A	3343	1/1	0.79	0.16	56,56,56,56	0
58	MG	2x	102	1/1	0.79	0.24	64,64,64,64	0
58	MG	2A	3053	1/1	0.79	0.18	63,63,63,63	0
58	MG	2A	3291	1/1	0.80	0.25	61,61,61,61	0
58	MG	1A	3167	1/1	0.80	0.23	45,45,45,45	0
58	MG	1a	1769	1/1	0.80	0.15	62,62,62,62	0
58	MG	1a	1622	1/1	0.80	0.22	61,61,61,61	0
58	MG	2A	3201	1/1	0.80	0.30	67,67,67,67	0
58	MG	2A	3740	1/1	0.80	0.17	47,47,47,47	0
58	MG	2A	3419	1/1	0.80	0.19	55,55,55,55	0
58	MG	1A	3495	1/1	0.80	0.12	56,56,56,56	0
58	MG	2A	3207	1/1	0.80	0.25	58,58,58,58	0
58	MG	1A	3838	1/1	0.80	0.19	80,80,80,80	0
58	MG	2A	3212	1/1	0.80	0.18	66,66,66,66	0
58	MG	2a	1735	1/1	0.80	0.18	57,57,57,57	0
58	MG	2a	1739	1/1	0.80	0.18	51,51,51,51	0
58	MG	2a	1603	1/1	0.80	0.29	58,58,58,58	0
58	MG	1A	3413	1/1	0.80	0.18	60,60,60,60	0
58	MG	1b	301	1/1	0.80	0.14	75,75,75,75	0
58	MG	1A	3520	1/1	0.80	0.14	55,55,55,55	0
58	MG	1A	3300	1/1	0.80	0.31	62,62,62,62	0
58	MG	11	104	1/1	0.80	0.13	44,44,44,44	0
58	MG	2A	3541	1/1	0.80	0.16	45,45,45,45	0
58	MG	1a	1643	1/1	0.80	0.16	56,56,56,56	0
58	MG	2A	3575	1/1	0.80	0.14	43,43,43,43	0
58	MG	2a	1794	1/1	0.80	0.15	68,68,68,68	0
58	MG	2A	3580	1/1	0.80	0.24	62,62,62,62	0
58	MG	2A	3328	1/1	0.80	0.16	68,68,68,68	0
58	MG	1A	3163	1/1	0.80	0.13	47,47,47,47	0
58	MG	2A	3612	1/1	0.80	0.20	53,53,53,53	0
58	MG	2A	3846	1/1	0.80	0.13	49,49,49,49	0
58	MG	2B	202	1/1	0.80	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3636	1/1	0.80	0.18	48,48,48,48	0
58	MG	1A	3615	1/1	0.80	0.13	31,31,31,31	0
58	MG	1a	1670	1/1	0.80	0.17	62,62,62,62	0
58	MG	1x	111	1/1	0.80	0.20	60,60,60,60	0
58	MG	1a	1741	1/1	0.80	0.24	68,68,68,68	0
58	MG	2A	3281	1/1	0.80	0.21	60,60,60,60	0
58	MG	2q	201	1/1	0.80	0.18	60,60,60,60	0
58	MG	2q	202	1/1	0.80	0.17	71,71,71,71	0
58	MG	1A	3541	1/1	0.80	0.17	48,48,48,48	0
58	MG	2A	3356	1/1	0.80	0.18	58,58,58,58	0
58	MG	2A	3368	1/1	0.80	0.25	68,68,68,68	0
58	MG	1a	1619	1/1	0.80	0.24	50,50,50,50	0
58	MG	2A	3471	1/1	0.81	0.13	50,50,50,50	0
58	MG	2A	3313	1/1	0.81	0.26	50,50,50,50	0
58	MG	1A	3431	1/1	0.81	0.16	38,38,38,38	0
58	MG	2A	3484	1/1	0.81	0.25	66,66,66,66	0
58	MG	1A	3600	1/1	0.81	0.22	61,61,61,61	0
58	MG	1a	1802	1/1	0.81	0.24	69,69,69,69	0
58	MG	2A	3106	1/1	0.81	0.15	56,56,56,56	0
58	MG	2a	1680	1/1	0.81	0.19	58,58,58,58	0
58	MG	2A	3235	1/1	0.81	0.14	54,54,54,54	0
58	MG	1A	3471	1/1	0.81	0.16	59,59,59,59	0
58	MG	10	108	1/1	0.81	0.18	64,64,64,64	0
58	MG	2A	3587	1/1	0.81	0.14	62,62,62,62	0
58	MG	2A	3244	1/1	0.81	0.19	60,60,60,60	0
58	MG	2A	3609	1/1	0.81	0.17	38,38,38,38	0
58	MG	1A	3252	1/1	0.81	0.18	67,67,67,67	0
58	MG	2A	3137	1/1	0.81	0.22	66,66,66,66	0
58	MG	2B	212	1/1	0.81	0.22	61,61,61,61	0
58	MG	2B	214	1/1	0.81	0.15	56,56,56,56	0
58	MG	2A	3617	1/1	0.81	0.21	60,60,60,60	0
58	MG	14	101	1/1	0.81	0.14	64,64,64,64	0
58	MG	16	101	1/1	0.81	0.15	56,56,56,56	0
58	MG	2A	3644	1/1	0.81	0.26	63,63,63,63	0
58	MG	1A	3486	1/1	0.81	0.20	58,58,58,58	0
58	MG	1x	102	1/1	0.81	0.32	70,70,70,70	0
58	MG	1x	104	1/1	0.81	0.14	60,60,60,60	0
58	MG	1A	3529	1/1	0.81	0.17	58,58,58,58	0
58	MG	1a	1669	1/1	0.81	0.17	56,56,56,56	0
58	MG	1A	3305	1/1	0.81	0.31	52,52,52,52	0
58	MG	2A	3382	1/1	0.81	0.14	50,50,50,50	0
58	MG	2A	3689	1/1	0.81	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4058	1/1	0.81	0.12	48,48,48,48	0
58	MG	2A	3692	1/1	0.81	0.12	55,55,55,55	0
58	MG	2a	1783	1/1	0.81	0.26	69,69,69,69	0
58	MG	1A	3947	1/1	0.81	0.28	69,69,69,69	0
58	MG	2A	3697	1/1	0.81	0.25	71,71,71,71	0
58	MG	2A	3702	1/1	0.81	0.12	41,41,41,41	0
58	MG	2A	3712	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3406	1/1	0.81	0.23	61,61,61,61	0
58	MG	2A	3186	1/1	0.81	0.24	58,58,58,58	0
58	MG	2A	3409	1/1	0.81	0.19	62,62,62,62	0
58	MG	2A	3413	1/1	0.81	0.29	60,60,60,60	0
58	MG	2A	3015	1/1	0.81	0.21	62,62,62,62	0
58	MG	1A	3592	1/1	0.81	0.26	66,66,66,66	0
58	MG	2a	1620	1/1	0.81	0.18	74,74,74,74	0
58	MG	2a	1816	1/1	0.81	0.26	65,65,65,65	0
58	MG	2A	3748	1/1	0.81	0.20	54,54,54,54	0
58	MG	2A	3423	1/1	0.81	0.20	58,58,58,58	0
58	MG	2A	3194	1/1	0.81	0.13	53,53,53,53	0
58	MG	2l	203	1/1	0.81	0.10	57,57,57,57	0
58	MG	1a	1686	1/1	0.81	0.26	59,59,59,59	0
58	MG	1a	1761	1/1	0.81	0.19	68,68,68,68	0
58	MG	1a	1687	1/1	0.81	0.30	53,53,53,53	0
58	MG	2q	203	1/1	0.81	0.17	70,70,70,70	0
58	MG	2a	1641	1/1	0.81	0.17	50,50,50,50	0
58	MG	2A	3779	1/1	0.81	0.19	54,54,54,54	0
58	MG	2A	3042	1/1	0.81	0.15	51,51,51,51	0
58	MG	2a	1647	1/1	0.81	0.19	69,69,69,69	0
58	MG	2a	1654	1/1	0.82	0.18	60,60,60,60	0
58	MG	2a	1660	1/1	0.82	0.18	65,65,65,65	0
58	MG	2A	3001	1/1	0.82	0.29	62,62,62,62	0
58	MG	1a	1720	1/1	0.82	0.25	66,66,66,66	0
58	MG	2A	3571	1/1	0.82	0.19	56,56,56,56	0
58	MG	2a	1677	1/1	0.82	0.14	56,56,56,56	0
58	MG	1A	3714	1/1	0.82	0.17	50,50,50,50	0
58	MG	1A	3027	1/1	0.82	0.14	63,63,63,63	0
58	MG	1a	1656	1/1	0.82	0.21	64,64,64,64	0
58	MG	2A	3209	1/1	0.82	0.28	62,62,62,62	0
58	MG	1A	3944	1/1	0.82	0.12	33,33,33,33	0
58	MG	1A	3034	1/1	0.82	0.16	32,32,32,32	0
58	MG	1A	3299	1/1	0.82	0.23	49,49,49,49	0
58	MG	2A	3615	1/1	0.82	0.22	63,63,63,63	0
58	MG	2A	3225	1/1	0.82	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
58	MG	2A	3336	1/1	0.82	0.20	49,49,49,49	0
58	MG	2A	3340	1/1	0.82	0.14	66,66,66,66	0
58	MG	2A	3234	1/1	0.82	0.16	63,63,63,63	0
58	MG	1A	3222	1/1	0.82	0.28	54,54,54,54	0
58	MG	2A	3650	1/1	0.82	0.14	61,61,61,61	0
58	MG	2A	3071	1/1	0.82	0.22	59,59,59,59	0
58	MG	2A	3088	1/1	0.82	0.20	48,48,48,48	0
58	MG	2A	3669	1/1	0.82	0.17	58,58,58,58	0
58	MG	1a	1764	1/1	0.82	0.18	59,59,59,59	0
58	MG	2P	201	1/1	0.82	0.20	58,58,58,58	0
58	MG	2A	3371	1/1	0.82	0.23	61,61,61,61	0
58	MG	1A	3456	1/1	0.82	0.17	62,62,62,62	0
58	MG	2a	1768	1/1	0.82	0.17	69,69,69,69	0
58	MG	2A	3255	1/1	0.82	0.19	60,60,60,60	0
58	MG	2a	1775	1/1	0.82	0.24	62,62,62,62	0
58	MG	2A	3687	1/1	0.82	0.20	68,68,68,68	0
58	MG	2A	3108	1/1	0.82	0.30	64,64,64,64	0
58	MG	2A	3384	1/1	0.82	0.19	68,68,68,68	0
58	MG	1a	1679	1/1	0.82	0.18	62,62,62,62	0
58	MG	17	105	1/1	0.82	0.17	52,52,52,52	0
58	MG	2a	1786	1/1	0.82	0.16	67,67,67,67	0
58	MG	2a	1788	1/1	0.82	0.16	66,66,66,66	0
58	MG	2a	1790	1/1	0.82	0.17	60,60,60,60	0
58	MG	2A	3395	1/1	0.82	0.20	52,52,52,52	0
58	MG	1a	1795	1/1	0.82	0.21	65,65,65,65	0
58	MG	1a	1800	1/1	0.82	0.21	68,68,68,68	0
58	MG	2A	3408	1/1	0.82	0.17	56,56,56,56	0
58	MG	1A	3985	1/1	0.82	0.14	42,42,42,42	0
58	MG	1a	1682	1/1	0.82	0.18	71,71,71,71	0
58	MG	1a	1602	1/1	0.82	0.19	64,64,64,64	0
58	MG	1B	206	1/1	0.82	0.21	47,47,47,47	0
58	MG	1B	223	1/1	0.82	0.20	65,65,65,65	0
58	MG	1a	1689	1/1	0.82	0.27	55,55,55,55	0
58	MG	2A	3168	1/1	0.82	0.13	52,52,52,52	0
58	MG	2a	1817	1/1	0.82	0.13	65,65,65,65	0
58	MG	2a	1636	1/1	0.82	0.28	64,64,64,64	0
58	MG	2A	3442	1/1	0.82	0.13	55,55,55,55	0
58	MG	2A	3445	1/1	0.82	0.14	58,58,58,58	0
58	MG	1A	3517	1/1	0.82	0.19	61,61,61,61	0
58	MG	1A	3462	1/1	0.82	0.20	62,62,62,62	0
58	MG	1A	3563	1/1	0.82	0.17	46,46,46,46	0
58	MG	1E	308	1/1	0.82	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4017	1/1	0.82	0.15	46,46,46,46	0
58	MG	1A	3378	1/1	0.82	0.14	39,39,39,39	0
58	MG	1R	204	1/1	0.82	0.25	53,53,53,53	0
58	MG	1A	3522	1/1	0.82	0.15	60,60,60,60	0
58	MG	2A	3196	1/1	0.82	0.21	65,65,65,65	0
58	MG	1A	3571	1/1	0.83	0.28	52,52,52,52	0
58	MG	1E	305	1/1	0.83	0.24	54,54,54,54	0
58	MG	1A	3441	1/1	0.83	0.15	44,44,44,44	0
58	MG	1A	3874	1/1	0.83	0.20	41,41,41,41	0
58	MG	1a	1633	1/1	0.83	0.26	58,58,58,58	0
58	MG	2A	3839	1/1	0.83	0.18	66,66,66,66	0
58	MG	1a	1635	1/1	0.83	0.14	49,49,49,49	0
58	MG	1a	1636	1/1	0.83	0.17	53,53,53,53	0
58	MG	2a	1697	1/1	0.83	0.18	63,63,63,63	0
58	MG	2A	3331	1/1	0.83	0.18	70,70,70,70	0
58	MG	2a	1699	1/1	0.83	0.22	70,70,70,70	0
58	MG	1A	3255	1/1	0.83	0.23	58,58,58,58	0
58	MG	1a	1640	1/1	0.83	0.24	59,59,59,59	0
58	MG	1A	4049	1/1	0.83	0.19	62,62,62,62	0
58	MG	1A	3716	1/1	0.83	0.19	51,51,51,51	0
58	MG	1A	3717	1/1	0.83	0.17	54,54,54,54	0
58	MG	2a	1715	1/1	0.83	0.22	65,65,65,65	0
58	MG	2A	3224	1/1	0.83	0.21	60,60,60,60	0
58	MG	2A	3056	1/1	0.83	0.13	60,60,60,60	0
58	MG	2A	3230	1/1	0.83	0.15	68,68,68,68	0
58	MG	1a	1659	1/1	0.83	0.24	68,68,68,68	0
58	MG	2A	3366	1/1	0.83	0.20	67,67,67,67	0
58	MG	2A	3086	1/1	0.83	0.22	68,68,68,68	0
58	MG	1A	3450	1/1	0.83	0.32	65,65,65,65	0
58	MG	2a	1736	1/1	0.83	0.26	62,62,62,62	0
58	MG	2A	3665	1/1	0.83	0.23	61,61,61,61	0
58	MG	2A	3667	1/1	0.83	0.11	51,51,51,51	0
58	MG	1A	3168	1/1	0.83	0.12	46,46,46,46	0
58	MG	2A	3099	1/1	0.83	0.23	60,60,60,60	0
58	MG	1A	3385	1/1	0.83	0.21	68,68,68,68	0
58	MG	1A	4089	1/1	0.83	0.18	50,50,50,50	0
58	MG	1a	1786	1/1	0.83	0.12	59,59,59,59	0
58	MG	1A	3633	1/1	0.83	0.14	57,57,57,57	0
58	MG	1a	1678	1/1	0.83	0.24	65,65,65,65	0
58	MG	28	102	1/1	0.83	0.19	61,61,61,61	0
58	MG	2A	3266	1/1	0.83	0.19	67,67,67,67	0
58	MG	2A	3136	1/1	0.83	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3315	1/1	0.83	0.25	59,59,59,59	0
58	MG	2A	3143	1/1	0.83	0.17	51,51,51,51	0
58	MG	1A	4100	1/1	0.83	0.11	41,41,41,41	0
58	MG	1A	3437	1/1	0.83	0.22	56,56,56,56	0
58	MG	2A	3282	1/1	0.83	0.17	70,70,70,70	0
58	MG	1a	1807	1/1	0.83	0.20	56,56,56,56	0
58	MG	18	107	1/1	0.83	0.17	62,62,62,62	0
58	MG	2a	1622	1/1	0.83	0.19	59,59,59,59	0
58	MG	2A	3161	1/1	0.83	0.11	60,60,60,60	0
58	MG	1B	212	1/1	0.83	0.21	58,58,58,58	0
58	MG	2A	3743	1/1	0.83	0.22	59,59,59,59	0
58	MG	1d	301	1/1	0.83	0.26	55,55,55,55	0
58	MG	2A	3446	1/1	0.83	0.25	57,57,57,57	0
58	MG	1B	213	1/1	0.83	0.16	57,57,57,57	0
58	MG	2a	1639	1/1	0.83	0.27	67,67,67,67	0
58	MG	2a	1818	1/1	0.83	0.22	54,54,54,54	0
58	MG	1A	3993	1/1	0.83	0.14	45,45,45,45	0
58	MG	2A	3465	1/1	0.83	0.11	59,59,59,59	0
58	MG	2A	3466	1/1	0.83	0.28	59,59,59,59	0
58	MG	1A	3358	1/1	0.83	0.18	43,43,43,43	0
58	MG	1A	3527	1/1	0.83	0.24	37,37,37,37	0
58	MG	1a	1692	1/1	0.83	0.15	51,51,51,51	0
58	MG	2A	3183	1/1	0.83	0.15	66,66,66,66	0
58	MG	1a	1693	1/1	0.83	0.25	61,61,61,61	0
58	MG	2v	101	1/1	0.83	0.18	58,58,58,58	0
58	MG	2A	3493	1/1	0.83	0.26	61,61,61,61	0
58	MG	1B	231	1/1	0.83	0.20	66,66,66,66	0
58	MG	2a	1658	1/1	0.83	0.21	70,70,70,70	0
58	MG	2A	3514	1/1	0.83	0.20	54,54,54,54	0
58	MG	2a	1646	1/1	0.84	0.14	66,66,66,66	0
58	MG	1A	3598	1/1	0.84	0.13	48,48,48,48	0
58	MG	1B	225	1/1	0.84	0.19	52,52,52,52	0
58	MG	1a	1637	1/1	0.84	0.19	55,55,55,55	0
58	MG	1A	3401	1/1	0.84	0.20	41,41,41,41	0
58	MG	2A	3275	1/1	0.84	0.15	62,62,62,62	0
58	MG	2A	3758	1/1	0.84	0.16	64,64,64,64	0
58	MG	1A	3487	1/1	0.84	0.11	42,42,42,42	0
58	MG	2A	3774	1/1	0.84	0.20	62,62,62,62	0
58	MG	1A	3738	1/1	0.84	0.23	77,77,77,77	0
58	MG	1D	313	1/1	0.84	0.16	40,40,40,40	0
58	MG	1A	3040	1/1	0.84	0.25	62,62,62,62	0
58	MG	1A	3745	1/1	0.84	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1E	310	1/1	0.84	0.19	62,62,62,62	0
58	MG	2A	3460	1/1	0.84	0.27	62,62,62,62	0
58	MG	2a	1688	1/1	0.84	0.25	65,65,65,65	0
58	MG	2A	3463	1/1	0.84	0.15	52,52,52,52	0
58	MG	1A	4010	1/1	0.84	0.08	36,36,36,36	0
58	MG	1A	3755	1/1	0.84	0.12	61,61,61,61	0
58	MG	2A	3294	1/1	0.84	0.21	65,65,65,65	0
58	MG	1O	204	1/1	0.84	0.14	43,43,43,43	0
58	MG	2A	3807	1/1	0.84	0.11	63,63,63,63	0
58	MG	1Q	206	1/1	0.84	0.16	58,58,58,58	0
58	MG	2A	3820	1/1	0.84	0.12	50,50,50,50	0
58	MG	1A	3770	1/1	0.84	0.10	30,30,30,30	0
58	MG	2A	3301	1/1	0.84	0.15	63,63,63,63	0
58	MG	1W	201	1/1	0.84	0.24	53,53,53,53	0
58	MG	1A	3268	1/1	0.84	0.17	60,60,60,60	0
58	MG	2A	3506	1/1	0.84	0.12	55,55,55,55	0
58	MG	2A	3181	1/1	0.84	0.20	61,61,61,61	0
58	MG	2a	1723	1/1	0.84	0.26	64,64,64,64	0
58	MG	2A	3182	1/1	0.84	0.32	60,60,60,60	0
58	MG	2A	3536	1/1	0.84	0.16	47,47,47,47	0
58	MG	2a	1730	1/1	0.84	0.28	55,55,55,55	0
58	MG	1A	4023	1/1	0.84	0.12	52,52,52,52	0
58	MG	1A	3793	1/1	0.84	0.10	36,36,36,36	0
58	MG	2A	3320	1/1	0.84	0.20	57,57,57,57	0
58	MG	1A	3805	1/1	0.84	0.14	64,64,64,64	0
58	MG	1x	106	1/1	0.84	0.17	54,54,54,54	0
58	MG	1A	3644	1/1	0.84	0.10	36,36,36,36	0
58	MG	2A	3195	1/1	0.84	0.31	60,60,60,60	0
58	MG	2A	3602	1/1	0.84	0.13	57,57,57,57	0
58	MG	1A	3549	1/1	0.84	0.19	59,59,59,59	0
58	MG	1A	4059	1/1	0.84	0.15	56,56,56,56	0
58	MG	1A	3357	1/1	0.84	0.14	53,53,53,53	0
58	MG	2G	201	1/1	0.84	0.13	62,62,62,62	0
58	MG	2A	3330	1/1	0.84	0.15	59,59,59,59	0
58	MG	1A	3862	1/1	0.84	0.12	47,47,47,47	0
58	MG	1A	3069	1/1	0.84	0.24	61,61,61,61	0
58	MG	1A	4081	1/1	0.84	0.15	56,56,56,56	0
58	MG	1a	1601	1/1	0.84	0.23	56,56,56,56	0
58	MG	1A	4085	1/1	0.84	0.28	69,69,69,69	0
58	MG	2A	3337	1/1	0.84	0.22	57,57,57,57	0
58	MG	1A	3039	1/1	0.84	0.24	35,35,35,35	0
58	MG	1A	3100	1/1	0.84	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3222	1/1	0.84	0.19	58,58,58,58	0
58	MG	1A	3707	1/1	0.84	0.11	30,30,30,30	0
58	MG	1a	1713	1/1	0.84	0.20	71,71,71,71	0
58	MG	2A	3363	1/1	0.84	0.28	61,61,61,61	0
58	MG	1A	4095	1/1	0.84	0.16	57,57,57,57	0
58	MG	2A	3233	1/1	0.84	0.18	63,63,63,63	0
58	MG	2A	3370	1/1	0.84	0.13	57,57,57,57	0
58	MG	2a	1815	1/1	0.84	0.22	61,61,61,61	0
58	MG	2a	1615	1/1	0.84	0.14	57,57,57,57	0
58	MG	2A	3059	1/1	0.84	0.24	51,51,51,51	0
58	MG	1A	3888	1/1	0.84	0.23	43,43,43,43	0
58	MG	2A	3237	1/1	0.84	0.22	70,70,70,70	0
58	MG	2a	1628	1/1	0.84	0.17	65,65,65,65	0
58	MG	1a	1724	1/1	0.84	0.20	50,50,50,50	0
58	MG	2l	202	1/1	0.84	0.18	59,59,59,59	0
58	MG	2A	3240	1/1	0.84	0.16	67,67,67,67	0
58	MG	2A	3385	1/1	0.84	0.15	56,56,56,56	0
58	MG	1A	3929	1/1	0.84	0.11	32,32,32,32	0
58	MG	2A	3705	1/1	0.84	0.17	52,52,52,52	0
58	MG	2A	3243	1/1	0.84	0.18	62,62,62,62	0
58	MG	1a	1625	1/1	0.84	0.23	58,58,58,58	0
58	MG	1A	3469	1/1	0.84	0.13	53,53,53,53	0
58	MG	1A	3588	1/1	0.84	0.11	29,29,29,29	0
58	MG	1A	3435	1/1	0.84	0.12	42,42,42,42	0
58	MG	1A	3297	1/1	0.84	0.29	56,56,56,56	0
58	MG	2A	3482	1/1	0.85	0.15	56,56,56,56	0
58	MG	1B	215	1/1	0.85	0.12	63,63,63,63	0
58	MG	1a	1663	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3498	1/1	0.85	0.33	65,65,65,65	0
58	MG	1a	1664	1/1	0.85	0.13	50,50,50,50	0
58	MG	2A	3082	1/1	0.85	0.18	51,51,51,51	0
58	MG	2a	1670	1/1	0.85	0.16	56,56,56,56	0
58	MG	2A	3791	1/1	0.85	0.17	52,52,52,52	0
58	MG	2a	1674	1/1	0.85	0.34	68,68,68,68	0
58	MG	2A	3508	1/1	0.85	0.18	38,38,38,38	0
58	MG	2a	1678	1/1	0.85	0.17	59,59,59,59	0
58	MG	15	107	1/1	0.85	0.11	54,54,54,54	0
58	MG	1a	1666	1/1	0.85	0.21	63,63,63,63	0
58	MG	2A	3223	1/1	0.85	0.32	66,66,66,66	0
58	MG	2A	3091	1/1	0.85	0.15	58,58,58,58	0
58	MG	2A	3822	1/1	0.85	0.12	63,63,63,63	0
58	MG	1A	3940	1/1	0.85	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3229	1/1	0.85	0.20	41,41,41,41	0
58	MG	1A	4031	1/1	0.85	0.14	49,49,49,49	0
58	MG	2A	3842	1/1	0.85	0.15	49,49,49,49	0
58	MG	2A	3100	1/1	0.85	0.16	58,58,58,58	0
58	MG	1A	3631	1/1	0.85	0.22	61,61,61,61	0
58	MG	2a	1708	1/1	0.85	0.18	60,60,60,60	0
58	MG	2A	3594	1/1	0.85	0.16	61,61,61,61	0
58	MG	1a	1676	1/1	0.85	0.23	58,58,58,58	0
58	MG	2A	3601	1/1	0.85	0.21	58,58,58,58	0
58	MG	2A	3114	1/1	0.85	0.23	56,56,56,56	0
58	MG	1A	3801	1/1	0.85	0.14	31,31,31,31	0
58	MG	2A	3349	1/1	0.85	0.21	61,61,61,61	0
58	MG	1A	3020	1/1	0.85	0.18	46,46,46,46	0
58	MG	2A	3353	1/1	0.85	0.12	71,71,71,71	0
58	MG	2A	3123	1/1	0.85	0.17	59,59,59,59	0
58	MG	1A	3814	1/1	0.85	0.17	38,38,38,38	0
58	MG	1D	303	1/1	0.85	0.33	58,58,58,58	0
58	MG	2A	3252	1/1	0.85	0.13	61,61,61,61	0
58	MG	1A	3582	1/1	0.85	0.12	57,57,57,57	0
58	MG	2A	3141	1/1	0.85	0.18	58,58,58,58	0
58	MG	2a	1740	1/1	0.85	0.25	63,63,63,63	0
58	MG	2A	3257	1/1	0.85	0.33	69,69,69,69	0
58	MG	1a	1810	1/1	0.85	0.17	55,55,55,55	0
58	MG	1A	3974	1/1	0.85	0.12	72,72,72,72	0
58	MG	2a	1753	1/1	0.85	0.25	77,77,77,77	0
58	MG	2A	3261	1/1	0.85	0.16	57,57,57,57	0
58	MG	2a	1773	1/1	0.85	0.10	50,50,50,50	0
58	MG	1A	4074	1/1	0.85	0.18	53,53,53,53	0
58	MG	1A	3975	1/1	0.85	0.12	56,56,56,56	0
58	MG	2A	3268	1/1	0.85	0.15	51,51,51,51	0
58	MG	1A	3096	1/1	0.85	0.11	40,40,40,40	0
58	MG	1I	201	1/1	0.85	0.13	55,55,55,55	0
58	MG	25	103	1/1	0.85	0.18	65,65,65,65	0
58	MG	2A	3162	1/1	0.85	0.14	58,58,58,58	0
58	MG	1A	3480	1/1	0.85	0.16	36,36,36,36	0
58	MG	1a	1627	1/1	0.85	0.12	52,52,52,52	0
58	MG	1A	3671	1/1	0.85	0.12	33,33,33,33	0
58	MG	1A	3395	1/1	0.85	0.21	51,51,51,51	0
58	MG	1A	3691	1/1	0.85	0.19	65,65,65,65	0
58	MG	1V	204	1/1	0.85	0.20	54,54,54,54	0
58	MG	2a	1800	1/1	0.85	0.29	57,57,57,57	0
58	MG	1A	4094	1/1	0.85	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1612	1/1	0.85	0.15	59,59,59,59	0
58	MG	2A	3709	1/1	0.85	0.19	55,55,55,55	0
58	MG	2a	1806	1/1	0.85	0.21	68,68,68,68	0
58	MG	2A	3430	1/1	0.85	0.22	54,54,54,54	0
58	MG	2a	1619	1/1	0.85	0.16	61,61,61,61	0
58	MG	2a	1809	1/1	0.85	0.16	47,47,47,47	0
58	MG	2A	3714	1/1	0.85	0.16	53,53,53,53	0
58	MG	1A	3311	1/1	0.85	0.13	63,63,63,63	0
58	MG	2A	3722	1/1	0.85	0.22	68,68,68,68	0
58	MG	1A	4011	1/1	0.85	0.15	44,44,44,44	0
58	MG	2a	1631	1/1	0.85	0.17	64,64,64,64	0
58	MG	1A	3884	1/1	0.85	0.10	57,57,57,57	0
58	MG	2A	3016	1/1	0.85	0.23	51,51,51,51	0
58	MG	1a	1718	1/1	0.85	0.21	66,66,66,66	0
58	MG	2e	201	1/1	0.85	0.15	71,71,71,71	0
58	MG	1Z	304	1/1	0.85	0.17	58,58,58,58	0
58	MG	2k	201	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3744	1/1	0.85	0.17	61,61,61,61	0
58	MG	2A	3456	1/1	0.85	0.19	54,54,54,54	0
58	MG	1A	3239	1/1	0.85	0.14	29,29,29,29	0
58	MG	2A	3038	1/1	0.85	0.24	54,54,54,54	0
58	MG	2A	3040	1/1	0.85	0.19	64,64,64,64	0
58	MG	1a	1646	1/1	0.85	0.11	42,42,42,42	0
58	MG	2A	3311	1/1	0.85	0.19	59,59,59,59	0
58	MG	1a	1654	1/1	0.85	0.20	53,53,53,53	0
58	MG	2A	3315	1/1	0.85	0.23	68,68,68,68	0
58	MG	1A	3436	1/1	0.85	0.23	56,56,56,56	0
58	MG	2x	104	1/1	0.85	0.22	64,64,64,64	0
58	MG	1A	3352	1/1	0.85	0.18	62,62,62,62	0
58	MG	2A	3603	1/1	0.86	0.14	67,67,67,67	0
58	MG	2A	3836	1/1	0.86	0.11	48,48,48,48	0
58	MG	2A	3604	1/1	0.86	0.12	41,41,41,41	0
58	MG	1A	3360	1/1	0.86	0.21	52,52,52,52	0
58	MG	1A	3237	1/1	0.86	0.11	39,39,39,39	0
58	MG	2a	1683	1/1	0.86	0.24	57,57,57,57	0
58	MG	1Q	208	1/1	0.86	0.21	42,42,42,42	0
58	MG	2a	1691	1/1	0.86	0.17	50,50,50,50	0
58	MG	2A	3851	1/1	0.86	0.16	61,61,61,61	0
58	MG	1A	3104	1/1	0.86	0.19	32,32,32,32	0
58	MG	1a	1638	1/1	0.86	0.24	62,62,62,62	0
58	MG	2B	204	1/1	0.86	0.14	72,72,72,72	0
58	MG	1S	203	1/1	0.86	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2B	207	1/1	0.86	0.12	60,60,60,60	0
58	MG	1A	3121	1/1	0.86	0.13	39,39,39,39	0
58	MG	1A	3607	1/1	0.86	0.19	46,46,46,46	0
58	MG	1A	3479	1/1	0.86	0.24	49,49,49,49	0
58	MG	1A	3432	1/1	0.86	0.20	62,62,62,62	0
58	MG	1a	1647	1/1	0.86	0.16	58,58,58,58	0
58	MG	2a	1713	1/1	0.86	0.12	43,43,43,43	0
58	MG	1A	3248	1/1	0.86	0.13	56,56,56,56	0
58	MG	2A	3410	1/1	0.86	0.18	57,57,57,57	0
58	MG	1A	3639	1/1	0.86	0.13	55,55,55,55	0
58	MG	1A	3398	1/1	0.86	0.13	29,29,29,29	0
58	MG	2A	3079	1/1	0.86	0.16	59,59,59,59	0
58	MG	1A	3653	1/1	0.86	0.09	29,29,29,29	0
58	MG	1a	1662	1/1	0.86	0.18	55,55,55,55	0
58	MG	2a	1729	1/1	0.86	0.21	61,61,61,61	0
58	MG	1A	3060	1/1	0.86	0.13	48,48,48,48	0
58	MG	1A	3403	1/1	0.86	0.14	40,40,40,40	0
58	MG	2A	3092	1/1	0.86	0.18	70,70,70,70	0
58	MG	15	102	1/1	0.86	0.16	44,44,44,44	0
58	MG	2A	3218	1/1	0.86	0.19	51,51,51,51	0
58	MG	2A	3694	1/1	0.86	0.12	30,30,30,30	0
58	MG	2a	1744	1/1	0.86	0.13	81,81,81,81	0
58	MG	1A	3006	1/1	0.86	0.26	66,66,66,66	0
58	MG	2A	3454	1/1	0.86	0.18	47,47,47,47	0
58	MG	1a	1667	1/1	0.86	0.27	68,68,68,68	0
58	MG	1A	3407	1/1	0.86	0.17	37,37,37,37	0
58	MG	1A	3817	1/1	0.86	0.14	59,59,59,59	0
58	MG	2a	1772	1/1	0.86	0.16	48,48,48,48	0
58	MG	2A	3228	1/1	0.86	0.20	52,52,52,52	0
58	MG	2A	3113	1/1	0.86	0.17	50,50,50,50	0
58	MG	2A	3717	1/1	0.86	0.14	64,64,64,64	0
58	MG	1A	3819	1/1	0.86	0.17	63,63,63,63	0
58	MG	2A	3326	1/1	0.86	0.28	66,66,66,66	0
58	MG	2a	1607	1/1	0.86	0.18	56,56,56,56	0
58	MG	2A	3726	1/1	0.86	0.13	39,39,39,39	0
58	MG	2a	1609	1/1	0.86	0.19	64,64,64,64	0
58	MG	2A	3727	1/1	0.86	0.14	63,63,63,63	0
58	MG	1A	3821	1/1	0.86	0.12	54,54,54,54	0
58	MG	1A	3689	1/1	0.86	0.12	40,40,40,40	0
58	MG	2a	1616	1/1	0.86	0.27	58,58,58,58	0
58	MG	1A	3502	1/1	0.86	0.11	51,51,51,51	0
58	MG	2A	3236	1/1	0.86	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3742	1/1	0.86	0.11	38,38,38,38	0
58	MG	1a	1606	1/1	0.86	0.27	52,52,52,52	0
58	MG	2a	1624	1/1	0.86	0.14	60,60,60,60	0
58	MG	2A	3135	1/1	0.86	0.21	50,50,50,50	0
58	MG	2a	1629	1/1	0.86	0.14	52,52,52,52	0
58	MG	2A	3495	1/1	0.86	0.21	64,64,64,64	0
58	MG	1A	3581	1/1	0.86	0.21	32,32,32,32	0
58	MG	1l	202	1/1	0.86	0.10	58,58,58,58	0
58	MG	1a	1611	1/1	0.86	0.11	52,52,52,52	0
58	MG	1A	3854	1/1	0.86	0.14	51,51,51,51	0
58	MG	2A	3510	1/1	0.86	0.15	63,63,63,63	0
58	MG	2A	3247	1/1	0.86	0.20	60,60,60,60	0
58	MG	2A	3521	1/1	0.86	0.12	40,40,40,40	0
58	MG	2A	3527	1/1	0.86	0.09	29,29,29,29	0
58	MG	1A	3696	1/1	0.86	0.11	27,27,27,27	0
58	MG	2d	301	1/1	0.86	0.17	51,51,51,51	0
58	MG	1A	3408	1/1	0.86	0.23	56,56,56,56	0
58	MG	2a	1643	1/1	0.86	0.16	61,61,61,61	0
58	MG	2A	3540	1/1	0.86	0.12	48,48,48,48	0
58	MG	2A	3351	1/1	0.86	0.16	54,54,54,54	0
58	MG	1A	4038	1/1	0.86	0.10	48,48,48,48	0
58	MG	2A	3561	1/1	0.86	0.13	59,59,59,59	0
58	MG	1A	4041	1/1	0.86	0.17	41,41,41,41	0
58	MG	1A	3584	1/1	0.86	0.17	40,40,40,40	0
58	MG	2A	3799	1/1	0.86	0.09	34,34,34,34	0
58	MG	1A	3452	1/1	0.86	0.12	48,48,48,48	0
58	MG	1G	202	1/1	0.86	0.21	63,63,63,63	0
58	MG	2v	102	1/1	0.86	0.34	68,68,68,68	0
58	MG	1a	1696	1/1	0.86	0.38	56,56,56,56	0
58	MG	1A	3711	1/1	0.86	0.12	35,35,35,35	0
58	MG	2A	3815	1/1	0.86	0.11	44,44,44,44	0
58	MG	1A	3313	1/1	0.86	0.13	45,45,45,45	0
58	MG	2A	3269	1/1	0.86	0.13	47,47,47,47	0
58	MG	1A	3848	1/1	0.87	0.11	61,61,61,61	0
58	MG	2A	3200	1/1	0.87	0.28	71,71,71,71	0
58	MG	1A	3427	1/1	0.87	0.13	50,50,50,50	0
58	MG	2A	3677	1/1	0.87	0.20	68,68,68,68	0
58	MG	1A	3367	1/1	0.87	0.16	42,42,42,42	0
58	MG	1A	3698	1/1	0.87	0.17	67,67,67,67	0
58	MG	2A	3685	1/1	0.87	0.22	59,59,59,59	0
58	MG	1A	3702	1/1	0.87	0.09	33,33,33,33	0
58	MG	2A	3210	1/1	0.87	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1674	1/1	0.87	0.23	55,55,55,55	0
58	MG	2A	3364	1/1	0.87	0.15	59,59,59,59	0
58	MG	1A	3149	1/1	0.87	0.18	32,32,32,32	0
58	MG	1A	3180	1/1	0.87	0.21	48,48,48,48	0
58	MG	1A	4077	1/1	0.87	0.12	30,30,30,30	0
58	MG	11	105	1/1	0.87	0.12	63,63,63,63	0
58	MG	2a	1648	1/1	0.87	0.22	61,61,61,61	0
58	MG	2A	3003	1/1	0.87	0.32	56,56,56,56	0
58	MG	12	101	1/1	0.87	0.14	50,50,50,50	0
58	MG	2A	3378	1/1	0.87	0.11	55,55,55,55	0
58	MG	2A	3380	1/1	0.87	0.14	53,53,53,53	0
58	MG	2a	1653	1/1	0.87	0.15	55,55,55,55	0
58	MG	2A	3381	1/1	0.87	0.12	57,57,57,57	0
58	MG	13	104	1/1	0.87	0.13	48,48,48,48	0
58	MG	1a	1684	1/1	0.87	0.20	67,67,67,67	0
58	MG	1A	3883	1/1	0.87	0.14	36,36,36,36	0
58	MG	1A	3489	1/1	0.87	0.17	45,45,45,45	0
58	MG	1A	3181	1/1	0.87	0.10	54,54,54,54	0
58	MG	1A	3309	1/1	0.87	0.22	57,57,57,57	0
58	MG	2A	3403	1/1	0.87	0.16	46,46,46,46	0
58	MG	1A	3184	1/1	0.87	0.18	38,38,38,38	0
58	MG	1A	3594	1/1	0.87	0.29	59,59,59,59	0
58	MG	1A	3350	1/1	0.87	0.24	59,59,59,59	0
58	MG	1A	3351	1/1	0.87	0.20	59,59,59,59	0
58	MG	2A	3239	1/1	0.87	0.27	68,68,68,68	0
58	MG	1a	1695	1/1	0.87	0.19	55,55,55,55	0
58	MG	2A	3414	1/1	0.87	0.31	64,64,64,64	0
58	MG	1A	3726	1/1	0.87	0.14	43,43,43,43	0
58	MG	2A	3060	1/1	0.87	0.17	62,62,62,62	0
58	MG	2A	3062	1/1	0.87	0.23	59,59,59,59	0
58	MG	2A	3245	1/1	0.87	0.18	49,49,49,49	0
58	MG	2A	3063	1/1	0.87	0.15	60,60,60,60	0
58	MG	2A	3064	1/1	0.87	0.21	63,63,63,63	0
58	MG	1a	1603	1/1	0.87	0.13	53,53,53,53	0
58	MG	2A	3077	1/1	0.87	0.12	47,47,47,47	0
58	MG	2a	1707	1/1	0.87	0.23	66,66,66,66	0
58	MG	1a	1699	1/1	0.87	0.20	48,48,48,48	0
58	MG	2A	3448	1/1	0.87	0.16	68,68,68,68	0
58	MG	1A	3404	1/1	0.87	0.19	54,54,54,54	0
58	MG	1B	208	1/1	0.87	0.14	60,60,60,60	0
58	MG	1a	1709	1/1	0.87	0.19	56,56,56,56	0
58	MG	1A	3129	1/1	0.87	0.13	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3263	1/1	0.87	0.17	66,66,66,66	0
58	MG	1A	3962	1/1	0.87	0.10	58,58,58,58	0
58	MG	2A	3267	1/1	0.87	0.14	64,64,64,64	0
58	MG	1A	3524	1/1	0.87	0.13	47,47,47,47	0
58	MG	1B	216	1/1	0.87	0.14	65,65,65,65	0
58	MG	2a	1726	1/1	0.87	0.16	57,57,57,57	0
58	MG	2A	3470	1/1	0.87	0.20	54,54,54,54	0
58	MG	1A	3744	1/1	0.87	0.14	47,47,47,47	0
58	MG	1A	3195	1/1	0.87	0.14	38,38,38,38	0
58	MG	2A	3480	1/1	0.87	0.10	45,45,45,45	0
58	MG	2A	3107	1/1	0.87	0.28	62,62,62,62	0
58	MG	1A	3984	1/1	0.87	0.12	23,23,23,23	0
58	MG	1a	1728	1/1	0.87	0.10	64,64,64,64	0
58	MG	2a	1742	1/1	0.87	0.11	55,55,55,55	0
58	MG	1a	1729	1/1	0.87	0.12	55,55,55,55	0
58	MG	1B	227	1/1	0.87	0.14	46,46,46,46	0
58	MG	1A	3752	1/1	0.87	0.12	55,55,55,55	0
58	MG	1A	3354	1/1	0.87	0.19	59,59,59,59	0
58	MG	1A	3287	1/1	0.87	0.14	53,53,53,53	0
58	MG	2a	1759	1/1	0.87	0.15	63,63,63,63	0
58	MG	1a	1747	1/1	0.87	0.21	66,66,66,66	0
58	MG	2B	205	1/1	0.87	0.13	59,59,59,59	0
58	MG	1A	3536	1/1	0.87	0.26	55,55,55,55	0
58	MG	2A	3512	1/1	0.87	0.20	50,50,50,50	0
58	MG	2B	208	1/1	0.87	0.18	55,55,55,55	0
58	MG	1A	4009	1/1	0.87	0.08	40,40,40,40	0
58	MG	2a	1778	1/1	0.87	0.15	67,67,67,67	0
58	MG	2A	3518	1/1	0.87	0.16	51,51,51,51	0
58	MG	1A	3772	1/1	0.87	0.11	29,29,29,29	0
58	MG	1A	3776	1/1	0.87	0.11	60,60,60,60	0
58	MG	2A	3528	1/1	0.87	0.20	63,63,63,63	0
58	MG	1A	3323	1/1	0.87	0.11	38,38,38,38	0
58	MG	2A	3146	1/1	0.87	0.14	52,52,52,52	0
58	MG	1a	1771	1/1	0.87	0.13	45,45,45,45	0
58	MG	1E	311	1/1	0.87	0.16	43,43,43,43	0
58	MG	2A	3551	1/1	0.87	0.10	65,65,65,65	0
58	MG	1a	1776	1/1	0.87	0.14	43,43,43,43	0
58	MG	2a	1799	1/1	0.87	0.21	62,62,62,62	0
58	MG	1a	1784	1/1	0.87	0.10	52,52,52,52	0
58	MG	2A	3567	1/1	0.87	0.14	49,49,49,49	0
58	MG	2A	3570	1/1	0.87	0.16	67,67,67,67	0
58	MG	1E	312	1/1	0.87	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3035	1/1	0.87	0.18	44,44,44,44	0
58	MG	2A	3577	1/1	0.87	0.21	73,73,73,73	0
58	MG	1A	3655	1/1	0.87	0.15	65,65,65,65	0
58	MG	1G	204	1/1	0.87	0.12	59,59,59,59	0
58	MG	1A	4020	1/1	0.87	0.09	52,52,52,52	0
58	MG	1a	1652	1/1	0.87	0.23	61,61,61,61	0
58	MG	2A	3323	1/1	0.87	0.22	66,66,66,66	0
58	MG	1a	1806	1/1	0.87	0.10	54,54,54,54	0
58	MG	1A	3472	1/1	0.87	0.14	51,51,51,51	0
58	MG	1A	3544	1/1	0.87	0.29	64,64,64,64	0
58	MG	2A	3608	1/1	0.87	0.12	34,34,34,34	0
58	MG	1A	3548	1/1	0.87	0.16	64,64,64,64	0
58	MG	1Q	207	1/1	0.87	0.21	58,58,58,58	0
58	MG	2a	1606	1/1	0.87	0.24	59,59,59,59	0
58	MG	1A	4034	1/1	0.87	0.16	42,42,42,42	0
58	MG	2A	3187	1/1	0.87	0.18	59,59,59,59	0
58	MG	1e	201	1/1	0.87	0.10	63,63,63,63	0
58	MG	2A	3192	1/1	0.87	0.18	48,48,48,48	0
58	MG	2A	3637	1/1	0.87	0.15	46,46,46,46	0
58	MG	2A	3333	1/1	0.87	0.36	50,50,50,50	0
58	MG	2A	3641	1/1	0.87	0.14	57,57,57,57	0
58	MG	1f	202	1/1	0.87	0.27	60,60,60,60	0
58	MG	2a	1618	1/1	0.87	0.27	73,73,73,73	0
58	MG	1A	3476	1/1	0.87	0.16	58,58,58,58	0
58	MG	1A	3415	1/1	0.87	0.19	69,69,69,69	0
58	MG	2v	104	1/1	0.87	0.15	62,62,62,62	0
58	MG	1t	201	1/1	0.87	0.11	49,49,49,49	0
58	MG	1A	3206	1/1	0.87	0.17	51,51,51,51	0
58	MG	2A	3343	1/1	0.87	0.14	63,63,63,63	0
58	MG	2A	3344	1/1	0.87	0.24	62,62,62,62	0
58	MG	1a	1691	1/1	0.88	0.23	49,49,49,49	0
58	MG	2A	3751	1/1	0.88	0.16	56,56,56,56	0
58	MG	1A	3370	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3813	1/1	0.88	0.13	56,56,56,56	0
58	MG	1A	3419	1/1	0.88	0.15	49,49,49,49	0
58	MG	2A	3770	1/1	0.88	0.13	60,60,60,60	0
58	MG	2a	1655	1/1	0.88	0.20	56,56,56,56	0
58	MG	2A	3314	1/1	0.88	0.21	70,70,70,70	0
58	MG	2A	3494	1/1	0.88	0.26	58,58,58,58	0
58	MG	1a	1609	1/1	0.88	0.15	57,57,57,57	0
58	MG	2A	3497	1/1	0.88	0.18	46,46,46,46	0
58	MG	2a	1666	1/1	0.88	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3190	1/1	0.88	0.10	49,49,49,49	0
58	MG	1A	3135	1/1	0.88	0.12	53,53,53,53	0
58	MG	1A	3597	1/1	0.88	0.12	45,45,45,45	0
58	MG	1A	4007	1/1	0.88	0.12	33,33,33,33	0
58	MG	2A	3014	1/1	0.88	0.17	38,38,38,38	0
58	MG	1A	3382	1/1	0.88	0.15	48,48,48,48	0
58	MG	1a	1706	1/1	0.88	0.28	63,63,63,63	0
58	MG	2a	1682	1/1	0.88	0.26	60,60,60,60	0
58	MG	2A	3793	1/1	0.88	0.11	46,46,46,46	0
58	MG	2a	1685	1/1	0.88	0.24	54,54,54,54	0
58	MG	1B	235	1/1	0.88	0.14	70,70,70,70	0
58	MG	2A	3199	1/1	0.88	0.14	47,47,47,47	0
58	MG	1A	3823	1/1	0.88	0.10	39,39,39,39	0
58	MG	1A	3227	1/1	0.88	0.12	24,24,24,24	0
58	MG	1A	3840	1/1	0.88	0.07	37,37,37,37	0
58	MG	2A	3206	1/1	0.88	0.21	53,53,53,53	0
58	MG	1A	3843	1/1	0.88	0.15	58,58,58,58	0
58	MG	2A	3208	1/1	0.88	0.18	60,60,60,60	0
58	MG	2A	3550	1/1	0.88	0.17	51,51,51,51	0
58	MG	2A	3833	1/1	0.88	0.12	52,52,52,52	0
58	MG	1A	4018	1/1	0.88	0.12	49,49,49,49	0
58	MG	1A	3231	1/1	0.88	0.16	40,40,40,40	0
58	MG	2A	3838	1/1	0.88	0.17	60,60,60,60	0
58	MG	1A	3158	1/1	0.88	0.12	50,50,50,50	0
58	MG	2A	3048	1/1	0.88	0.14	57,57,57,57	0
58	MG	2A	3050	1/1	0.88	0.18	58,58,58,58	0
58	MG	2a	1716	1/1	0.88	0.27	53,53,53,53	0
58	MG	2A	3847	1/1	0.88	0.13	61,61,61,61	0
58	MG	1A	3197	1/1	0.88	0.09	36,36,36,36	0
58	MG	1A	3626	1/1	0.88	0.10	26,26,26,26	0
58	MG	2a	1722	1/1	0.88	0.27	58,58,58,58	0
58	MG	1F	306	1/1	0.88	0.07	28,28,28,28	0
58	MG	1A	4027	1/1	0.88	0.10	47,47,47,47	0
58	MG	1a	1735	1/1	0.88	0.25	61,61,61,61	0
58	MG	1A	3308	1/1	0.88	0.35	64,64,64,64	0
58	MG	1A	4033	1/1	0.88	0.10	41,41,41,41	0
58	MG	2A	3600	1/1	0.88	0.14	58,58,58,58	0
58	MG	1A	3724	1/1	0.88	0.21	50,50,50,50	0
58	MG	2A	3232	1/1	0.88	0.17	47,47,47,47	0
58	MG	1a	1746	1/1	0.88	0.10	57,57,57,57	0
58	MG	1A	3438	1/1	0.88	0.14	51,51,51,51	0
58	MG	1a	1752	1/1	0.88	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2B	218	1/1	0.88	0.15	70,70,70,70	0
58	MG	2A	3367	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3872	1/1	0.88	0.14	42,42,42,42	0
58	MG	1A	3336	1/1	0.88	0.16	53,53,53,53	0
58	MG	1a	1759	1/1	0.88	0.19	61,61,61,61	0
58	MG	1A	3881	1/1	0.88	0.17	42,42,42,42	0
58	MG	1A	3641	1/1	0.88	0.08	19,19,19,19	0
58	MG	2a	1764	1/1	0.88	0.13	74,74,74,74	0
58	MG	2a	1767	1/1	0.88	0.12	61,61,61,61	0
58	MG	2F	303	1/1	0.88	0.11	58,58,58,58	0
58	MG	2A	3097	1/1	0.88	0.23	55,55,55,55	0
58	MG	1a	1768	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3552	1/1	0.88	0.28	49,49,49,49	0
58	MG	2A	3104	1/1	0.88	0.14	58,58,58,58	0
58	MG	1U	206	1/1	0.88	0.15	44,44,44,44	0
58	MG	1A	3885	1/1	0.88	0.13	38,38,38,38	0
58	MG	2A	3651	1/1	0.88	0.14	63,63,63,63	0
58	MG	2A	3652	1/1	0.88	0.12	49,49,49,49	0
58	MG	1A	4062	1/1	0.88	0.12	18,18,18,18	0
58	MG	2A	3110	1/1	0.88	0.16	50,50,50,50	0
58	MG	1a	1779	1/1	0.88	0.14	55,55,55,55	0
58	MG	1Y	201	1/1	0.88	0.14	49,49,49,49	0
58	MG	2A	3405	1/1	0.88	0.13	51,51,51,51	0
58	MG	2a	1791	1/1	0.88	0.17	75,75,75,75	0
58	MG	1A	3405	1/1	0.88	0.13	41,41,41,41	0
58	MG	2A	3260	1/1	0.88	0.12	58,58,58,58	0
58	MG	1A	3340	1/1	0.88	0.12	51,51,51,51	0
58	MG	1a	1789	1/1	0.88	0.11	59,59,59,59	0
58	MG	1a	1792	1/1	0.88	0.11	79,79,79,79	0
58	MG	2A	3129	1/1	0.88	0.17	41,41,41,41	0
58	MG	2A	3131	1/1	0.88	0.19	72,72,72,72	0
58	MG	1A	3908	1/1	0.88	0.17	51,51,51,51	0
58	MG	1A	3919	1/1	0.88	0.13	34,34,34,34	0
58	MG	2A	3271	1/1	0.88	0.23	60,60,60,60	0
58	MG	2a	1614	1/1	0.88	0.15	58,58,58,58	0
58	MG	2A	3426	1/1	0.88	0.15	50,50,50,50	0
58	MG	1A	3341	1/1	0.88	0.24	39,39,39,39	0
58	MG	1A	3504	1/1	0.88	0.16	48,48,48,48	0
58	MG	2a	1814	1/1	0.88	0.17	52,52,52,52	0
58	MG	2A	3699	1/1	0.88	0.17	57,57,57,57	0
58	MG	1A	3761	1/1	0.88	0.23	51,51,51,51	0
58	MG	1A	3762	1/1	0.88	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3706	1/1	0.88	0.10	49,49,49,49	0
58	MG	2a	1819	1/1	0.88	0.10	56,56,56,56	0
58	MG	1a	1675	1/1	0.88	0.15	44,44,44,44	0
58	MG	2a	1627	1/1	0.88	0.25	66,66,66,66	0
58	MG	1A	3506	1/1	0.88	0.14	49,49,49,49	0
58	MG	13	102	1/1	0.88	0.14	37,37,37,37	0
58	MG	2i	201	1/1	0.88	0.22	61,61,61,61	0
58	MG	2A	3283	1/1	0.88	0.17	62,62,62,62	0
58	MG	2A	3718	1/1	0.88	0.24	62,62,62,62	0
58	MG	1A	3017	1/1	0.88	0.21	59,59,59,59	0
58	MG	2A	3455	1/1	0.88	0.17	59,59,59,59	0
58	MG	2A	3725	1/1	0.88	0.10	54,54,54,54	0
58	MG	1A	3362	1/1	0.88	0.18	61,61,61,61	0
58	MG	1A	3958	1/1	0.88	0.16	43,43,43,43	0
58	MG	1A	3961	1/1	0.88	0.09	41,41,41,41	0
58	MG	1A	3583	1/1	0.88	0.10	29,29,29,29	0
58	MG	1A	3966	1/1	0.88	0.12	51,51,51,51	0
58	MG	1A	3182	1/1	0.88	0.18	72,72,72,72	0
58	MG	2A	3468	1/1	0.88	0.14	56,56,56,56	0
58	MG	2w	102	1/1	0.88	0.12	62,62,62,62	0
58	MG	1A	3795	1/1	0.88	0.12	68,68,68,68	0
58	MG	2w	104	1/1	0.88	0.14	70,70,70,70	0
58	MG	1w	106	1/1	0.88	0.15	71,71,71,71	0
58	MG	1B	214	1/1	0.88	0.11	61,61,61,61	0
58	MG	1A	3142	1/1	0.88	0.12	42,42,42,42	0
58	MG	1A	3518	1/1	0.89	0.23	40,40,40,40	0
58	MG	2A	3654	1/1	0.89	0.16	68,68,68,68	0
58	MG	2a	1621	1/1	0.89	0.31	70,70,70,70	0
58	MG	1B	211	1/1	0.89	0.12	50,50,50,50	0
58	MG	1A	3076	1/1	0.89	0.09	27,27,27,27	0
58	MG	2a	1626	1/1	0.89	0.20	65,65,65,65	0
58	MG	2A	3659	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3660	1/1	0.89	0.14	59,59,59,59	0
58	MG	2A	3379	1/1	0.89	0.24	57,57,57,57	0
58	MG	1a	1613	1/1	0.89	0.09	47,47,47,47	0
58	MG	1A	3804	1/1	0.89	0.09	44,44,44,44	0
58	MG	2a	1633	1/1	0.89	0.23	54,54,54,54	0
58	MG	2A	3061	1/1	0.89	0.16	66,66,66,66	0
58	MG	1a	1727	1/1	0.89	0.11	52,52,52,52	0
58	MG	2A	3676	1/1	0.89	0.09	40,40,40,40	0
58	MG	1A	3585	1/1	0.89	0.10	48,48,48,48	0
58	MG	1A	3809	1/1	0.89	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3070	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3394	1/1	0.89	0.20	54,54,54,54	0
58	MG	1A	3329	1/1	0.89	0.16	45,45,45,45	0
58	MG	2A	3688	1/1	0.89	0.10	59,59,59,59	0
58	MG	2A	3397	1/1	0.89	0.23	46,46,46,46	0
58	MG	2A	3074	1/1	0.89	0.13	40,40,40,40	0
58	MG	1B	221	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3693	1/1	0.89	0.16	66,66,66,66	0
58	MG	1A	3460	1/1	0.89	0.17	40,40,40,40	0
58	MG	1A	3701	1/1	0.89	0.09	36,36,36,36	0
58	MG	1A	3818	1/1	0.89	0.09	53,53,53,53	0
58	MG	1a	1743	1/1	0.89	0.14	54,54,54,54	0
58	MG	1a	1745	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3412	1/1	0.89	0.10	49,49,49,49	0
58	MG	1A	3384	1/1	0.89	0.13	47,47,47,47	0
58	MG	1a	1629	1/1	0.89	0.25	55,55,55,55	0
58	MG	2A	3415	1/1	0.89	0.29	56,56,56,56	0
58	MG	2a	1659	1/1	0.89	0.22	71,71,71,71	0
58	MG	2A	3417	1/1	0.89	0.25	52,52,52,52	0
58	MG	1a	1751	1/1	0.89	0.10	45,45,45,45	0
58	MG	2a	1663	1/1	0.89	0.18	53,53,53,53	0
58	MG	1A	3986	1/1	0.89	0.13	38,38,38,38	0
58	MG	1A	3417	1/1	0.89	0.26	42,42,42,42	0
58	MG	1B	234	1/1	0.89	0.11	41,41,41,41	0
58	MG	2A	3428	1/1	0.89	0.17	51,51,51,51	0
58	MG	1A	3596	1/1	0.89	0.14	54,54,54,54	0
58	MG	2a	1676	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3256	1/1	0.89	0.12	62,62,62,62	0
58	MG	2A	3436	1/1	0.89	0.12	43,43,43,43	0
58	MG	2a	1679	1/1	0.89	0.14	54,54,54,54	0
58	MG	1a	1762	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3734	1/1	0.89	0.20	50,50,50,50	0
58	MG	1A	3386	1/1	0.89	0.18	38,38,38,38	0
58	MG	1D	307	1/1	0.89	0.13	42,42,42,42	0
58	MG	1A	3841	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3447	1/1	0.89	0.15	48,48,48,48	0
58	MG	1a	1770	1/1	0.89	0.11	62,62,62,62	0
58	MG	2A	3451	1/1	0.89	0.14	40,40,40,40	0
58	MG	2A	3270	1/1	0.89	0.14	58,58,58,58	0
58	MG	1A	3392	1/1	0.89	0.23	37,37,37,37	0
58	MG	2A	3119	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3273	1/1	0.89	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3429	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1645	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3762	1/1	0.89	0.16	66,66,66,66	0
58	MG	2A	3462	1/1	0.89	0.16	53,53,53,53	0
58	MG	1a	1777	1/1	0.89	0.10	50,50,50,50	0
58	MG	2A	3775	1/1	0.89	0.17	54,54,54,54	0
58	MG	2A	3279	1/1	0.89	0.18	49,49,49,49	0
58	MG	1A	3606	1/1	0.89	0.13	54,54,54,54	0
58	MG	2A	3134	1/1	0.89	0.26	57,57,57,57	0
58	MG	1A	3851	1/1	0.89	0.11	44,44,44,44	0
58	MG	1A	3539	1/1	0.89	0.21	50,50,50,50	0
58	MG	1A	3853	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3472	1/1	0.89	0.11	56,56,56,56	0
58	MG	2A	3786	1/1	0.89	0.12	70,70,70,70	0
58	MG	1A	3610	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3478	1/1	0.89	0.19	54,54,54,54	0
58	MG	1A	3614	1/1	0.89	0.11	54,54,54,54	0
58	MG	1A	3868	1/1	0.89	0.11	44,44,44,44	0
58	MG	1H	201	1/1	0.89	0.15	42,42,42,42	0
58	MG	1A	3301	1/1	0.89	0.20	43,43,43,43	0
58	MG	2A	3488	1/1	0.89	0.17	61,61,61,61	0
58	MG	2A	3804	1/1	0.89	0.12	49,49,49,49	0
58	MG	2A	3155	1/1	0.89	0.09	33,33,33,33	0
58	MG	1N	205	1/1	0.89	0.14	45,45,45,45	0
58	MG	2A	3158	1/1	0.89	0.09	37,37,37,37	0
58	MG	1A	3622	1/1	0.89	0.09	10,10,10,10	0
58	MG	1A	3235	1/1	0.89	0.27	32,32,32,32	0
58	MG	1A	3873	1/1	0.89	0.11	33,33,33,33	0
58	MG	2A	3827	1/1	0.89	0.09	41,41,41,41	0
58	MG	2A	3504	1/1	0.89	0.12	35,35,35,35	0
58	MG	1A	3107	1/1	0.89	0.11	24,24,24,24	0
58	MG	2a	1755	1/1	0.89	0.08	41,41,41,41	0
58	MG	2A	3507	1/1	0.89	0.11	49,49,49,49	0
58	MG	1A	3402	1/1	0.89	0.14	48,48,48,48	0
58	MG	2a	1765	1/1	0.89	0.14	60,60,60,60	0
58	MG	1A	3635	1/1	0.89	0.08	47,47,47,47	0
58	MG	2A	3511	1/1	0.89	0.11	35,35,35,35	0
58	MG	1a	1672	1/1	0.89	0.10	50,50,50,50	0
58	MG	1A	4042	1/1	0.89	0.10	28,28,28,28	0
58	MG	2A	3177	1/1	0.89	0.15	47,47,47,47	0
58	MG	2A	3519	1/1	0.89	0.11	49,49,49,49	0
58	MG	1A	4044	1/1	0.89	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3747	1/1	0.89	0.10	19,19,19,19	0
58	MG	1A	3166	1/1	0.89	0.09	28,28,28,28	0
58	MG	2A	3530	1/1	0.89	0.09	32,32,32,32	0
58	MG	1A	3359	1/1	0.89	0.15	59,59,59,59	0
58	MG	1A	3493	1/1	0.89	0.14	43,43,43,43	0
58	MG	1w	105	1/1	0.89	0.19	64,64,64,64	0
58	MG	1A	3890	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3188	1/1	0.89	0.15	51,51,51,51	0
58	MG	1A	3899	1/1	0.89	0.09	20,20,20,20	0
58	MG	1A	3902	1/1	0.89	0.17	41,41,41,41	0
58	MG	1A	3906	1/1	0.89	0.13	52,52,52,52	0
58	MG	2A	3564	1/1	0.89	0.15	40,40,40,40	0
58	MG	1A	3055	1/1	0.89	0.12	43,43,43,43	0
58	MG	1A	3766	1/1	0.89	0.12	25,25,25,25	0
58	MG	2a	1802	1/1	0.89	0.12	68,68,68,68	0
58	MG	1A	4082	1/1	0.89	0.16	56,56,56,56	0
58	MG	1l	106	1/1	0.89	0.14	51,51,51,51	0
58	MG	2E	308	1/1	0.89	0.13	50,50,50,50	0
58	MG	2E	309	1/1	0.89	0.11	48,48,48,48	0
58	MG	2A	3576	1/1	0.89	0.09	52,52,52,52	0
58	MG	1A	4083	1/1	0.89	0.16	50,50,50,50	0
58	MG	1A	3213	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3931	1/1	0.89	0.17	50,50,50,50	0
58	MG	2N	201	1/1	0.89	0.15	51,51,51,51	0
58	MG	2a	1813	1/1	0.89	0.15	54,54,54,54	0
58	MG	2A	3593	1/1	0.89	0.12	50,50,50,50	0
58	MG	2A	3004	1/1	0.89	0.18	45,45,45,45	0
58	MG	2R	202	1/1	0.89	0.18	50,50,50,50	0
58	MG	2A	3341	1/1	0.89	0.18	54,54,54,54	0
58	MG	2A	3598	1/1	0.89	0.20	50,50,50,50	0
58	MG	2A	3342	1/1	0.89	0.27	63,63,63,63	0
58	MG	2A	3005	1/1	0.89	0.18	54,54,54,54	0
58	MG	1A	3130	1/1	0.89	0.15	57,57,57,57	0
58	MG	2W	201	1/1	0.89	0.20	61,61,61,61	0
58	MG	1A	3448	1/1	0.89	0.17	55,55,55,55	0
58	MG	1A	4092	1/1	0.89	0.25	56,56,56,56	0
58	MG	27	102	1/1	0.89	0.14	52,52,52,52	0
58	MG	2A	3350	1/1	0.89	0.18	68,68,68,68	0
58	MG	2A	3018	1/1	0.89	0.17	64,64,64,64	0
58	MG	1A	3251	1/1	0.89	0.16	59,59,59,59	0
58	MG	2A	3027	1/1	0.89	0.19	58,58,58,58	0
58	MG	1A	3945	1/1	0.89	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4098	1/1	0.89	0.14	56,56,56,56	0
58	MG	2A	3618	1/1	0.89	0.09	45,45,45,45	0
58	MG	2r	101	1/1	0.89	0.15	63,63,63,63	0
58	MG	2A	3623	1/1	0.89	0.16	34,34,34,34	0
58	MG	2A	3358	1/1	0.89	0.11	52,52,52,52	0
58	MG	1a	1705	1/1	0.89	0.16	57,57,57,57	0
58	MG	2A	3216	1/1	0.89	0.16	52,52,52,52	0
58	MG	1A	3784	1/1	0.89	0.15	35,35,35,35	0
58	MG	1A	3178	1/1	0.89	0.17	36,36,36,36	0
58	MG	2A	3645	1/1	0.89	0.28	66,66,66,66	0
58	MG	1B	202	1/1	0.89	0.15	52,52,52,52	0
58	MG	1B	204	1/1	0.89	0.23	59,59,59,59	0
58	MG	1A	3950	1/1	0.89	0.10	57,57,57,57	0
58	MG	1U	202	1/1	0.90	0.22	46,46,46,46	0
58	MG	2A	3461	1/1	0.90	0.08	38,38,38,38	0
58	MG	1A	3618	1/1	0.90	0.13	39,39,39,39	0
58	MG	1A	4051	1/1	0.90	0.19	59,59,59,59	0
58	MG	2A	3715	1/1	0.90	0.12	62,62,62,62	0
58	MG	2A	3167	1/1	0.90	0.15	37,37,37,37	0
58	MG	1A	3467	1/1	0.90	0.11	37,37,37,37	0
58	MG	2A	3171	1/1	0.90	0.24	54,54,54,54	0
58	MG	2A	3721	1/1	0.90	0.12	55,55,55,55	0
58	MG	1A	3088	1/1	0.90	0.13	32,32,32,32	0
58	MG	1x	101	1/1	0.90	0.20	66,66,66,66	0
58	MG	1a	1683	1/1	0.90	0.18	57,57,57,57	0
58	MG	1x	103	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3728	1/1	0.90	0.17	49,49,49,49	0
58	MG	1A	3416	1/1	0.90	0.10	49,49,49,49	0
58	MG	2A	3476	1/1	0.90	0.11	50,50,50,50	0
58	MG	2A	3477	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3372	1/1	0.90	0.21	54,54,54,54	0
58	MG	2A	3736	1/1	0.90	0.14	51,51,51,51	0
58	MG	1A	3543	1/1	0.90	0.17	54,54,54,54	0
58	MG	1A	3900	1/1	0.90	0.14	66,66,66,66	0
58	MG	1A	3474	1/1	0.90	0.12	42,42,42,42	0
58	MG	1A	3545	1/1	0.90	0.15	54,54,54,54	0
58	MG	11	103	1/1	0.90	0.12	41,41,41,41	0
58	MG	2A	3490	1/1	0.90	0.11	56,56,56,56	0
58	MG	2A	3491	1/1	0.90	0.31	59,59,59,59	0
58	MG	1A	3642	1/1	0.90	0.10	49,49,49,49	0
58	MG	1A	3911	1/1	0.90	0.15	49,49,49,49	0
58	MG	1A	3373	1/1	0.90	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3924	1/1	0.90	0.11	64,64,64,64	0
58	MG	2A	3761	1/1	0.90	0.11	44,44,44,44	0
58	MG	1A	3774	1/1	0.90	0.10	30,30,30,30	0
58	MG	1A	3775	1/1	0.90	0.07	22,22,22,22	0
58	MG	1A	3645	1/1	0.90	0.13	56,56,56,56	0
58	MG	1A	4091	1/1	0.90	0.14	44,44,44,44	0
58	MG	1A	3781	1/1	0.90	0.11	45,45,45,45	0
58	MG	1A	3089	1/1	0.90	0.20	40,40,40,40	0
58	MG	1A	3791	1/1	0.90	0.07	52,52,52,52	0
58	MG	1A	4096	1/1	0.90	0.09	40,40,40,40	0
58	MG	1A	3004	1/1	0.90	0.18	36,36,36,36	0
58	MG	1A	3068	1/1	0.90	0.08	27,27,27,27	0
58	MG	2A	3338	1/1	0.90	0.17	59,59,59,59	0
58	MG	2A	3785	1/1	0.90	0.16	65,65,65,65	0
58	MG	2a	1686	1/1	0.90	0.19	56,56,56,56	0
58	MG	1A	3430	1/1	0.90	0.12	59,59,59,59	0
58	MG	1B	201	1/1	0.90	0.16	45,45,45,45	0
58	MG	2A	3522	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3790	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3525	1/1	0.90	0.12	37,37,37,37	0
58	MG	1a	1605	1/1	0.90	0.11	50,50,50,50	0
58	MG	2A	3797	1/1	0.90	0.12	47,47,47,47	0
58	MG	1A	3952	1/1	0.90	0.09	52,52,52,52	0
58	MG	1A	3953	1/1	0.90	0.13	48,48,48,48	0
58	MG	1A	3955	1/1	0.90	0.09	48,48,48,48	0
58	MG	2A	3532	1/1	0.90	0.18	52,52,52,52	0
58	MG	2A	3535	1/1	0.90	0.21	62,62,62,62	0
58	MG	2A	3348	1/1	0.90	0.13	57,57,57,57	0
58	MG	2a	1710	1/1	0.90	0.22	59,59,59,59	0
58	MG	2A	3054	1/1	0.90	0.17	63,63,63,63	0
58	MG	1A	3802	1/1	0.90	0.14	24,24,24,24	0
58	MG	2a	1714	1/1	0.90	0.14	59,59,59,59	0
58	MG	2A	3547	1/1	0.90	0.10	46,46,46,46	0
58	MG	2A	3058	1/1	0.90	0.10	38,38,38,38	0
58	MG	1A	3561	1/1	0.90	0.16	38,38,38,38	0
58	MG	1A	3675	1/1	0.90	0.10	39,39,39,39	0
58	MG	1a	1617	1/1	0.90	0.11	41,41,41,41	0
58	MG	1a	1618	1/1	0.90	0.11	53,53,53,53	0
58	MG	2A	3357	1/1	0.90	0.18	54,54,54,54	0
58	MG	1A	3807	1/1	0.90	0.17	46,46,46,46	0
58	MG	1A	3041	1/1	0.90	0.09	33,33,33,33	0
58	MG	2A	3844	1/1	0.90	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3969	1/1	0.90	0.23	53,53,53,53	0
58	MG	1A	3001	1/1	0.90	0.09	34,34,34,34	0
58	MG	2A	3848	1/1	0.90	0.17	59,59,59,59	0
58	MG	1A	3057	1/1	0.90	0.12	44,44,44,44	0
58	MG	1A	3262	1/1	0.90	0.17	68,68,68,68	0
58	MG	2A	3581	1/1	0.90	0.22	58,58,58,58	0
58	MG	2A	3585	1/1	0.90	0.17	59,59,59,59	0
58	MG	1A	3977	1/1	0.90	0.11	43,43,43,43	0
58	MG	1A	3978	1/1	0.90	0.10	65,65,65,65	0
58	MG	1a	1755	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3376	1/1	0.90	0.24	57,57,57,57	0
58	MG	2B	210	1/1	0.90	0.18	75,75,75,75	0
58	MG	2a	1751	1/1	0.90	0.12	64,64,64,64	0
58	MG	2a	1752	1/1	0.90	0.15	69,69,69,69	0
58	MG	1A	3118	1/1	0.90	0.11	29,29,29,29	0
58	MG	2A	3599	1/1	0.90	0.15	56,56,56,56	0
58	MG	2a	1758	1/1	0.90	0.10	66,66,66,66	0
58	MG	1A	3312	1/1	0.90	0.10	43,43,43,43	0
58	MG	1A	3700	1/1	0.90	0.09	47,47,47,47	0
58	MG	2A	3093	1/1	0.90	0.13	43,43,43,43	0
58	MG	2a	1766	1/1	0.90	0.10	65,65,65,65	0
58	MG	2A	3095	1/1	0.90	0.24	64,64,64,64	0
58	MG	1A	3233	1/1	0.90	0.20	44,44,44,44	0
58	MG	1A	3824	1/1	0.90	0.10	39,39,39,39	0
58	MG	2D	304	1/1	0.90	0.13	55,55,55,55	0
58	MG	1A	3086	1/1	0.90	0.15	28,28,28,28	0
58	MG	2A	3248	1/1	0.90	0.16	48,48,48,48	0
58	MG	2A	3249	1/1	0.90	0.19	64,64,64,64	0
58	MG	2E	304	1/1	0.90	0.20	65,65,65,65	0
58	MG	2A	3393	1/1	0.90	0.15	39,39,39,39	0
58	MG	2a	1780	1/1	0.90	0.20	67,67,67,67	0
58	MG	2A	3251	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	4005	1/1	0.90	0.07	26,26,26,26	0
58	MG	2A	3103	1/1	0.90	0.20	56,56,56,56	0
58	MG	2a	1785	1/1	0.90	0.14	60,60,60,60	0
58	MG	2A	3400	1/1	0.90	0.35	60,60,60,60	0
58	MG	1A	3703	1/1	0.90	0.15	29,29,29,29	0
58	MG	1A	3194	1/1	0.90	0.30	51,51,51,51	0
58	MG	1A	3445	1/1	0.90	0.10	36,36,36,36	0
58	MG	1A	3275	1/1	0.90	0.17	40,40,40,40	0
58	MG	1A	3122	1/1	0.90	0.17	35,35,35,35	0
58	MG	1A	3327	1/1	0.90	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3242	1/1	0.90	0.14	48,48,48,48	0
58	MG	2A	3411	1/1	0.90	0.22	59,59,59,59	0
58	MG	1A	3523	1/1	0.90	0.09	68,68,68,68	0
58	MG	2V	201	1/1	0.90	0.30	45,45,45,45	0
58	MG	2A	3264	1/1	0.90	0.11	54,54,54,54	0
58	MG	1A	3332	1/1	0.90	0.24	55,55,55,55	0
58	MG	2Z	301	1/1	0.90	0.15	68,68,68,68	0
58	MG	1A	4021	1/1	0.90	0.13	51,51,51,51	0
58	MG	2I	101	1/1	0.90	0.27	55,55,55,55	0
58	MG	23	101	1/1	0.90	0.15	63,63,63,63	0
58	MG	23	102	1/1	0.90	0.11	48,48,48,48	0
58	MG	25	102	1/1	0.90	0.10	43,43,43,43	0
58	MG	1a	1658	1/1	0.90	0.20	47,47,47,47	0
58	MG	2A	3125	1/1	0.90	0.18	45,45,45,45	0
58	MG	1A	3601	1/1	0.90	0.25	56,56,56,56	0
58	MG	1A	3863	1/1	0.90	0.23	37,37,37,37	0
58	MG	1a	1797	1/1	0.90	0.10	45,45,45,45	0
58	MG	2A	3427	1/1	0.90	0.24	43,43,43,43	0
58	MG	2A	3671	1/1	0.90	0.22	58,58,58,58	0
58	MG	1A	3866	1/1	0.90	0.17	52,52,52,52	0
58	MG	2A	3675	1/1	0.90	0.27	55,55,55,55	0
58	MG	1A	3458	1/1	0.90	0.25	51,51,51,51	0
58	MG	1A	3528	1/1	0.90	0.13	41,41,41,41	0
58	MG	2f	201	1/1	0.90	0.07	42,42,42,42	0
58	MG	2A	3434	1/1	0.90	0.28	53,53,53,53	0
58	MG	2a	1610	1/1	0.90	0.14	52,52,52,52	0
58	MG	2A	3680	1/1	0.90	0.12	52,52,52,52	0
58	MG	2A	3681	1/1	0.90	0.21	47,47,47,47	0
58	MG	2a	1613	1/1	0.90	0.17	62,62,62,62	0
58	MG	2A	3277	1/1	0.90	0.17	63,63,63,63	0
58	MG	1a	1805	1/1	0.90	0.14	58,58,58,58	0
58	MG	1A	3290	1/1	0.90	0.12	48,48,48,48	0
58	MG	1O	205	1/1	0.90	0.11	54,54,54,54	0
58	MG	1P	203	1/1	0.90	0.19	32,32,32,32	0
58	MG	2t	201	1/1	0.90	0.14	59,59,59,59	0
58	MG	2t	202	1/1	0.90	0.12	48,48,48,48	0
58	MG	1A	3730	1/1	0.90	0.16	59,59,59,59	0
58	MG	1A	3532	1/1	0.90	0.20	55,55,55,55	0
58	MG	2A	3449	1/1	0.90	0.15	39,39,39,39	0
58	MG	2A	3285	1/1	0.90	0.24	56,56,56,56	0
58	MG	2w	101	1/1	0.90	0.24	52,52,52,52	0
58	MG	1A	3461	1/1	0.90	0.37	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1625	1/1	0.90	0.16	61,61,61,61	0
58	MG	1R	201	1/1	0.90	0.20	31,31,31,31	0
58	MG	1A	3743	1/1	0.90	0.08	46,46,46,46	0
58	MG	1S	201	1/1	0.90	0.19	38,38,38,38	0
58	MG	1A	3291	1/1	0.90	0.12	52,52,52,52	0
58	MG	1A	3733	1/1	0.91	0.22	68,68,68,68	0
58	MG	2a	1623	1/1	0.91	0.19	55,55,55,55	0
58	MG	1A	3296	1/1	0.91	0.08	41,41,41,41	0
58	MG	1A	3199	1/1	0.91	0.10	36,36,36,36	0
58	MG	1V	207	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3742	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3241	1/1	0.91	0.12	72,72,72,72	0
58	MG	1A	3447	1/1	0.91	0.15	38,38,38,38	0
58	MG	2A	3052	1/1	0.91	0.12	46,46,46,46	0
58	MG	1Y	202	1/1	0.91	0.13	51,51,51,51	0
58	MG	1A	4054	1/1	0.91	0.10	36,36,36,36	0
58	MG	2A	3055	1/1	0.91	0.33	68,68,68,68	0
58	MG	1A	3400	1/1	0.91	0.10	35,35,35,35	0
58	MG	2A	3429	1/1	0.91	0.15	52,52,52,52	0
58	MG	1A	3896	1/1	0.91	0.10	30,30,30,30	0
58	MG	1a	1700	1/1	0.91	0.13	45,45,45,45	0
58	MG	1a	1702	1/1	0.91	0.10	51,51,51,51	0
58	MG	1A	3201	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3438	1/1	0.91	0.13	33,33,33,33	0
58	MG	2A	3254	1/1	0.91	0.12	47,47,47,47	0
58	MG	10	102	1/1	0.91	0.14	45,45,45,45	0
58	MG	1A	3525	1/1	0.91	0.11	43,43,43,43	0
58	MG	2A	3716	1/1	0.91	0.12	38,38,38,38	0
58	MG	1A	3092	1/1	0.91	0.12	54,54,54,54	0
58	MG	1A	4073	1/1	0.91	0.12	45,45,45,45	0
58	MG	1a	1710	1/1	0.91	0.19	53,53,53,53	0
58	MG	1A	3616	1/1	0.91	0.10	52,52,52,52	0
58	MG	2A	3450	1/1	0.91	0.12	58,58,58,58	0
58	MG	2A	3076	1/1	0.91	0.11	46,46,46,46	0
58	MG	1A	3907	1/1	0.91	0.09	32,32,32,32	0
58	MG	1A	3123	1/1	0.91	0.09	36,36,36,36	0
58	MG	1A	4080	1/1	0.91	0.07	32,32,32,32	0
58	MG	2A	3083	1/1	0.91	0.13	53,53,53,53	0
58	MG	1A	3620	1/1	0.91	0.10	28,28,28,28	0
58	MG	1A	3304	1/1	0.91	0.12	43,43,43,43	0
58	MG	1a	1722	1/1	0.91	0.33	55,55,55,55	0
58	MG	1A	3531	1/1	0.91	0.28	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3737	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3738	1/1	0.91	0.18	65,65,65,65	0
58	MG	1A	4084	1/1	0.91	0.15	45,45,45,45	0
58	MG	2a	1671	1/1	0.91	0.11	41,41,41,41	0
58	MG	15	104	1/1	0.91	0.15	26,26,26,26	0
58	MG	2a	1673	1/1	0.91	0.16	57,57,57,57	0
58	MG	1A	3629	1/1	0.91	0.11	46,46,46,46	0
58	MG	2a	1675	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	4086	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	3094	1/1	0.91	0.15	42,42,42,42	0
58	MG	18	103	1/1	0.91	0.09	35,35,35,35	0
58	MG	1a	1740	1/1	0.91	0.11	40,40,40,40	0
58	MG	18	105	1/1	0.91	0.16	50,50,50,50	0
58	MG	2A	3474	1/1	0.91	0.09	29,29,29,29	0
58	MG	1A	3632	1/1	0.91	0.07	23,23,23,23	0
58	MG	1A	3212	1/1	0.91	0.14	42,42,42,42	0
58	MG	19	101	1/1	0.91	0.16	52,52,52,52	0
58	MG	2A	3284	1/1	0.91	0.18	56,56,56,56	0
58	MG	1A	3634	1/1	0.91	0.07	33,33,33,33	0
58	MG	1A	3050	1/1	0.91	0.17	40,40,40,40	0
58	MG	2a	1694	1/1	0.91	0.20	67,67,67,67	0
58	MG	2A	3287	1/1	0.91	0.19	55,55,55,55	0
58	MG	1A	3097	1/1	0.91	0.08	28,28,28,28	0
58	MG	1A	3463	1/1	0.91	0.23	63,63,63,63	0
58	MG	1A	3465	1/1	0.91	0.21	66,66,66,66	0
58	MG	1A	3078	1/1	0.91	0.09	30,30,30,30	0
58	MG	1A	3265	1/1	0.91	0.23	58,58,58,58	0
58	MG	2a	1701	1/1	0.91	0.13	61,61,61,61	0
58	MG	2A	3297	1/1	0.91	0.16	63,63,63,63	0
58	MG	2A	3124	1/1	0.91	0.12	65,65,65,65	0
58	MG	2a	1705	1/1	0.91	0.26	65,65,65,65	0
58	MG	1A	3954	1/1	0.91	0.12	53,53,53,53	0
58	MG	1A	4102	1/1	0.91	0.36	55,55,55,55	0
58	MG	1A	3649	1/1	0.91	0.09	64,64,64,64	0
58	MG	2A	3502	1/1	0.91	0.11	53,53,53,53	0
58	MG	2A	3503	1/1	0.91	0.20	53,53,53,53	0
58	MG	1A	3267	1/1	0.91	0.16	45,45,45,45	0
58	MG	1A	3080	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3661	1/1	0.91	0.07	43,43,43,43	0
58	MG	1a	1620	1/1	0.91	0.09	38,38,38,38	0
58	MG	1A	3665	1/1	0.91	0.07	24,24,24,24	0
58	MG	2A	3138	1/1	0.91	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	210	1/1	0.91	0.15	52,52,52,52	0
58	MG	2A	3317	1/1	0.91	0.15	67,67,67,67	0
58	MG	2A	3517	1/1	0.91	0.15	58,58,58,58	0
58	MG	1A	3547	1/1	0.91	0.15	57,57,57,57	0
58	MG	1A	3968	1/1	0.91	0.11	33,33,33,33	0
58	MG	2A	3821	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3473	1/1	0.91	0.10	51,51,51,51	0
58	MG	2A	3147	1/1	0.91	0.23	54,54,54,54	0
58	MG	1a	1781	1/1	0.91	0.11	44,44,44,44	0
58	MG	2A	3154	1/1	0.91	0.07	54,54,54,54	0
58	MG	1A	3971	1/1	0.91	0.14	65,65,65,65	0
58	MG	1A	3361	1/1	0.91	0.19	56,56,56,56	0
58	MG	1A	3475	1/1	0.91	0.14	53,53,53,53	0
58	MG	1A	3556	1/1	0.91	0.17	40,40,40,40	0
58	MG	1a	1631	1/1	0.91	0.23	57,57,57,57	0
58	MG	2A	3843	1/1	0.91	0.14	47,47,47,47	0
58	MG	1A	3558	1/1	0.91	0.12	33,33,33,33	0
58	MG	2A	3164	1/1	0.91	0.26	58,58,58,58	0
58	MG	1a	1634	1/1	0.91	0.21	59,59,59,59	0
58	MG	1a	1798	1/1	0.91	0.09	57,57,57,57	0
58	MG	1A	3320	1/1	0.91	0.20	26,26,26,26	0
58	MG	2B	201	1/1	0.91	0.18	59,59,59,59	0
58	MG	1A	3982	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	3983	1/1	0.91	0.19	53,53,53,53	0
58	MG	2A	3558	1/1	0.91	0.11	59,59,59,59	0
58	MG	1A	3365	1/1	0.91	0.17	32,32,32,32	0
58	MG	1A	3830	1/1	0.91	0.08	34,34,34,34	0
58	MG	2A	3339	1/1	0.91	0.32	74,74,74,74	0
58	MG	1A	3420	1/1	0.91	0.21	61,61,61,61	0
58	MG	2a	1771	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3839	1/1	0.91	0.11	34,34,34,34	0
58	MG	1A	3992	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3269	1/1	0.91	0.27	49,49,49,49	0
58	MG	1A	3324	1/1	0.91	0.21	55,55,55,55	0
58	MG	2A	3578	1/1	0.91	0.11	30,30,30,30	0
58	MG	1A	4001	1/1	0.91	0.10	59,59,59,59	0
58	MG	2A	3184	1/1	0.91	0.24	73,73,73,73	0
58	MG	1A	3138	1/1	0.91	0.10	29,29,29,29	0
58	MG	1l	201	1/1	0.91	0.09	66,66,66,66	0
58	MG	2A	3588	1/1	0.91	0.21	53,53,53,53	0
58	MG	1a	1653	1/1	0.91	0.09	41,41,41,41	0
58	MG	1A	3578	1/1	0.91	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1655	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3274	1/1	0.91	0.07	41,41,41,41	0
58	MG	2E	305	1/1	0.91	0.12	35,35,35,35	0
58	MG	1A	3082	1/1	0.91	0.14	34,34,34,34	0
58	MG	1A	3491	1/1	0.91	0.13	43,43,43,43	0
58	MG	1A	3374	1/1	0.91	0.15	40,40,40,40	0
58	MG	2F	302	1/1	0.91	0.10	44,44,44,44	0
58	MG	2a	1796	1/1	0.91	0.12	57,57,57,57	0
58	MG	2A	3361	1/1	0.91	0.10	45,45,45,45	0
58	MG	1A	3710	1/1	0.91	0.09	30,30,30,30	0
58	MG	1A	3858	1/1	0.91	0.07	53,53,53,53	0
58	MG	2A	3365	1/1	0.91	0.14	66,66,66,66	0
58	MG	1G	203	1/1	0.91	0.12	61,61,61,61	0
58	MG	1A	3433	1/1	0.91	0.12	43,43,43,43	0
58	MG	1A	3053	1/1	0.91	0.10	41,41,41,41	0
58	MG	2A	3614	1/1	0.91	0.23	52,52,52,52	0
58	MG	1A	3590	1/1	0.91	0.09	48,48,48,48	0
58	MG	1N	201	1/1	0.91	0.28	47,47,47,47	0
58	MG	2T	202	1/1	0.91	0.21	65,65,65,65	0
58	MG	2A	3373	1/1	0.91	0.10	49,49,49,49	0
58	MG	2A	3205	1/1	0.91	0.30	66,66,66,66	0
58	MG	2A	3632	1/1	0.91	0.11	39,39,39,39	0
58	MG	2A	3633	1/1	0.91	0.10	46,46,46,46	0
58	MG	2Y	201	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3635	1/1	0.91	0.14	41,41,41,41	0
58	MG	2A	3375	1/1	0.91	0.17	70,70,70,70	0
58	MG	1A	4022	1/1	0.91	0.11	65,65,65,65	0
58	MG	2A	3639	1/1	0.91	0.13	41,41,41,41	0
58	MG	1A	3867	1/1	0.91	0.16	38,38,38,38	0
58	MG	25	101	1/1	0.91	0.11	46,46,46,46	0
58	MG	1O	203	1/1	0.91	0.30	57,57,57,57	0
58	MG	1A	4024	1/1	0.91	0.11	46,46,46,46	0
58	MG	1A	3285	1/1	0.91	0.11	43,43,43,43	0
58	MG	2A	3647	1/1	0.91	0.09	49,49,49,49	0
58	MG	1A	3143	1/1	0.91	0.19	51,51,51,51	0
58	MG	1P	206	1/1	0.91	0.09	46,46,46,46	0
58	MG	2A	3383	1/1	0.91	0.18	58,58,58,58	0
58	MG	2A	3213	1/1	0.91	0.26	36,36,36,36	0
58	MG	2A	3653	1/1	0.91	0.13	51,51,51,51	0
58	MG	2A	3006	1/1	0.91	0.17	58,58,58,58	0
58	MG	2A	3009	1/1	0.91	0.18	55,55,55,55	0
58	MG	2A	3011	1/1	0.91	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
58	MG	2A	3219	1/1	0.91	0.18	44,44,44,44	0
58	MG	1A	3012	1/1	0.91	0.08	26,26,26,26	0
58	MG	2A	3662	1/1	0.91	0.10	56,56,56,56	0
58	MG	1A	4032	1/1	0.91	0.09	38,38,38,38	0
58	MG	1A	3508	1/1	0.91	0.08	41,41,41,41	0
58	MG	2A	3017	1/1	0.91	0.14	38,38,38,38	0
58	MG	1A	3514	1/1	0.91	0.27	28,28,28,28	0
58	MG	1R	203	1/1	0.91	0.08	33,33,33,33	0
58	MG	1A	3026	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	4037	1/1	0.91	0.15	40,40,40,40	0
58	MG	2x	101	1/1	0.91	0.20	44,44,44,44	0
58	MG	2A	3034	1/1	0.91	0.16	52,52,52,52	0
58	MG	1A	3246	1/1	0.91	0.13	48,48,48,48	0
58	MG	1T	202	1/1	0.91	0.15	49,49,49,49	0
58	MG	1A	3530	1/1	0.92	0.24	48,48,48,48	0
58	MG	1A	4002	1/1	0.92	0.11	57,57,57,57	0
58	MG	1A	4003	1/1	0.92	0.07	62,62,62,62	0
58	MG	1B	238	1/1	0.92	0.07	29,29,29,29	0
58	MG	1a	1787	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3713	1/1	0.92	0.13	40,40,40,40	0
58	MG	2a	1632	1/1	0.92	0.20	51,51,51,51	0
58	MG	1D	304	1/1	0.92	0.10	43,43,43,43	0
58	MG	1D	306	1/1	0.92	0.11	18,18,18,18	0
58	MG	1A	3193	1/1	0.92	0.22	35,35,35,35	0
58	MG	1A	3715	1/1	0.92	0.11	46,46,46,46	0
58	MG	1A	3083	1/1	0.92	0.17	41,41,41,41	0
58	MG	1E	307	1/1	0.92	0.11	50,50,50,50	0
58	MG	2A	3299	1/1	0.92	0.13	58,58,58,58	0
58	MG	2A	3149	1/1	0.92	0.11	43,43,43,43	0
58	MG	1a	1801	1/1	0.92	0.31	66,66,66,66	0
58	MG	2A	3304	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3306	1/1	0.92	0.08	43,43,43,43	0
58	MG	2A	3483	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3048	1/1	0.92	0.10	36,36,36,36	0
58	MG	2A	3739	1/1	0.92	0.09	43,43,43,43	0
58	MG	1E	309	1/1	0.92	0.12	32,32,32,32	0
58	MG	2A	3741	1/1	0.92	0.33	48,48,48,48	0
58	MG	2A	3489	1/1	0.92	0.27	53,53,53,53	0
58	MG	1A	4013	1/1	0.92	0.16	53,53,53,53	0
58	MG	1A	3718	1/1	0.92	0.10	65,65,65,65	0
58	MG	2A	3159	1/1	0.92	0.17	55,55,55,55	0
58	MG	1A	4016	1/1	0.92	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3613	1/1	0.92	0.11	25,25,25,25	0
58	MG	1F	305	1/1	0.92	0.08	30,30,30,30	0
58	MG	2A	3163	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3019	1/1	0.92	0.12	34,34,34,34	0
58	MG	1F	307	1/1	0.92	0.08	25,25,25,25	0
58	MG	1F	308	1/1	0.92	0.12	31,31,31,31	0
58	MG	1A	3345	1/1	0.92	0.18	30,30,30,30	0
58	MG	1A	3434	1/1	0.92	0.14	31,31,31,31	0
58	MG	2A	3773	1/1	0.92	0.10	60,60,60,60	0
58	MG	2A	3169	1/1	0.92	0.23	73,73,73,73	0
58	MG	1A	3310	1/1	0.92	0.08	45,45,45,45	0
58	MG	2A	3509	1/1	0.92	0.23	66,66,66,66	0
58	MG	2A	3172	1/1	0.92	0.17	47,47,47,47	0
58	MG	1A	3348	1/1	0.92	0.15	29,29,29,29	0
58	MG	1A	3484	1/1	0.92	0.11	39,39,39,39	0
58	MG	2A	3176	1/1	0.92	0.15	64,64,64,64	0
58	MG	1A	3625	1/1	0.92	0.10	59,59,59,59	0
58	MG	1A	3879	1/1	0.92	0.11	30,30,30,30	0
58	MG	1A	3485	1/1	0.92	0.14	35,35,35,35	0
58	MG	1A	3271	1/1	0.92	0.15	38,38,38,38	0
58	MG	1A	3546	1/1	0.92	0.14	59,59,59,59	0
58	MG	1A	3016	1/1	0.92	0.16	52,52,52,52	0
58	MG	1A	3175	1/1	0.92	0.08	26,26,26,26	0
58	MG	1A	3440	1/1	0.92	0.13	46,46,46,46	0
58	MG	2A	3792	1/1	0.92	0.13	46,46,46,46	0
58	MG	2a	1689	1/1	0.92	0.33	67,67,67,67	0
58	MG	1A	3277	1/1	0.92	0.14	37,37,37,37	0
58	MG	1A	3753	1/1	0.92	0.13	41,41,41,41	0
58	MG	1A	3898	1/1	0.92	0.04	26,26,26,26	0
58	MG	2A	3800	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	3555	1/1	0.92	0.13	36,36,36,36	0
58	MG	2A	3802	1/1	0.92	0.13	39,39,39,39	0
58	MG	2A	3191	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3760	1/1	0.92	0.10	53,53,53,53	0
58	MG	1A	3176	1/1	0.92	0.10	19,19,19,19	0
58	MG	2A	3810	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	4050	1/1	0.92	0.09	12,12,12,12	0
58	MG	2A	3814	1/1	0.92	0.12	56,56,56,56	0
58	MG	2a	1706	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3548	1/1	0.92	0.09	32,32,32,32	0
58	MG	2A	3002	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3904	1/1	0.92	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3905	1/1	0.92	0.08	37,37,37,37	0
58	MG	2a	1711	1/1	0.92	0.31	60,60,60,60	0
58	MG	2A	3824	1/1	0.92	0.12	73,73,73,73	0
58	MG	1A	3444	1/1	0.92	0.16	41,41,41,41	0
58	MG	1A	3643	1/1	0.92	0.12	46,46,46,46	0
58	MG	2A	3828	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3007	1/1	0.92	0.14	47,47,47,47	0
58	MG	2a	1717	1/1	0.92	0.30	58,58,58,58	0
58	MG	2a	1718	1/1	0.92	0.10	64,64,64,64	0
58	MG	2A	3834	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3316	1/1	0.92	0.09	35,35,35,35	0
58	MG	2A	3202	1/1	0.92	0.11	55,55,55,55	0
58	MG	1A	3909	1/1	0.92	0.17	24,24,24,24	0
58	MG	2A	3572	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3204	1/1	0.92	0.14	49,49,49,49	0
58	MG	1A	3498	1/1	0.92	0.08	50,50,50,50	0
58	MG	1A	4072	1/1	0.92	0.09	44,44,44,44	0
58	MG	1A	3501	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3921	1/1	0.92	0.16	36,36,36,36	0
58	MG	1A	3177	1/1	0.92	0.11	35,35,35,35	0
58	MG	2a	1732	1/1	0.92	0.28	65,65,65,65	0
58	MG	2a	1733	1/1	0.92	0.24	55,55,55,55	0
58	MG	1A	3926	1/1	0.92	0.10	35,35,35,35	0
58	MG	1A	3002	1/1	0.92	0.12	55,55,55,55	0
58	MG	2a	1738	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3656	1/1	0.92	0.15	48,48,48,48	0
58	MG	10	105	1/1	0.92	0.22	58,58,58,58	0
58	MG	1a	1698	1/1	0.92	0.17	52,52,52,52	0
58	MG	1A	3935	1/1	0.92	0.14	60,60,60,60	0
58	MG	2A	3597	1/1	0.92	0.18	67,67,67,67	0
58	MG	2A	3217	1/1	0.92	0.17	36,36,36,36	0
58	MG	1A	3657	1/1	0.92	0.09	28,28,28,28	0
58	MG	2B	209	1/1	0.92	0.15	58,58,58,58	0
58	MG	1A	3660	1/1	0.92	0.17	45,45,45,45	0
58	MG	1a	1703	1/1	0.92	0.21	49,49,49,49	0
58	MG	2A	3044	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3786	1/1	0.92	0.14	48,48,48,48	0
58	MG	1A	3569	1/1	0.92	0.13	30,30,30,30	0
58	MG	2a	1760	1/1	0.92	0.09	74,74,74,74	0
58	MG	2A	3606	1/1	0.92	0.12	56,56,56,56	0
58	MG	2A	3226	1/1	0.92	0.15	49,49,49,49	0
58	MG	1A	3663	1/1	0.92	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3505	1/1	0.92	0.09	46,46,46,46	0
58	MG	1A	3796	1/1	0.92	0.18	60,60,60,60	0
58	MG	2a	1769	1/1	0.92	0.28	68,68,68,68	0
58	MG	1A	3179	1/1	0.92	0.20	53,53,53,53	0
58	MG	1A	3148	1/1	0.92	0.18	42,42,42,42	0
58	MG	2A	3392	1/1	0.92	0.24	52,52,52,52	0
58	MG	1A	3803	1/1	0.92	0.09	39,39,39,39	0
58	MG	15	103	1/1	0.92	0.10	33,33,33,33	0
58	MG	2E	306	1/1	0.92	0.14	51,51,51,51	0
58	MG	2a	1777	1/1	0.92	0.10	53,53,53,53	0
58	MG	1a	1715	1/1	0.92	0.16	34,34,34,34	0
58	MG	1a	1716	1/1	0.92	0.10	29,29,29,29	0
58	MG	2E	310	1/1	0.92	0.19	41,41,41,41	0
58	MG	2a	1781	1/1	0.92	0.24	72,72,72,72	0
58	MG	1A	3512	1/1	0.92	0.13	27,27,27,27	0
58	MG	2A	3402	1/1	0.92	0.11	36,36,36,36	0
58	MG	15	105	1/1	0.92	0.10	30,30,30,30	0
58	MG	2F	304	1/1	0.92	0.14	42,42,42,42	0
58	MG	1a	1719	1/1	0.92	0.36	54,54,54,54	0
58	MG	15	106	1/1	0.92	0.12	50,50,50,50	0
58	MG	2A	3068	1/1	0.92	0.18	51,51,51,51	0
58	MG	2O	201	1/1	0.92	0.18	59,59,59,59	0
58	MG	2A	3642	1/1	0.92	0.20	65,65,65,65	0
58	MG	1A	3672	1/1	0.92	0.09	34,34,34,34	0
58	MG	2Q	203	1/1	0.92	0.23	62,62,62,62	0
58	MG	2R	201	1/1	0.92	0.12	55,55,55,55	0
58	MG	2a	1798	1/1	0.92	0.13	53,53,53,53	0
58	MG	1A	3806	1/1	0.92	0.07	45,45,45,45	0
58	MG	17	104	1/1	0.92	0.17	49,49,49,49	0
58	MG	1A	3959	1/1	0.92	0.12	55,55,55,55	0
58	MG	18	102	1/1	0.92	0.21	36,36,36,36	0
58	MG	1A	3960	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3250	1/1	0.92	0.21	57,57,57,57	0
58	MG	2T	204	1/1	0.92	0.12	51,51,51,51	0
58	MG	1A	3293	1/1	0.92	0.13	32,32,32,32	0
58	MG	2A	3416	1/1	0.92	0.13	56,56,56,56	0
58	MG	1a	1736	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3682	1/1	0.92	0.09	27,27,27,27	0
58	MG	1A	3684	1/1	0.92	0.13	53,53,53,53	0
58	MG	2A	3420	1/1	0.92	0.22	49,49,49,49	0
58	MG	2A	3421	1/1	0.92	0.18	53,53,53,53	0
58	MG	2A	3664	1/1	0.92	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3422	1/1	0.92	0.19	63,63,63,63	0
58	MG	1B	203	1/1	0.92	0.10	40,40,40,40	0
58	MG	2A	3424	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3217	1/1	0.92	0.15	40,40,40,40	0
58	MG	1B	205	1/1	0.92	0.09	49,49,49,49	0
58	MG	28	101	1/1	0.92	0.13	58,58,58,58	0
58	MG	1A	3816	1/1	0.92	0.12	41,41,41,41	0
58	MG	28	104	1/1	0.92	0.21	55,55,55,55	0
58	MG	1A	3457	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3364	1/1	0.92	0.10	41,41,41,41	0
58	MG	1A	3259	1/1	0.92	0.10	38,38,38,38	0
58	MG	1A	3521	1/1	0.92	0.21	68,68,68,68	0
58	MG	2A	3435	1/1	0.92	0.14	55,55,55,55	0
58	MG	1A	3073	1/1	0.92	0.07	12,12,12,12	0
58	MG	1A	3334	1/1	0.92	0.23	55,55,55,55	0
58	MG	2A	3105	1/1	0.92	0.17	43,43,43,43	0
58	MG	1A	3153	1/1	0.92	0.11	39,39,39,39	0
58	MG	1A	3095	1/1	0.92	0.11	52,52,52,52	0
58	MG	1B	220	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3109	1/1	0.92	0.15	49,49,49,49	0
58	MG	1A	3338	1/1	0.92	0.18	53,53,53,53	0
58	MG	1A	3599	1/1	0.92	0.09	32,32,32,32	0
58	MG	1A	3706	1/1	0.92	0.10	32,32,32,32	0
58	MG	1A	3842	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3276	1/1	0.92	0.17	66,66,66,66	0
58	MG	2A	3698	1/1	0.92	0.14	61,61,61,61	0
58	MG	1B	226	1/1	0.92	0.12	62,62,62,62	0
58	MG	1A	3162	1/1	0.92	0.11	48,48,48,48	0
58	MG	1a	1772	1/1	0.92	0.14	57,57,57,57	0
58	MG	1A	3428	1/1	0.92	0.11	45,45,45,45	0
58	MG	1A	3602	1/1	0.92	0.33	55,55,55,55	0
58	MG	2x	103	1/1	0.92	0.08	53,53,53,53	0
58	MG	2A	3710	1/1	0.92	0.10	40,40,40,40	0
58	MG	1B	233	1/1	0.92	0.18	59,59,59,59	0
58	MG	2A	3303	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	3223	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3148	1/1	0.93	0.12	36,36,36,36	0
58	MG	1a	1791	1/1	0.93	0.09	59,59,59,59	0
58	MG	2A	3485	1/1	0.93	0.19	53,53,53,53	0
58	MG	1A	3732	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3627	1/1	0.93	0.11	29,29,29,29	0
58	MG	1A	3063	1/1	0.93	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1E	301	1/1	0.93	0.12	46,46,46,46	0
58	MG	2A	3312	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3739	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3337	1/1	0.93	0.22	61,61,61,61	0
58	MG	2A	3496	1/1	0.93	0.27	60,60,60,60	0
58	MG	1A	3229	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3339	1/1	0.93	0.29	65,65,65,65	0
58	MG	1A	3230	1/1	0.93	0.17	44,44,44,44	0
58	MG	1A	3880	1/1	0.93	0.14	38,38,38,38	0
58	MG	1A	3288	1/1	0.93	0.08	38,38,38,38	0
58	MG	1A	3289	1/1	0.93	0.15	54,54,54,54	0
58	MG	1a	1648	1/1	0.93	0.16	58,58,58,58	0
58	MG	1a	1650	1/1	0.93	0.11	38,38,38,38	0
58	MG	1A	3064	1/1	0.93	0.20	39,39,39,39	0
58	MG	2a	1656	1/1	0.93	0.08	62,62,62,62	0
58	MG	1A	3105	1/1	0.93	0.14	43,43,43,43	0
58	MG	1e	202	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3011	1/1	0.93	0.10	42,42,42,42	0
58	MG	1A	3411	1/1	0.93	0.10	43,43,43,43	0
58	MG	1F	309	1/1	0.93	0.09	37,37,37,37	0
58	MG	2A	3515	1/1	0.93	0.12	39,39,39,39	0
58	MG	1F	311	1/1	0.93	0.15	29,29,29,29	0
58	MG	1n	102	1/1	0.93	0.11	43,43,43,43	0
58	MG	1G	201	1/1	0.93	0.10	40,40,40,40	0
58	MG	1A	3294	1/1	0.93	0.24	47,47,47,47	0
58	MG	1a	1661	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3894	1/1	0.93	0.06	42,42,42,42	0
58	MG	1A	4030	1/1	0.93	0.10	46,46,46,46	0
58	MG	1w	107	1/1	0.93	0.10	35,35,35,35	0
58	MG	2A	3185	1/1	0.93	0.25	49,49,49,49	0
58	MG	1A	3895	1/1	0.93	0.10	23,23,23,23	0
58	MG	2A	3789	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3144	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	3554	1/1	0.93	0.18	29,29,29,29	0
58	MG	1N	203	1/1	0.93	0.11	47,47,47,47	0
58	MG	2A	3539	1/1	0.93	0.07	38,38,38,38	0
58	MG	2A	3794	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	3768	1/1	0.93	0.07	27,27,27,27	0
58	MG	1A	3183	1/1	0.93	0.10	39,39,39,39	0
58	MG	2A	3543	1/1	0.93	0.07	38,38,38,38	0
58	MG	1A	3241	1/1	0.93	0.10	40,40,40,40	0
58	MG	2a	1693	1/1	0.93	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3418	1/1	0.93	0.21	52,52,52,52	0
58	MG	1A	4039	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3659	1/1	0.93	0.13	38,38,38,38	0
58	MG	2A	3805	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3552	1/1	0.93	0.11	39,39,39,39	0
58	MG	2A	3553	1/1	0.93	0.11	40,40,40,40	0
58	MG	1A	3110	1/1	0.93	0.18	27,27,27,27	0
58	MG	1Q	204	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	4043	1/1	0.93	0.12	42,42,42,42	0
58	MG	2A	3817	1/1	0.93	0.17	45,45,45,45	0
58	MG	1A	3186	1/1	0.93	0.12	40,40,40,40	0
58	MG	1A	4046	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3568	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	4047	1/1	0.93	0.06	25,25,25,25	0
58	MG	2A	3360	1/1	0.93	0.24	55,55,55,55	0
58	MG	1A	3778	1/1	0.93	0.07	28,28,28,28	0
58	MG	1A	3421	1/1	0.93	0.10	47,47,47,47	0
58	MG	2A	3832	1/1	0.93	0.12	54,54,54,54	0
58	MG	1A	3910	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	4053	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3664	1/1	0.93	0.10	29,29,29,29	0
58	MG	1A	3913	1/1	0.93	0.09	45,45,45,45	0
58	MG	1U	203	1/1	0.93	0.31	40,40,40,40	0
58	MG	2A	3582	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3840	1/1	0.93	0.10	54,54,54,54	0
58	MG	2A	3583	1/1	0.93	0.15	46,46,46,46	0
58	MG	1A	3916	1/1	0.93	0.12	32,32,32,32	0
58	MG	1A	3187	1/1	0.93	0.26	38,38,38,38	0
58	MG	2A	3022	1/1	0.93	0.12	50,50,50,50	0
58	MG	2A	3592	1/1	0.93	0.09	45,45,45,45	0
58	MG	1V	206	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3028	1/1	0.93	0.11	38,38,38,38	0
58	MG	2a	1727	1/1	0.93	0.32	47,47,47,47	0
58	MG	2a	1728	1/1	0.93	0.33	69,69,69,69	0
58	MG	1A	3788	1/1	0.93	0.08	59,59,59,59	0
58	MG	2A	3033	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	4065	1/1	0.93	0.20	58,58,58,58	0
58	MG	1W	202	1/1	0.93	0.10	41,41,41,41	0
58	MG	1A	3922	1/1	0.93	0.13	48,48,48,48	0
58	MG	2a	1734	1/1	0.93	0.39	67,67,67,67	0
58	MG	2A	3039	1/1	0.93	0.27	55,55,55,55	0
58	MG	1A	3355	1/1	0.93	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1737	1/1	0.93	0.38	62,62,62,62	0
58	MG	1A	3925	1/1	0.93	0.07	35,35,35,35	0
58	MG	1A	3117	1/1	0.93	0.23	39,39,39,39	0
58	MG	1A	3927	1/1	0.93	0.09	44,44,44,44	0
58	MG	2a	1741	1/1	0.93	0.20	63,63,63,63	0
58	MG	2A	3227	1/1	0.93	0.16	39,39,39,39	0
58	MG	1A	3492	1/1	0.93	0.10	42,42,42,42	0
58	MG	2a	1746	1/1	0.93	0.11	66,66,66,66	0
58	MG	2a	1747	1/1	0.93	0.15	63,63,63,63	0
58	MG	1A	3014	1/1	0.93	0.08	26,26,26,26	0
58	MG	1A	3932	1/1	0.93	0.07	33,33,33,33	0
58	MG	1A	3797	1/1	0.93	0.14	46,46,46,46	0
58	MG	2B	217	1/1	0.93	0.11	52,52,52,52	0
58	MG	1a	1707	1/1	0.93	0.12	41,41,41,41	0
58	MG	1A	3937	1/1	0.93	0.07	32,32,32,32	0
58	MG	2A	3398	1/1	0.93	0.20	54,54,54,54	0
58	MG	2a	1756	1/1	0.93	0.23	58,58,58,58	0
58	MG	2D	303	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3620	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3622	1/1	0.93	0.12	56,56,56,56	0
58	MG	2a	1762	1/1	0.93	0.09	67,67,67,67	0
58	MG	10	109	1/1	0.93	0.09	53,53,53,53	0
58	MG	2A	3624	1/1	0.93	0.16	58,58,58,58	0
58	MG	2A	3625	1/1	0.93	0.08	38,38,38,38	0
58	MG	2A	3627	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	3939	1/1	0.93	0.17	52,52,52,52	0
58	MG	1A	3674	1/1	0.93	0.12	32,32,32,32	0
58	MG	2A	3404	1/1	0.93	0.28	63,63,63,63	0
58	MG	1A	3156	1/1	0.93	0.23	24,24,24,24	0
58	MG	1A	3677	1/1	0.93	0.09	23,23,23,23	0
58	MG	1A	4088	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3042	1/1	0.93	0.17	27,27,27,27	0
58	MG	13	103	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	3253	1/1	0.93	0.14	48,48,48,48	0
58	MG	1A	3029	1/1	0.93	0.12	30,30,30,30	0
58	MG	1A	3075	1/1	0.93	0.07	19,19,19,19	0
58	MG	1A	3951	1/1	0.93	0.07	54,54,54,54	0
58	MG	2O	202	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3808	1/1	0.93	0.07	21,21,21,21	0
58	MG	1A	3690	1/1	0.93	0.06	27,27,27,27	0
58	MG	1A	3503	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3257	1/1	0.93	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3080	1/1	0.93	0.12	45,45,45,45	0
58	MG	1A	3815	1/1	0.93	0.08	34,34,34,34	0
58	MG	1A	3164	1/1	0.93	0.13	34,34,34,34	0
58	MG	2A	3656	1/1	0.93	0.14	58,58,58,58	0
58	MG	1A	3202	1/1	0.93	0.14	20,20,20,20	0
58	MG	18	101	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3089	1/1	0.93	0.12	40,40,40,40	0
58	MG	2U	201	1/1	0.93	0.18	44,44,44,44	0
58	MG	2a	1797	1/1	0.93	0.15	47,47,47,47	0
58	MG	2A	3090	1/1	0.93	0.11	42,42,42,42	0
58	MG	1A	3059	1/1	0.93	0.11	42,42,42,42	0
58	MG	1A	3510	1/1	0.93	0.17	54,54,54,54	0
58	MG	2a	1801	1/1	0.93	0.17	59,59,59,59	0
58	MG	1A	3318	1/1	0.93	0.12	52,52,52,52	0
58	MG	1A	3371	1/1	0.93	0.16	47,47,47,47	0
58	MG	1a	1744	1/1	0.93	0.12	58,58,58,58	0
58	MG	1A	3967	1/1	0.93	0.11	25,25,25,25	0
58	MG	1B	207	1/1	0.93	0.08	46,46,46,46	0
58	MG	1A	3516	1/1	0.93	0.10	44,44,44,44	0
58	MG	23	103	1/1	0.93	0.07	43,43,43,43	0
58	MG	1a	1748	1/1	0.93	0.19	36,36,36,36	0
58	MG	2A	3437	1/1	0.93	0.11	53,53,53,53	0
58	MG	1B	209	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3679	1/1	0.93	0.11	52,52,52,52	0
58	MG	1A	3205	1/1	0.93	0.10	31,31,31,31	0
58	MG	1a	1753	1/1	0.93	0.08	49,49,49,49	0
58	MG	28	103	1/1	0.93	0.20	60,60,60,60	0
58	MG	2A	3682	1/1	0.93	0.17	67,67,67,67	0
58	MG	1A	3321	1/1	0.93	0.12	50,50,50,50	0
58	MG	1A	3443	1/1	0.93	0.11	31,31,31,31	0
58	MG	1A	3077	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	3049	1/1	0.93	0.06	19,19,19,19	0
58	MG	1A	3211	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3170	1/1	0.93	0.08	39,39,39,39	0
58	MG	1A	3979	1/1	0.93	0.07	59,59,59,59	0
58	MG	2f	202	1/1	0.93	0.22	66,66,66,66	0
58	MG	1a	1765	1/1	0.93	0.09	45,45,45,45	0
58	MG	1a	1767	1/1	0.93	0.10	54,54,54,54	0
58	MG	2j	202	1/1	0.93	0.12	61,61,61,61	0
58	MG	2A	3121	1/1	0.93	0.15	44,44,44,44	0
58	MG	2l	201	1/1	0.93	0.17	66,66,66,66	0
58	MG	2A	3696	1/1	0.93	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3062	1/1	0.93	0.07	41,41,41,41	0
58	MG	1A	3451	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3330	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3131	1/1	0.93	0.15	44,44,44,44	0
58	MG	1A	3220	1/1	0.93	0.10	41,41,41,41	0
58	MG	2A	3288	1/1	0.93	0.13	52,52,52,52	0
58	MG	1a	1774	1/1	0.93	0.10	56,56,56,56	0
58	MG	2A	3290	1/1	0.93	0.11	47,47,47,47	0
58	MG	1A	3101	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3856	1/1	0.93	0.10	20,20,20,20	0
58	MG	1A	3857	1/1	0.93	0.12	44,44,44,44	0
58	MG	2A	3295	1/1	0.93	0.12	46,46,46,46	0
58	MG	1A	3621	1/1	0.93	0.08	27,27,27,27	0
58	MG	1A	3997	1/1	0.93	0.07	10,10,10,10	0
58	MG	1A	3399	1/1	0.93	0.11	46,46,46,46	0
58	MG	1A	3459	1/1	0.93	0.15	56,56,56,56	0
58	MG	1A	3865	1/1	0.93	0.09	47,47,47,47	0
58	MG	2A	3723	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	4004	1/1	0.93	0.06	31,31,31,31	0
58	MG	2A	3479	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3302	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	3115	1/1	0.94	0.08	40,40,40,40	0
58	MG	1T	201	1/1	0.94	0.18	55,55,55,55	0
58	MG	1A	3003	1/1	0.94	0.12	23,23,23,23	0
58	MG	1A	3844	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3745	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3746	1/1	0.94	0.09	59,59,59,59	0
58	MG	1A	3507	1/1	0.94	0.08	22,22,22,22	0
58	MG	2A	3180	1/1	0.94	0.30	67,67,67,67	0
58	MG	1U	204	1/1	0.94	0.11	44,44,44,44	0
58	MG	1A	3847	1/1	0.94	0.08	30,30,30,30	0
58	MG	2A	3753	1/1	0.94	0.13	41,41,41,41	0
58	MG	1U	209	1/1	0.94	0.16	32,32,32,32	0
58	MG	2A	3756	1/1	0.94	0.08	60,60,60,60	0
58	MG	2A	3520	1/1	0.94	0.12	39,39,39,39	0
58	MG	1A	3008	1/1	0.94	0.07	20,20,20,20	0
58	MG	2A	3760	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3849	1/1	0.94	0.11	57,57,57,57	0
58	MG	1x	112	1/1	0.94	0.16	58,58,58,58	0
58	MG	2A	3765	1/1	0.94	0.06	45,45,45,45	0
58	MG	2A	3768	1/1	0.94	0.10	63,63,63,63	0
58	MG	2a	1657	1/1	0.94	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3769	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3850	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3031	1/1	0.94	0.10	25,25,25,25	0
58	MG	1A	3511	1/1	0.94	0.13	28,28,28,28	0
58	MG	2a	1662	1/1	0.94	0.31	54,54,54,54	0
58	MG	1X	103	1/1	0.94	0.09	35,35,35,35	0
58	MG	2a	1664	1/1	0.94	0.07	47,47,47,47	0
58	MG	1X	104	1/1	0.94	0.07	46,46,46,46	0
58	MG	2A	3534	1/1	0.94	0.15	50,50,50,50	0
58	MG	2a	1668	1/1	0.94	0.11	61,61,61,61	0
58	MG	1A	3377	1/1	0.94	0.11	50,50,50,50	0
58	MG	2A	3347	1/1	0.94	0.23	65,65,65,65	0
58	MG	2A	3537	1/1	0.94	0.07	38,38,38,38	0
58	MG	1A	3574	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3973	1/1	0.94	0.07	44,44,44,44	0
58	MG	1Y	204	1/1	0.94	0.25	39,39,39,39	0
58	MG	1A	3741	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3544	1/1	0.94	0.11	48,48,48,48	0
58	MG	1A	3576	1/1	0.94	0.16	49,49,49,49	0
58	MG	1A	3577	1/1	0.94	0.11	37,37,37,37	0
58	MG	2A	3354	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	3066	1/1	0.94	0.16	47,47,47,47	0
58	MG	1a	1701	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3579	1/1	0.94	0.13	34,34,34,34	0
58	MG	1A	3864	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3556	1/1	0.94	0.10	31,31,31,31	0
58	MG	2A	3798	1/1	0.94	0.10	47,47,47,47	0
58	MG	2A	3557	1/1	0.94	0.17	52,52,52,52	0
58	MG	2A	3026	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	3464	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3563	1/1	0.94	0.09	44,44,44,44	0
58	MG	1A	3749	1/1	0.94	0.09	22,22,22,22	0
58	MG	1l	101	1/1	0.94	0.21	40,40,40,40	0
58	MG	1A	3379	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3381	1/1	0.94	0.15	36,36,36,36	0
58	MG	1A	3150	1/1	0.94	0.12	27,27,27,27	0
58	MG	2A	3811	1/1	0.94	0.11	65,65,65,65	0
58	MG	2A	3812	1/1	0.94	0.09	54,54,54,54	0
58	MG	1A	3757	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3991	1/1	0.94	0.09	48,48,48,48	0
58	MG	1A	3662	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3470	1/1	0.94	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3995	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3579	1/1	0.94	0.17	56,56,56,56	0
58	MG	2A	3215	1/1	0.94	0.10	53,53,53,53	0
58	MG	2A	3043	1/1	0.94	0.27	63,63,63,63	0
58	MG	2A	3825	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3586	1/1	0.94	0.08	44,44,44,44	0
58	MG	2A	3045	1/1	0.94	0.11	29,29,29,29	0
58	MG	2A	3046	1/1	0.94	0.10	38,38,38,38	0
58	MG	2A	3829	1/1	0.94	0.09	37,37,37,37	0
58	MG	1A	3875	1/1	0.94	0.28	35,35,35,35	0
58	MG	1A	3999	1/1	0.94	0.11	26,26,26,26	0
58	MG	2A	3591	1/1	0.94	0.11	63,63,63,63	0
58	MG	2A	3835	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3152	1/1	0.94	0.36	42,42,42,42	0
58	MG	2A	3051	1/1	0.94	0.20	63,63,63,63	0
58	MG	1A	3666	1/1	0.94	0.05	22,22,22,22	0
58	MG	2A	3595	1/1	0.94	0.10	53,53,53,53	0
58	MG	1a	1721	1/1	0.94	0.29	49,49,49,49	0
58	MG	2A	3841	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3387	1/1	0.94	0.12	64,64,64,64	0
58	MG	1A	3589	1/1	0.94	0.06	29,29,29,29	0
58	MG	1A	3067	1/1	0.94	0.06	26,26,26,26	0
58	MG	2A	3845	1/1	0.94	0.11	63,63,63,63	0
58	MG	2A	3390	1/1	0.94	0.17	43,43,43,43	0
58	MG	1a	1726	1/1	0.94	0.11	54,54,54,54	0
58	MG	1A	3022	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3849	1/1	0.94	0.18	57,57,57,57	0
58	MG	1A	3389	1/1	0.94	0.08	31,31,31,31	0
58	MG	1A	3390	1/1	0.94	0.09	49,49,49,49	0
58	MG	1a	1733	1/1	0.94	0.08	57,57,57,57	0
58	MG	1A	3216	1/1	0.94	0.11	45,45,45,45	0
58	MG	1A	3393	1/1	0.94	0.18	63,63,63,63	0
58	MG	1A	3892	1/1	0.94	0.08	28,28,28,28	0
58	MG	2A	3067	1/1	0.94	0.11	51,51,51,51	0
58	MG	18	104	1/1	0.94	0.16	41,41,41,41	0
58	MG	1A	3780	1/1	0.94	0.07	57,57,57,57	0
58	MG	1A	3679	1/1	0.94	0.05	23,23,23,23	0
58	MG	2A	3073	1/1	0.94	0.10	38,38,38,38	0
58	MG	2A	3619	1/1	0.94	0.07	39,39,39,39	0
58	MG	1A	3783	1/1	0.94	0.06	24,24,24,24	0
58	MG	2B	213	1/1	0.94	0.27	58,58,58,58	0
58	MG	1A	3680	1/1	0.94	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3394	1/1	0.94	0.09	45,45,45,45	0
58	MG	2A	3078	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3481	1/1	0.94	0.17	36,36,36,36	0
58	MG	1A	3286	1/1	0.94	0.12	33,33,33,33	0
58	MG	2A	3081	1/1	0.94	0.10	50,50,50,50	0
58	MG	1a	1604	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3634	1/1	0.94	0.12	35,35,35,35	0
58	MG	1A	3483	1/1	0.94	0.14	52,52,52,52	0
58	MG	2A	3085	1/1	0.94	0.10	51,51,51,51	0
58	MG	1D	302	1/1	0.94	0.14	46,46,46,46	0
58	MG	2A	3638	1/1	0.94	0.15	40,40,40,40	0
58	MG	2A	3256	1/1	0.94	0.07	42,42,42,42	0
58	MG	1A	3533	1/1	0.94	0.17	43,43,43,43	0
58	MG	1A	3126	1/1	0.94	0.08	25,25,25,25	0
58	MG	1A	3694	1/1	0.94	0.06	33,33,33,33	0
58	MG	1A	3798	1/1	0.94	0.07	32,32,32,32	0
58	MG	1D	310	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3425	1/1	0.94	0.17	47,47,47,47	0
58	MG	1D	312	1/1	0.94	0.17	32,32,32,32	0
58	MG	1A	3604	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3605	1/1	0.94	0.26	47,47,47,47	0
58	MG	2A	3265	1/1	0.94	0.10	54,54,54,54	0
58	MG	1E	304	1/1	0.94	0.11	33,33,33,33	0
58	MG	1A	3697	1/1	0.94	0.06	27,27,27,27	0
58	MG	1A	3159	1/1	0.94	0.10	31,31,31,31	0
58	MG	2A	3101	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3254	1/1	0.94	0.14	19,19,19,19	0
58	MG	2Q	201	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3056	1/1	0.94	0.08	30,30,30,30	0
58	MG	1A	3611	1/1	0.94	0.11	24,24,24,24	0
58	MG	2A	3661	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3540	1/1	0.94	0.09	47,47,47,47	0
58	MG	2a	1789	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3923	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	4040	1/1	0.94	0.12	30,30,30,30	0
58	MG	2a	1792	1/1	0.94	0.16	63,63,63,63	0
58	MG	1A	3704	1/1	0.94	0.07	21,21,21,21	0
58	MG	1A	3810	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3103	1/1	0.94	0.11	35,35,35,35	0
58	MG	1A	3326	1/1	0.94	0.11	58,58,58,58	0
58	MG	1a	1780	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3292	1/1	0.94	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1F	310	1/1	0.94	0.16	54,54,54,54	0
58	MG	2A	3120	1/1	0.94	0.28	53,53,53,53	0
58	MG	1A	3225	1/1	0.94	0.08	44,44,44,44	0
58	MG	1F	312	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	4048	1/1	0.94	0.08	54,54,54,54	0
58	MG	1A	3045	1/1	0.94	0.08	34,34,34,34	0
58	MG	1A	3260	1/1	0.94	0.15	51,51,51,51	0
58	MG	1A	3261	1/1	0.94	0.12	48,48,48,48	0
58	MG	1a	1644	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3464	1/1	0.94	0.09	37,37,37,37	0
58	MG	1G	205	1/1	0.94	0.17	61,61,61,61	0
58	MG	2A	3292	1/1	0.94	0.10	57,57,57,57	0
58	MG	1A	4052	1/1	0.94	0.07	47,47,47,47	0
58	MG	2a	1812	1/1	0.94	0.13	57,57,57,57	0
58	MG	2A	3691	1/1	0.94	0.09	62,62,62,62	0
58	MG	1a	1799	1/1	0.94	0.12	46,46,46,46	0
58	MG	1A	3820	1/1	0.94	0.09	24,24,24,24	0
58	MG	1A	3624	1/1	0.94	0.07	26,26,26,26	0
58	MG	29	101	1/1	0.94	0.10	61,61,61,61	0
58	MG	1N	202	1/1	0.94	0.10	46,46,46,46	0
58	MG	2A	3473	1/1	0.94	0.06	34,34,34,34	0
58	MG	1A	4055	1/1	0.94	0.13	49,49,49,49	0
58	MG	1A	3941	1/1	0.94	0.09	49,49,49,49	0
58	MG	2d	302	1/1	0.94	0.08	62,62,62,62	0
58	MG	1A	3046	1/1	0.94	0.08	26,26,26,26	0
58	MG	1O	202	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3499	1/1	0.94	0.11	33,33,33,33	0
58	MG	1a	1809	1/1	0.94	0.09	39,39,39,39	0
58	MG	2A	3707	1/1	0.94	0.15	61,61,61,61	0
58	MG	1A	3828	1/1	0.94	0.11	29,29,29,29	0
58	MG	2A	3305	1/1	0.94	0.10	59,59,59,59	0
58	MG	2A	3711	1/1	0.94	0.11	41,41,41,41	0
58	MG	1A	4063	1/1	0.94	0.13	38,38,38,38	0
58	MG	1A	3500	1/1	0.94	0.21	56,56,56,56	0
58	MG	1P	204	1/1	0.94	0.07	29,29,29,29	0
58	MG	2A	3157	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3832	1/1	0.94	0.07	46,46,46,46	0
58	MG	1f	201	1/1	0.94	0.12	47,47,47,47	0
58	MG	1A	4071	1/1	0.94	0.06	40,40,40,40	0
58	MG	1Q	205	1/1	0.94	0.13	56,56,56,56	0
58	MG	2A	3492	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3834	1/1	0.94	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1m	3001	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3091	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3013	1/1	0.94	0.11	23,23,23,23	0
58	MG	2A	3319	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3111	1/1	0.94	0.10	36,36,36,36	0
58	MG	1R	202	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	4076	1/1	0.94	0.10	36,36,36,36	0
58	MG	1w	104	1/1	0.94	0.22	64,64,64,64	0
58	MG	2A	3170	1/1	0.94	0.07	41,41,41,41	0
58	MG	2A	3505	1/1	0.94	0.11	71,71,71,71	0
58	MG	1A	3266	1/1	0.94	0.20	41,41,41,41	0
58	MG	1A	4079	1/1	0.94	0.14	37,37,37,37	0
58	MG	1S	202	1/1	0.94	0.13	49,49,49,49	0
58	MG	1A	3882	1/1	0.95	0.08	28,28,28,28	0
58	MG	2A	3649	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3723	1/1	0.95	0.07	36,36,36,36	0
58	MG	1N	204	1/1	0.95	0.08	48,48,48,48	0
58	MG	1A	3084	1/1	0.95	0.19	39,39,39,39	0
58	MG	1A	3725	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3047	1/1	0.95	0.05	20,20,20,20	0
58	MG	1A	3557	1/1	0.95	0.16	39,39,39,39	0
58	MG	1A	3889	1/1	0.95	0.07	28,28,28,28	0
58	MG	1A	3079	1/1	0.95	0.09	24,24,24,24	0
58	MG	1A	3990	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3731	1/1	0.95	0.10	56,56,56,56	0
58	MG	1a	1749	1/1	0.95	0.12	50,50,50,50	0
58	MG	2a	1692	1/1	0.95	0.22	60,60,60,60	0
58	MG	1P	205	1/1	0.95	0.25	30,30,30,30	0
58	MG	2A	3663	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3852	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3188	1/1	0.95	0.12	30,30,30,30	0
58	MG	1Q	201	1/1	0.95	0.21	38,38,38,38	0
58	MG	1A	4093	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3478	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3486	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3174	1/1	0.95	0.07	27,27,27,27	0
58	MG	1A	3244	1/1	0.95	0.24	62,62,62,62	0
58	MG	2A	3674	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3317	1/1	0.95	0.31	54,54,54,54	0
58	MG	1A	3132	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3901	1/1	0.95	0.07	35,35,35,35	0
58	MG	1a	1641	1/1	0.95	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
58	MG	1A	3570	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	3375	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3065	1/1	0.95	0.13	52,52,52,52	0
58	MG	1A	3346	1/1	0.95	0.11	35,35,35,35	0
58	MG	1A	3623	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	3134	1/1	0.95	0.07	32,32,32,32	0
58	MG	1A	3526	1/1	0.95	0.08	42,42,42,42	0
58	MG	1a	1773	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3827	1/1	0.95	0.07	20,20,20,20	0
58	MG	1A	3054	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3220	1/1	0.95	0.15	44,44,44,44	0
58	MG	2A	3221	1/1	0.95	0.10	34,34,34,34	0
58	MG	1a	1651	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	3829	1/1	0.95	0.11	39,39,39,39	0
58	MG	1A	3380	1/1	0.95	0.09	25,25,25,25	0
58	MG	1A	3831	1/1	0.95	0.07	39,39,39,39	0
58	MG	2E	307	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3349	1/1	0.95	0.07	38,38,38,38	0
58	MG	1a	1782	1/1	0.95	0.06	51,51,51,51	0
58	MG	1V	201	1/1	0.95	0.18	27,27,27,27	0
58	MG	2A	3516	1/1	0.95	0.09	43,43,43,43	0
58	MG	2A	3084	1/1	0.95	0.15	44,44,44,44	0
58	MG	1a	1657	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3920	1/1	0.95	0.06	37,37,37,37	0
58	MG	1V	205	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3693	1/1	0.95	0.06	30,30,30,30	0
58	MG	2A	3369	1/1	0.95	0.19	58,58,58,58	0
58	MG	2A	3524	1/1	0.95	0.17	61,61,61,61	0
58	MG	2A	3713	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3835	1/1	0.95	0.10	45,45,45,45	0
58	MG	2P	202	1/1	0.95	0.09	64,64,64,64	0
58	MG	1A	3759	1/1	0.95	0.15	29,29,29,29	0
58	MG	1a	1793	1/1	0.95	0.15	58,58,58,58	0
58	MG	2A	3529	1/1	0.95	0.10	43,43,43,43	0
58	MG	2Q	204	1/1	0.95	0.09	42,42,42,42	0
58	MG	1a	1794	1/1	0.95	0.08	60,60,60,60	0
58	MG	1A	3630	1/1	0.95	0.07	43,43,43,43	0
58	MG	1a	1796	1/1	0.95	0.07	39,39,39,39	0
58	MG	1X	101	1/1	0.95	0.05	34,34,34,34	0
58	MG	1B	217	1/1	0.95	0.07	50,50,50,50	0
58	MG	1A	3322	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3455	1/1	0.95	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	222	1/1	0.95	0.08	37,37,37,37	0
58	MG	2A	3246	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3729	1/1	0.95	0.06	60,60,60,60	0
58	MG	2a	1757	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3763	1/1	0.95	0.09	27,27,27,27	0
58	MG	1A	3928	1/1	0.95	0.10	55,55,55,55	0
58	MG	1A	3764	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3930	1/1	0.95	0.12	41,41,41,41	0
58	MG	1A	3765	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	3845	1/1	0.95	0.09	39,39,39,39	0
58	MG	1a	1677	1/1	0.95	0.16	58,58,58,58	0
58	MG	2A	3391	1/1	0.95	0.20	59,59,59,59	0
58	MG	10	103	1/1	0.95	0.08	32,32,32,32	0
58	MG	1B	229	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3196	1/1	0.95	0.13	30,30,30,30	0
58	MG	1A	3137	1/1	0.95	0.27	33,33,33,33	0
58	MG	2A	3117	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3560	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3938	1/1	0.95	0.09	39,39,39,39	0
58	MG	2A	3399	1/1	0.95	0.30	51,51,51,51	0
58	MG	1A	3769	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3749	1/1	0.95	0.13	49,49,49,49	0
58	MG	2A	3401	1/1	0.95	0.26	50,50,50,50	0
58	MG	11	102	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3752	1/1	0.95	0.05	36,36,36,36	0
58	MG	1A	3699	1/1	0.95	0.10	23,23,23,23	0
58	MG	1B	237	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3109	1/1	0.95	0.11	33,33,33,33	0
58	MG	2A	3757	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3574	1/1	0.95	0.11	35,35,35,35	0
58	MG	2a	1787	1/1	0.95	0.10	58,58,58,58	0
58	MG	1A	3638	1/1	0.95	0.09	25,25,25,25	0
58	MG	1A	3773	1/1	0.95	0.08	36,36,36,36	0
58	MG	12	102	1/1	0.95	0.08	34,34,34,34	0
58	MG	2A	3133	1/1	0.95	0.08	54,54,54,54	0
58	MG	13	101	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3767	1/1	0.95	0.09	52,52,52,52	0
58	MG	1A	3090	1/1	0.95	0.14	43,43,43,43	0
58	MG	1A	3640	1/1	0.95	0.09	33,33,33,33	0
58	MG	1A	3424	1/1	0.95	0.08	30,30,30,30	0
58	MG	1A	3948	1/1	0.95	0.08	56,56,56,56	0
58	MG	2A	3139	1/1	0.95	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	15	101	1/1	0.95	0.13	27,27,27,27	0
58	MG	2A	3142	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3777	1/1	0.95	0.15	24,24,24,24	0
58	MG	1A	3071	1/1	0.95	0.08	15,15,15,15	0
58	MG	2A	3780	1/1	0.95	0.08	39,39,39,39	0
58	MG	1A	3859	1/1	0.95	0.10	23,23,23,23	0
58	MG	1E	302	1/1	0.95	0.09	36,36,36,36	0
58	MG	1A	3860	1/1	0.95	0.13	21,21,21,21	0
58	MG	1A	3203	1/1	0.95	0.07	29,29,29,29	0
58	MG	2A	3150	1/1	0.95	0.06	52,52,52,52	0
58	MG	2A	3151	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3302	1/1	0.95	0.14	34,34,34,34	0
58	MG	1A	3127	1/1	0.95	0.10	35,35,35,35	0
58	MG	1A	3957	1/1	0.95	0.08	58,58,58,58	0
58	MG	1A	4056	1/1	0.95	0.05	31,31,31,31	0
58	MG	1A	3648	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3785	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3433	1/1	0.95	0.32	57,57,57,57	0
58	MG	1A	3279	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3795	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3466	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3789	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3611	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3963	1/1	0.95	0.09	30,30,30,30	0
58	MG	1A	3397	1/1	0.95	0.08	26,26,26,26	0
58	MG	2a	1645	1/1	0.95	0.18	57,57,57,57	0
58	MG	1A	4067	1/1	0.95	0.07	19,19,19,19	0
58	MG	2A	3440	1/1	0.95	0.08	52,52,52,52	0
58	MG	1A	3468	1/1	0.95	0.08	38,38,38,38	0
58	MG	1A	3307	1/1	0.95	0.06	31,31,31,31	0
58	MG	2A	3012	1/1	0.95	0.08	39,39,39,39	0
58	MG	2A	3808	1/1	0.95	0.08	50,50,50,50	0
58	MG	1A	3281	1/1	0.95	0.23	31,31,31,31	0
58	MG	1A	3970	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3509	1/1	0.95	0.11	42,42,42,42	0
58	MG	1A	3876	1/1	0.95	0.07	39,39,39,39	0
58	MG	1a	1723	1/1	0.95	0.18	50,50,50,50	0
58	MG	2A	3452	1/1	0.95	0.11	50,50,50,50	0
58	MG	2A	3020	1/1	0.95	0.11	36,36,36,36	0
58	MG	1a	1608	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3878	1/1	0.95	0.12	32,32,32,32	0
58	MG	2A	3023	1/1	0.95	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4078	1/1	0.95	0.12	34,34,34,34	0
58	MG	1a	1612	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3009	1/1	0.95	0.06	24,24,24,24	0
58	MG	1a	1731	1/1	0.95	0.11	37,37,37,37	0
58	MG	2A	3030	1/1	0.95	0.10	44,44,44,44	0
58	MG	2a	1667	1/1	0.95	0.10	51,51,51,51	0
58	MG	2A	3031	1/1	0.95	0.15	38,38,38,38	0
58	MG	2A	3830	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3831	1/1	0.95	0.09	55,55,55,55	0
58	MG	2A	3643	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3258	1/1	0.95	0.09	37,37,37,37	0
58	MG	1a	1616	1/1	0.95	0.08	40,40,40,40	0
58	MG	1A	3722	1/1	0.95	0.08	34,34,34,34	0
58	MG	2x	106	1/1	0.95	0.09	51,51,51,51	0
59	K	2A	3443	1/1	0.95	0.07	51,51,51,51	0
60	ZN	24	501	1/1	0.95	0.12	103,103,103,103	0
61	SF4	1d	302	8/8	0.95	0.08	52,54,59,62	0
58	MG	1A	3612	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3553	1/1	0.96	0.07	27,27,27,27	0
58	MG	1A	3683	1/1	0.96	0.06	31,31,31,31	0
58	MG	1U	205	1/1	0.96	0.18	33,33,33,33	0
58	MG	1A	3215	1/1	0.96	0.09	38,38,38,38	0
58	MG	1U	208	1/1	0.96	0.28	29,29,29,29	0
58	MG	2A	3658	1/1	0.96	0.05	32,32,32,32	0
58	MG	2a	1684	1/1	0.96	0.14	49,49,49,49	0
58	MG	2A	3057	1/1	0.96	0.16	40,40,40,40	0
58	MG	1A	3686	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3099	1/1	0.96	0.07	36,36,36,36	0
58	MG	1V	202	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3487	1/1	0.96	0.12	27,27,27,27	0
58	MG	1A	3112	1/1	0.96	0.09	29,29,29,29	0
58	MG	1A	4025	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3850	1/1	0.96	0.10	46,46,46,46	0
58	MG	2A	3666	1/1	0.96	0.09	36,36,36,36	0
58	MG	1B	219	1/1	0.96	0.07	41,41,41,41	0
58	MG	1A	3391	1/1	0.96	0.23	38,38,38,38	0
58	MG	1A	3319	1/1	0.96	0.09	36,36,36,36	0
58	MG	2A	3066	1/1	0.96	0.08	33,33,33,33	0
58	MG	2A	3346	1/1	0.96	0.13	63,63,63,63	0
58	MG	1A	4028	1/1	0.96	0.04	19,19,19,19	0
58	MG	1A	4029	1/1	0.96	0.07	42,42,42,42	0
58	MG	2a	1703	1/1	0.96	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3069	1/1	0.96	0.07	42,42,42,42	0
58	MG	1X	102	1/1	0.96	0.08	46,46,46,46	0
58	MG	1A	3934	1/1	0.96	0.04	11,11,11,11	0
58	MG	2A	3501	1/1	0.96	0.08	59,59,59,59	0
58	MG	2A	3072	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3767	1/1	0.96	0.09	37,37,37,37	0
58	MG	1A	3692	1/1	0.96	0.08	32,32,32,32	0
58	MG	2A	3075	1/1	0.96	0.08	22,22,22,22	0
58	MG	2A	3684	1/1	0.96	0.07	61,61,61,61	0
58	MG	1A	3513	1/1	0.96	0.14	30,30,30,30	0
58	MG	2A	3686	1/1	0.96	0.15	46,46,46,46	0
58	MG	1a	1783	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3218	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3515	1/1	0.96	0.07	33,33,33,33	0
58	MG	1Z	301	1/1	0.96	0.14	43,43,43,43	0
58	MG	2A	3362	1/1	0.96	0.20	49,49,49,49	0
58	MG	2D	306	1/1	0.96	0.14	40,40,40,40	0
58	MG	1B	230	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	4036	1/1	0.96	0.07	29,29,29,29	0
58	MG	1a	1790	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3192	1/1	0.96	0.11	27,27,27,27	0
58	MG	1A	3564	1/1	0.96	0.10	53,53,53,53	0
58	MG	1A	3943	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3855	1/1	0.96	0.09	49,49,49,49	0
58	MG	1A	3565	1/1	0.96	0.08	35,35,35,35	0
58	MG	2A	3701	1/1	0.96	0.10	35,35,35,35	0
58	MG	1a	1673	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3703	1/1	0.96	0.11	47,47,47,47	0
58	MG	2A	3372	1/1	0.96	0.15	38,38,38,38	0
58	MG	1A	3146	1/1	0.96	0.18	32,32,32,32	0
58	MG	1A	3147	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3526	1/1	0.96	0.04	38,38,38,38	0
58	MG	1A	3224	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3010	1/1	0.96	0.06	30,30,30,30	0
58	MG	1D	305	1/1	0.96	0.08	36,36,36,36	0
58	MG	1A	3572	1/1	0.96	0.16	31,31,31,31	0
58	MG	1A	3023	1/1	0.96	0.06	13,13,13,13	0
58	MG	1a	1804	1/1	0.96	0.16	52,52,52,52	0
58	MG	1D	308	1/1	0.96	0.07	28,28,28,28	0
58	MG	2a	1743	1/1	0.96	0.07	56,56,56,56	0
58	MG	2A	3102	1/1	0.96	0.13	50,50,50,50	0
58	MG	2a	1745	1/1	0.96	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3782	1/1	0.96	0.09	32,32,32,32	0
58	MG	2A	3719	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3575	1/1	0.96	0.40	34,34,34,34	0
58	MG	2A	3538	1/1	0.96	0.13	47,47,47,47	0
58	MG	1A	3015	1/1	0.96	0.10	32,32,32,32	0
58	MG	2A	3386	1/1	0.96	0.14	43,43,43,43	0
58	MG	1a	1685	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3133	1/1	0.96	0.06	38,38,38,38	0
58	MG	2a	1754	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	3200	1/1	0.96	0.09	31,31,31,31	0
58	MG	2A	3545	1/1	0.96	0.07	46,46,46,46	0
58	MG	1A	3331	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3298	1/1	0.96	0.08	28,28,28,28	0
58	MG	2A	3112	1/1	0.96	0.08	29,29,29,29	0
58	MG	1A	3232	1/1	0.96	0.07	44,44,44,44	0
58	MG	1A	4057	1/1	0.96	0.05	18,18,18,18	0
58	MG	1A	3368	1/1	0.96	0.14	49,49,49,49	0
58	MG	2A	3396	1/1	0.96	0.22	48,48,48,48	0
58	MG	20	102	1/1	0.96	0.08	50,50,50,50	0
58	MG	2A	3555	1/1	0.96	0.05	40,40,40,40	0
58	MG	1A	3005	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	4060	1/1	0.96	0.08	45,45,45,45	0
58	MG	2A	3118	1/1	0.96	0.09	60,60,60,60	0
58	MG	1A	3154	1/1	0.96	0.12	33,33,33,33	0
58	MG	1F	303	1/1	0.96	0.07	28,28,28,28	0
58	MG	2A	3562	1/1	0.96	0.06	38,38,38,38	0
58	MG	27	101	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3964	1/1	0.96	0.06	57,57,57,57	0
58	MG	17	102	1/1	0.96	0.06	29,29,29,29	0
58	MG	17	103	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3646	1/1	0.96	0.04	22,22,22,22	0
58	MG	2A	3569	1/1	0.96	0.07	42,42,42,42	0
58	MG	2A	3126	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3127	1/1	0.96	0.11	44,44,44,44	0
58	MG	1A	3058	1/1	0.96	0.10	22,22,22,22	0
58	MG	1A	3587	1/1	0.96	0.24	43,43,43,43	0
58	MG	1A	3720	1/1	0.96	0.05	13,13,13,13	0
58	MG	1A	3650	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3303	1/1	0.96	0.06	22,22,22,22	0
58	MG	1A	3654	1/1	0.96	0.05	27,27,27,27	0
58	MG	1A	3136	1/1	0.96	0.10	21,21,21,21	0
58	MG	1A	3534	1/1	0.96	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3454	1/1	0.96	0.15	39,39,39,39	0
58	MG	1A	3658	1/1	0.96	0.06	37,37,37,37	0
58	MG	2A	3763	1/1	0.96	0.11	41,41,41,41	0
58	MG	1x	107	1/1	0.96	0.05	47,47,47,47	0
58	MG	1A	3729	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	3812	1/1	0.96	0.18	18,18,18,18	0
58	MG	1A	3891	1/1	0.96	0.14	25,25,25,25	0
58	MG	2A	3145	1/1	0.96	0.12	50,50,50,50	0
58	MG	2A	3771	1/1	0.96	0.08	71,71,71,71	0
58	MG	1a	1714	1/1	0.96	0.18	41,41,41,41	0
58	MG	1A	3043	1/1	0.96	0.12	35,35,35,35	0
58	MG	1A	3051	1/1	0.96	0.09	22,22,22,22	0
58	MG	1A	3496	1/1	0.96	0.10	26,26,26,26	0
58	MG	1A	3497	1/1	0.96	0.10	27,27,27,27	0
58	MG	1A	3987	1/1	0.96	0.12	29,29,29,29	0
58	MG	1a	1610	1/1	0.96	0.10	23,23,23,23	0
58	MG	1A	3735	1/1	0.96	0.10	48,48,48,48	0
58	MG	2A	3431	1/1	0.96	0.26	58,58,58,58	0
58	MG	1A	3243	1/1	0.96	0.12	40,40,40,40	0
58	MG	2A	3008	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3052	1/1	0.96	0.09	24,24,24,24	0
58	MG	2A	3010	1/1	0.96	0.06	43,43,43,43	0
58	MG	2A	3605	1/1	0.96	0.10	55,55,55,55	0
58	MG	1a	1614	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3208	1/1	0.96	0.07	37,37,37,37	0
58	MG	1A	3185	1/1	0.96	0.20	40,40,40,40	0
58	MG	1A	3994	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3278	1/1	0.96	0.06	28,28,28,28	0
58	MG	1a	1730	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3444	1/1	0.96	0.10	25,25,25,25	0
58	MG	1A	3422	1/1	0.96	0.08	44,44,44,44	0
58	MG	1a	1732	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3825	1/1	0.96	0.05	20,20,20,20	0
58	MG	1A	3998	1/1	0.96	0.11	19,19,19,19	0
58	MG	1P	207	1/1	0.96	0.12	34,34,34,34	0
58	MG	2A	3621	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3025	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	3826	1/1	0.96	0.08	34,34,34,34	0
58	MG	1a	1624	1/1	0.96	0.15	50,50,50,50	0
58	MG	2A	3173	1/1	0.96	0.09	39,39,39,39	0
58	MG	2A	3626	1/1	0.96	0.09	60,60,60,60	0
58	MG	1a	1738	1/1	0.96	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3809	1/1	0.96	0.07	51,51,51,51	0
58	MG	2A	3628	1/1	0.96	0.08	37,37,37,37	0
58	MG	2A	3629	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1739	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3670	1/1	0.96	0.07	35,35,35,35	0
58	MG	1A	3247	1/1	0.96	0.13	33,33,33,33	0
58	MG	1A	3036	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	4101	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3819	1/1	0.96	0.06	56,56,56,56	0
58	MG	1A	3426	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3912	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3750	1/1	0.96	0.08	16,16,16,16	0
58	MG	1a	1632	1/1	0.96	0.12	24,24,24,24	0
58	MG	1A	3915	1/1	0.96	0.14	34,34,34,34	0
58	MG	1A	3751	1/1	0.96	0.13	50,50,50,50	0
58	MG	1a	1750	1/1	0.96	0.19	52,52,52,52	0
58	MG	1A	3550	1/1	0.96	0.10	33,33,33,33	0
58	MG	2a	1669	1/1	0.96	0.10	35,35,35,35	0
58	MG	1A	3551	1/1	0.96	0.08	32,32,32,32	0
58	MG	2A	3646	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3836	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3837	1/1	0.96	0.08	50,50,50,50	0
58	MG	1a	1756	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3049	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3165	1/1	0.96	0.12	30,30,30,30	0
61	SF4	2d	304	8/8	0.96	0.08	61,70,76,84	0
58	MG	1A	3209	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3306	1/1	0.97	0.07	30,30,30,30	0
58	MG	2A	3764	1/1	0.97	0.07	50,50,50,50	0
58	MG	1a	1778	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	3708	1/1	0.97	0.04	15,15,15,15	0
58	MG	2A	3630	1/1	0.97	0.12	39,39,39,39	0
58	MG	2A	3631	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3499	1/1	0.97	0.11	66,66,66,66	0
58	MG	1A	3914	1/1	0.97	0.05	34,34,34,34	0
58	MG	2A	3772	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3651	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3652	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3917	1/1	0.97	0.09	34,34,34,34	0
58	MG	2A	3776	1/1	0.97	0.06	66,66,66,66	0
58	MG	1A	3918	1/1	0.97	0.04	28,28,28,28	0
58	MG	1a	1785	1/1	0.97	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3113	1/1	0.97	0.09	28,28,28,28	0
58	MG	1A	3712	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3272	1/1	0.97	0.10	46,46,46,46	0
58	MG	1A	3145	1/1	0.97	0.14	27,27,27,27	0
58	MG	1A	3114	1/1	0.97	0.07	28,28,28,28	0
58	MG	1A	4006	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3383	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3513	1/1	0.97	0.10	23,23,23,23	0
58	MG	1A	3425	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3214	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	3061	1/1	0.97	0.09	36,36,36,36	0
58	MG	1A	4012	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3191	1/1	0.97	0.13	30,30,30,30	0
58	MG	1A	4014	1/1	0.97	0.06	59,59,59,59	0
58	MG	1A	3608	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3787	1/1	0.97	0.11	28,28,28,28	0
58	MG	1A	3609	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3796	1/1	0.97	0.05	36,36,36,36	0
58	MG	2A	3523	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3280	1/1	0.97	0.20	37,37,37,37	0
58	MG	1P	201	1/1	0.97	0.18	29,29,29,29	0
58	MG	1A	3790	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3116	1/1	0.97	0.15	29,29,29,29	0
58	MG	1A	3282	1/1	0.97	0.09	28,28,28,28	0
58	MG	1A	3861	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3794	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3283	1/1	0.97	0.17	35,35,35,35	0
58	MG	1Q	202	1/1	0.97	0.12	36,36,36,36	0
58	MG	2A	3533	1/1	0.97	0.07	43,43,43,43	0
58	MG	1Q	203	1/1	0.97	0.04	24,24,24,24	0
58	MG	2A	3668	1/1	0.97	0.09	63,63,63,63	0
58	MG	2a	1763	1/1	0.97	0.15	59,59,59,59	0
58	MG	1A	3727	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3249	1/1	0.97	0.06	28,28,28,28	0
58	MG	1A	3028	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3799	1/1	0.97	0.08	18,18,18,18	0
58	MG	2A	3673	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3816	1/1	0.97	0.08	51,51,51,51	0
58	MG	2a	1770	1/1	0.97	0.11	51,51,51,51	0
58	MG	1A	3219	1/1	0.97	0.08	37,37,37,37	0
58	MG	1A	3567	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3673	1/1	0.97	0.05	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3542	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3396	1/1	0.97	0.10	35,35,35,35	0
58	MG	2A	3087	1/1	0.97	0.10	40,40,40,40	0
58	MG	1A	3949	1/1	0.97	0.04	45,45,45,45	0
58	MG	1B	218	1/1	0.97	0.05	45,45,45,45	0
58	MG	1A	3171	1/1	0.97	0.07	19,19,19,19	0
58	MG	2A	3549	1/1	0.97	0.12	39,39,39,39	0
58	MG	1A	3737	1/1	0.97	0.10	20,20,20,20	0
58	MG	2A	3316	1/1	0.97	0.06	44,44,44,44	0
58	MG	1w	102	1/1	0.97	0.13	46,46,46,46	0
58	MG	1A	3676	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3221	1/1	0.97	0.08	33,33,33,33	0
58	MG	1U	201	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3877	1/1	0.97	0.20	33,33,33,33	0
58	MG	1A	3172	1/1	0.97	0.14	27,27,27,27	0
58	MG	1a	1725	1/1	0.97	0.14	56,56,56,56	0
58	MG	2A	3559	1/1	0.97	0.06	46,46,46,46	0
58	MG	1A	3085	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3811	1/1	0.97	0.04	22,22,22,22	0
58	MG	1A	3120	1/1	0.97	0.07	44,44,44,44	0
58	MG	1U	207	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3024	1/1	0.97	0.13	45,45,45,45	0
58	MG	2A	3441	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3030	1/1	0.97	0.14	31,31,31,31	0
58	MG	1A	3685	1/1	0.97	0.08	58,58,58,58	0
58	MG	1A	3746	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3704	1/1	0.97	0.05	43,43,43,43	0
58	MG	1B	232	1/1	0.97	0.05	61,61,61,61	0
58	MG	1A	3228	1/1	0.97	0.07	28,28,28,28	0
58	MG	2A	3573	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3111	1/1	0.97	0.19	49,49,49,49	0
58	MG	1A	3155	1/1	0.97	0.09	39,39,39,39	0
58	MG	1A	3965	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3446	1/1	0.97	0.26	28,28,28,28	0
58	MG	1A	3366	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3098	1/1	0.97	0.10	18,18,18,18	0
58	MG	1D	301	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3449	1/1	0.97	0.09	42,42,42,42	0
58	MG	2A	3231	1/1	0.97	0.10	54,54,54,54	0
58	MG	1A	3893	1/1	0.97	0.08	47,47,47,47	0
58	MG	1A	3754	1/1	0.97	0.08	37,37,37,37	0
58	MG	2A	3586	1/1	0.97	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3972	1/1	0.97	0.07	53,53,53,53	0
58	MG	2A	3122	1/1	0.97	0.14	39,39,39,39	0
58	MG	2A	3589	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3157	1/1	0.97	0.06	33,33,33,33	0
58	MG	1a	1649	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3636	1/1	0.97	0.04	22,22,22,22	0
58	MG	2A	3013	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3467	1/1	0.97	0.06	49,49,49,49	0
58	MG	2D	301	1/1	0.97	0.10	34,34,34,34	0
58	MG	1A	3897	1/1	0.97	0.06	25,25,25,25	0
58	MG	2A	3731	1/1	0.97	0.05	48,48,48,48	0
58	MG	1A	3637	1/1	0.97	0.04	27,27,27,27	0
58	MG	2D	305	1/1	0.97	0.09	29,29,29,29	0
58	MG	1D	311	1/1	0.97	0.06	38,38,38,38	0
58	MG	2A	3130	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3072	1/1	0.97	0.28	31,31,31,31	0
58	MG	2a	1687	1/1	0.97	0.10	59,59,59,59	0
58	MG	10	101	1/1	0.97	0.11	37,37,37,37	0
58	MG	2E	303	1/1	0.97	0.13	48,48,48,48	0
58	MG	1A	3538	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3125	1/1	0.97	0.14	25,25,25,25	0
58	MG	10	104	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3980	1/1	0.97	0.04	40,40,40,40	0
58	MG	10	106	1/1	0.97	0.12	45,45,45,45	0
58	MG	2A	3607	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	3234	1/1	0.97	0.05	56,56,56,56	0
58	MG	1A	4070	1/1	0.97	0.05	37,37,37,37	0
58	MG	1E	306	1/1	0.97	0.08	29,29,29,29	0
58	MG	1A	3903	1/1	0.97	0.08	49,49,49,49	0
58	MG	1a	1766	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3412	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3833	1/1	0.97	0.10	39,39,39,39	0
58	MG	2A	3616	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3160	1/1	0.97	0.04	19,19,19,19	0
58	MG	2A	3035	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3036	1/1	0.97	0.04	22,22,22,22	0
58	MG	2A	3755	1/1	0.97	0.10	53,53,53,53	0
58	MG	1a	1668	1/1	0.97	0.15	55,55,55,55	0
58	MG	1A	3414	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3236	1/1	0.97	0.10	27,27,27,27	0
60	ZN	1Y	205	1/1	0.97	0.05	56,56,56,56	0
60	ZN	14	102	1/1	0.97	0.07	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	15	108	1/1	0.97	0.11	41,41,41,41	0
60	ZN	1n	103	1/1	0.97	0.05	51,51,51,51	0
60	ZN	2Y	202	1/1	0.97	0.05	85,85,85,85	0
58	MG	1F	302	1/1	0.97	0.07	30,30,30,30	0
60	ZN	26	501	1/1	0.97	0.06	57,57,57,57	0
60	ZN	2n	102	1/1	0.97	0.05	86,86,86,86	0
58	MG	1A	3065	1/1	0.97	0.19	39,39,39,39	0
58	MG	1A	3025	1/1	0.97	0.07	25,25,25,25	0
58	MG	1A	3007	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3328	1/1	0.98	0.07	42,42,42,42	0
58	MG	1A	3119	1/1	0.98	0.05	33,33,33,33	0
58	MG	1U	210	1/1	0.98	0.28	32,32,32,32	0
58	MG	1A	3161	1/1	0.98	0.09	24,24,24,24	0
58	MG	1A	4064	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3238	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3198	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3546	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3748	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	4068	1/1	0.98	0.07	44,44,44,44	0
58	MG	2A	3132	1/1	0.98	0.12	38,38,38,38	0
58	MG	1A	4069	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3667	1/1	0.98	0.04	20,20,20,20	0
58	MG	2B	219	1/1	0.98	0.14	54,54,54,54	0
58	MG	1W	204	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3591	1/1	0.98	0.10	31,31,31,31	0
58	MG	1A	3240	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3593	1/1	0.98	0.28	40,40,40,40	0
58	MG	1A	3108	1/1	0.98	0.06	37,37,37,37	0
58	MG	2A	3140	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3081	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	3044	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3886	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	3756	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	3800	1/1	0.98	0.10	17,17,17,17	0
58	MG	1A	3933	1/1	0.98	0.04	36,36,36,36	0
58	MG	1A	3387	1/1	0.98	0.11	30,30,30,30	0
58	MG	2A	3565	1/1	0.98	0.10	34,34,34,34	0
58	MG	2A	3566	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3981	1/1	0.98	0.07	56,56,56,56	0
58	MG	2A	3724	1/1	0.98	0.14	52,52,52,52	0
58	MG	1A	3758	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3388	1/1	0.98	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3019	1/1	0.98	0.04	23,23,23,23	0
58	MG	2A	3152	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3070	1/1	0.98	0.08	22,22,22,22	0
58	MG	2F	305	1/1	0.98	0.10	47,47,47,47	0
58	MG	1A	3018	1/1	0.98	0.19	27,27,27,27	0
58	MG	2A	3359	1/1	0.98	0.04	30,30,30,30	0
58	MG	2A	3732	1/1	0.98	0.08	35,35,35,35	0
58	MG	1P	202	1/1	0.98	0.06	27,27,27,27	0
58	MG	1A	3566	1/1	0.98	0.12	28,28,28,28	0
58	MG	2A	3024	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3363	1/1	0.98	0.14	31,31,31,31	0
58	MG	2A	3818	1/1	0.98	0.06	32,32,32,32	0
58	MG	1A	3151	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3477	1/1	0.98	0.06	42,42,42,42	0
58	MG	1A	3093	1/1	0.98	0.06	22,22,22,22	0
58	MG	1A	3226	1/1	0.98	0.06	23,23,23,23	0
58	MG	2A	3823	1/1	0.98	0.07	23,23,23,23	0
58	MG	2A	3094	1/1	0.98	0.05	40,40,40,40	0
58	MG	2A	3584	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3032	1/1	0.98	0.09	31,31,31,31	0
58	MG	1A	3573	1/1	0.98	0.07	35,35,35,35	0
58	MG	2A	3032	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3037	1/1	0.98	0.07	19,19,19,19	0
58	MG	1D	309	1/1	0.98	0.09	33,33,33,33	0
58	MG	2A	3590	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3189	1/1	0.98	0.13	34,34,34,34	0
58	MG	1A	4097	1/1	0.98	0.04	41,41,41,41	0
58	MG	2X	3500	1/1	0.98	0.03	52,52,52,52	0
58	MG	1A	4045	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3140	1/1	0.98	0.11	26,26,26,26	0
58	MG	1A	3276	1/1	0.98	0.10	40,40,40,40	0
58	MG	1A	3173	1/1	0.98	0.10	29,29,29,29	0
58	MG	1E	303	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	4000	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3141	1/1	0.98	0.10	13,13,13,13	0
58	MG	2a	1761	1/1	0.98	0.11	48,48,48,48	0
58	MG	1a	1760	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3580	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3087	1/1	0.98	0.05	32,32,32,32	0
58	MG	1a	1763	1/1	0.98	0.05	37,37,37,37	0
58	MG	2A	3457	1/1	0.98	0.04	19,19,19,19	0
58	MG	1A	3822	1/1	0.98	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	K	1A	3562	1/1	0.98	0.10	43,43,43,43	0
58	MG	2A	3459	1/1	0.98	0.16	46,46,46,46	0
58	MG	1A	3617	1/1	0.98	0.13	32,32,32,32	0
58	MG	2A	3766	1/1	0.98	0.06	52,52,52,52	0
58	MG	1A	3106	1/1	0.98	0.07	33,33,33,33	0
60	ZN	16	102	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3619	1/1	0.98	0.05	44,44,44,44	0
58	MG	17	101	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	4008	1/1	0.98	0.09	23,23,23,23	0
58	MG	1A	3376	1/1	0.98	0.15	31,31,31,31	0
58	MG	2A	3613	1/1	0.98	0.10	35,35,35,35	0
58	MG	2a	1690	1/1	0.98	0.18	36,36,36,36	0
58	MG	1A	3490	1/1	0.98	0.06	27,27,27,27	0
58	MG	2A	3708	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3936	1/1	0.99	0.06	33,33,33,33	0
58	MG	2A	3806	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3988	1/1	0.99	0.04	30,30,30,30	0
58	MG	1A	3628	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3273	1/1	0.99	0.08	27,27,27,27	0
58	MG	1A	3021	1/1	0.99	0.03	20,20,20,20	0
58	MG	1A	3169	1/1	0.99	0.12	11,11,11,11	0
58	MG	1V	203	1/1	0.99	0.14	25,25,25,25	0
58	MG	1A	3688	1/1	0.99	0.05	18,18,18,18	0
58	MG	2A	3098	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3678	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3734	1/1	0.99	0.07	39,39,39,39	0
58	MG	1A	3210	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3736	1/1	0.99	0.04	22,22,22,22	0
58	MG	1A	3647	1/1	0.99	0.10	17,17,17,17	0
58	MG	1W	203	1/1	0.99	0.07	31,31,31,31	0
58	MG	2A	3700	1/1	0.99	0.09	31,31,31,31	0
60	ZN	19	102	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3681	1/1	0.99	0.07	23,23,23,23	0
58	MG	1A	3792	1/1	0.99	0.03	35,35,35,35	0
58	MG	1A	3033	1/1	0.99	0.27	30,30,30,30	0
60	ZN	25	104	1/1	0.99	0.07	59,59,59,59	0
58	MG	1A	3779	1/1	0.99	0.03	37,37,37,37	0
60	ZN	29	102	1/1	0.99	0.03	57,57,57,57	0
58	MG	1A	3870	1/1	0.99	0.02	19,19,19,19	0
58	MG	1F	301	1/1	0.99	0.06	35,35,35,35	0
58	MG	1A	3038	1/1	0.99	0.05	26,26,26,26	0
58	MG	1a	1754	1/1	1.00	0.11	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.