



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 03:37 am BST

PDB ID : 6UO1  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA (containing pseudouridine at the first position of the codon) and deacylated A-, P-, and E-site tRNAs at 2.95Å resolution  
Authors : Batool, Z.; Dobosz-Bartoszek, M.; Polikanov, Y.S.  
Deposited on : 2019-10-14  
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

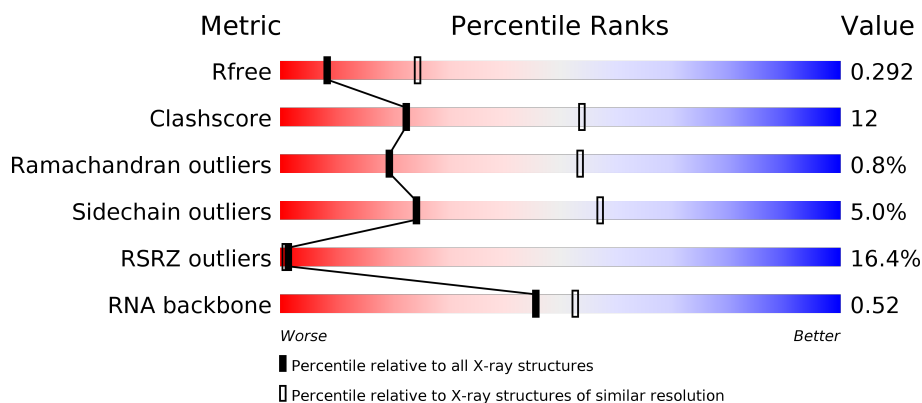
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>7%</div> </div> </div>
1	2A	2915	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>9%</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>62%</div> <div>34%</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>52%</div> <div>40%</div> <div>7%</div> </div> </div>

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

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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3036	-	-	-	X
56	MG	1A	3098	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3114	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3318	-	-	-	X
56	MG	1A	3359	-	-	-	X
56	MG	1A	3368	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3433	-	-	-	X
56	MG	1A	3506	-	-	-	X
56	MG	1A	3513	-	-	-	X
56	MG	1a	3016	-	-	-	X
56	MG	1a	3037	-	-	-	X
56	MG	1a	3043	-	-	-	X
56	MG	1a	3053	-	-	-	X
56	MG	1a	3082	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	3092	-	-	-	X
56	MG	1a	3094	-	-	-	X
56	MG	1a	3111	-	-	-	X
56	MG	1a	3116	-	-	-	X
56	MG	1a	3122	-	-	-	X
56	MG	1a	3163	-	-	-	X
56	MG	1a	3167	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3099	-	-	-	X
56	MG	2A	3101	-	-	-	X
56	MG	2A	3111	-	-	-	X
56	MG	2A	3142	-	-	-	X
56	MG	2A	3158	-	-	-	X
56	MG	2A	3234	-	-	-	X
56	MG	2A	3245	-	-	-	X
56	MG	2A	3315	-	-	-	X
56	MG	2A	3316	-	-	-	X
56	MG	2A	3317	-	-	-	X
56	MG	2a	3007	-	-	-	X
56	MG	2a	3017	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3053	-	-	-	X
56	MG	2a	3058	-	-	-	X
56	MG	2a	3059	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3087	-	-	-	X



## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 295398 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	50	89	13			
53	2v	8	Total	C	N	O	P	0	0	0
			167	75	25	59	8			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2a	183	Total	Mg	0	0
			183	183		
56	1A	680	Total	Mg	0	0
			680	680		
56	2A	351	Total	Mg	0	0
			351	351		
56	1a	238	Total	Mg	0	0
			238	238		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

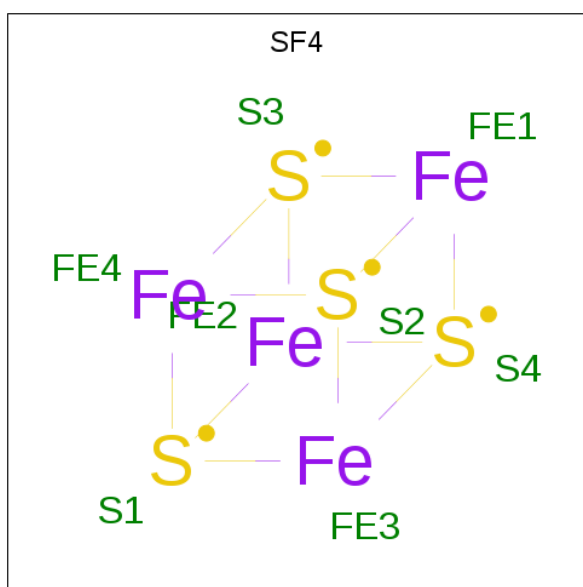
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total 8	Fe 4	S 4	0	0
58	2d	1	Total 8	Fe 4	S 4	0	0

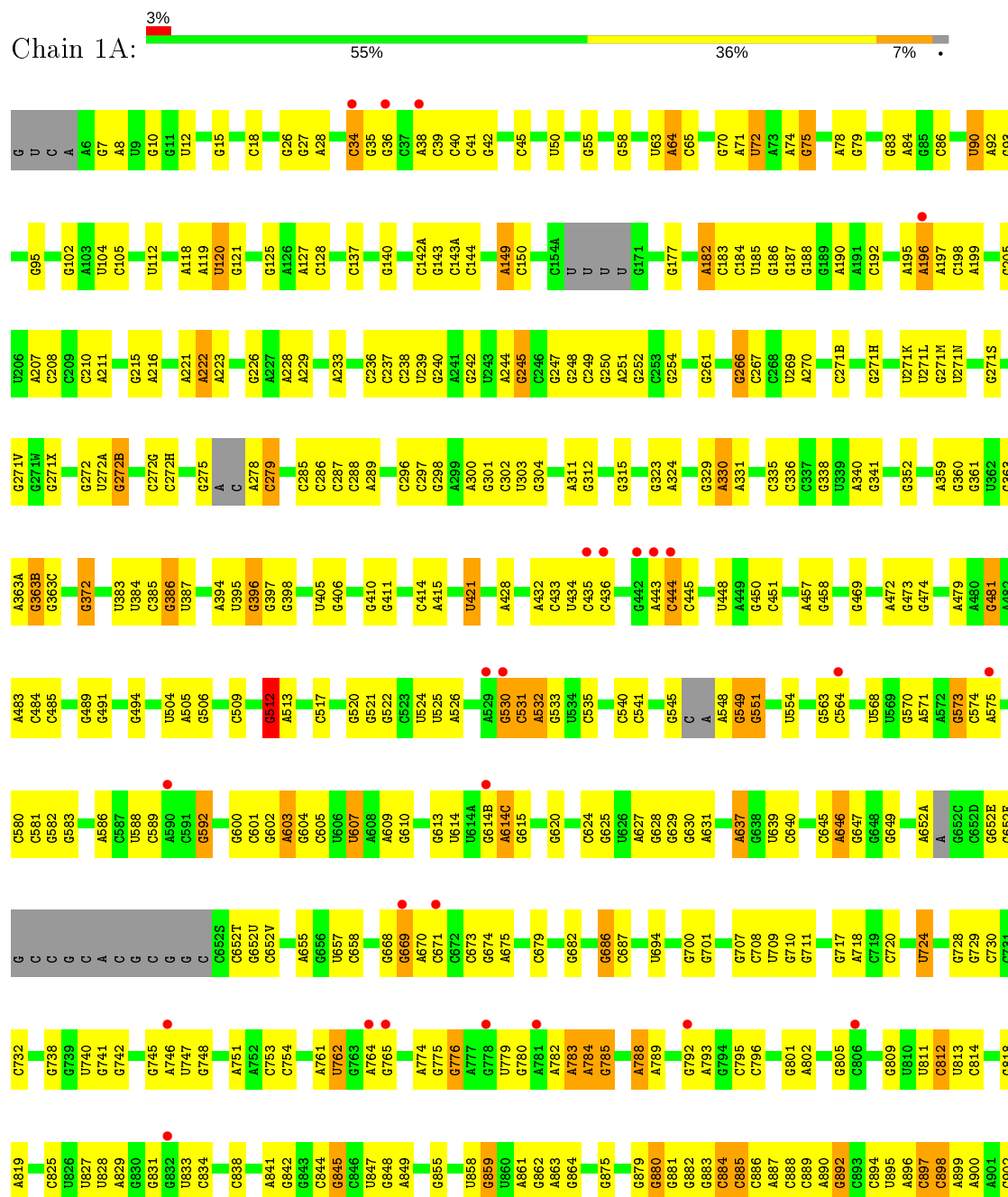
- Molecule 59 is water.

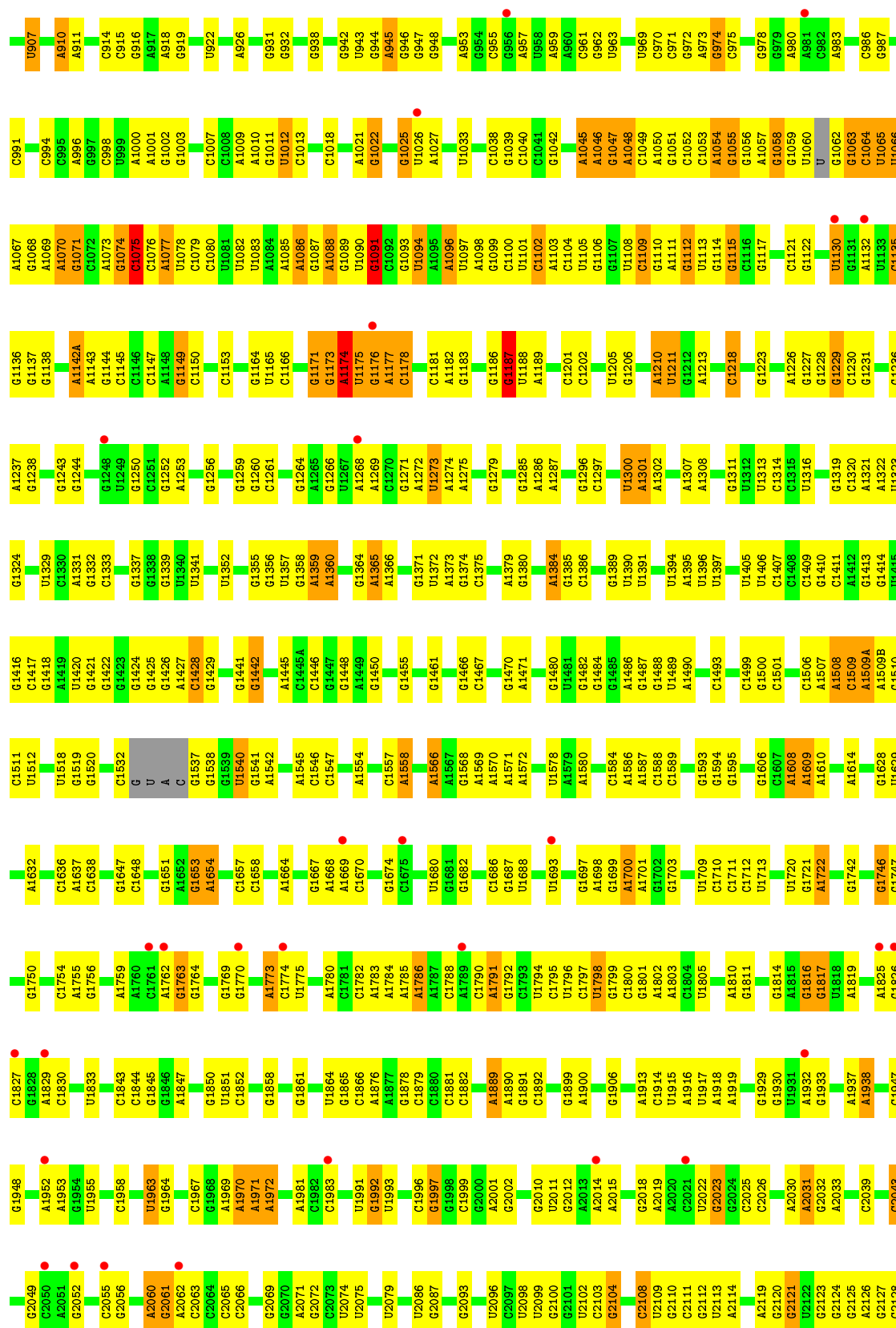
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	585	Total 585	O 585	0	0
59	1a	181	Total 181	O 181	0	0
59	2A	234	Total 234	O 234	0	0
59	2a	167	Total 167	O 167	0	0

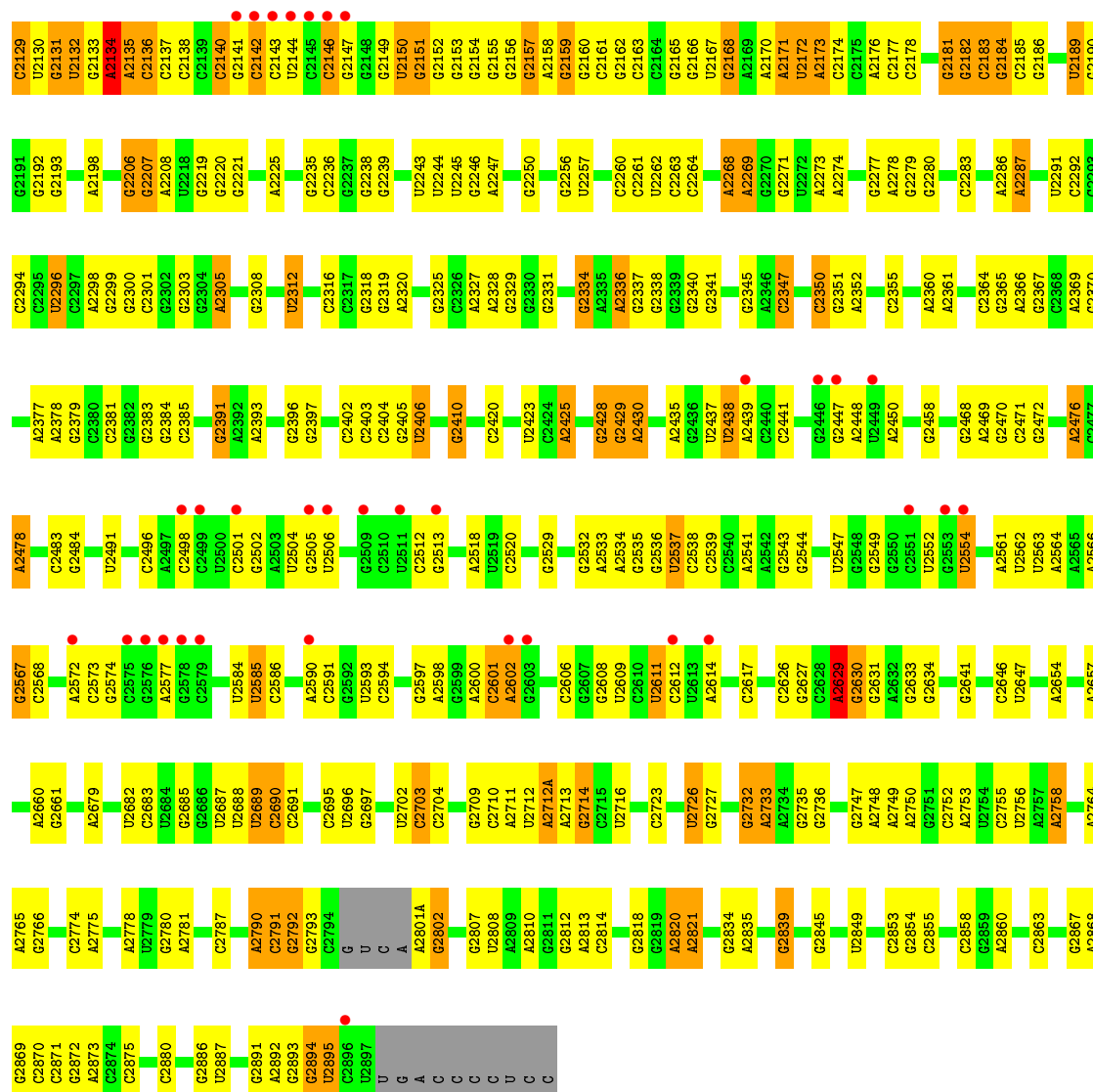
### 3 Residue-property plots

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

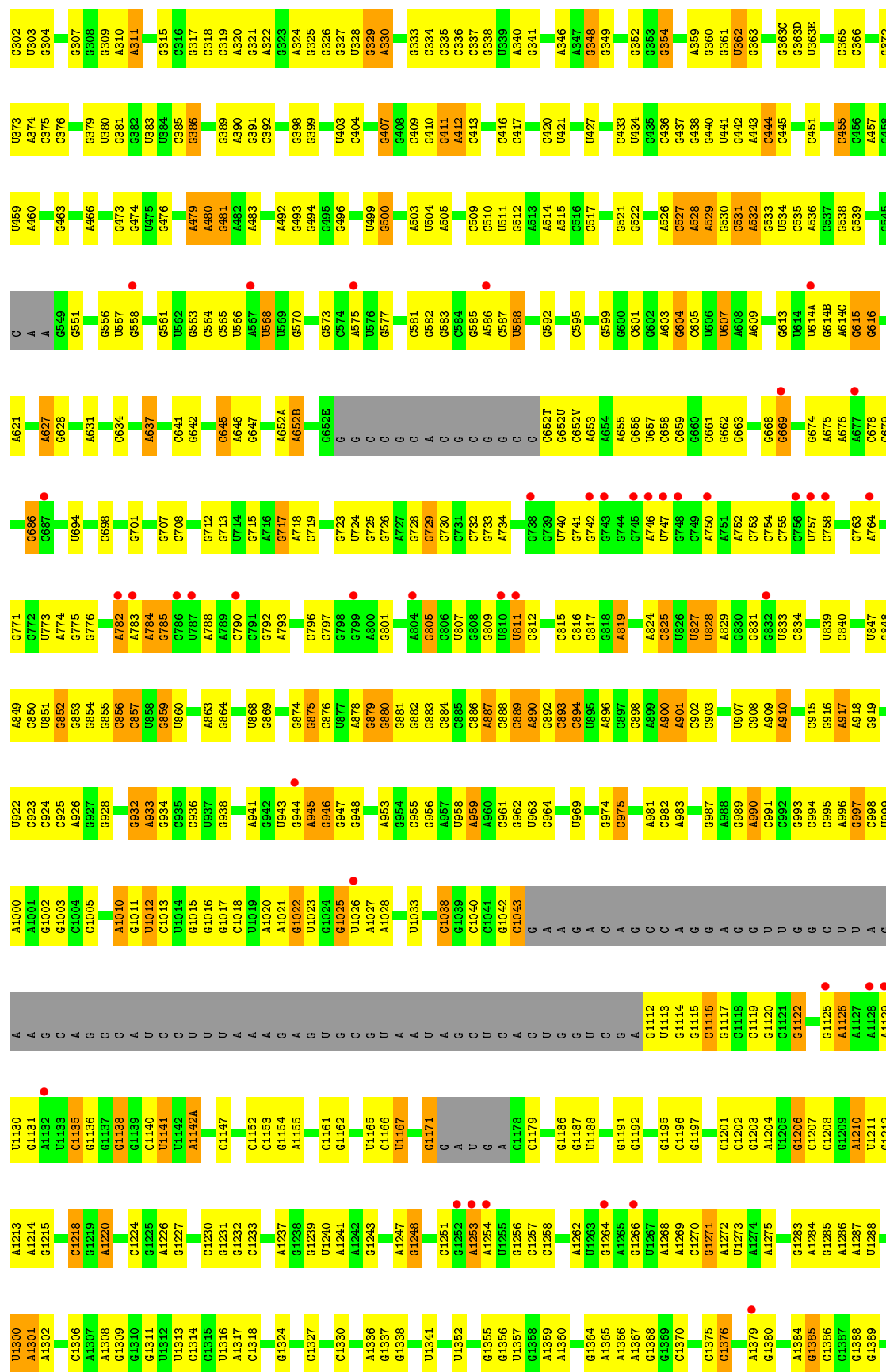
- Molecule 1: 23S Ribosomal RNA



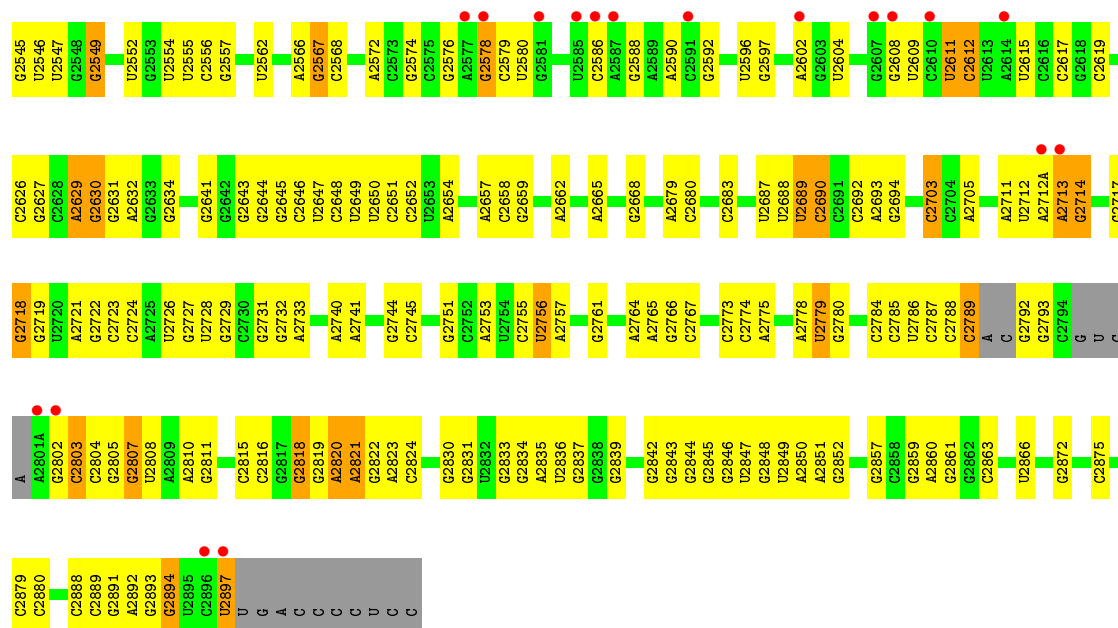






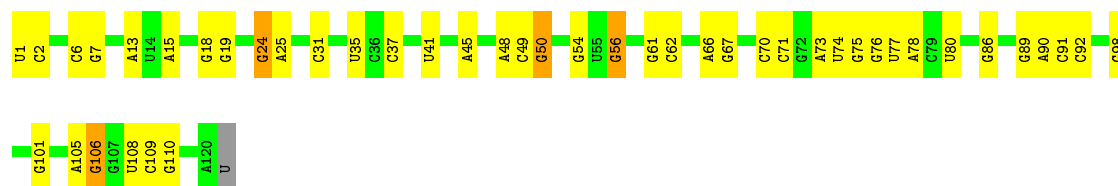


G2468	G2469	C2474	G2475	G2476	G2477	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2494	G2495	G2496	G2497	G2498	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2527	G2528	G2529	G2530	G2533	G2536	G2537	G2538	G2539	G2544																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C2395	G2396	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2419	G2420	G2421	G2422	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2439	G2440	G2441	G2442	G2443	G2446	G2447	G2448	G2449	G2450	G2454	G2455	G2456	G2457	G2462	G2463	G2464	G2465	G2466	G2467																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2351	G2352	G2353	G2354	G2355	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2388	G2389	G2390	G2391	G2392	G2393	G2394																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C2248	G2249	G2250	G2251	C2258	C2261	C2262	C2263	C2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2278	G2279	G2283	G2284	G2285	G2286	G2287	G2288	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2197	G2198	G2206	G2207	G2208	G2224	G2225	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2242	G2243	G2244																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G2018	G2019	U2022	G2023	G2024	G2025	G2026	G2027	G2030	G2031	G2032	G2033	G2036	G2037	G2038	G2039	G2040	U2041	G2042	G2043	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2061	G2062	G2066	G2067	G2068	G2069	G2070	G2071	U2074	U2075	G2078	U2079	U2086	G2087	G2088	U2089	G2090	U2091	U2092	G2093	G2094																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A1927	A1928	G1929	G1930	U1931	G1935	A1936	A1937	A1938	U1939	C1942	U1943	U1944	U1945	U1955	U1960	C1961	U1962	U1963	U1964	C1967	A1968	A1969	A1970	A1971	A1972	G1973	G1974	A1977	G1983	G1984	G1985	A1986	G1988	G1989	C1990	U1991	G1992	U1993	G1997	G1998	G1999	G2000	A2001	G2002	A2005	A2006	G2010	A2015	A2016	A2017	A2018	A2019																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G1811	G1812	G1813	G1814	G1815	G1816	G1817	A1821	G1827	G1828	A1829	G1835	G1838	G1839	G1843	G1846	A1847	A1848	A1853	A1854	G1858	A1859	A1860	A1861	G1862	G1865	A1877	G1878	C1882	G1883	A1889	A1890	G1894	G1899	A1900	G1906	A1913	C1914	U1915	A1916	C1920	G1921	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806



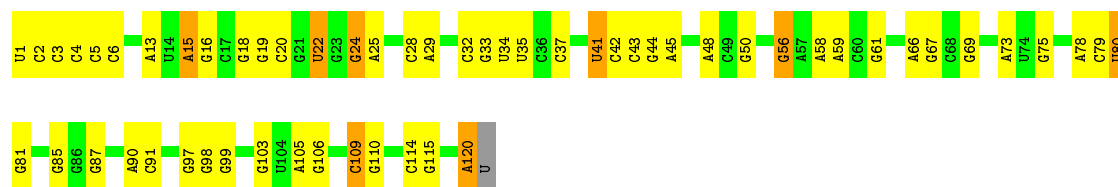
### • Molecule 2: 5S Ribosomal RNA

Chain 1B: 62% 34%



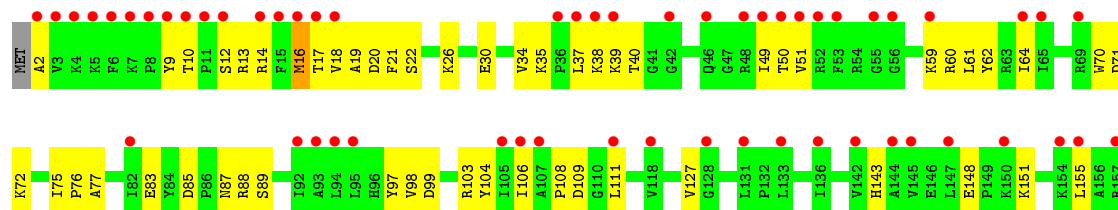
### • Molecule 2: 5S Ribosomal RNA

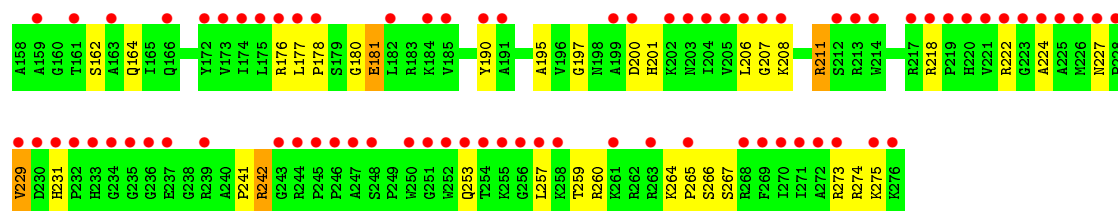
Chain 2B: 52% 40% 7%



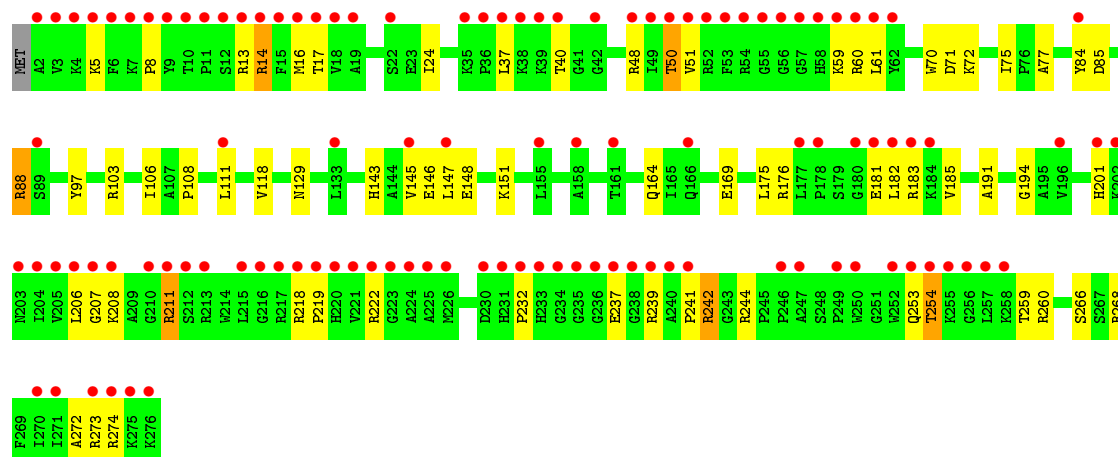
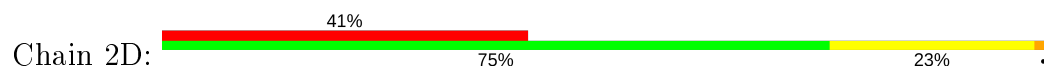
### • Molecule 3: 50S ribosomal protein L2

Chain 1D: 48% 67% 30%

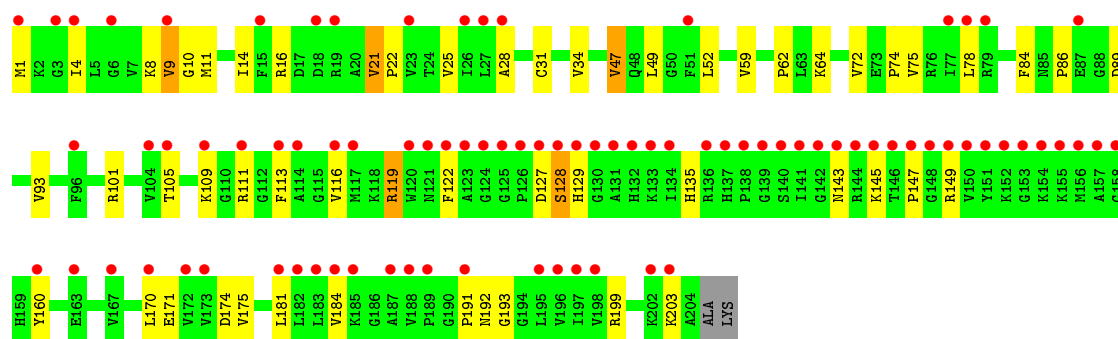
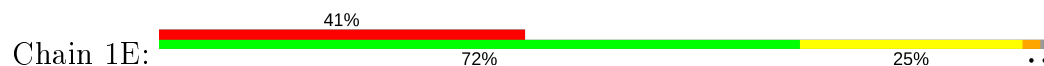




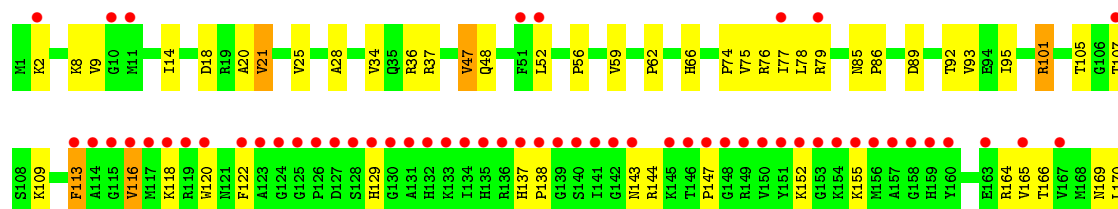
• Molecule 3: 50S ribosomal protein L2

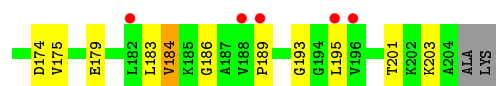


• Molecule 4: 50S ribosomal protein L3

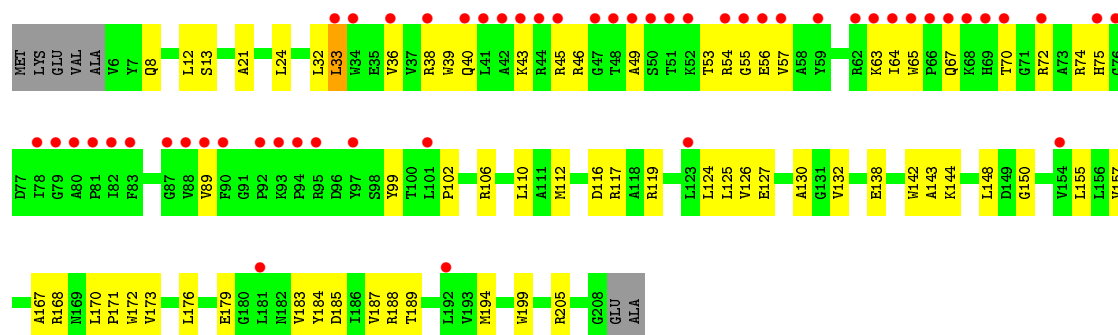


• Molecule 4: 50S ribosomal protein L3

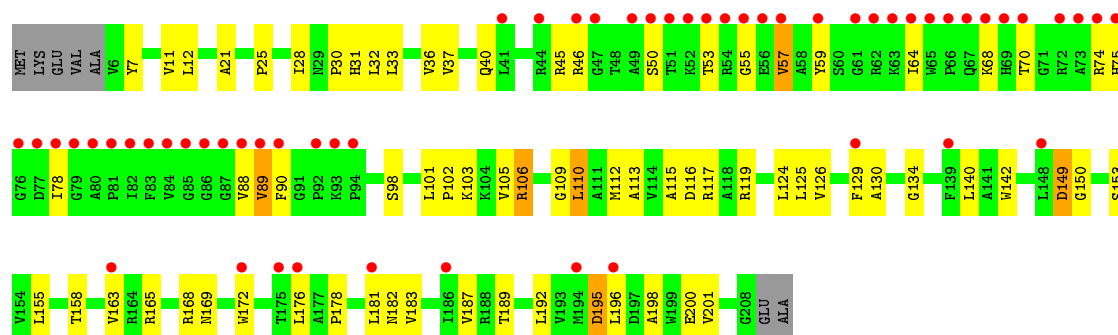




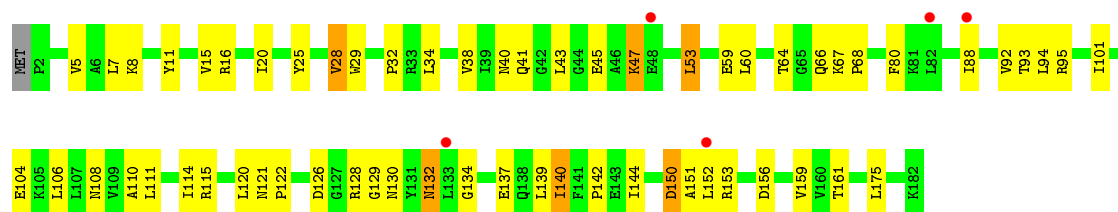
- Molecule 5: 50S ribosomal protein L4



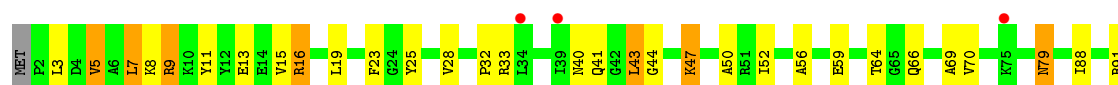
- Molecule 5: 50S ribosomal protein L4

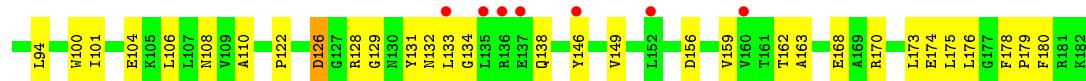


- Molecule 6: 50S ribosomal protein L5

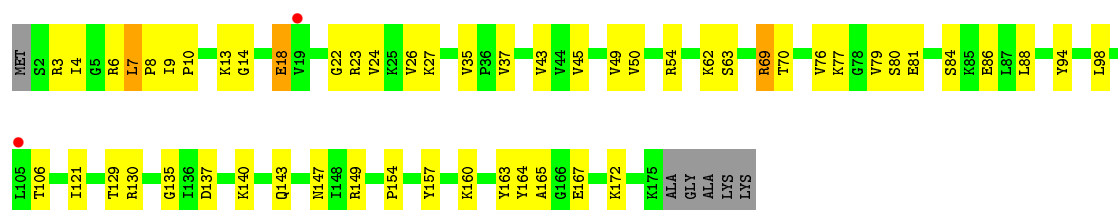


- Molecule 6: 50S ribosomal protein L5

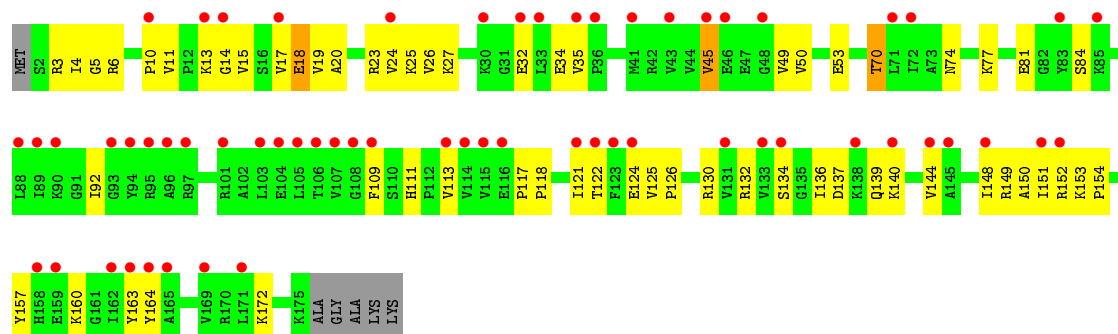




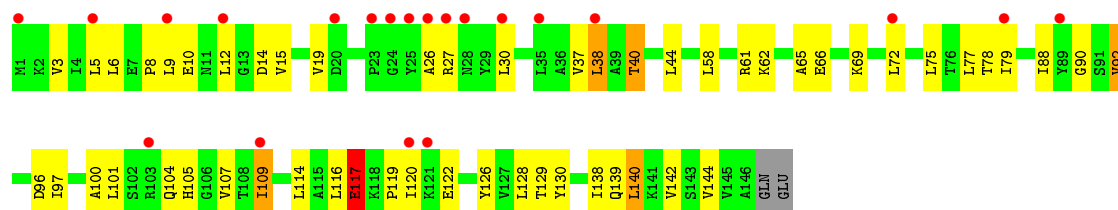
- Molecule 7: 50S ribosomal protein L6



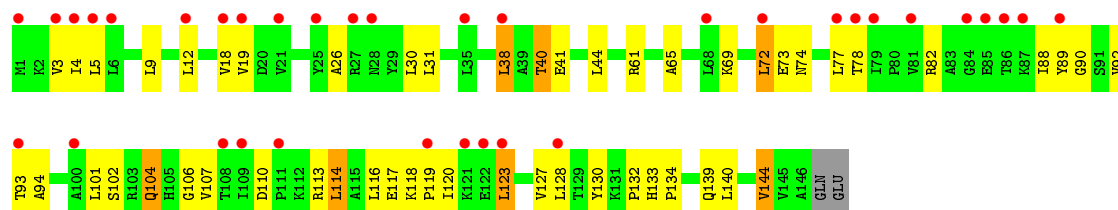
- Molecule 7: 50S ribosomal protein L6

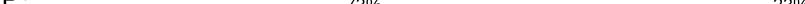


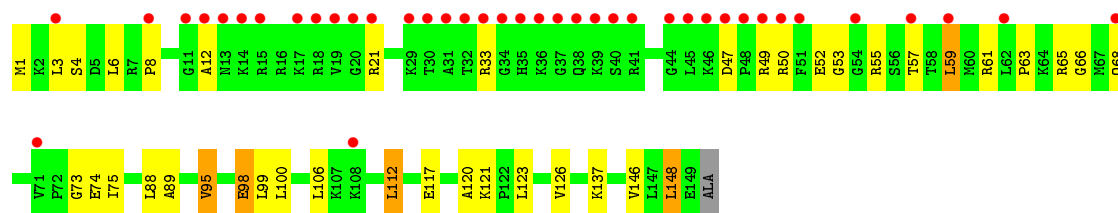
- Molecule 8: 50S ribosomal protein L9



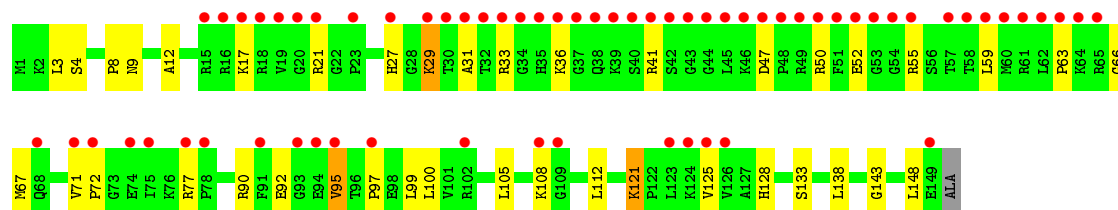
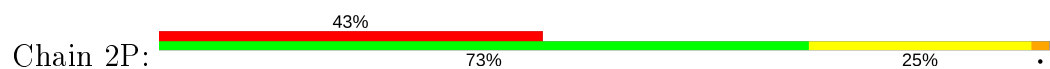
- Molecule 8: 50S ribosomal protein L9



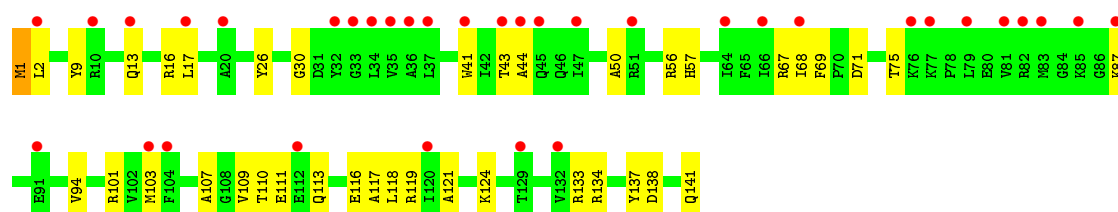
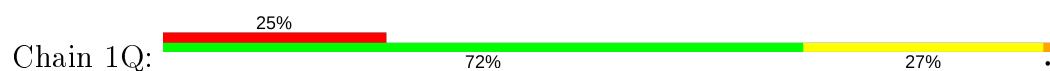
- Chain 1P:  27% 73% 23%



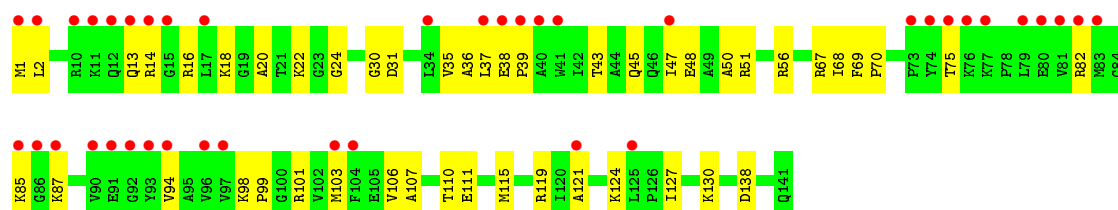
• Molecule 11: 50S ribosomal protein L15



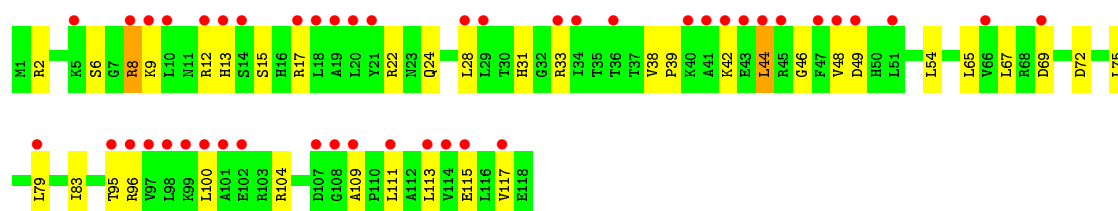
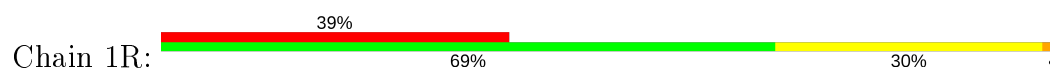
• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16

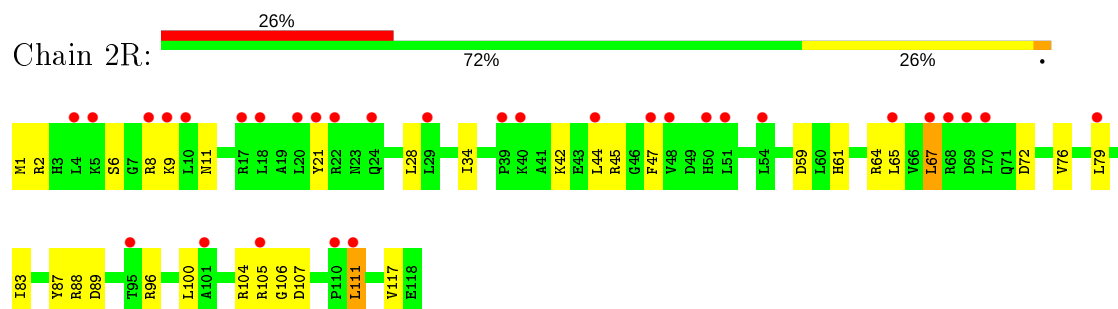


• Molecule 13: 50S ribosomal protein L17

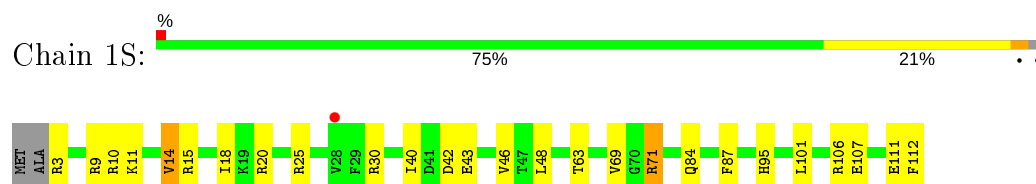




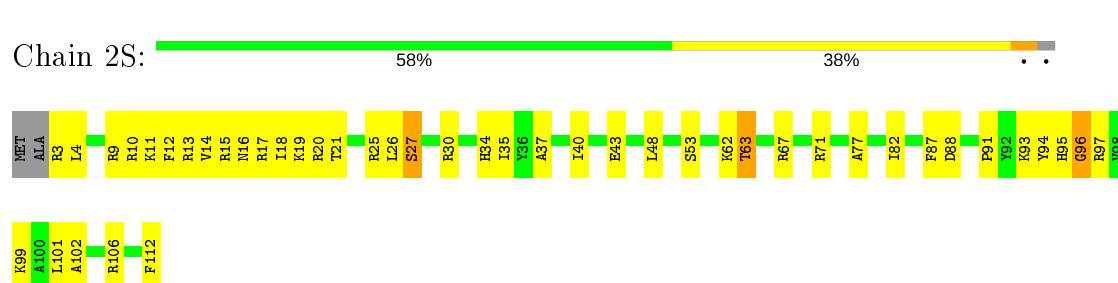
- Molecule 13: 50S ribosomal protein L17



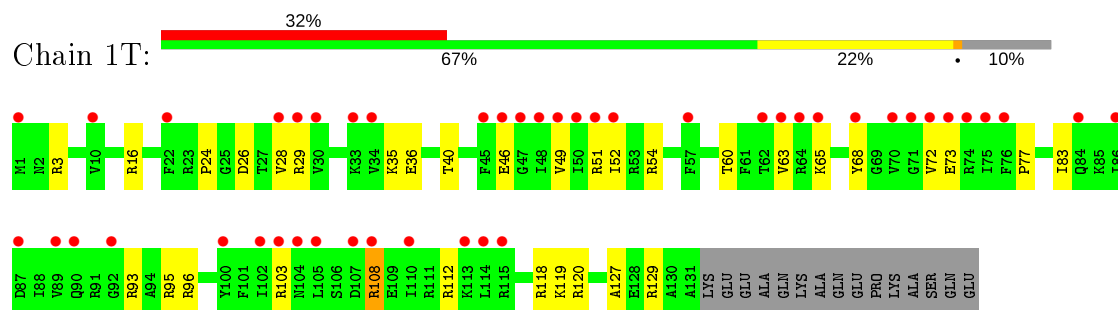
- Molecule 14: 50S ribosomal protein L18



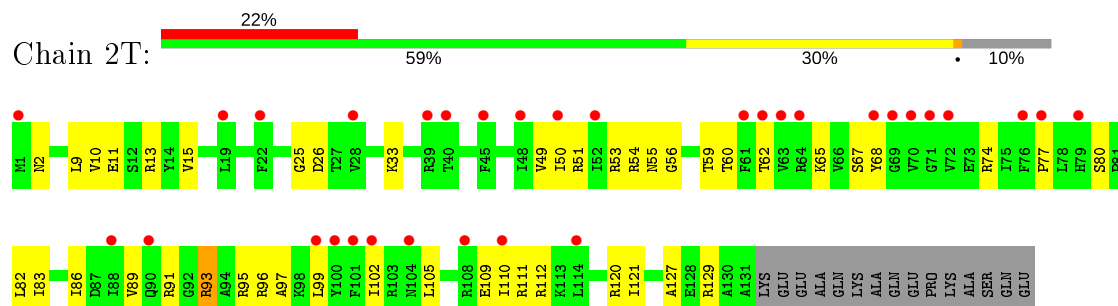
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

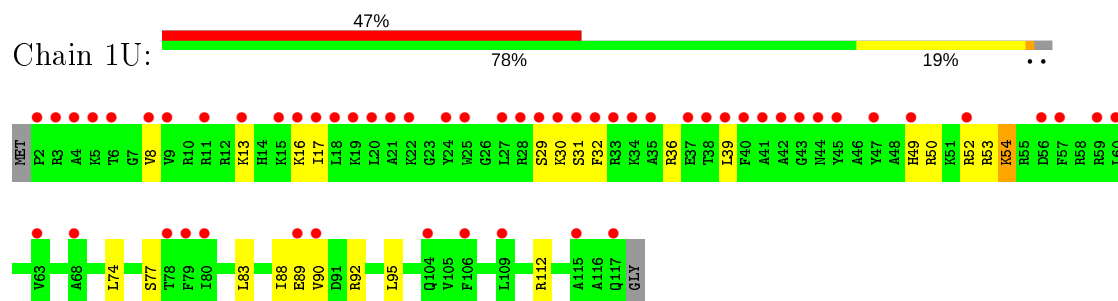


- Molecule 15: 50S ribosomal protein L19



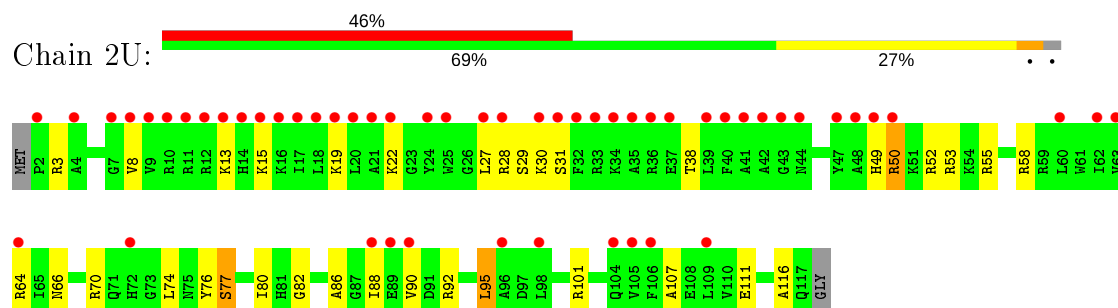
- Molecule 16: 50S ribosomal protein L20

Chain 1U:



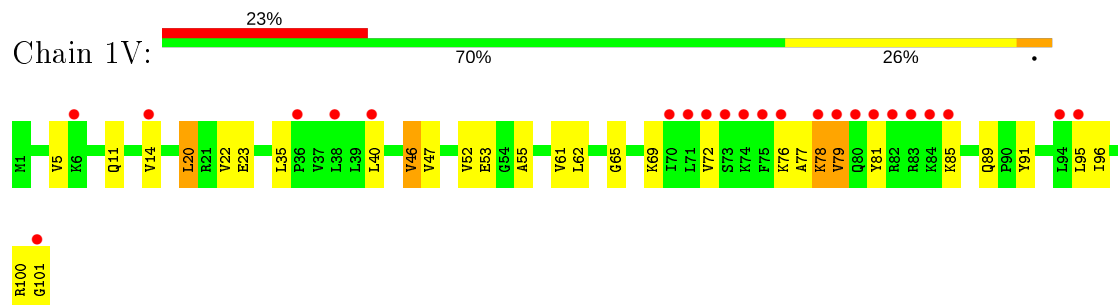
- Molecule 16: 50S ribosomal protein L20

Chain 2U:



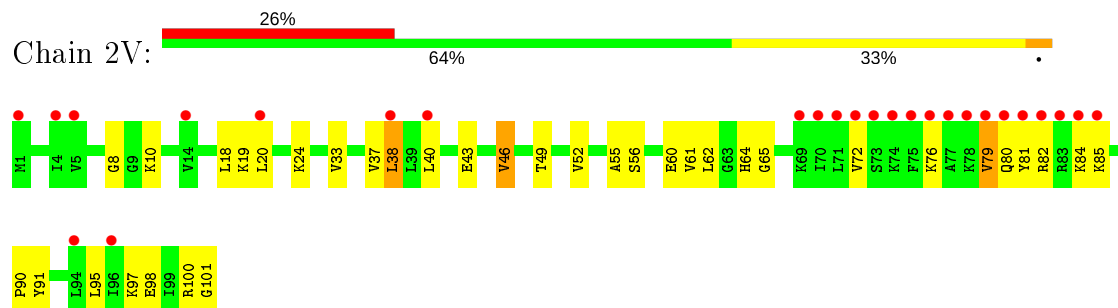
- Molecule 17: 50S ribosomal protein L21

Chain 1V:



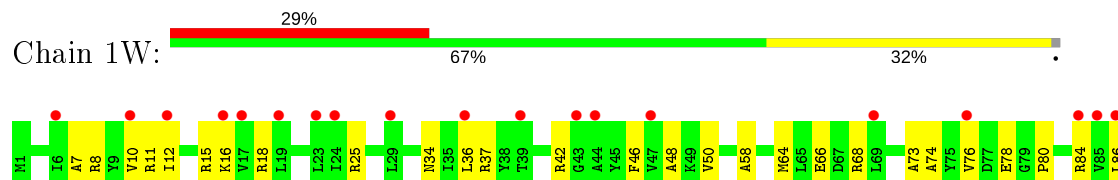
- Molecule 17: 50S ribosomal protein L21

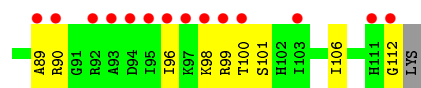
Chain 2V:



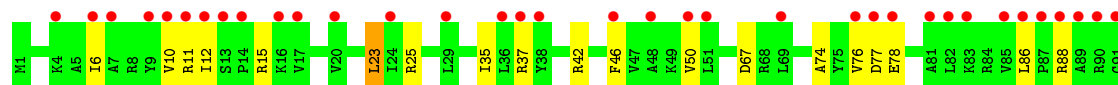
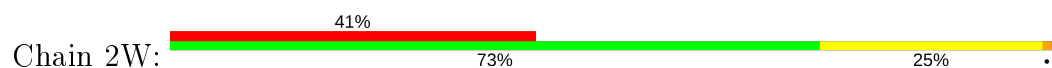
- Molecule 18: 50S ribosomal protein L22

Chain 1W:

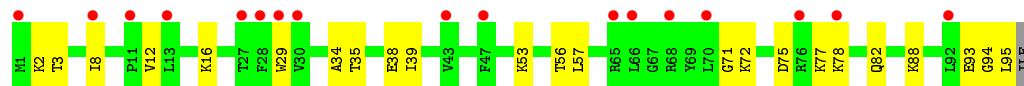
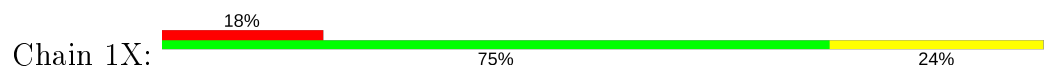




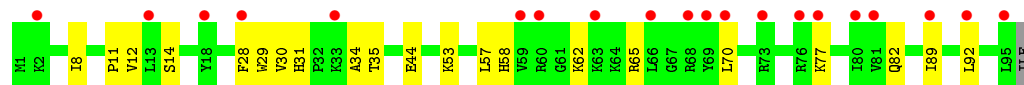
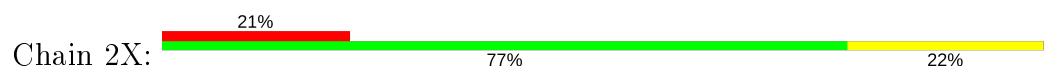
- Molecule 18: 50S ribosomal protein L22



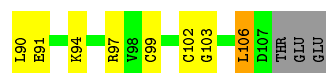
- Molecule 19: 50S ribosomal protein L23



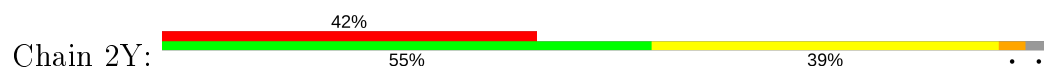
- Molecule 19: 50S ribosomal protein L23

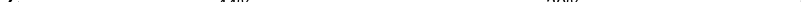


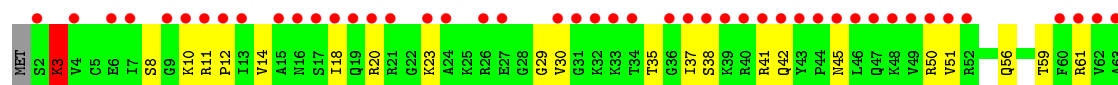
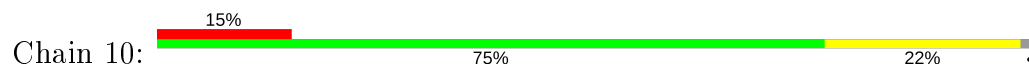
- Molecule 20: 50S ribosomal protein L24

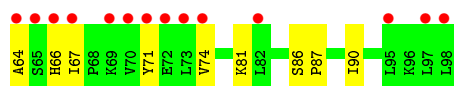


- Molecule 20: 50S ribosomal protein L24

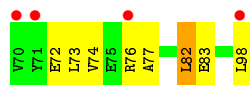
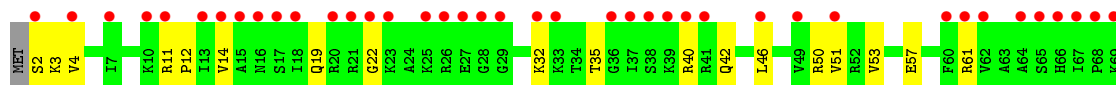
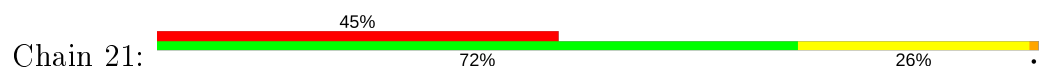


- Chain 1Z: 

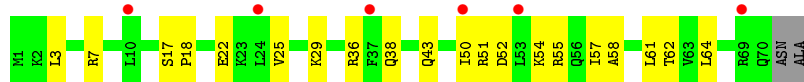




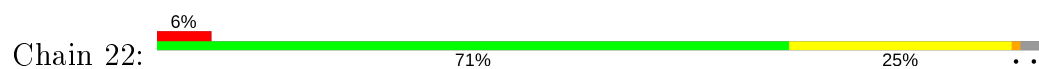
- Molecule 23: 50S ribosomal protein L28



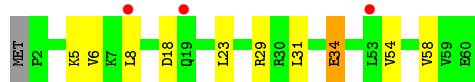
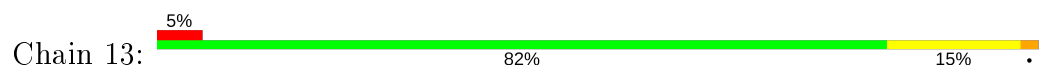
- Molecule 24: 50S ribosomal protein L29



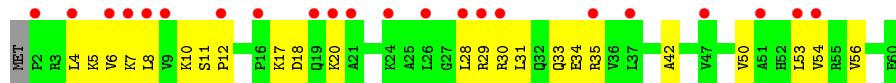
- Molecule 24: 50S ribosomal protein L29



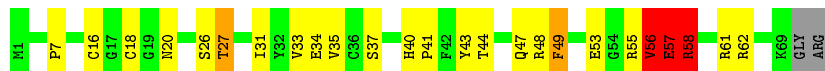
- Molecule 25: 50S ribosomal protein L30



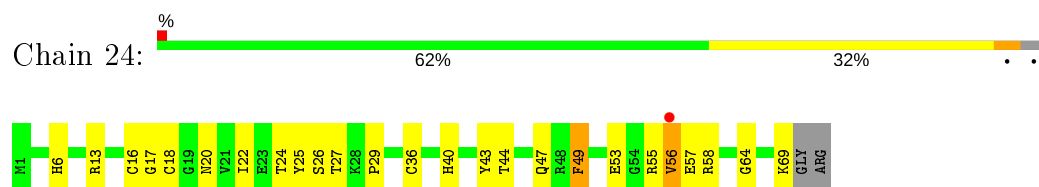
- Molecule 25: 50S ribosomal protein L30



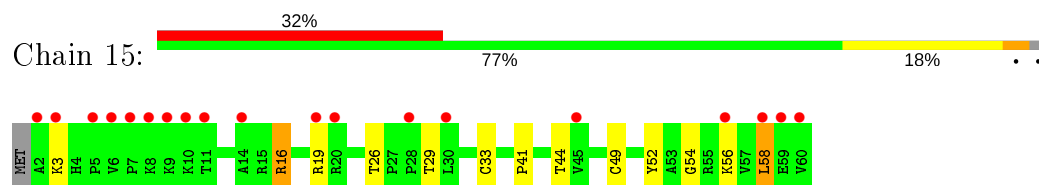
- Molecule 26: 50S ribosomal protein L31



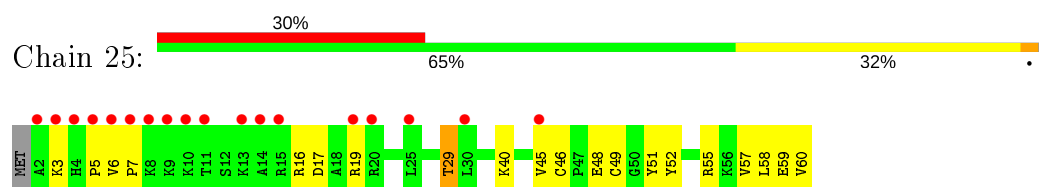
- Molecule 26: 50S ribosomal protein L31



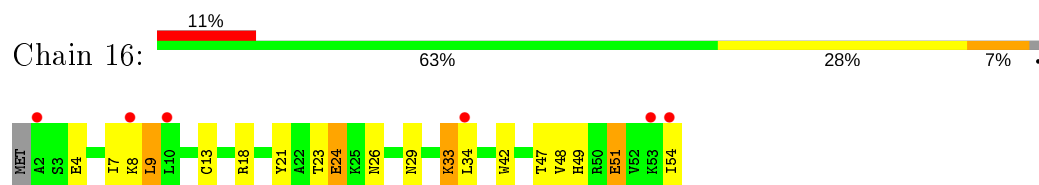
- Molecule 27: 50S ribosomal protein L32



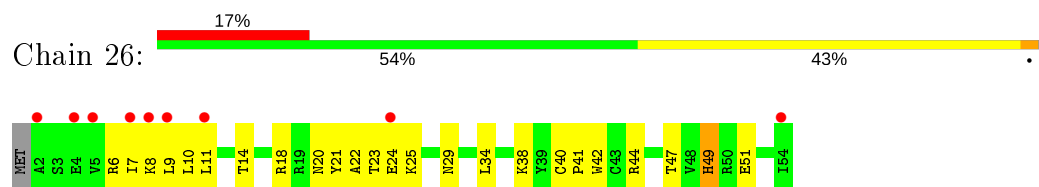
- Molecule 27: 50S ribosomal protein L32



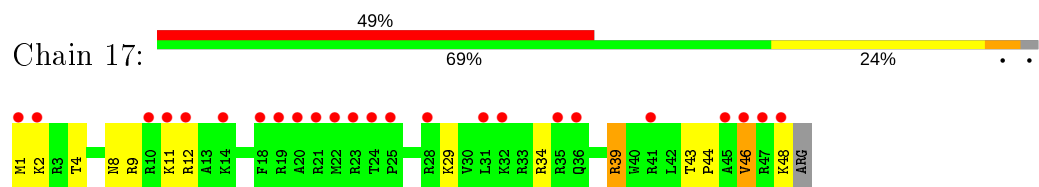
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

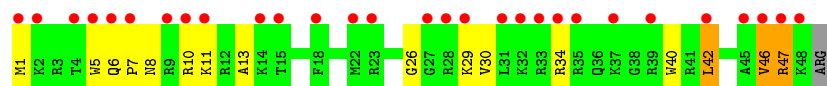


- Molecule 29: 50S ribosomal protein L34

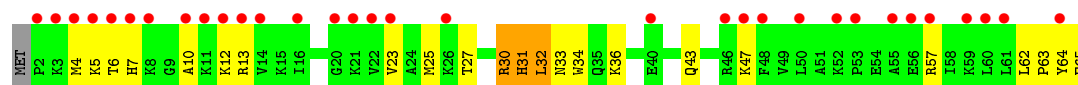


- Molecule 29: 50S ribosomal protein L34

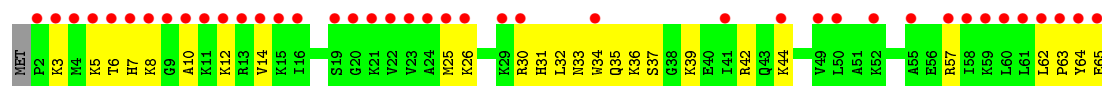




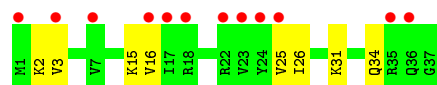
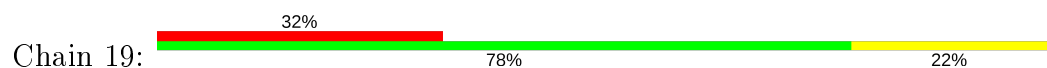
- Molecule 30: 50S ribosomal protein L35



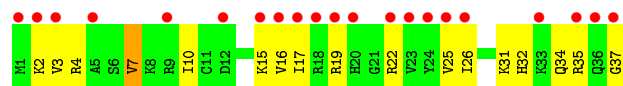
- Molecule 30: 50S ribosomal protein L35



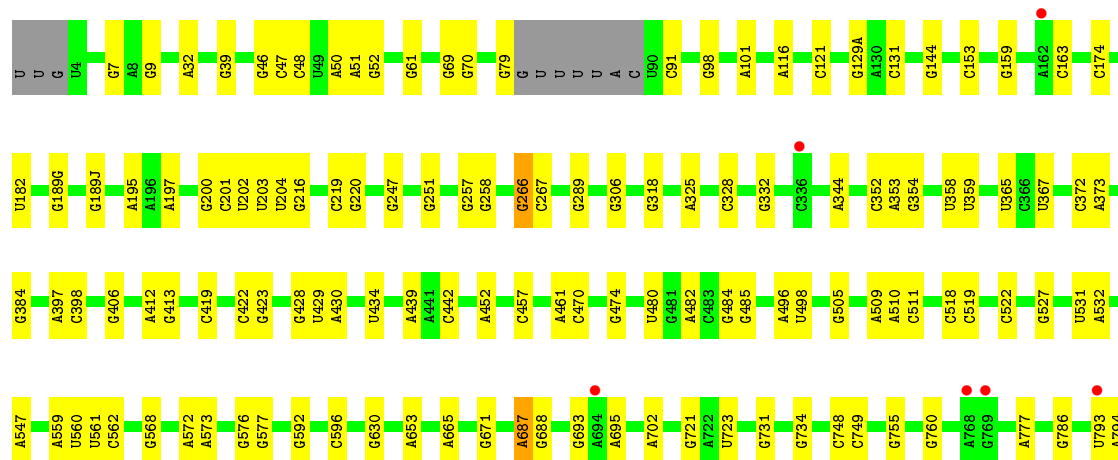
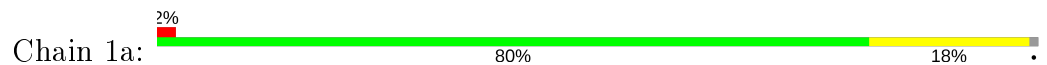
- Molecule 31: 50S ribosomal protein L36

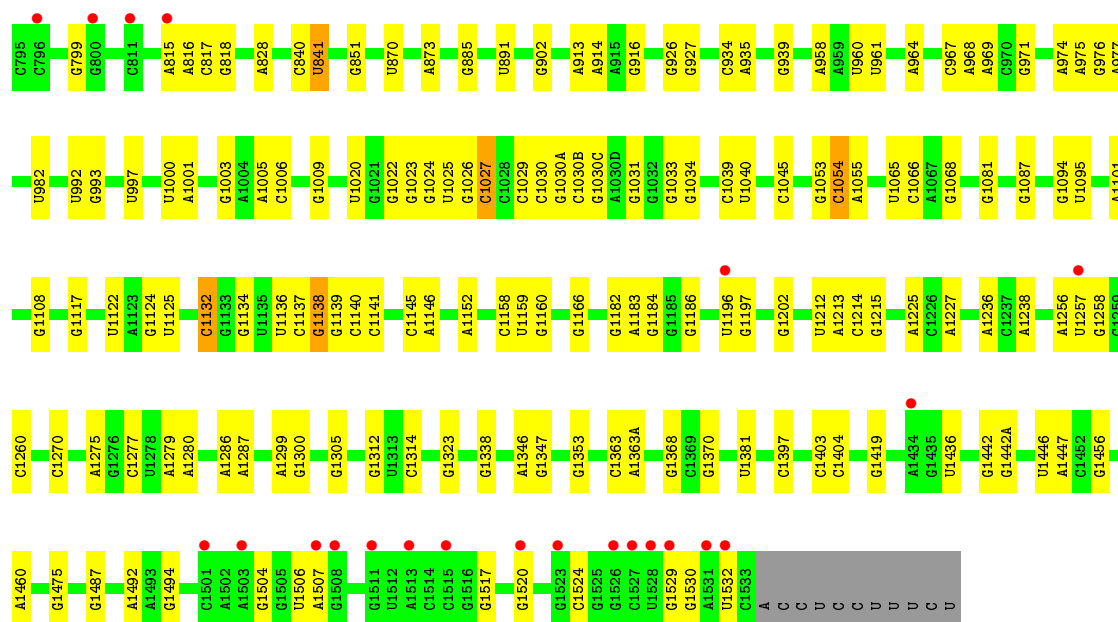


- Molecule 31: 50S ribosomal protein L36

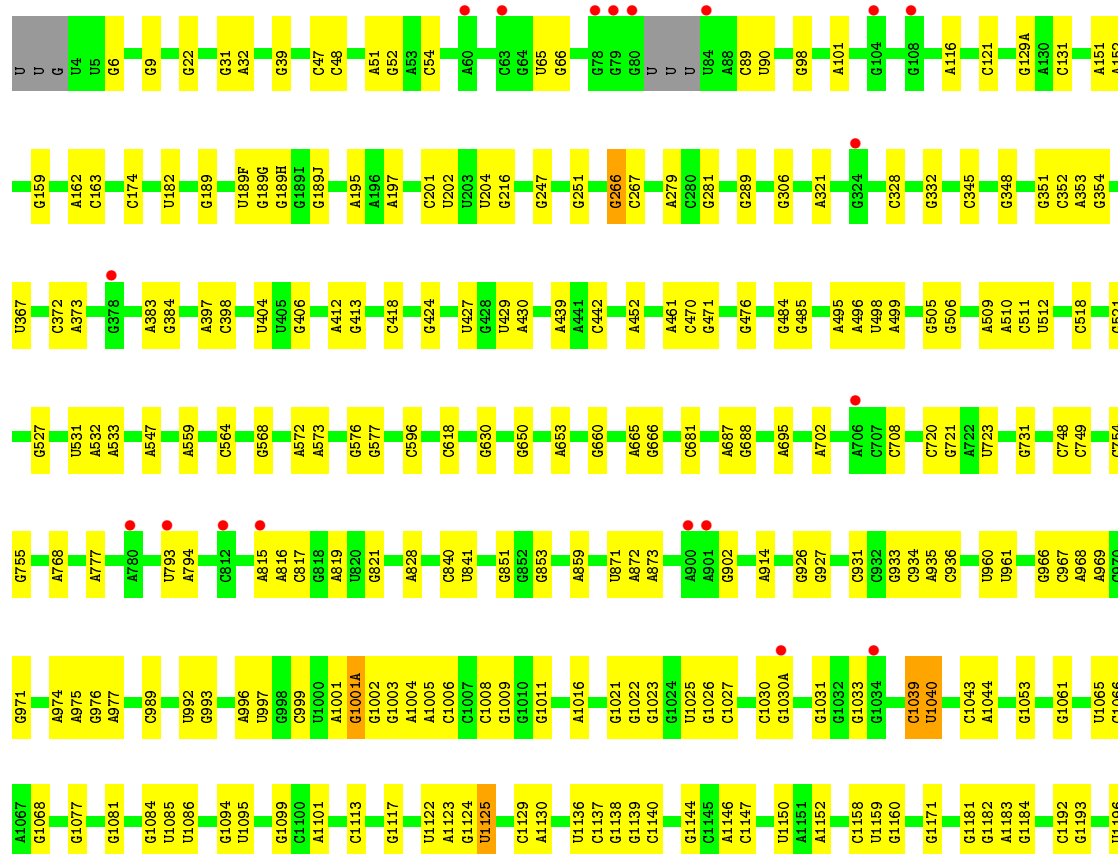
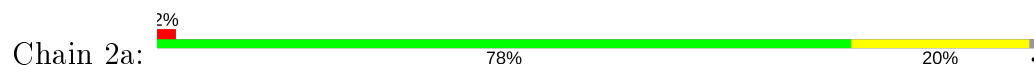


- Molecule 32: 16S Ribosomal RNA

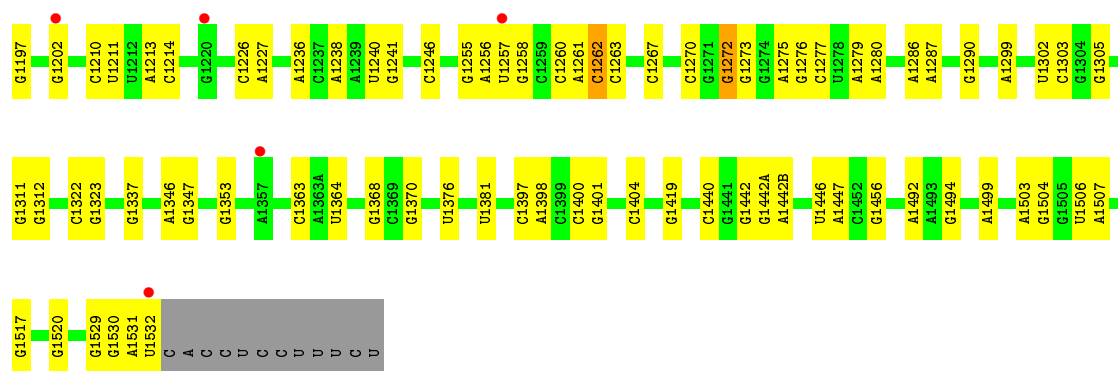




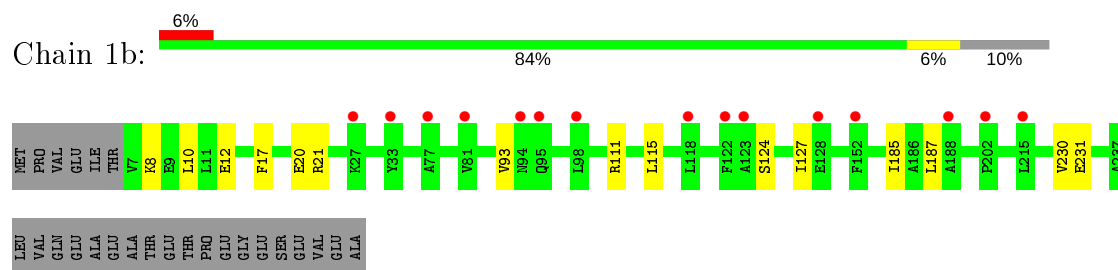
• Molecule 32: 16S Ribosomal RNA



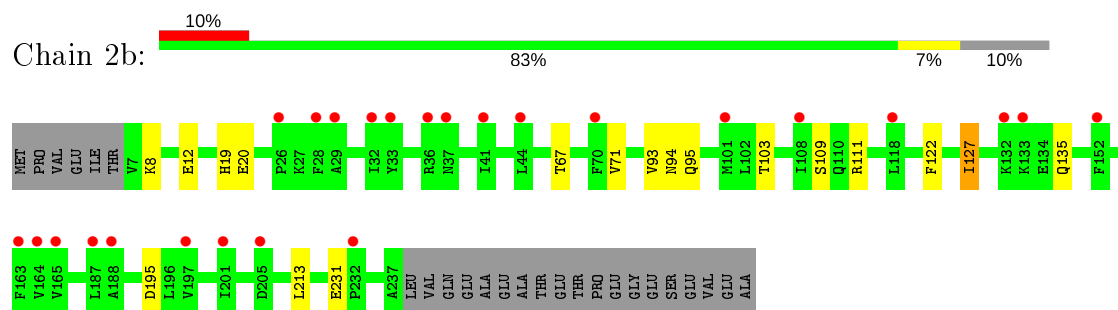




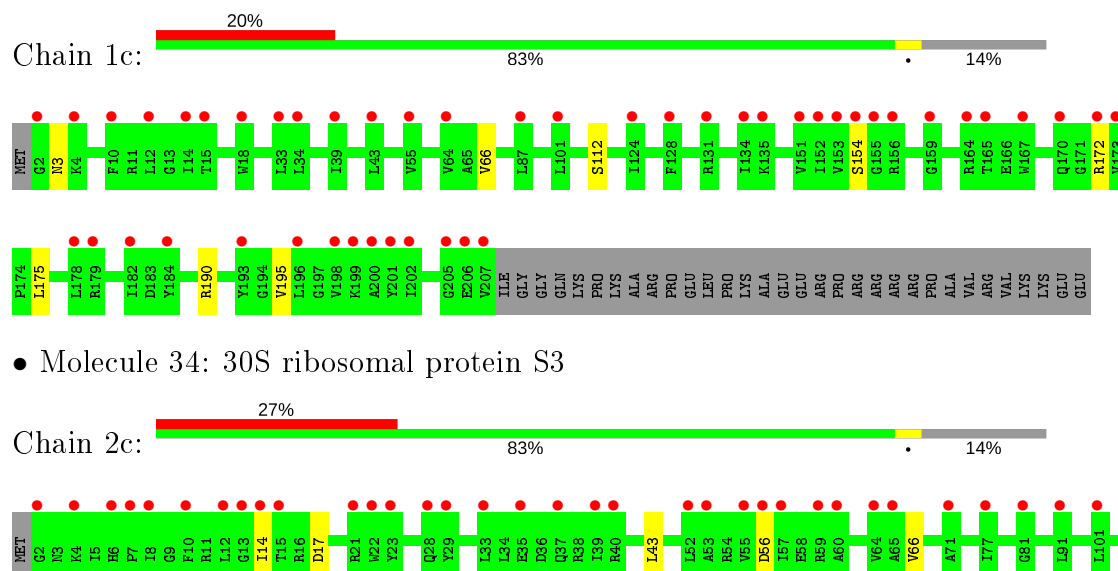
• Molecule 33: 30S ribosomal protein S2



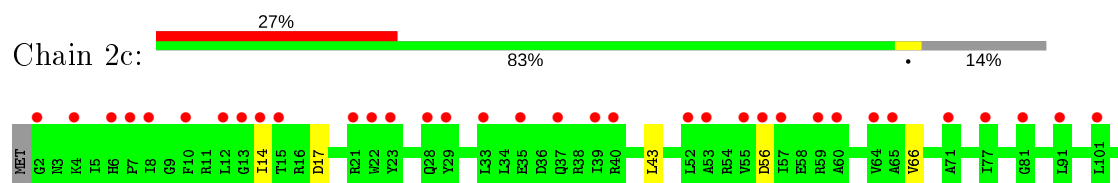
• Molecule 33: 30S ribosomal protein S2

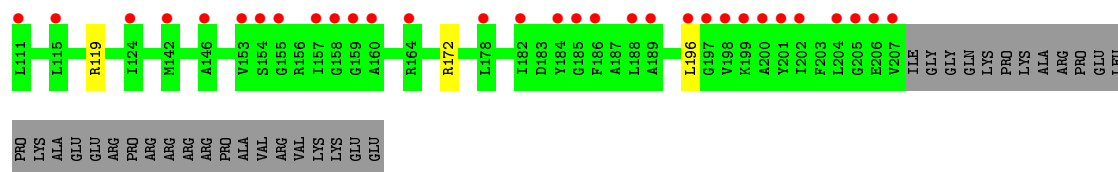


• Molecule 34: 30S ribosomal protein S3

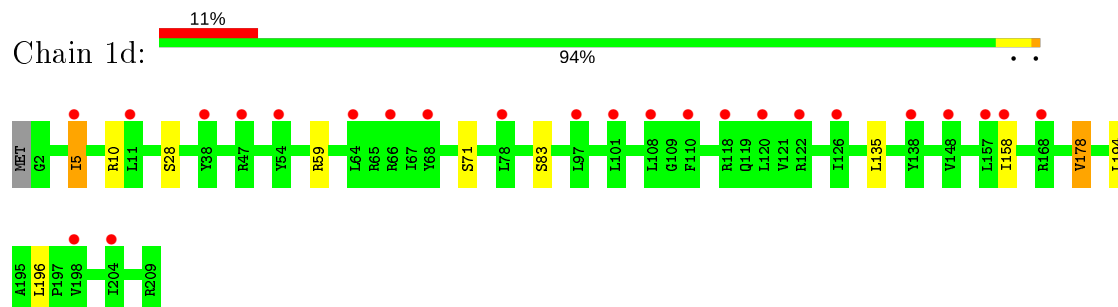


• Molecule 34: 30S ribosomal protein S3

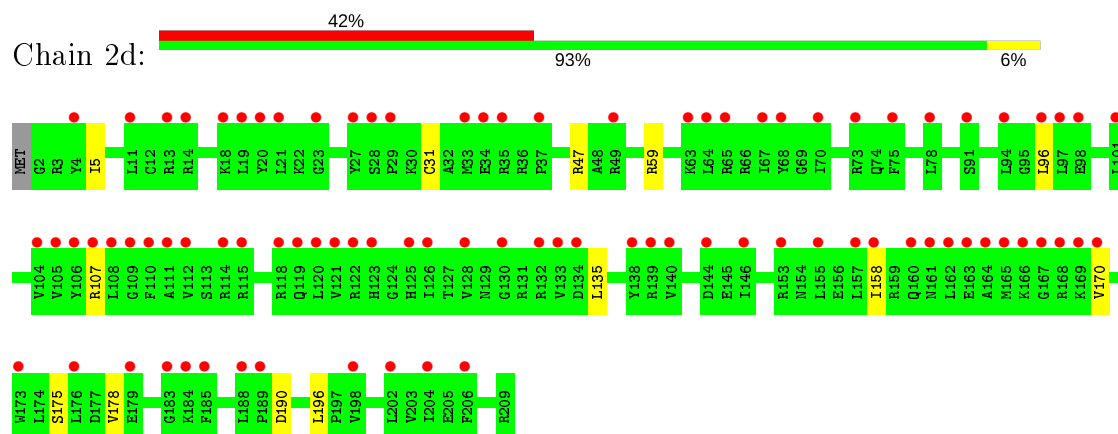




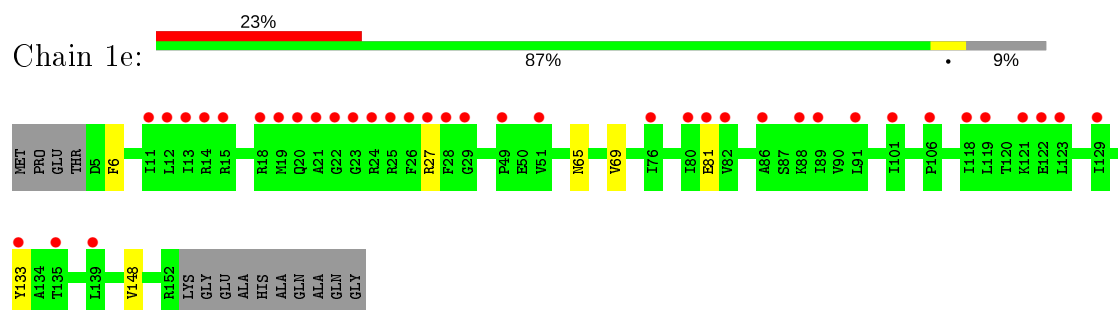
- Molecule 35: 30S ribosomal protein S4



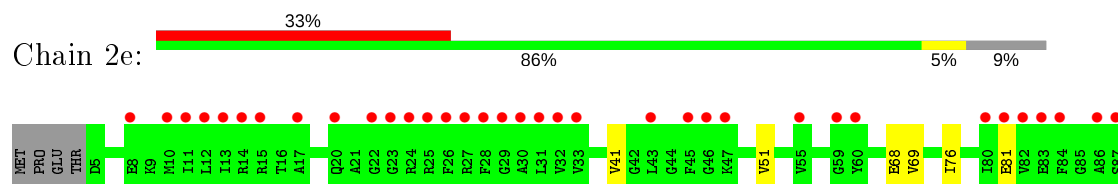
- Molecule 35: 30S ribosomal protein S4

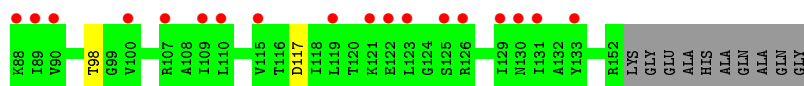


- Molecule 36: 30S ribosomal protein S5

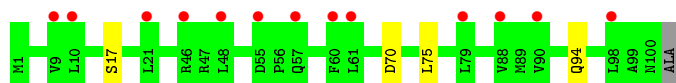


- Molecule 36: 30S ribosomal protein S5





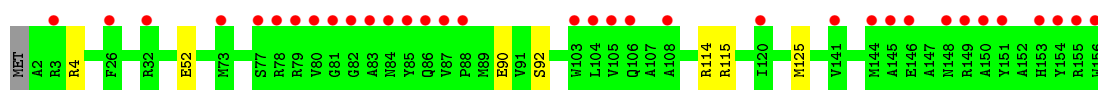
- Molecule 37: 30S ribosomal protein S6



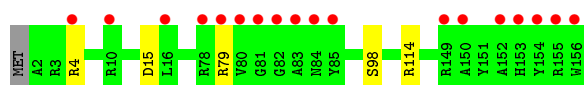
- Molecule 37: 30S ribosomal protein S6



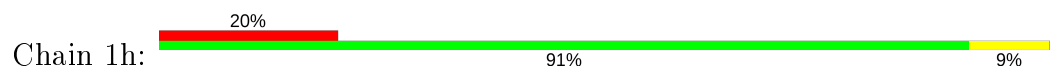
- Molecule 38: 30S ribosomal protein S7



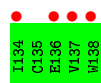
- Molecule 38: 30S ribosomal protein S7

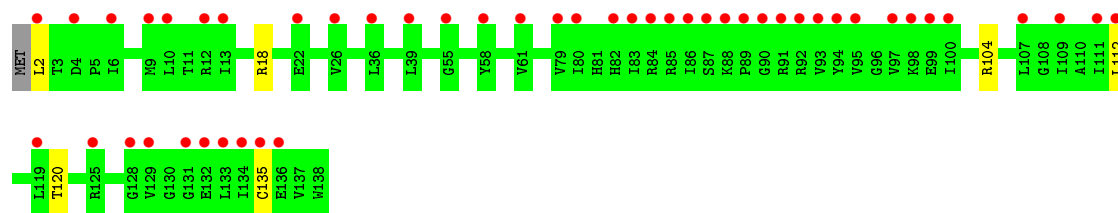


- Molecule 39: 30S ribosomal protein S8

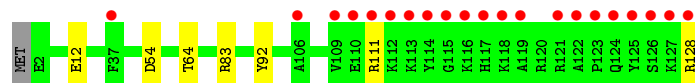


- Molecule 39: 30S ribosomal protein S8

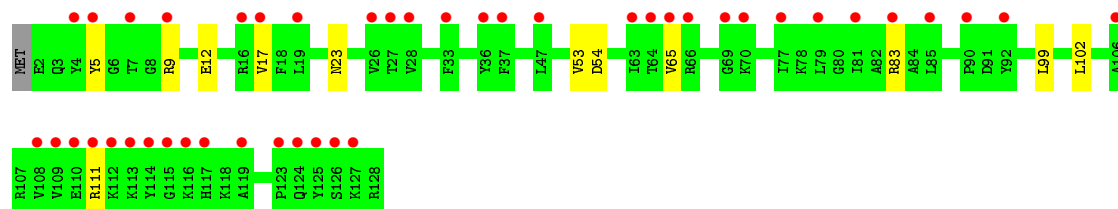
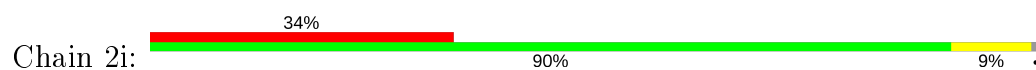




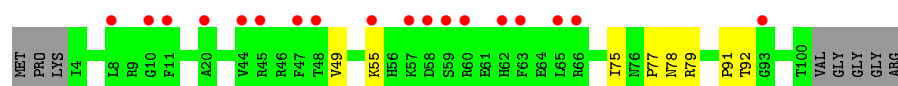
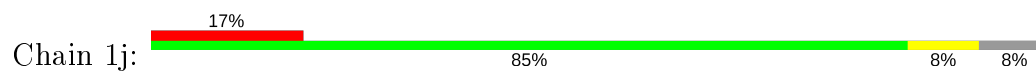
- Molecule 40: 30S ribosomal protein S9



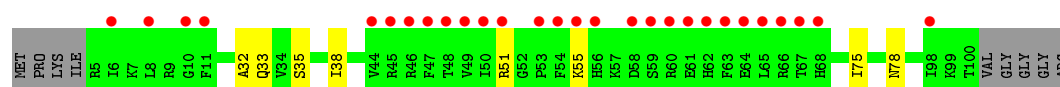
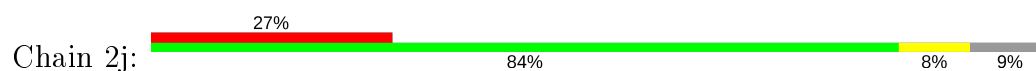
- Molecule 40: 30S ribosomal protein S9



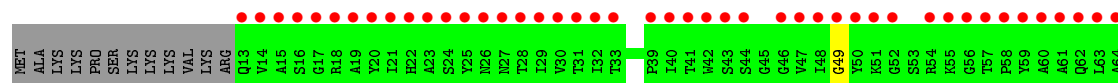
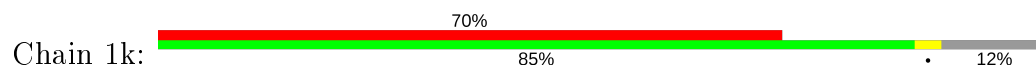
- Molecule 41: 30S ribosomal protein S10

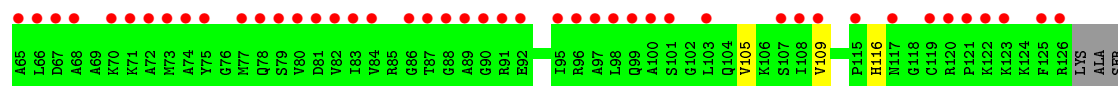


- Molecule 41: 30S ribosomal protein S10

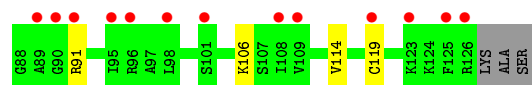
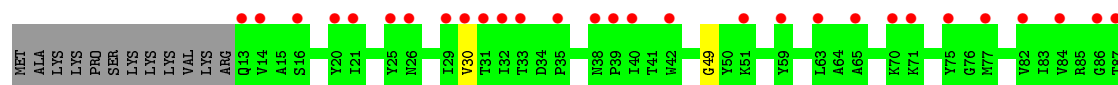
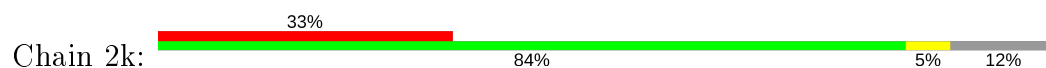


- Molecule 42: 30S ribosomal protein S11

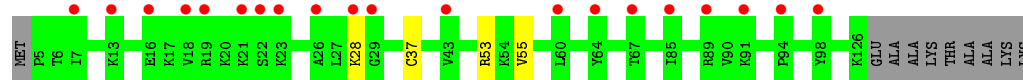
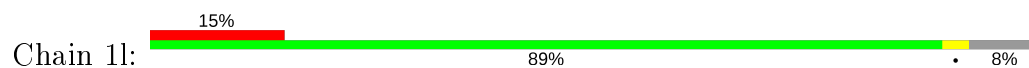




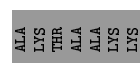
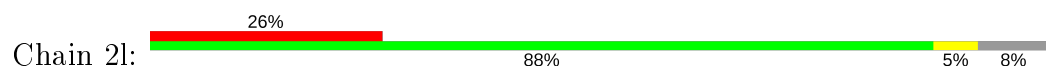
- Molecule 42: 30S ribosomal protein S11



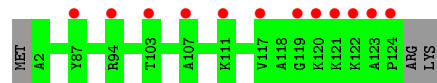
- Molecule 43: 30S ribosomal protein S12



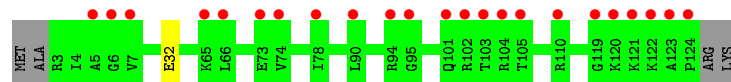
- Molecule 43: 30S ribosomal protein S12



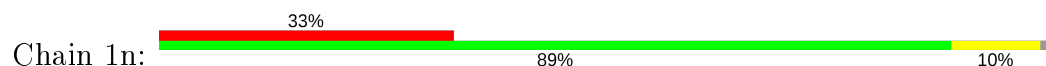
- Molecule 44: 30S ribosomal protein S13

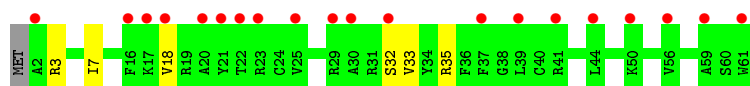


- Molecule 44: 30S ribosomal protein S13

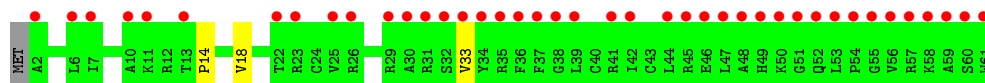


- Molecule 45: 30S ribosomal protein S14 type Z

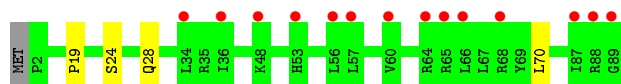




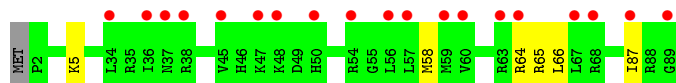
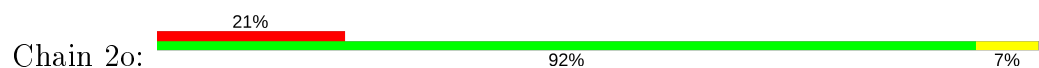
- Molecule 45: 30S ribosomal protein S14 type Z



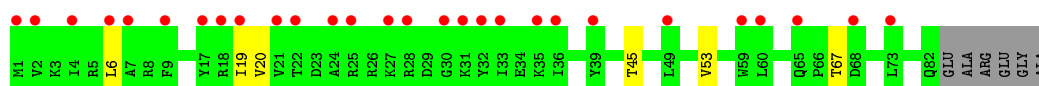
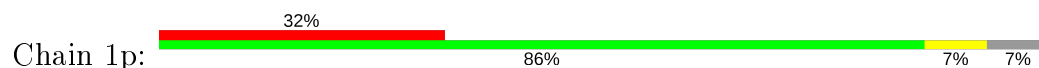
- Molecule 46: 30S ribosomal protein S15



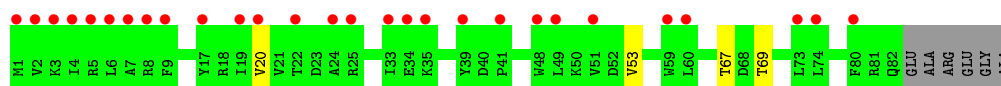
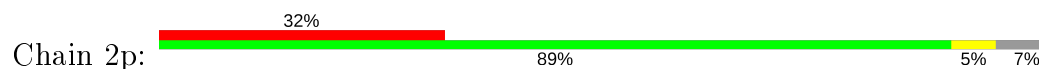
- Molecule 46: 30S ribosomal protein S15



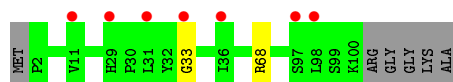
- Molecule 47: 30S ribosomal protein S16



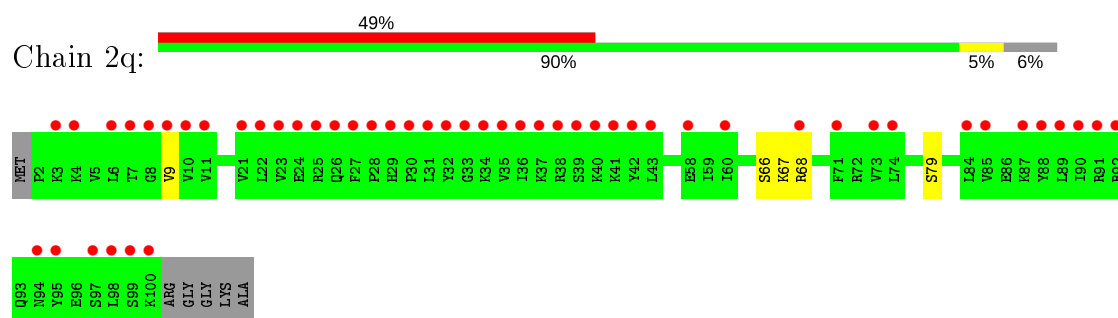
- Molecule 47: 30S ribosomal protein S16



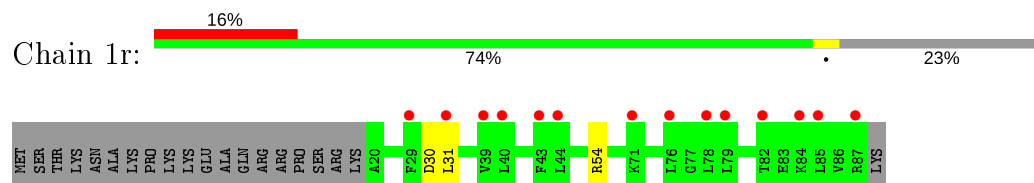
- Molecule 48: 30S ribosomal protein S17



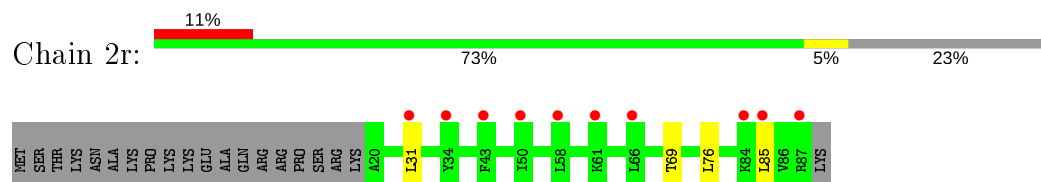
- Molecule 48: 30S ribosomal protein S17



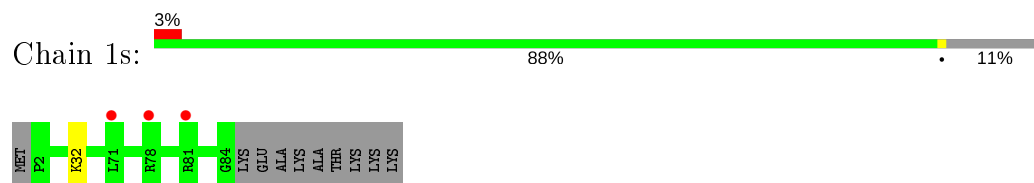
- Molecule 49: 30S ribosomal protein S18



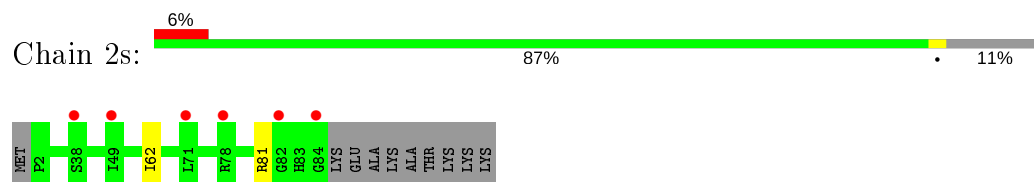
- Molecule 49: 30S ribosomal protein S18



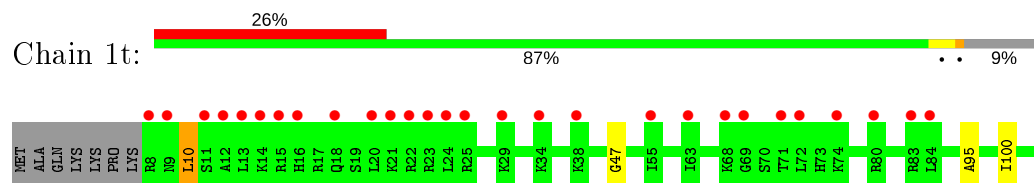
- Molecule 50: 30S ribosomal protein S19



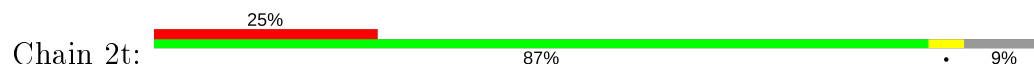
- Molecule 50: 30S ribosomal protein S19

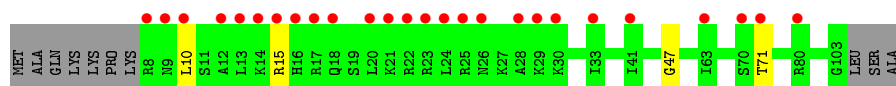


- Molecule 51: 30S ribosomal protein S20

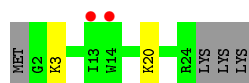
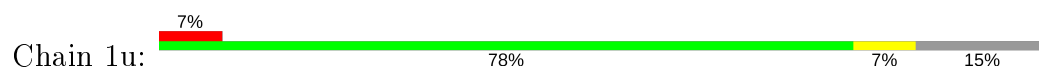


- Molecule 51: 30S ribosomal protein S20

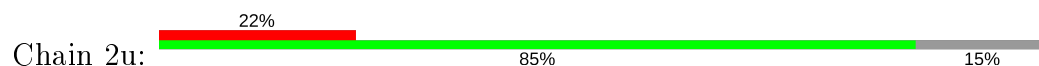




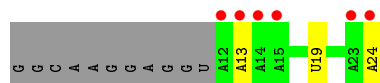
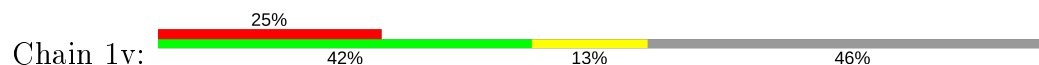
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



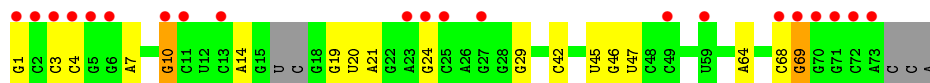
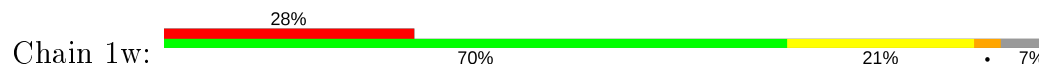
- Molecule 53: mRNA



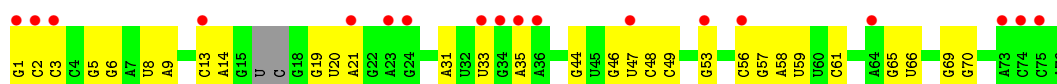
- Molecule 53: mRNA



- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

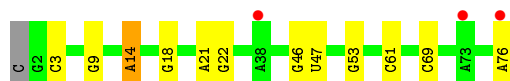
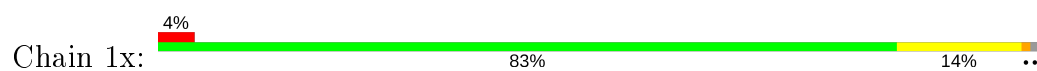




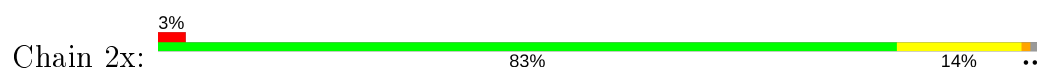
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.73Å 445.10Å 613.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	360.30 – 2.95 360.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (360.30-2.95) 99.7 (360.30-2.95)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.238 , 0.292 0.238 , 0.292	Depositor DCC
$R_{free}$ test set	59210 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	295398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, PSU

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	0.30	0/69009	0.79	27/107712 (0.0%)
1	2A	0.26	0/67293	0.79	22/105034 (0.0%)
2	1B	0.31	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.28	0/2186	0.48	0/2944
3	2D	0.27	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.47	0/2149
4	2E	0.26	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.45	0/2193
5	2F	0.27	0/1615	0.43	0/2188
6	1G	0.26	0/1448	0.45	0/1957
6	2G	0.26	0/1453	0.44	0/1963
7	1H	0.28	0/1356	0.46	0/1834
7	2H	0.26	0/1356	0.45	0/1834
8	1I	0.25	0/1112	0.45	0/1514
8	2I	0.26	0/1079	0.47	0/1475
9	1N	0.27	0/1144	0.45	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.49	0/1269
10	2O	0.28	0/943	0.49	0/1269
11	1P	0.29	0/1152	0.51	0/1533
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.29	0/1143	0.45	0/1527
12	2Q	0.26	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.45	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.26	0/883	0.42	0/1176
14	2S	0.27	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.46	0/1468
16	1U	0.26	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.25	0/977	0.40	0/1301
17	1V	0.30	0/782	0.51	0/1049
17	2V	0.27	0/782	0.50	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.26	0/897	0.43	0/1205
19	1X	0.29	0/764	0.50	0/1025
19	2X	0.25	0/764	0.44	0/1025
20	1Y	0.29	0/819	0.47	0/1095
20	2Y	0.28	0/819	0.47	0/1095
21	1Z	0.26	0/1267	0.46	0/1717
21	2Z	0.26	0/1299	0.47	0/1763
22	10	0.27	0/662	0.46	0/881
22	20	0.27	0/662	0.47	0/881
23	11	0.29	0/762	0.47	0/1014
23	21	0.27	0/762	0.48	0/1014
24	12	0.25	0/590	0.40	0/781
24	22	0.25	0/590	0.38	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.25	0/469	0.42	0/630
26	14	0.28	0/565	0.51	0/761
26	24	0.30	0/545	0.51	0/737
27	15	0.26	0/469	0.47	0/635
27	25	0.29	0/469	0.44	0/635
28	16	0.29	0/460	0.46	0/613
28	26	0.25	0/456	0.46	0/608
29	17	0.25	0/426	0.43	0/561
29	27	0.24	0/426	0.46	0/561
30	18	0.27	0/525	0.45	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.31	0/310	0.49	0/407
31	29	0.28	0/310	0.51	0/407
32	1a	0.26	0/35795	0.82	25/55864 (0.0%)
32	2a	0.27	2/35886 (0.0%)	0.85	31/56005 (0.1%)
33	1b	0.26	0/1881	0.46	0/2542
33	2b	0.26	0/1860	0.46	0/2518
34	1c	0.28	0/1572	0.44	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.26	0/1685	0.43	0/2262
35	2d	0.25	0/1704	0.43	0/2284
36	1e	0.26	0/1145	0.48	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.27	0/823	0.47	0/1115
37	2f	0.27	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.25	0/1250	0.43	0/1679
38	2g	0.25	0/1254	0.41	0/1683
39	1h	0.26	0/1108	0.45	0/1494
39	2h	0.26	0/1108	0.44	0/1494
40	1i	0.27	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.49	0/1343
41	1j	0.25	0/722	0.48	0/982
41	2j	0.26	0/727	0.47	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.28	0/848	0.45	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.26	0/969	0.46	0/1302
44	2m	0.25	0/961	0.47	0/1291
45	1n	0.28	0/501	0.42	0/664
45	2n	0.26	0/501	0.44	0/664
46	1o	0.24	0/739	0.41	0/985
46	2o	0.24	0/739	0.42	0/985
47	1p	0.25	0/697	0.46	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.26	0/836	0.46	0/1117
48	2q	0.26	0/836	0.46	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.24	0/560	0.45	0/746
50	1s	0.25	0/667	0.50	0/900
50	2s	0.27	0/661	0.50	0/893
51	1t	0.26	0/730	0.41	0/965
51	2t	0.24	0/729	0.39	0/965
52	1u	0.23	0/203	0.43	0/266
52	2u	0.24	0/203	0.43	0/266
53	1v	0.27	0/288	0.85	0/446
53	2v	0.33	0/163	0.84	0/251
54	1w	0.46	1/1537 (0.1%)	1.06	6/2390 (0.3%)
54	1y	0.44	1/1606 (0.1%)	1.06	5/2497 (0.2%)
54	2w	0.36	0/1487	1.05	1/2311 (0.0%)
54	2y	0.50	1/1583 (0.1%)	1.15	7/2459 (0.3%)
55	1x	0.40	0/1725	1.05	9/2689 (0.3%)
55	2x	0.36	0/1725	0.99	9/2689 (0.3%)
All	All	0.28	7/316379 (0.0%)	0.74	143/473636 (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
26	24	0	1
41	2j	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.52	1.48	1.61
54	2y	1	G	OP3-P	-10.49	1.48	1.61
54	1w	1	G	OP3-P	-10.38	1.48	1.61
2	1B	1	U	OP3-P	-10.34	1.48	1.61
54	1y	1	G	OP3-P	-10.27	1.48	1.61

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	N3-C2-N2	18.40	132.78	119.90
32	2a	1263	C	N1-C2-O2	17.88	129.63	118.90
32	2a	1272	G	C5-C6-O6	16.95	138.77	128.60
32	2a	1272	G	N1-C2-N2	-14.73	102.94	116.20
2	2B	80	U	O4'-C1'-N1	12.03	117.82	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide
41	2j	32	ALA	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	31193	824	0
1	2A	60322	0	30421	1007	0
2	1B	2577	0	1305	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2575	0	1303	39	0
3	1D	2136	0	2218	73	0
3	2D	2136	0	2218	56	0
4	1E	1559	0	1618	39	0
4	2E	1559	0	1618	49	0
5	1F	1584	0	1625	52	0
5	2F	1580	0	1619	53	0
6	1G	1423	0	1436	43	0
6	2G	1428	0	1438	50	0
7	1H	1330	0	1407	34	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	38	0
8	2I	1064	0	1082	42	0
9	1N	1117	0	1184	21	0
9	2N	1117	0	1184	34	0
10	1O	933	0	996	25	0
10	2O	933	0	996	28	0
11	1P	1135	0	1212	42	0
11	2P	1135	0	1212	35	0
12	1Q	1122	0	1179	28	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	21	0
14	1S	873	0	927	21	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	29	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	32	0
17	1V	771	0	830	19	0
17	2V	771	0	830	23	0
18	1W	886	0	940	23	0
18	2W	886	0	940	18	0
19	1X	750	0	814	16	0
19	2X	750	0	814	12	0
20	1Y	806	0	881	24	0
20	2Y	806	0	881	33	0
21	1Z	1240	0	1240	39	0
21	2Z	1271	0	1273	31	0
22	10	653	0	674	17	0
22	20	653	0	674	19	0
23	11	755	0	826	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	755	0	826	20	0
24	12	588	0	643	15	0
24	22	588	0	643	16	0
25	13	469	0	518	7	0
25	23	464	0	514	17	0
26	14	552	0	533	19	0
26	24	532	0	503	17	0
27	15	455	0	465	7	0
27	25	455	0	465	16	0
28	16	453	0	473	11	0
28	26	449	0	469	17	0
29	17	418	0	467	9	0
29	27	418	0	467	12	0
30	18	517	0	582	22	0
30	28	517	0	582	22	0
31	19	307	0	335	6	0
31	29	307	0	335	15	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	139	0	0
53	2v	167	0	84	0	0
54	1w	1530	0	786	0	0
54	1y	1585	0	804	0	0
54	2w	1482	0	755	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	1A	680	0	0	0	0
56	1a	238	0	0	0	0
56	2A	351	0	0	0	0
56	2a	183	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2d	8	0	0	0	0
59	1A	585	0	0	27	0
59	1a	181	0	0	0	0
59	2A	234	0	0	14	0
59	2a	167	0	0	0	0
All	All	295398	0	196565	2965	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 12.

The worst 5 of 2965 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.19	1.34
1:2A:2138:C:N4	1:2A:2153:G:H1	1.36	1.24
1:1A:1082:U:O4	1:1A:1086:A:N1	1.89	1.05
1:1A:1054:A:H61	1:1A:1105:U:H3	1.03	0.98
1:1A:765:G:H1	1:1A:812:C:HO2'	84.79	0.96

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%)	262 (96%)	10 (4%)	1 (0%)	34	69
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	64
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	48
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	48
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	60
6	2G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	60
7	1H	172/180 (96%)	159 (92%)	13 (8%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	43
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22	56
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22	56
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	53
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11	39
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	51
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	53
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	20
17	2V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	48
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22	56
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	46
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	7
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	7
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	6	28
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	23 (10%)	4 (2%)	9	34
33	2b	229/256 (90%)	205 (90%)	20 (9%)	4 (2%)	9	34
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	64
34	2c	204/239 (85%)	192 (94%)	10 (5%)	2 (1%)	15	48
35	1d	206/209 (99%)	200 (97%)	4 (2%)	2 (1%)	15	48
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	64
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	39
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	39
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	7	30
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22	56
39	1h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	56
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	9	36
40	2i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	9	36
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	6
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	12
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	33
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	33
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	34
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	43
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	48
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	48
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	43
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	12
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	29
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11370/12128 (94%)	10654 (94%)	629 (6%)	87 (1%)	19	53

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
35	1d	5	ILE
40	1i	54	ASP
5	2F	130	ALA

### 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%)	207 (96%)	8 (4%)	34	66
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	59
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	58
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	53
5	1F	160/166 (96%)	155 (97%)	5 (3%)	40	71
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	44
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	63
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	53
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	53
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	37
8	2I	105/124 (85%)	97 (92%)	8 (8%)	13	39
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	50
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	45
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	50
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	62
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	61
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	37
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	78
14	2S	85/88 (97%)	82 (96%)	3 (4%)	36	68
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	68
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	62
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	54
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	48
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	48
18	1W	90/92 (98%)	88 (98%)	2 (2%)	52	79
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	62
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	65
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	16
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	50
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	50
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	79
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	71
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	66
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	76
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	71
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	65
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	80
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	81
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	26
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	50
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	15
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	26
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	27
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	41
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	53
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	81
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	73
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	50
33	1b	192/220 (87%)	181 (94%)	11 (6%)	20	52
33	2b	187/220 (85%)	172 (92%)	15 (8%)	12	37
34	1c	142/188 (76%)	135 (95%)	7 (5%)	25	58
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	62
35	1d	169/181 (93%)	158 (94%)	11 (6%)	17	46
35	2d	173/181 (96%)	161 (93%)	12 (7%)	15	44
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	62
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	55
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	59
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	69
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38	70
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	28
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22	55
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21	53
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	22
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	72
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	62
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	77
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	63
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	48
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	89
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	19
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	64
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	66
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	39
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	42
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	62
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	89
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	62
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	56
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	86
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	85
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42	73
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	22
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8839 (95%)	464 (5%)	24	57

5 of 464 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	1n	18	VAL
6	2G	5	VAL
41	2j	35	SER
47	1p	6	LEU
3	2D	211	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
40	1i	124	GLN
5	2F	75	HIS
42	2k	116	HIS
41	1j	56	HIS
49	1r	63	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	474 (16%)	22 (0%)
1	2A	2788/2915 (95%)	531 (19%)	22 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1494/1521 (98%)	279 (18%)	0
32	2a	1498/1521 (98%)	311 (20%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	7/24 (29%)	3 (42%)	0
54	1w	68/76 (89%)	15 (22%)	0
54	1y	71/76 (93%)	27 (38%)	0
54	2w	65/76 (85%)	18 (27%)	0
54	2y	69/76 (90%)	24 (34%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	10 (13%)	0
All	All	9319/9620 (96%)	1736 (18%)	44 (0%)

5 of 1736 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2601	C
1	2A	266	G
1	2A	2156	G
1	1A	2629	A
1	2A	195	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.65	4 (22%)
32	M2G	2a	966	32	20,27,28	1.41	3 (15%)	22,40,43	2.12	5 (22%)
55	PSU	2x	55	55	17,21,22	1.50	2 (11%)	20,30,33	3.11	6 (30%)
43	0TD	1l	92	43	4,9,10	3.08	1 (25%)	3,11,13	9.13	1 (33%)
54	5MU	1y	54	54	15,22,23	1.04	1 (6%)	16,32,35	1.72	2 (12%)
54	PSU	2w	32	54	17,21,22	1.58	2 (11%)	20,30,33	3.16	6 (30%)
55	4SU	1x	8	55,56	14,21,22	1.44	2 (14%)	15,30,33	2.13	2 (13%)
54	PSU	1w	32	54	17,21,22	1.55	2 (11%)	20,30,33	3.12	6 (30%)
1	5MC	2A	1962	1	15,22,23	1.30	1 (6%)	19,32,35	1.39	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.60	5 (27%)
32	5MC	1a	967	32	15,22,23	1.27	1 (6%)	19,32,35	1.31	3 (15%)
54	MIA	2y	37	54,32	18,24,32	1.13	2 (11%)	18,35,47	1.22	2 (11%)
54	4SU	1y	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.41	2 (13%)
53	PSU	2v	19	54,56,53	17,21,22	1.68	2 (11%)	20,30,33	3.41	6 (30%)
55	4SU	2x	8	55,56	14,21,22	1.27	2 (14%)	15,30,33	2.21	2 (13%)
32	2MG	1a	1207	32	19,26,27	1.21	2 (10%)	21,38,41	2.21	8 (38%)
54	5MU	2y	54	54	15,22,23	1.07	1 (6%)	16,32,35	1.92	2 (12%)
32	4OC	2a	1402	32,56	16,23,24	0.58	0	17,32,35	1.39	1 (5%)
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.77	9 (32%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.54	10 (38%)
1	2MU	1A	2552	1,56	14,22,24	0.88	0	14,31,36	0.84	1 (7%)
54	MIA	2w	37	54	20,27,32	1.84	2 (10%)	22,39,47	1.87	7 (31%)
54	PSU	2y	55	54	17,21,22	1.50	3 (17%)	20,30,33	3.13	7 (35%)
54	4SU	2y	8	54,56	14,21,22	1.33	1 (7%)	15,30,33	1.26	2 (13%)
54	PSU	1w	55	54	17,21,22	1.46	2 (11%)	20,30,33	3.40	6 (30%)
54	PSU	2w	39	54	17,21,22	1.40	2 (11%)	20,30,33	2.85	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	1A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.83	2 (12%)
54	PSU	2y	32	54	17,21,22	1.47	3 (17%)	20,30,33	3.09	6 (30%)
1	2MU	2A	2552	1,56	14,22,24	0.89	0	14,31,36	0.81	1 (7%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.73	9 (32%)
54	5MU	1w	54	54	15,22,23	1.04	2 (13%)	16,32,35	2.28	1 (6%)
1	5MU	2A	1939	1	15,22,23	1.08	1 (6%)	16,32,35	1.80	2 (12%)
54	7MG	2y	46	54	22,26,27	1.85	4 (18%)	28,39,42	3.07	10 (35%)
1	OMG	2A	2251	1,55	18,26,27	1.16	2 (11%)	20,38,41	2.05	6 (30%)
55	5MU	1x	54	55	15,22,23	1.09	1 (6%)	16,32,35	1.91	1 (6%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.18	5 (22%)
54	7MG	1y	46	54	22,26,27	1.85	4 (18%)	28,39,42	3.04	10 (35%)
1	5MC	1A	1962	1	15,22,23	1.36	1 (6%)	19,32,35	1.30	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.72	6 (33%)
32	5MC	2a	1407	32,56	15,22,23	1.33	1 (6%)	19,32,35	1.29	2 (10%)
1	PSU	1A	2605	1	17,21,22	1.46	2 (11%)	20,30,33	3.11	6 (30%)
1	PSU	1A	1911	1	17,21,22	1.61	3 (17%)	20,30,33	3.11	6 (30%)
54	PSU	2w	55	54	17,21,22	1.48	2 (11%)	20,30,33	3.45	7 (35%)
54	PSU	1y	39	54	17,21,22	1.48	2 (11%)	20,30,33	2.96	5 (25%)
54	4SU	2w	8	54	14,21,22	1.31	1 (7%)	15,30,33	1.40	2 (13%)
32	2MG	2a	1207	32,56	19,26,27	1.25	2 (10%)	21,38,41	2.13	6 (28%)
32	5MC	1a	1407	32	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
1	5MC	1A	1942	1	15,22,23	1.23	1 (6%)	19,32,35	1.39	3 (15%)
1	PSU	2A	2605	1	17,21,22	1.56	3 (17%)	20,30,33	3.18	6 (30%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	10.39	1 (33%)
1	2MA	1A	2503	1,56	17,25,26	1.37	2 (11%)	19,37,40	2.07	3 (15%)
32	5MC	1a	1404	32	15,22,23	1.34	1 (6%)	19,32,35	1.33	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.30	1 (6%)	19,32,35	1.40	3 (15%)
32	PSU	1a	516	32	17,21,22	1.51	3 (17%)	20,30,33	3.20	5 (25%)
1	2MA	2A	2503	1	17,25,26	1.29	2 (11%)	19,37,40	2.07	3 (15%)
1	5MU	1A	1939	1	15,22,23	1.12	2 (13%)	16,32,35	1.89	2 (12%)
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.63	0
1	4OC	2A	1920	1	15,22,24	0.64	0	17,31,35	1.46	2 (11%)
1	PSU	1A	1917	1	17,21,22	1.54	2 (11%)	20,30,33	3.06	6 (30%)
54	MIA	1y	37	54	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
53	PSU	1v	19	54,53	17,21,22	1.46	3 (17%)	20,30,33	3.56	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.34	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.27	1 (6%)	19,32,35	1.49	4 (21%)
32	5MC	2a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.46	2 (10%)
32	4OC	1a	1402	32	16,23,24	0.63	0	17,32,35	1.16	1 (5%)
54	PSU	2y	39	54	17,21,22	1.47	2 (11%)	20,30,33	3.36	7 (35%)
55	PSU	1x	55	55	17,21,22	1.61	2 (11%)	20,30,33	3.09	6 (30%)
54	PSU	1w	39	54	17,21,22	1.51	2 (11%)	20,30,33	2.82	5 (25%)
1	4OC	1A	1920	1	15,22,24	0.69	0	17,31,35	1.43	2 (11%)
55	5MC	1x	32	55	15,22,23	1.31	1 (6%)	19,32,35	1.33	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.57	2 (11%)	20,30,33	3.15	6 (30%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.68	4 (22%)
1	PSU	2A	1917	1	17,21,22	1.55	2 (11%)	20,30,33	3.09	6 (30%)
54	PSU	1y	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.09	7 (35%)
32	UR3	2a	1498	32	14,22,23	0.80	1 (7%)	15,32,35	0.72	0
54	5MU	2w	54	54	15,22,23	1.09	2 (13%)	16,32,35	2.04	2 (12%)
55	5MC	2x	32	55	15,22,23	1.37	1 (6%)	19,32,35	1.33	3 (15%)
55	5MU	2x	54	55	15,22,23	1.07	1 (6%)	16,32,35	1.80	2 (12%)
54	PSU	1y	32	54	17,21,22	1.54	2 (11%)	20,30,33	3.22	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.47	4 (21%)
32	7MG	1a	527	32,56	22,26,27	1.81	4 (18%)	28,39,42	2.76	8 (28%)
1	5MU	2A	1915	1	15,22,23	1.11	1 (6%)	16,32,35	1.81	2 (12%)
54	4SU	1w	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.50	2 (13%)
54	7MG	1w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.77	9 (32%)
1	OMG	1A	2251	1,55,56	18,26,27	1.23	2 (11%)	20,38,41	2.12	6 (30%)
32	PSU	2a	516	32	17,21,22	1.57	3 (17%)	20,30,33	3.16	7 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
54	5MU	1y	54	54	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
55	4SU	1x	8	55,56	-	0/5/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	2/3/25/34	0/3/3/3
54	4SU	1y	8	54	-	2/5/25/26	0/2/2/2
53	PSU	2v	19	54,56,53	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	5MU	2y	54	54	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
54	4SU	2y	8	54,56	-	1/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/5/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	2/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
32	5MC	2a	1407	32,56	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
53	PSU	1v	19	54,53	-	3/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/5/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
54	PSU	1y	32	54	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
54	1w	37	MIA	C2-S10	-7.02	1.69	1.75
54	2w	37	MIA	C2-S10	-6.89	1.69	1.75
43	2l	92	0TD	CB-SB	-5.91	1.69	1.84
43	1l	92	0TD	CB-SB	-5.88	1.69	1.84

The worst 5 of 365 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.95	66.54	101.85
43	1l	92	0TD	CSB-SB-CB	-15.74	70.90	101.85
54	2y	46	7MG	N3-C4-N9	10.22	140.03	126.91
54	1y	46	7MG	N3-C4-N9	10.18	139.99	126.91
53	1v	19	PSU	N1-C2-N3	-9.84	120.61	128.43

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1962	5MC	2	0
1	1A	2552	2MU	2	0
1	1A	1915	5MU	2	0
1	2A	2552	2MU	2	0
1	2A	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2251	OMG	1	0
1	2A	2503	2MA	2	0
1	2A	1920	4OC	1	0
1	1A	1917	PSU	1	0
1	2A	1942	5MC	1	0
1	2A	1915	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1466 ligands modelled in this entry, 1464 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	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	-		
58	SF4	2d	501	35	0,12,12	0.00	-	-		

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
58	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	501	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.51	88 (3%)	49	32	67, 83, 117, 127	0
1	2A	2789/2915 (95%)	0.33	106 (3%)	40	26	79, 94, 115, 128	0
2	1B	120/121 (99%)	0.15	0	100	100	77, 89, 99, 110	0
2	2B	120/121 (99%)	-0.20	0	100	100	96, 106, 115, 119	0
3	1D	275/276 (99%)	2.13	132 (48%)	0	0	71, 84, 93, 110	0
3	2D	275/276 (99%)	1.87	112 (40%)	0	0	78, 89, 98, 106	0
4	1E	204/206 (99%)	1.87	85 (41%)	0	0	70, 85, 96, 106	0
4	2E	204/206 (99%)	1.43	62 (30%)	0	0	82, 92, 100, 104	0
5	1F	203/210 (96%)	1.22	53 (26%)	0	0	72, 87, 101, 111	0
5	2F	203/210 (96%)	1.42	57 (28%)	0	0	82, 96, 105, 111	0
6	1G	181/182 (99%)	0.18	5 (2%)	53	36	77, 95, 104, 116	0
6	2G	181/182 (99%)	0.17	10 (5%)	25	15	97, 106, 113, 116	0
7	1H	174/180 (96%)	0.26	2 (1%)	80	65	81, 90, 98, 104	0
7	2H	174/180 (96%)	1.77	61 (35%)	0	0	95, 106, 112, 115	0
8	1I	146/148 (98%)	0.55	21 (14%)	2	1	86, 101, 107, 111	0
8	2I	146/148 (98%)	1.16	35 (23%)	0	0	92, 109, 117, 126	0
9	1N	140/140 (100%)	2.05	67 (47%)	0	0	74, 86, 97, 103	0
9	2N	140/140 (100%)	3.26	102 (72%)	0	0	82, 96, 104, 115	0
10	1O	122/122 (100%)	2.25	65 (53%)	0	0	73, 84, 92, 100	0
10	2O	122/122 (100%)	1.78	45 (36%)	0	0	82, 92, 99, 106	0
11	1P	149/150 (99%)	1.29	40 (26%)	0	0	67, 87, 100, 108	0
11	2P	149/150 (99%)	1.88	65 (43%)	0	0	81, 98, 111, 116	0
12	1Q	141/141 (100%)	1.36	35 (24%)	0	0	76, 86, 94, 105	0
12	2Q	141/141 (100%)	1.36	40 (28%)	0	0	85, 97, 105, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	1.62	46 (38%)	0	0	72, 83, 95, 97	0
13	2R	118/118 (100%)	1.44	31 (26%)	0	0	82, 90, 97, 99	0
14	1S	110/112 (98%)	0.16	1 (0%)	84	71	80, 89, 94, 102	0
14	2S	110/112 (98%)	-0.14	0	100	100	92, 99, 104, 108	0
15	1T	131/146 (89%)	1.46	46 (35%)	0	0	78, 87, 99, 107	0
15	2T	131/146 (89%)	1.19	32 (24%)	0	0	83, 93, 104, 108	0
16	1U	116/118 (98%)	1.94	56 (48%)	0	0	71, 83, 92, 104	0
16	2U	116/118 (98%)	1.84	54 (46%)	0	0	81, 95, 105, 111	0
17	1V	101/101 (100%)	1.20	23 (22%)	0	0	72, 86, 95, 99	0
17	2V	101/101 (100%)	1.38	26 (25%)	0	0	88, 99, 106, 109	0
18	1W	112/113 (99%)	1.52	33 (29%)	0	0	72, 82, 93, 111	0
18	2W	112/113 (99%)	1.90	46 (41%)	0	0	80, 90, 100, 112	0
19	1X	95/96 (98%)	1.13	17 (17%)	1	1	71, 84, 96, 108	0
19	2X	95/96 (98%)	1.24	20 (21%)	1	0	87, 97, 105, 111	0
20	1Y	107/110 (97%)	0.81	7 (6%)	18	11	79, 89, 102, 106	0
20	2Y	107/110 (97%)	1.95	46 (42%)	0	0	92, 99, 108, 114	0
21	1Z	154/206 (74%)	0.13	2 (1%)	77	61	85, 96, 110, 116	0
21	2Z	160/206 (77%)	-0.23	0	100	100	95, 105, 112, 120	0
22	10	83/85 (97%)	1.70	13 (15%)	2	1	75, 85, 101, 110	0
22	20	83/85 (97%)	2.11	25 (30%)	0	0	90, 97, 109, 113	0
23	11	97/98 (98%)	2.76	60 (61%)	0	0	75, 86, 102, 108	0
23	21	97/98 (98%)	1.66	44 (45%)	0	0	81, 92, 103, 107	0
24	12	70/72 (97%)	0.65	6 (8%)	10	6	80, 89, 97, 104	0
24	22	70/72 (97%)	0.19	4 (5%)	23	14	90, 100, 106, 110	0
25	13	59/60 (98%)	0.76	3 (5%)	28	17	75, 85, 94, 97	0
25	23	59/60 (98%)	1.53	22 (37%)	0	0	91, 97, 106, 110	0
26	14	69/71 (97%)	-0.38	0	100	100	91, 102, 113, 117	0
26	24	69/71 (97%)	-0.51	1 (1%)	75	59	98, 110, 116, 121	0
27	15	59/60 (98%)	1.76	19 (32%)	0	0	74, 82, 93, 98	0
27	25	59/60 (98%)	1.60	18 (30%)	0	0	79, 88, 99, 105	0
28	16	53/54 (98%)	0.78	6 (11%)	5	3	76, 85, 92, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.87	9 (16%)	1	1	88, 95, 102, 105	0
29	17	48/49 (97%)	2.53	24 (50%)	0	0	73, 79, 94, 102	0
29	27	48/49 (97%)	2.92	29 (60%)	0	0	80, 86, 97, 107	0
30	18	64/65 (98%)	2.01	32 (50%)	0	0	72, 82, 88, 91	0
30	28	64/65 (98%)	2.68	41 (64%)	0	0	84, 92, 99, 100	0
31	19	37/37 (100%)	1.26	12 (32%)	0	0	78, 84, 92, 94	0
31	29	37/37 (100%)	2.47	21 (56%)	0	0	93, 101, 105, 110	0
32	1a	1488/1521 (97%)	0.11	28 (1%)	66	49	80, 97, 114, 122	0
32	2a	1491/1521 (98%)	-0.01	24 (1%)	72	55	89, 105, 116, 125	0
33	1b	231/256 (90%)	0.29	15 (6%)	18	11	92, 103, 111, 120	0
33	2b	231/256 (90%)	0.30	25 (10%)	5	3	96, 109, 115, 120	0
34	1c	206/239 (86%)	1.02	47 (22%)	0	0	89, 99, 106, 109	0
34	2c	206/239 (86%)	1.44	65 (31%)	0	0	97, 107, 111, 114	0
35	1d	208/209 (99%)	0.57	24 (11%)	4	3	87, 97, 105, 115	0
35	2d	208/209 (99%)	1.79	88 (42%)	0	0	91, 102, 111, 116	0
36	1e	148/162 (91%)	1.19	38 (25%)	0	0	86, 95, 101, 106	0
36	2e	148/162 (91%)	1.28	53 (35%)	0	0	93, 103, 110, 111	0
37	1f	100/101 (99%)	0.60	13 (13%)	3	2	89, 98, 104, 108	0
37	2f	100/101 (99%)	-0.13	2 (2%)	65	48	91, 99, 105, 110	0
38	1g	155/156 (99%)	1.08	34 (21%)	0	0	91, 98, 109, 112	0
38	2g	155/156 (99%)	0.50	18 (11%)	4	2	94, 104, 111, 114	0
39	1h	137/138 (99%)	0.96	27 (19%)	1	0	88, 97, 103, 108	0
39	2h	137/138 (99%)	1.59	48 (35%)	0	0	94, 104, 109, 116	0
40	1i	127/128 (99%)	0.47	21 (16%)	1	1	88, 99, 106, 110	0
40	2i	127/128 (99%)	1.30	44 (34%)	0	0	93, 107, 113, 115	0
41	1j	97/105 (92%)	0.58	18 (18%)	1	0	86, 102, 109, 116	0
41	2j	96/105 (91%)	1.50	28 (29%)	0	0	98, 109, 114, 117	0
42	1k	114/129 (88%)	3.55	90 (78%)	0	0	89, 99, 106, 111	0
42	2k	114/129 (88%)	1.79	42 (36%)	0	0	91, 101, 107, 110	0
43	1l	121/132 (91%)	0.82	20 (16%)	1	1	83, 91, 98, 103	0
43	2l	121/132 (91%)	1.17	34 (28%)	0	0	91, 100, 106, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.52	12 (9%) 7 4	86, 99, 107, 117	0
44	2m	122/126 (96%)	0.97	23 (18%) 1 0	97, 107, 115, 120	0
45	1n	60/61 (98%)	1.56	20 (33%) 0 0	88, 95, 101, 102	0
45	2n	60/61 (98%)	3.52	41 (68%) 0 0	96, 108, 113, 115	0
46	1o	88/89 (98%)	0.71	14 (15%) 1 1	83, 96, 104, 109	0
46	2o	88/89 (98%)	0.94	19 (21%) 0 0	94, 102, 109, 111	0
47	1p	82/88 (93%)	1.37	28 (34%) 0 0	92, 100, 106, 108	0
47	2p	82/88 (93%)	1.55	28 (34%) 0 0	90, 99, 104, 109	0
48	1q	99/105 (94%)	0.52	7 (7%) 16 9	88, 97, 103, 107	0
48	2q	99/105 (94%)	2.11	51 (51%) 0 0	91, 99, 107, 111	0
49	1r	68/88 (77%)	1.20	14 (20%) 1 0	88, 97, 104, 106	0
49	2r	68/88 (77%)	0.65	10 (14%) 2 1	91, 101, 106, 111	0
50	1s	83/93 (89%)	0.03	3 (3%) 42 28	93, 99, 106, 113	0
50	2s	83/93 (89%)	0.17	6 (7%) 15 8	102, 107, 112, 114	0
51	1t	96/106 (90%)	1.08	28 (29%) 0 0	90, 100, 105, 108	0
51	2t	96/106 (90%)	1.36	26 (27%) 0 0	91, 99, 107, 111	0
52	1u	23/27 (85%)	0.89	2 (8%) 10 6	93, 98, 101, 102	0
52	2u	23/27 (85%)	1.53	6 (26%) 0 0	102, 106, 109, 112	0
53	1v	12/24 (50%)	2.46	6 (50%) 0 0	88, 98, 119, 119	0
53	2v	7/24 (29%)	0.77	2 (28%) 0 0	100, 103, 118, 118	0
54	1w	64/76 (84%)	1.63	21 (32%) 0 0	94, 117, 124, 127	0
54	1y	67/76 (88%)	1.27	18 (26%) 0 0	83, 120, 124, 126	0
54	2w	62/76 (81%)	0.53	6 (9%) 7 4	107, 122, 127, 130	0
54	2y	66/76 (86%)	0.59	9 (13%) 3 1	97, 119, 123, 126	0
55	1x	72/77 (93%)	0.24	3 (4%) 36 23	85, 97, 110, 112	0
55	2x	72/77 (93%)	-0.12	2 (2%) 53 36	95, 108, 115, 119	0
All	All	20862/21748 (95%)	0.82	3414 (16%) 1 1	67, 96, 113, 130	0

The worst 5 of 3414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	18.6
22	10	6	GLY	15.7

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Mol	Chain	Res	Type	RSRZ
22	20	7	LEU	14.7
44	2m	124	PRO	14.2
44	1m	123	ALA	13.8

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	5MU	2y	54	21/22	0.66	0.34	101,120,137,154	0
54	PSU	2w	55	20/21	0.68	0.16	105,120,127,131	0
54	PSU	2w	39	20/21	0.72	0.40	115,123,126,127	0
54	4SU	2w	8	20/21	0.75	0.16	122,126,137,146	0
54	PSU	2y	55	20/21	0.76	0.39	114,121,139,154	0
54	PSU	1y	55	20/21	0.76	0.35	119,126,131,138	0
54	4SU	1y	8	20/21	0.77	0.15	115,120,127,132	0
54	4SU	2y	8	20/21	0.77	0.13	115,120,129,132	0
54	PSU	1w	55	20/21	0.80	0.21	102,112,115,117	0
54	7MG	2y	46	24/25	0.81	0.36	114,121,128,137	0
54	PSU	2y	32	20/21	0.82	0.37	109,122,134,138	0
54	PSU	2y	39	20/21	0.82	0.33	110,119,130,143	0
54	PSU	1y	39	20/21	0.82	0.36	107,116,137,143	0
54	4SU	1w	8	20/21	0.82	0.22	112,119,134,134	0
54	MIA	2y	37	22/30	0.84	0.29	107,116,130,143	0
54	7MG	2w	46	24/25	0.85	0.15	113,122,129,141	0
54	MIA	2w	37	25/30	0.85	0.19	91,115,118,133	0
32	5MC	2a	1400	21/22	0.86	0.33	87,108,118,120	0
53	PSU	2v	19	20/21	0.86	0.18	105,112,119,120	0
54	7MG	1w	46	24/25	0.86	0.17	105,115,124,133	0
54	5MU	2w	54	21/22	0.88	0.13	103,113,118,121	0
55	PSU	2x	55	20/21	0.89	0.11	106,112,122,123	0
54	5MU	1y	54	21/22	0.89	0.25	114,120,132,137	0
54	7MG	1y	46	24/25	0.89	0.26	109,119,125,130	0
54	PSU	1w	32	20/21	0.90	0.24	90,101,108,117	0
54	PSU	1y	32	20/21	0.90	0.29	105,113,128,129	0
54	MIA	1w	37	29/30	0.90	0.26	78,99,107,108	0
32	2MG	2a	1207	24/25	0.90	0.16	100,107,116,125	0
32	PSU	2a	516	20/21	0.90	0.16	92,103,111,114	0
54	MIA	1y	37	22/30	0.91	0.24	108,117,123,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	5MC	2a	967	21/22	0.91	0.16	99,102,110,118	0
32	5MC	2a	1404	21/22	0.91	0.17	84,99,105,110	0
55	4SU	2x	8	20/21	0.91	0.11	97,110,116,120	0
54	PSU	2w	32	20/21	0.91	0.29	108,114,123,126	0
54	PSU	1w	39	20/21	0.91	0.29	97,105,119,120	0
43	0TD	1l	92	10/11	0.93	0.22	88,91,97,113	0
55	4SU	1x	8	20/21	0.93	0.15	93,100,106,110	0
53	PSU	1v	19	20/21	0.93	0.14	79,95,102,102	0
55	5MC	2x	32	21/22	0.93	0.22	99,105,110,112	0
1	PSU	1A	2605	20/21	0.93	0.28	66,79,85,86	0
1	5MU	1A	1915	21/22	0.93	0.17	82,100,104,110	0
32	4OC	2a	1402	22/23	0.93	0.17	97,104,109,114	0
32	7MG	2a	527	24/25	0.93	0.18	89,95,101,112	0
43	0TD	2l	92	10/11	0.94	0.15	95,101,103,110	0
32	PSU	1a	516	20/21	0.94	0.17	84,92,98,104	0
1	PSU	2A	1911	20/21	0.94	0.14	86,98,105,106	0
1	PSU	2A	1917	20/21	0.94	0.13	86,103,108,111	0
1	4OC	2A	1920	21/23	0.94	0.15	89,98,103,108	0
32	UR3	2a	1498	21/22	0.94	0.24	88,98,102,106	0
1	5MC	2A	1962	21/22	0.94	0.17	77,89,95,99	0
32	MA6	2a	1519	24/25	0.94	0.30	86,99,103,105	0
55	5MU	2x	54	21/22	0.94	0.13	103,111,114,124	0
54	5MU	1w	54	21/22	0.94	0.25	104,108,117,119	0
1	5MU	2A	1915	21/22	0.94	0.13	101,107,111,116	0
1	PSU	1A	1911	20/21	0.94	0.18	70,90,95,100	0
32	5MC	1a	1407	21/22	0.94	0.23	76,88,93,97	0
32	4OC	1a	1402	22/23	0.94	0.26	82,92,98,100	0
32	M2G	2a	966	25/26	0.95	0.19	93,99,106,113	0
1	PSU	1A	1917	20/21	0.95	0.18	83,90,95,96	0
1	5MC	1A	1962	21/22	0.95	0.22	72,83,91,94	0
32	5MC	2a	1407	21/22	0.95	0.16	93,98,101,106	0
32	2MG	1a	1207	24/25	0.95	0.17	77,95,102,105	0
1	PSU	2A	2605	20/21	0.95	0.25	79,88,93,96	0
1	OMG	2A	2251	24/25	0.95	0.33	74,88,94,96	0
32	5MC	1a	1404	21/22	0.95	0.28	74,83,96,97	0
1	5MC	2A	1942	21/22	0.95	0.17	88,94,99,106	0
55	5MU	1x	54	21/22	0.95	0.14	86,97,101,105	0
55	PSU	1x	55	20/21	0.95	0.12	94,100,107,116	0
1	2MA	2A	2503	23/24	0.95	0.27	70,81,88,92	0
55	5MC	1x	32	21/22	0.95	0.23	84,95,100,102	0
1	2MU	1A	2552	21/23	0.96	0.31	58,78,84,92	0
32	5MC	1a	1400	21/22	0.96	0.26	81,91,96,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	4OC	1A	1920	21/23	0.96	0.21	76,89,95,96	0
32	5MC	1a	967	21/22	0.96	0.23	77,88,95,101	0
1	5MC	1A	1942	21/22	0.96	0.20	65,81,86,88	0
32	7MG	1a	527	24/25	0.96	0.20	78,89,96,98	0
32	MA6	2a	1518	24/25	0.96	0.22	90,97,101,102	0
1	5MU	1A	1939	21/22	0.96	0.26	66,78,86,90	0
1	5MU	2A	1939	21/22	0.96	0.23	75,86,91,95	0
32	M2G	1a	966	25/26	0.96	0.26	81,87,96,98	0
32	MA6	1a	1518	24/25	0.97	0.24	58,85,89,93	0
32	UR3	1a	1498	21/22	0.97	0.28	78,85,89,93	0
1	2MU	2A	2552	21/23	0.97	0.17	74,84,89,91	0
32	MA6	1a	1519	24/25	0.97	0.34	82,87,92,99	0
1	OMG	1A	2251	24/25	0.97	0.25	66,80,85,86	0
1	2MA	1A	2503	23/24	0.97	0.32	58,74,81,83	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3317	1/1	0.32	0.65	92,92,92,92	0
56	MG	2A	3201	1/1	0.34	0.22	102,102,102,102	0
56	MG	1A	3190	1/1	0.34	0.48	118,118,118,118	0
56	MG	1A	3242	1/1	0.37	0.33	78,78,78,78	0
56	MG	2a	3060	1/1	0.37	0.43	101,101,101,101	0
56	MG	2a	3082	1/1	0.37	0.31	109,109,109,109	0
56	MG	2a	3154	1/1	0.38	0.16	101,101,101,101	0
56	MG	2A	3315	1/1	0.40	0.84	103,103,103,103	0
56	MG	1A	3557	1/1	0.40	0.36	89,89,89,89	0
56	MG	1a	3094	1/1	0.44	1.77	96,96,96,96	0
56	MG	2A	3031	1/1	0.45	0.20	100,100,100,100	0
56	MG	1a	3214	1/1	0.45	0.26	103,103,103,103	0
56	MG	1A	3497	1/1	0.46	0.22	96,96,96,96	0
56	MG	1A	3104	1/1	0.46	0.98	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3017	1/1	0.48	0.30	98,98,98,98	0
56	MG	1A	3377	1/1	0.48	0.45	102,102,102,102	0
56	MG	1A	3429	1/1	0.50	0.25	87,87,87,87	0
56	MG	1a	3111	1/1	0.51	0.42	103,103,103,103	0
56	MG	1A	3240	1/1	0.53	0.37	101,101,101,101	0
56	MG	1A	3194	1/1	0.53	0.26	72,72,72,72	0
56	MG	1A	3157	1/1	0.54	0.13	92,92,92,92	0
56	MG	1A	3036	1/1	0.54	0.80	99,99,99,99	0
56	MG	1A	3099	1/1	0.55	0.40	77,77,77,77	0
56	MG	1A	3133	1/1	0.55	0.36	76,76,76,76	0
56	MG	2a	3080	1/1	0.56	0.28	85,85,85,85	0
56	MG	1A	3433	1/1	0.56	1.77	97,97,97,97	0
56	MG	1A	3359	1/1	0.56	0.77	89,89,89,89	0
56	MG	1A	3041	1/1	0.56	0.23	105,105,105,105	0
56	MG	1A	3534	1/1	0.56	0.30	86,86,86,86	0
56	MG	2A	3205	1/1	0.57	0.32	111,111,111,111	0
56	MG	1A	3441	1/1	0.57	0.38	103,103,103,103	0
56	MG	2a	3059	1/1	0.57	0.46	79,79,79,79	0
56	MG	1a	3077	1/1	0.58	0.22	84,84,84,84	0
56	MG	1A	3367	1/1	0.58	0.25	104,104,104,104	0
56	MG	1A	3148	1/1	0.58	0.42	79,79,79,79	0
56	MG	2a	3034	1/1	0.59	0.23	79,79,79,79	0
56	MG	1a	3005	1/1	0.60	0.21	80,80,80,80	0
56	MG	2a	3107	1/1	0.60	0.10	106,106,106,106	0
56	MG	2A	3146	1/1	0.60	0.23	79,79,79,79	0
56	MG	1A	3615	1/1	0.60	0.22	95,95,95,95	0
56	MG	2A	3057	1/1	0.61	0.71	89,89,89,89	0
56	MG	2A	3074	1/1	0.61	0.30	102,102,102,102	0
56	MG	1A	3651	1/1	0.61	0.19	90,90,90,90	0
56	MG	2A	3034	1/1	0.61	0.17	71,71,71,71	0
56	MG	2a	3102	1/1	0.61	0.23	90,90,90,90	0
56	MG	1A	3527	1/1	0.61	0.24	74,74,74,74	0
56	MG	1a	3211	1/1	0.61	0.30	77,77,77,77	0
56	MG	2A	3111	1/1	0.61	0.67	81,81,81,81	0
56	MG	2A	3316	1/1	0.62	0.48	93,93,93,93	0
56	MG	2A	3302	1/1	0.63	0.14	82,82,82,82	0
56	MG	2a	3007	1/1	0.64	0.54	99,99,99,99	0
56	MG	1a	3043	1/1	0.64	0.41	95,95,95,95	0
56	MG	1A	3142	1/1	0.64	0.53	73,73,73,73	0
56	MG	2a	3087	1/1	0.64	0.46	94,94,94,94	0
56	MG	1A	3105	1/1	0.64	0.25	74,74,74,74	0
56	MG	2a	3058	1/1	0.65	0.61	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3569	1/1	0.65	0.11	95,95,95,95	0
56	MG	1a	3167	1/1	0.65	0.48	109,109,109,109	0
56	MG	2a	3015	1/1	0.65	0.15	98,98,98,98	0
56	MG	2A	3158	1/1	0.65	0.67	78,78,78,78	0
56	MG	1a	3122	1/1	0.65	1.05	93,93,93,93	0
56	MG	2a	3017	1/1	0.66	2.14	89,89,89,89	0
56	MG	2A	3323	1/1	0.66	0.15	104,104,104,104	0
56	MG	2a	3051	1/1	0.66	0.31	79,79,79,79	0
56	MG	1A	3364	1/1	0.66	0.30	96,96,96,96	0
56	MG	2A	3160	1/1	0.67	0.13	88,88,88,88	0
56	MG	1A	3145	1/1	0.67	0.27	93,93,93,93	0
56	MG	2a	3106	1/1	0.67	0.22	124,124,124,124	0
56	MG	1a	3008	1/1	0.67	0.15	66,66,66,66	0
56	MG	1a	3116	1/1	0.67	0.47	90,90,90,90	0
56	MG	1a	3149	1/1	0.67	0.21	110,110,110,110	0
57	ZN	14	501	1/1	0.67	0.04	162,162,162,162	0
56	MG	1A	3123	1/1	0.67	0.47	93,93,93,93	0
56	MG	2A	3184	1/1	0.67	0.28	82,82,82,82	0
56	MG	1A	3191	1/1	0.67	0.26	90,90,90,90	0
56	MG	1A	3098	1/1	0.67	1.35	80,80,80,80	0
56	MG	1A	3524	1/1	0.68	0.36	84,84,84,84	0
56	MG	2a	3138	1/1	0.68	0.28	95,95,95,95	0
56	MG	2A	3287	1/1	0.68	0.16	83,83,83,83	0
56	MG	2a	3049	1/1	0.68	0.18	79,79,79,79	0
56	MG	1a	3085	1/1	0.68	0.34	89,89,89,89	0
56	MG	1A	3408	1/1	0.68	0.20	96,96,96,96	0
56	MG	1A	3034	1/1	0.69	0.10	79,79,79,79	0
56	MG	1A	3573	1/1	0.69	0.21	88,88,88,88	0
56	MG	1A	3565	1/1	0.69	0.28	83,83,83,83	0
56	MG	2a	3158	1/1	0.69	0.22	116,116,116,116	0
56	MG	2A	3162	1/1	0.69	0.23	77,77,77,77	0
56	MG	1A	3128	1/1	0.70	0.22	75,75,75,75	0
56	MG	2a	3100	1/1	0.71	0.26	94,94,94,94	0
56	MG	1A	3506	1/1	0.71	0.52	118,118,118,118	0
56	MG	2a	3070	1/1	0.71	0.21	87,87,87,87	0
56	MG	1A	3277	1/1	0.71	0.21	73,73,73,73	0
56	MG	2a	3053	1/1	0.71	0.82	90,90,90,90	0
56	MG	1a	3173	1/1	0.71	0.25	75,75,75,75	0
56	MG	1A	3303	1/1	0.71	0.27	78,78,78,78	0
56	MG	1A	3151	1/1	0.71	0.27	64,64,64,64	0
56	MG	1A	3585	1/1	0.71	0.19	76,76,76,76	0
56	MG	2A	3094	1/1	0.71	0.22	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3196	1/1	0.71	0.33	81,81,81,81	0
56	MG	2A	3278	1/1	0.71	0.16	89,89,89,89	0
56	MG	1A	3160	1/1	0.71	0.26	76,76,76,76	0
56	MG	1A	3572	1/1	0.71	0.18	85,85,85,85	0
56	MG	2A	3166	1/1	0.71	0.27	79,79,79,79	0
56	MG	2A	3290	1/1	0.72	0.14	94,94,94,94	0
56	MG	1A	3533	1/1	0.72	0.37	114,114,114,114	0
56	MG	1a	3028	1/1	0.72	0.20	76,76,76,76	0
56	MG	2A	3099	1/1	0.72	0.62	89,89,89,89	0
56	MG	1a	3082	1/1	0.72	0.80	75,75,75,75	0
56	MG	2a	3077	1/1	0.72	0.17	95,95,95,95	0
56	MG	2a	3006	1/1	0.72	0.31	104,104,104,104	0
56	MG	2A	3022	1/1	0.72	0.16	96,96,96,96	0
56	MG	1a	3162	1/1	0.72	0.31	93,93,93,93	0
56	MG	2A	3119	1/1	0.72	0.15	90,90,90,90	0
56	MG	1A	3239	1/1	0.72	0.25	93,93,93,93	0
56	MG	1A	3636	1/1	0.73	0.34	73,73,73,73	0
56	MG	2A	3019	1/1	0.73	0.21	101,101,101,101	0
56	MG	2a	3054	1/1	0.73	0.18	90,90,90,90	0
56	MG	2A	3245	1/1	0.73	0.41	94,94,94,94	0
56	MG	2a	3130	1/1	0.73	0.09	74,74,74,74	0
56	MG	1A	3612	1/1	0.73	0.24	95,95,95,95	0
56	MG	2a	3179	1/1	0.73	0.12	106,106,106,106	0
56	MG	2a	3037	1/1	0.73	0.21	106,106,106,106	0
56	MG	1A	3505	1/1	0.73	0.15	70,70,70,70	0
56	MG	2A	3092	1/1	0.73	0.48	99,99,99,99	0
56	MG	1A	3513	1/1	0.73	0.63	88,88,88,88	0
56	MG	2A	3193	1/1	0.74	0.35	86,86,86,86	0
56	MG	2a	3088	1/1	0.74	0.32	97,97,97,97	0
56	MG	1A	3390	1/1	0.74	0.27	87,87,87,87	0
56	MG	2A	3192	1/1	0.74	0.12	77,77,77,77	0
56	MG	2a	3031	1/1	0.74	0.88	109,109,109,109	0
56	MG	1a	3105	1/1	0.74	0.25	86,86,86,86	0
56	MG	2A	3244	1/1	0.74	0.11	90,90,90,90	0
56	MG	1A	3583	1/1	0.74	0.15	88,88,88,88	0
56	MG	2A	3070	1/1	0.74	0.35	74,74,74,74	0
56	MG	1A	3352	1/1	0.75	0.26	95,95,95,95	0
56	MG	2A	3087	1/1	0.75	0.28	88,88,88,88	0
56	MG	2A	3197	1/1	0.75	0.20	78,78,78,78	0
56	MG	1a	3163	1/1	0.75	0.41	66,66,66,66	0
56	MG	1A	3368	1/1	0.75	0.78	99,99,99,99	0
56	MG	1a	3092	1/1	0.75	0.71	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3097	1/1	0.75	0.31	89,89,89,89	0
56	MG	1A	3268	1/1	0.75	0.21	68,68,68,68	0
56	MG	1A	3423	1/1	0.76	0.38	78,78,78,78	0
56	MG	1a	3016	1/1	0.76	0.92	87,87,87,87	0
56	MG	2A	3156	1/1	0.76	0.17	69,69,69,69	0
56	MG	1A	3014	1/1	0.76	0.39	93,93,93,93	0
56	MG	1a	3182	1/1	0.76	0.21	102,102,102,102	0
56	MG	2a	3166	1/1	0.76	0.14	115,115,115,115	0
56	MG	2A	3123	1/1	0.76	0.18	81,81,81,81	0
56	MG	1A	3555	1/1	0.76	0.23	80,80,80,80	0
56	MG	2A	3058	1/1	0.76	0.32	78,78,78,78	0
56	MG	1A	3257	1/1	0.76	0.27	80,80,80,80	0
56	MG	1A	3149	1/1	0.76	0.53	76,76,76,76	0
56	MG	1A	3244	1/1	0.77	0.23	81,81,81,81	0
56	MG	1A	3629	1/1	0.77	0.28	106,106,106,106	0
56	MG	2A	3243	1/1	0.77	0.13	88,88,88,88	0
56	MG	1A	3280	1/1	0.77	0.20	77,77,77,77	0
56	MG	2A	3003	1/1	0.77	0.23	84,84,84,84	0
56	MG	1A	3304	1/1	0.77	0.21	76,76,76,76	0
56	MG	1A	3045	1/1	0.77	0.23	94,94,94,94	0
56	MG	1A	3518	1/1	0.77	0.27	97,97,97,97	0
56	MG	2A	3198	1/1	0.77	0.17	83,83,83,83	0
56	MG	1a	3027	1/1	0.77	0.18	76,76,76,76	0
56	MG	1a	3067	1/1	0.77	0.18	80,80,80,80	0
56	MG	1A	3415	1/1	0.77	0.21	78,78,78,78	0
56	MG	1A	3394	1/1	0.77	0.46	91,91,91,91	0
56	MG	2A	3138	1/1	0.77	0.20	102,102,102,102	0
56	MG	2A	3148	1/1	0.77	0.16	96,96,96,96	0
56	MG	1A	3442	1/1	0.77	0.15	77,77,77,77	0
56	MG	2A	3142	1/1	0.78	0.61	81,81,81,81	0
56	MG	2A	3297	1/1	0.78	0.19	93,93,93,93	0
56	MG	2A	3206	1/1	0.78	0.35	73,73,73,73	0
56	MG	1a	3051	1/1	0.78	0.33	99,99,99,99	0
56	MG	1A	3121	1/1	0.78	0.42	76,76,76,76	0
56	MG	1A	3318	1/1	0.78	0.46	99,99,99,99	0
56	MG	2A	3331	1/1	0.78	0.28	67,67,67,67	0
56	MG	1A	3428	1/1	0.78	0.26	79,79,79,79	0
56	MG	1A	3125	1/1	0.78	0.30	77,77,77,77	0
56	MG	2A	3249	1/1	0.78	0.11	81,81,81,81	0
56	MG	1A	3176	1/1	0.78	0.23	95,95,95,95	0
56	MG	1A	3320	1/1	0.78	0.23	65,65,65,65	0
56	MG	1A	3252	1/1	0.78	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3198	1/1	0.78	0.11	83,83,83,83	0
56	MG	2A	3110	1/1	0.78	0.15	79,79,79,79	0
56	MG	1A	3376	1/1	0.78	0.19	92,92,92,92	0
56	MG	1A	3549	1/1	0.78	0.26	83,83,83,83	0
56	MG	2a	3090	1/1	0.78	0.22	91,91,91,91	0
56	MG	2A	3318	1/1	0.78	0.21	87,87,87,87	0
56	MG	2A	3294	1/1	0.78	0.38	104,104,104,104	0
56	MG	2A	3078	1/1	0.79	0.23	75,75,75,75	0
56	MG	1a	3238	1/1	0.79	0.15	99,99,99,99	0
56	MG	1A	3479	1/1	0.79	0.14	86,86,86,86	0
56	MG	1A	3571	1/1	0.79	0.05	98,98,98,98	0
56	MG	1A	3554	1/1	0.79	0.14	109,109,109,109	0
56	MG	1A	3199	1/1	0.79	0.23	70,70,70,70	0
56	MG	2a	3169	1/1	0.79	0.25	78,78,78,78	0
56	MG	1a	3189	1/1	0.79	0.23	85,85,85,85	0
56	MG	2A	3101	1/1	0.79	0.46	83,83,83,83	0
56	MG	1a	3037	1/1	0.79	0.42	82,82,82,82	0
56	MG	1a	3134	1/1	0.79	0.39	77,77,77,77	0
56	MG	1a	3106	1/1	0.79	0.07	98,98,98,98	0
56	MG	1a	3152	1/1	0.79	0.18	102,102,102,102	0
56	MG	2a	3092	1/1	0.79	0.19	88,88,88,88	0
56	MG	2A	3143	1/1	0.79	0.24	93,93,93,93	0
56	MG	1A	3114	1/1	0.79	0.42	93,93,93,93	0
56	MG	2a	3141	1/1	0.79	0.10	82,82,82,82	0
56	MG	1A	3486	1/1	0.79	0.23	68,68,68,68	0
56	MG	1A	3161	1/1	0.79	0.17	90,90,90,90	0
56	MG	2a	3028	1/1	0.79	0.14	85,85,85,85	0
56	MG	2A	3310	1/1	0.79	0.06	91,91,91,91	0
56	MG	2A	3071	1/1	0.79	0.20	75,75,75,75	0
56	MG	2a	3036	1/1	0.80	0.10	95,95,95,95	0
56	MG	1a	3179	1/1	0.80	0.13	90,90,90,90	0
56	MG	1A	3056	1/1	0.80	0.27	80,80,80,80	0
56	MG	2A	3051	1/1	0.80	0.29	80,80,80,80	0
56	MG	1A	3579	1/1	0.80	0.51	118,118,118,118	0
56	MG	1A	3258	1/1	0.80	0.29	95,95,95,95	0
56	MG	1a	3053	1/1	0.80	1.62	79,79,79,79	0
56	MG	1A	3511	1/1	0.80	0.17	62,62,62,62	0
56	MG	1a	3230	1/1	0.80	0.23	84,84,84,84	0
56	MG	2A	3234	1/1	0.80	0.72	84,84,84,84	0
56	MG	1a	3222	1/1	0.80	0.11	91,91,91,91	0
56	MG	2a	3048	1/1	0.80	0.33	94,94,94,94	0
56	MG	1A	3420	1/1	0.80	0.36	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3063	1/1	0.80	0.25	83,83,83,83	0
56	MG	1A	3181	1/1	0.80	1.48	78,78,78,78	0
56	MG	2A	3112	1/1	0.80	0.31	89,89,89,89	0
56	MG	1a	3068	1/1	0.80	0.15	95,95,95,95	0
56	MG	1a	3072	1/1	0.80	0.20	94,94,94,94	0
56	MG	2A	3114	1/1	0.80	0.37	79,79,79,79	0
56	MG	2A	3237	1/1	0.80	0.18	92,92,92,92	0
56	MG	1A	3058	1/1	0.80	0.15	80,80,80,80	0
56	MG	1A	3661	1/1	0.80	0.35	87,87,87,87	0
56	MG	1a	3117	1/1	0.80	0.14	83,83,83,83	0
56	MG	2a	3050	1/1	0.80	0.29	105,105,105,105	0
56	MG	2A	3227	1/1	0.80	0.11	81,81,81,81	0
56	MG	2a	3144	1/1	0.80	0.24	101,101,101,101	0
56	MG	1A	3159	1/1	0.80	0.11	69,69,69,69	0
56	MG	1A	3002	1/1	0.81	0.17	72,72,72,72	0
56	MG	2A	3337	1/1	0.81	0.14	78,78,78,78	0
56	MG	1A	3015	1/1	0.81	0.13	86,86,86,86	0
56	MG	1A	3016	1/1	0.81	0.28	66,66,66,66	0
56	MG	2A	3258	1/1	0.81	0.34	103,103,103,103	0
56	MG	1a	3039	1/1	0.81	0.21	80,80,80,80	0
56	MG	1a	3033	1/1	0.81	0.28	87,87,87,87	0
56	MG	2A	3134	1/1	0.81	0.42	91,91,91,91	0
56	MG	1A	3174	1/1	0.81	0.39	77,77,77,77	0
56	MG	1A	3168	1/1	0.81	0.19	78,78,78,78	0
56	MG	1A	3580	1/1	0.81	0.15	74,74,74,74	0
56	MG	1a	3136	1/1	0.81	0.23	84,84,84,84	0
56	MG	1a	3203	1/1	0.81	0.34	105,105,105,105	0
56	MG	2A	3332	1/1	0.81	0.48	116,116,116,116	0
56	MG	1A	3291	1/1	0.81	0.18	79,79,79,79	0
56	MG	1A	3295	1/1	0.81	0.34	66,66,66,66	0
56	MG	2A	3055	1/1	0.81	0.13	92,92,92,92	0
56	MG	2A	3336	1/1	0.81	0.21	77,77,77,77	0
56	MG	1a	3004	1/1	0.81	0.19	101,101,101,101	0
56	MG	1a	3201	1/1	0.81	0.50	93,93,93,93	0
56	MG	2a	3167	1/1	0.81	0.30	101,101,101,101	0
56	MG	2a	3116	1/1	0.81	0.20	82,82,82,82	0
56	MG	1a	3069	1/1	0.81	0.18	81,81,81,81	0
56	MG	2a	3004	1/1	0.81	0.29	98,98,98,98	0
56	MG	1a	3019	1/1	0.81	0.53	96,96,96,96	0
56	MG	1a	3110	1/1	0.81	0.10	90,90,90,90	0
56	MG	2a	3099	1/1	0.81	0.20	93,93,93,93	0
56	MG	1A	3053	1/1	0.81	0.38	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3447	1/1	0.81	0.30	91,91,91,91	0
56	MG	2A	3216	1/1	0.81	0.75	87,87,87,87	0
56	MG	1A	3400	1/1	0.81	0.25	90,90,90,90	0
56	MG	1a	3030	1/1	0.81	0.47	105,105,105,105	0
56	MG	2A	3351	1/1	0.81	0.15	84,84,84,84	0
56	MG	2A	3298	1/1	0.82	0.56	76,76,76,76	0
56	MG	1A	3192	1/1	0.82	0.14	74,74,74,74	0
56	MG	1A	3196	1/1	0.82	0.23	81,81,81,81	0
56	MG	2A	3097	1/1	0.82	0.41	91,91,91,91	0
56	MG	2a	3177	1/1	0.82	0.16	86,86,86,86	0
56	MG	2A	3247	1/1	0.82	0.16	101,101,101,101	0
56	MG	1a	3133	1/1	0.82	0.15	90,90,90,90	0
56	MG	2a	3085	1/1	0.82	0.16	83,83,83,83	0
56	MG	1A	3249	1/1	0.82	0.34	77,77,77,77	0
56	MG	1A	3647	1/1	0.82	0.15	93,93,93,93	0
56	MG	2A	3217	1/1	0.82	0.52	82,82,82,82	0
56	MG	1A	3385	1/1	0.82	0.30	74,74,74,74	0
56	MG	1a	3090	1/1	0.82	0.53	87,87,87,87	0
56	MG	1A	3657	1/1	0.82	0.43	79,79,79,79	0
56	MG	1a	3220	1/1	0.82	0.35	80,80,80,80	0
56	MG	1A	3180	1/1	0.82	0.77	93,93,93,93	0
56	MG	2A	3344	1/1	0.82	0.10	106,106,106,106	0
56	MG	2A	3222	1/1	0.82	0.23	89,89,89,89	0
56	MG	2A	3165	1/1	0.82	0.14	77,77,77,77	0
56	MG	2A	3090	1/1	0.82	0.22	98,98,98,98	0
56	MG	2A	3098	1/1	0.82	0.57	79,79,79,79	0
56	MG	2a	3061	1/1	0.82	0.07	92,92,92,92	0
56	MG	1A	3567	1/1	0.82	0.13	87,87,87,87	0
56	MG	1A	3293	1/1	0.82	0.13	78,78,78,78	0
56	MG	1a	3233	1/1	0.82	0.19	76,76,76,76	0
56	MG	1a	3143	1/1	0.83	0.27	91,91,91,91	0
56	MG	1A	3147	1/1	0.83	0.15	86,86,86,86	0
56	MG	1A	3208	1/1	0.83	0.22	74,74,74,74	0
56	MG	2A	3186	1/1	0.83	0.20	79,79,79,79	0
56	MG	1A	3234	1/1	0.83	0.36	96,96,96,96	0
56	MG	2a	3010	1/1	0.83	0.08	86,86,86,86	0
56	MG	1a	3169	1/1	0.83	0.16	80,80,80,80	0
56	MG	1A	3144	1/1	0.83	0.18	85,85,85,85	0
56	MG	2a	3009	1/1	0.83	0.32	84,84,84,84	0
56	MG	1a	3063	1/1	0.83	0.27	89,89,89,89	0
56	MG	1a	3062	1/1	0.83	0.27	71,71,71,71	0
56	MG	1a	3187	1/1	0.83	0.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3161	1/1	0.83	0.14	104,104,104,104	0
56	MG	1A	3203	1/1	0.83	0.29	74,74,74,74	0
56	MG	2A	3011	1/1	0.83	0.21	87,87,87,87	0
56	MG	1A	3419	1/1	0.83	0.16	87,87,87,87	0
56	MG	1A	3319	1/1	0.83	0.54	100,100,100,100	0
56	MG	1A	3113	1/1	0.83	0.14	75,75,75,75	0
56	MG	1A	3620	1/1	0.83	0.51	91,91,91,91	0
56	MG	1a	3126	1/1	0.83	0.15	100,100,100,100	0
56	MG	2a	3047	1/1	0.83	0.14	83,83,83,83	0
56	MG	1A	3444	1/1	0.83	0.23	83,83,83,83	0
56	MG	1A	3459	1/1	0.83	0.11	62,62,62,62	0
56	MG	1A	3087	1/1	0.83	0.14	79,79,79,79	0
56	MG	2A	3060	1/1	0.83	0.17	79,79,79,79	0
56	MG	1a	3097	1/1	0.83	0.88	95,95,95,95	0
56	MG	1A	3197	1/1	0.83	0.25	72,72,72,72	0
56	MG	2A	3131	1/1	0.83	0.41	95,95,95,95	0
56	MG	2A	3277	1/1	0.83	0.40	93,93,93,93	0
56	MG	2A	3151	1/1	0.83	0.13	78,78,78,78	0
56	MG	2A	3104	1/1	0.83	0.16	98,98,98,98	0
56	MG	1A	3391	1/1	0.83	0.27	80,80,80,80	0
56	MG	2A	3283	1/1	0.83	0.20	84,84,84,84	0
56	MG	2A	3033	1/1	0.83	0.33	81,81,81,81	0
56	MG	2A	3313	1/1	0.83	0.15	96,96,96,96	0
57	ZN	24	501	1/1	0.83	0.06	168,168,168,168	0
56	MG	1a	3089	1/1	0.83	0.16	78,78,78,78	0
56	MG	1a	3165	1/1	0.83	0.49	87,87,87,87	0
56	MG	1A	3265	1/1	0.83	0.26	65,65,65,65	0
56	MG	2A	3153	1/1	0.83	0.35	81,81,81,81	0
56	MG	1a	3049	1/1	0.83	0.21	87,87,87,87	0
56	MG	2a	3089	1/1	0.83	0.14	86,86,86,86	0
56	MG	1a	3083	1/1	0.83	0.30	93,93,93,93	0
56	MG	2A	3127	1/1	0.84	0.10	78,78,78,78	0
56	MG	1A	3457	1/1	0.84	0.18	77,77,77,77	0
56	MG	2A	3100	1/1	0.84	0.21	86,86,86,86	0
56	MG	1a	3115	1/1	0.84	0.12	89,89,89,89	0
56	MG	1A	3343	1/1	0.84	0.20	72,72,72,72	0
56	MG	1A	3453	1/1	0.84	0.19	84,84,84,84	0
56	MG	1A	3674	1/1	0.84	0.33	81,81,81,81	0
56	MG	1a	3107	1/1	0.84	0.17	84,84,84,84	0
56	MG	1a	3174	1/1	0.84	0.15	87,87,87,87	0
56	MG	2A	3328	1/1	0.84	0.12	90,90,90,90	0
56	MG	2a	3121	1/1	0.84	0.26	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3617	1/1	0.84	0.14	69,69,69,69	0
56	MG	2A	3194	1/1	0.84	0.16	85,85,85,85	0
56	MG	1a	3205	1/1	0.84	0.11	102,102,102,102	0
56	MG	1A	3299	1/1	0.84	0.20	90,90,90,90	0
56	MG	2A	3018	1/1	0.84	0.20	85,85,85,85	0
56	MG	1a	3007	1/1	0.84	0.19	67,67,67,67	0
56	MG	1a	3191	1/1	0.84	0.12	93,93,93,93	0
56	MG	2A	3266	1/1	0.84	0.10	88,88,88,88	0
56	MG	2a	3159	1/1	0.84	0.33	92,92,92,92	0
56	MG	2A	3013	1/1	0.84	0.36	79,79,79,79	0
56	MG	1a	3052	1/1	0.84	0.15	84,84,84,84	0
56	MG	1A	3371	1/1	0.84	0.29	52,52,52,52	0
56	MG	1A	3633	1/1	0.84	0.22	75,75,75,75	0
56	MG	2A	3061	1/1	0.84	0.18	76,76,76,76	0
56	MG	1A	3658	1/1	0.84	0.23	98,98,98,98	0
56	MG	2A	3026	1/1	0.84	0.19	92,92,92,92	0
56	MG	1A	3287	1/1	0.84	0.13	80,80,80,80	0
56	MG	1A	3253	1/1	0.84	0.28	71,71,71,71	0
56	MG	1A	3601	1/1	0.84	0.91	102,102,102,102	0
56	MG	1A	3339	1/1	0.84	1.46	112,112,112,112	0
56	MG	1A	3622	1/1	0.84	0.19	91,91,91,91	0
56	MG	1A	3026	1/1	0.84	0.27	77,77,77,77	0
56	MG	1A	3001	1/1	0.84	0.10	70,70,70,70	0
56	MG	1a	3070	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3137	1/1	0.84	0.20	82,82,82,82	0
56	MG	1A	3030	1/1	0.84	0.50	69,69,69,69	0
56	MG	2A	3204	1/1	0.84	0.53	90,90,90,90	0
56	MG	2a	3160	1/1	0.84	0.11	104,104,104,104	0
56	MG	2A	3215	1/1	0.84	0.18	86,86,86,86	0
56	MG	2a	3012	1/1	0.84	0.14	79,79,79,79	0
56	MG	2a	3078	1/1	0.84	0.15	85,85,85,85	0
56	MG	1A	3012	1/1	0.84	0.13	78,78,78,78	0
56	MG	1A	3548	1/1	0.84	0.62	91,91,91,91	0
56	MG	2A	3152	1/1	0.85	0.68	85,85,85,85	0
56	MG	1A	3521	1/1	0.85	0.15	64,64,64,64	0
56	MG	1A	3372	1/1	0.85	0.17	63,63,63,63	0
56	MG	1a	3099	1/1	0.85	0.10	90,90,90,90	0
56	MG	1A	3019	1/1	0.85	0.19	81,81,81,81	0
56	MG	2A	3253	1/1	0.85	0.17	74,74,74,74	0
56	MG	1A	3063	1/1	0.85	0.16	80,80,80,80	0
56	MG	1A	3519	1/1	0.85	0.17	88,88,88,88	0
56	MG	2a	3062	1/1	0.85	0.32	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3181	1/1	0.85	0.69	90,90,90,90	0
56	MG	1A	3417	1/1	0.85	0.19	79,79,79,79	0
56	MG	1A	3219	1/1	0.85	0.13	84,84,84,84	0
56	MG	1A	3205	1/1	0.85	0.15	78,78,78,78	0
56	MG	2A	3024	1/1	0.85	0.22	95,95,95,95	0
56	MG	1A	3246	1/1	0.85	0.14	78,78,78,78	0
56	MG	2A	3207	1/1	0.85	0.46	68,68,68,68	0
56	MG	2A	3190	1/1	0.85	0.11	98,98,98,98	0
56	MG	1a	3127	1/1	0.85	0.21	82,82,82,82	0
56	MG	2a	3076	1/1	0.85	0.17	99,99,99,99	0
56	MG	1A	3543	1/1	0.85	0.28	86,86,86,86	0
56	MG	2A	3203	1/1	0.85	0.43	87,87,87,87	0
56	MG	2A	3080	1/1	0.85	0.08	80,80,80,80	0
56	MG	1A	3608	1/1	0.85	0.12	87,87,87,87	0
56	MG	1A	3007	1/1	0.85	0.12	91,91,91,91	0
56	MG	1a	3166	1/1	0.85	0.15	100,100,100,100	0
56	MG	1a	3108	1/1	0.85	0.24	93,93,93,93	0
56	MG	2A	3263	1/1	0.85	0.52	86,86,86,86	0
56	MG	2A	3028	1/1	0.85	0.40	68,68,68,68	0
56	MG	1A	3354	1/1	0.85	0.21	83,83,83,83	0
56	MG	2A	3041	1/1	0.85	0.23	69,69,69,69	0
56	MG	2a	3162	1/1	0.85	0.15	126,126,126,126	0
56	MG	1a	3224	1/1	0.85	0.21	77,77,77,77	0
56	MG	1A	3552	1/1	0.85	0.14	100,100,100,100	0
56	MG	1A	3455	1/1	0.85	0.15	63,63,63,63	0
56	MG	2A	3209	1/1	0.85	0.38	83,83,83,83	0
56	MG	1a	3036	1/1	0.85	0.14	90,90,90,90	0
56	MG	1a	3060	1/1	0.85	0.17	83,83,83,83	0
56	MG	2A	3295	1/1	0.85	0.31	91,91,91,91	0
56	MG	2A	3195	1/1	0.85	0.31	84,84,84,84	0
56	MG	1A	3153	1/1	0.85	0.37	72,72,72,72	0
56	MG	2a	3118	1/1	0.85	0.04	115,115,115,115	0
56	MG	2a	3120	1/1	0.85	0.67	103,103,103,103	0
56	MG	1a	3180	1/1	0.85	0.19	90,90,90,90	0
56	MG	1a	3213	1/1	0.86	1.10	117,117,117,117	0
56	MG	2A	3053	1/1	0.86	0.10	77,77,77,77	0
56	MG	1A	3621	1/1	0.86	0.13	69,69,69,69	0
56	MG	1a	3058	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3154	1/1	0.86	0.70	74,74,74,74	0
56	MG	2A	3072	1/1	0.86	0.18	74,74,74,74	0
56	MG	1A	3237	1/1	0.86	0.33	74,74,74,74	0
56	MG	1A	3122	1/1	0.86	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3025	1/1	0.86	0.21	88,88,88,88	0
56	MG	1A	3075	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3443	1/1	0.86	0.09	82,82,82,82	0
56	MG	1A	3154	1/1	0.86	0.18	59,59,59,59	0
56	MG	1A	3330	1/1	0.86	0.26	96,96,96,96	0
56	MG	2A	3084	1/1	0.86	0.26	90,90,90,90	0
56	MG	1A	3529	1/1	0.86	0.16	71,71,71,71	0
56	MG	2A	3048	1/1	0.86	0.23	83,83,83,83	0
56	MG	1A	3103	1/1	0.86	0.86	68,68,68,68	0
56	MG	2a	3066	1/1	0.86	0.22	106,106,106,106	0
56	MG	1A	3150	1/1	0.86	0.20	91,91,91,91	0
56	MG	1A	3425	1/1	0.86	0.31	62,62,62,62	0
56	MG	1A	3022	1/1	0.86	0.38	83,83,83,83	0
56	MG	1A	3609	1/1	0.86	0.67	74,74,74,74	0
56	MG	1A	3525	1/1	0.86	0.21	101,101,101,101	0
56	MG	2A	3144	1/1	0.86	0.42	75,75,75,75	0
56	MG	1A	3589	1/1	0.86	0.11	86,86,86,86	0
56	MG	2a	3043	1/1	0.86	0.66	70,70,70,70	0
56	MG	1A	3493	1/1	0.86	0.16	69,69,69,69	0
56	MG	1a	3140	1/1	0.86	0.33	84,84,84,84	0
56	MG	2A	3333	1/1	0.86	0.12	101,101,101,101	0
56	MG	1A	3566	1/1	0.86	0.10	93,93,93,93	0
56	MG	2a	3168	1/1	0.86	0.15	112,112,112,112	0
56	MG	1A	3065	1/1	0.86	0.43	71,71,71,71	0
56	MG	1A	3556	1/1	0.86	0.18	81,81,81,81	0
56	MG	1A	3251	1/1	0.86	0.43	69,69,69,69	0
56	MG	1A	3452	1/1	0.86	0.16	97,97,97,97	0
56	MG	1A	3139	1/1	0.86	0.21	79,79,79,79	0
56	MG	1A	3177	1/1	0.86	0.66	89,89,89,89	0
56	MG	1a	3103	1/1	0.86	0.19	79,79,79,79	0
56	MG	1a	3018	1/1	0.86	0.37	74,74,74,74	0
56	MG	2A	3286	1/1	0.86	0.15	93,93,93,93	0
56	MG	1A	3431	1/1	0.86	0.14	76,76,76,76	0
56	MG	2A	3188	1/1	0.86	0.12	92,92,92,92	0
56	MG	2a	3142	1/1	0.86	0.24	103,103,103,103	0
56	MG	1A	3011	1/1	0.86	0.38	65,65,65,65	0
56	MG	1A	3100	1/1	0.87	0.60	61,61,61,61	0
56	MG	1A	3186	1/1	0.87	0.15	95,95,95,95	0
56	MG	2a	3064	1/1	0.87	0.14	99,99,99,99	0
56	MG	1a	3170	1/1	0.87	0.13	76,76,76,76	0
56	MG	1a	3120	1/1	0.87	0.57	87,87,87,87	0
56	MG	2A	3157	1/1	0.87	0.84	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3023	1/1	0.87	1.07	88,88,88,88	0
56	MG	1A	3545	1/1	0.87	0.17	67,67,67,67	0
56	MG	2A	3140	1/1	0.87	0.45	81,81,81,81	0
56	MG	1a	3042	1/1	0.87	0.11	74,74,74,74	0
56	MG	1A	3167	1/1	0.87	0.20	90,90,90,90	0
56	MG	2a	3117	1/1	0.87	0.11	92,92,92,92	0
56	MG	2a	3024	1/1	0.87	0.10	90,90,90,90	0
56	MG	1A	3048	1/1	0.87	0.51	74,74,74,74	0
56	MG	2A	3038	1/1	0.87	0.39	65,65,65,65	0
56	MG	2A	3115	1/1	0.87	1.18	80,80,80,80	0
56	MG	2a	3183	1/1	0.87	0.07	98,98,98,98	0
56	MG	1A	3637	1/1	0.87	0.13	100,100,100,100	0
56	MG	2a	3042	1/1	0.87	0.19	82,82,82,82	0
56	MG	1A	3541	1/1	0.87	0.15	72,72,72,72	0
56	MG	2A	3106	1/1	0.87	0.25	73,73,73,73	0
56	MG	2A	3254	1/1	0.87	0.15	78,78,78,78	0
56	MG	1a	3071	1/1	0.87	0.84	75,75,75,75	0
56	MG	1A	3437	1/1	0.87	0.31	79,79,79,79	0
56	MG	1a	3139	1/1	0.87	0.41	81,81,81,81	0
56	MG	1a	3020	1/1	0.87	0.15	74,74,74,74	0
56	MG	2a	3176	1/1	0.87	0.14	83,83,83,83	0
56	MG	1A	3032	1/1	0.87	0.14	75,75,75,75	0
56	MG	1a	3184	1/1	0.87	0.27	71,71,71,71	0
56	MG	2A	3334	1/1	0.87	0.46	105,105,105,105	0
56	MG	1A	3613	1/1	0.87	0.15	64,64,64,64	0
56	MG	1A	3118	1/1	0.87	0.11	60,60,60,60	0
56	MG	2a	3055	1/1	0.87	0.23	95,95,95,95	0
56	MG	2a	3069	1/1	0.87	0.19	103,103,103,103	0
56	MG	1A	3183	1/1	0.87	0.42	74,74,74,74	0
56	MG	2A	3327	1/1	0.87	0.52	96,96,96,96	0
56	MG	1A	3288	1/1	0.87	0.12	70,70,70,70	0
56	MG	2a	3129	1/1	0.87	0.14	92,92,92,92	0
56	MG	1A	3600	1/1	0.87	0.10	77,77,77,77	0
56	MG	1a	3035	1/1	0.87	0.23	81,81,81,81	0
56	MG	1A	3358	1/1	0.87	0.19	83,83,83,83	0
56	MG	1A	3138	1/1	0.87	0.48	82,82,82,82	0
56	MG	1A	3322	1/1	0.87	0.15	92,92,92,92	0
56	MG	1A	3494	1/1	0.88	0.11	75,75,75,75	0
56	MG	1a	3217	1/1	0.88	0.10	85,85,85,85	0
56	MG	2a	3105	1/1	0.88	0.26	95,95,95,95	0
56	MG	2A	3343	1/1	0.88	0.23	99,99,99,99	0
56	MG	1A	3614	1/1	0.88	0.15	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3004	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3263	1/1	0.88	0.20	78,78,78,78	0
56	MG	1a	3146	1/1	0.88	0.20	79,79,79,79	0
56	MG	1A	3301	1/1	0.88	0.24	85,85,85,85	0
56	MG	1a	3113	1/1	0.88	0.13	86,86,86,86	0
56	MG	2a	3164	1/1	0.88	0.10	114,114,114,114	0
56	MG	1A	3481	1/1	0.88	0.22	83,83,83,83	0
56	MG	1a	3175	1/1	0.88	0.07	87,87,87,87	0
56	MG	2a	3096	1/1	0.88	0.27	84,84,84,84	0
56	MG	2A	3147	1/1	0.88	0.13	84,84,84,84	0
56	MG	1A	3436	1/1	0.88	0.18	68,68,68,68	0
56	MG	1A	3185	1/1	0.88	1.14	80,80,80,80	0
56	MG	1A	3465	1/1	0.88	0.18	80,80,80,80	0
56	MG	2a	3124	1/1	0.88	0.18	83,83,83,83	0
56	MG	1A	3066	1/1	0.88	0.37	78,78,78,78	0
56	MG	1a	3073	1/1	0.88	0.16	78,78,78,78	0
56	MG	1A	3286	1/1	0.88	0.12	96,96,96,96	0
56	MG	1a	3147	1/1	0.88	0.27	71,71,71,71	0
56	MG	1a	3153	1/1	0.88	0.15	84,84,84,84	0
56	MG	1A	3175	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	3279	1/1	0.88	0.15	82,82,82,82	0
56	MG	2A	3121	1/1	0.88	0.34	79,79,79,79	0
56	MG	2A	3296	1/1	0.88	0.21	102,102,102,102	0
56	MG	1A	3396	1/1	0.88	0.28	99,99,99,99	0
56	MG	1A	3645	1/1	0.88	0.24	82,82,82,82	0
56	MG	2A	3301	1/1	0.88	0.22	83,83,83,83	0
56	MG	1A	3184	1/1	0.88	1.24	73,73,73,73	0
56	MG	1A	3021	1/1	0.88	1.00	55,55,55,55	0
56	MG	1A	3267	1/1	0.88	0.22	76,76,76,76	0
56	MG	1A	3173	1/1	0.88	0.16	74,74,74,74	0
56	MG	1a	3064	1/1	0.88	0.32	87,87,87,87	0
56	MG	1A	3544	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3136	1/1	0.88	0.23	71,71,71,71	0
56	MG	1A	3052	1/1	0.88	0.21	77,77,77,77	0
56	MG	1A	3261	1/1	0.88	0.22	72,72,72,72	0
56	MG	2A	3150	1/1	0.88	0.43	88,88,88,88	0
56	MG	1A	3214	1/1	0.88	0.27	96,96,96,96	0
56	MG	1A	3347	1/1	0.88	0.23	70,70,70,70	0
56	MG	1a	3190	1/1	0.88	1.15	95,95,95,95	0
56	MG	1A	3210	1/1	0.88	0.15	71,71,71,71	0
56	MG	2A	3035	1/1	0.88	0.16	92,92,92,92	0
56	MG	2a	3101	1/1	0.88	0.80	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3143	1/1	0.88	0.10	107,107,107,107	0
56	MG	2A	3265	1/1	0.88	0.34	93,93,93,93	0
56	MG	2a	3074	1/1	0.88	0.14	98,98,98,98	0
56	MG	1a	3024	1/1	0.88	0.41	83,83,83,83	0
56	MG	1a	3032	1/1	0.88	0.07	76,76,76,76	0
56	MG	1A	3042	1/1	0.88	0.17	64,64,64,64	0
56	MG	2a	3180	1/1	0.88	0.26	102,102,102,102	0
56	MG	1A	3127	1/1	0.88	0.16	72,72,72,72	0
56	MG	2A	3223	1/1	0.88	0.21	72,72,72,72	0
56	MG	2a	3178	1/1	0.88	0.26	96,96,96,96	0
56	MG	1A	3639	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	3136	1/1	0.89	0.69	78,78,78,78	0
56	MG	1a	3192	1/1	0.89	0.19	85,85,85,85	0
56	MG	1A	3662	1/1	0.89	0.16	90,90,90,90	0
56	MG	2A	3047	1/1	0.89	0.26	89,89,89,89	0
56	MG	1A	3648	1/1	0.89	0.32	127,127,127,127	0
56	MG	2a	3005	1/1	0.89	0.43	96,96,96,96	0
56	MG	1A	3092	1/1	0.89	0.09	70,70,70,70	0
56	MG	1A	3308	1/1	0.89	0.13	80,80,80,80	0
56	MG	2A	3118	1/1	0.89	0.62	72,72,72,72	0
56	MG	1A	3575	1/1	0.89	0.25	83,83,83,83	0
56	MG	1a	3101	1/1	0.89	0.39	88,88,88,88	0
56	MG	2a	3003	1/1	0.89	0.48	69,69,69,69	0
56	MG	2a	3115	1/1	0.89	0.24	103,103,103,103	0
56	MG	2A	3042	1/1	0.89	0.12	89,89,89,89	0
56	MG	1A	3363	1/1	0.89	0.18	79,79,79,79	0
56	MG	2A	3105	1/1	0.89	0.18	71,71,71,71	0
56	MG	2A	3008	1/1	0.89	0.11	79,79,79,79	0
56	MG	1A	3560	1/1	0.89	0.27	88,88,88,88	0
56	MG	2A	3141	1/1	0.89	0.72	81,81,81,81	0
56	MG	1A	3353	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3346	1/1	0.89	0.41	92,92,92,92	0
56	MG	1A	3323	1/1	0.89	0.20	81,81,81,81	0
56	MG	1A	3062	1/1	0.89	0.84	92,92,92,92	0
56	MG	1a	3121	1/1	0.89	0.41	88,88,88,88	0
56	MG	2A	3039	1/1	0.89	0.32	88,88,88,88	0
56	MG	1A	3515	1/1	0.89	0.30	63,63,63,63	0
56	MG	1a	3048	1/1	0.89	0.20	73,73,73,73	0
56	MG	1A	3306	1/1	0.89	0.28	82,82,82,82	0
56	MG	2a	3175	1/1	0.89	0.20	76,76,76,76	0
56	MG	1A	3078	1/1	0.89	0.91	79,79,79,79	0
56	MG	1A	3407	1/1	0.89	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3079	1/1	0.89	0.37	90,90,90,90	0
56	MG	2A	3079	1/1	0.89	0.25	89,89,89,89	0
56	MG	2a	3163	1/1	0.89	0.19	103,103,103,103	0
56	MG	1A	3416	1/1	0.89	0.34	82,82,82,82	0
56	MG	1a	3124	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3169	1/1	0.89	0.25	84,84,84,84	0
56	MG	1A	3164	1/1	0.89	0.14	72,72,72,72	0
56	MG	1A	3503	1/1	0.89	0.27	90,90,90,90	0
56	MG	2A	3282	1/1	0.89	0.12	87,87,87,87	0
56	MG	1A	3588	1/1	0.89	0.23	82,82,82,82	0
56	MG	2a	3170	1/1	0.89	0.13	80,80,80,80	0
56	MG	1A	3676	1/1	0.89	0.15	84,84,84,84	0
56	MG	1a	3158	1/1	0.89	0.15	81,81,81,81	0
56	MG	1A	3434	1/1	0.89	0.10	81,81,81,81	0
56	MG	1A	3112	1/1	0.89	0.29	66,66,66,66	0
56	MG	2A	3126	1/1	0.89	0.21	80,80,80,80	0
56	MG	1a	3045	1/1	0.89	0.12	85,85,85,85	0
56	MG	1a	3236	1/1	0.89	0.15	85,85,85,85	0
56	MG	2A	3293	1/1	0.89	0.13	95,95,95,95	0
56	MG	1A	3165	1/1	0.89	0.41	86,86,86,86	0
56	MG	1a	3050	1/1	0.89	0.11	80,80,80,80	0
56	MG	2a	3014	1/1	0.90	0.30	89,89,89,89	0
56	MG	2A	3077	1/1	0.90	0.42	77,77,77,77	0
56	MG	2a	3029	1/1	0.90	0.20	87,87,87,87	0
56	MG	1a	3209	1/1	0.90	0.33	90,90,90,90	0
56	MG	1a	3065	1/1	0.90	0.19	87,87,87,87	0
56	MG	1A	3327	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3040	1/1	0.90	0.14	82,82,82,82	0
56	MG	2A	3130	1/1	0.90	0.24	90,90,90,90	0
56	MG	1A	3577	1/1	0.90	0.12	94,94,94,94	0
56	MG	2a	3040	1/1	0.90	0.14	78,78,78,78	0
56	MG	1a	3215	1/1	0.90	0.15	84,84,84,84	0
56	MG	1A	3472	1/1	0.90	0.14	72,72,72,72	0
56	MG	1A	3547	1/1	0.90	0.18	71,71,71,71	0
56	MG	1A	3374	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3568	1/1	0.90	0.09	79,79,79,79	0
57	ZN	2Y	501	1/1	0.90	0.13	138,138,138,138	0
56	MG	2A	3089	1/1	0.90	0.15	82,82,82,82	0
56	MG	1A	3489	1/1	0.90	0.34	78,78,78,78	0
56	MG	1A	3188	1/1	0.90	0.27	91,91,91,91	0
56	MG	1A	3520	1/1	0.90	0.10	88,88,88,88	0
56	MG	1A	3679	1/1	0.90	0.59	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3156	1/1	0.90	0.14	66,66,66,66	0
56	MG	1A	3049	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3324	1/1	0.90	0.36	67,67,67,67	0
56	MG	1A	3044	1/1	0.90	0.16	89,89,89,89	0
56	MG	1a	3009	1/1	0.90	0.36	91,91,91,91	0
56	MG	1A	3250	1/1	0.90	0.30	94,94,94,94	0
56	MG	1A	3009	1/1	0.90	0.28	75,75,75,75	0
56	MG	1A	3468	1/1	0.90	0.73	83,83,83,83	0
56	MG	1A	3531	1/1	0.90	0.20	92,92,92,92	0
56	MG	2A	3173	1/1	0.90	0.11	70,70,70,70	0
56	MG	2a	3139	1/1	0.90	0.15	81,81,81,81	0
56	MG	1a	3066	1/1	0.90	0.11	101,101,101,101	0
56	MG	1A	3218	1/1	0.90	0.21	96,96,96,96	0
56	MG	1a	3012	1/1	0.90	0.49	93,93,93,93	0
56	MG	2a	3151	1/1	0.90	0.20	111,111,111,111	0
56	MG	2A	3330	1/1	0.90	0.16	101,101,101,101	0
56	MG	2A	3213	1/1	0.90	0.14	90,90,90,90	0
56	MG	1a	3109	1/1	0.90	0.61	103,103,103,103	0
56	MG	1a	3093	1/1	0.90	0.39	88,88,88,88	0
56	MG	1A	3439	1/1	0.90	0.30	84,84,84,84	0
56	MG	2A	3004	1/1	0.90	0.16	91,91,91,91	0
56	MG	1A	3067	1/1	0.90	0.08	65,65,65,65	0
56	MG	2a	3157	1/1	0.90	0.29	114,114,114,114	0
56	MG	2A	3273	1/1	0.90	0.20	86,86,86,86	0
56	MG	1A	3405	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3256	1/1	0.90	0.08	98,98,98,98	0
56	MG	1a	3014	1/1	0.90	0.10	78,78,78,78	0
56	MG	2A	3076	1/1	0.90	0.47	77,77,77,77	0
56	MG	2a	3011	1/1	0.90	0.10	101,101,101,101	0
56	MG	1A	3584	1/1	0.90	0.16	92,92,92,92	0
56	MG	1a	3118	1/1	0.90	0.75	101,101,101,101	0
56	MG	1A	3094	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3665	1/1	0.90	0.21	74,74,74,74	0
56	MG	2a	3155	1/1	0.90	0.11	84,84,84,84	0
56	MG	2A	3139	1/1	0.90	0.25	101,101,101,101	0
56	MG	1A	3096	1/1	0.90	0.09	90,90,90,90	0
56	MG	2A	3159	1/1	0.90	0.14	91,91,91,91	0
56	MG	1A	3231	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3070	1/1	0.90	0.23	52,52,52,52	0
56	MG	1a	3046	1/1	0.90	0.24	73,73,73,73	0
56	MG	1A	3270	1/1	0.90	0.41	75,75,75,75	0
56	MG	1A	3607	1/1	0.90	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3072	1/1	0.90	0.12	107,107,107,107	0
56	MG	2A	3086	1/1	0.91	0.92	78,78,78,78	0
56	MG	1A	3024	1/1	0.91	0.82	83,83,83,83	0
56	MG	1A	3300	1/1	0.91	0.19	77,77,77,77	0
56	MG	1A	3140	1/1	0.91	0.20	89,89,89,89	0
56	MG	1a	3154	1/1	0.91	0.32	78,78,78,78	0
56	MG	1a	3226	1/1	0.91	0.27	89,89,89,89	0
56	MG	1A	3006	1/1	0.91	0.45	69,69,69,69	0
56	MG	1A	3095	1/1	0.91	0.17	81,81,81,81	0
56	MG	1a	3095	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3050	1/1	0.91	0.16	76,76,76,76	0
56	MG	2A	3124	1/1	0.91	0.20	86,86,86,86	0
56	MG	2a	3126	1/1	0.91	0.31	86,86,86,86	0
56	MG	2A	3246	1/1	0.91	0.88	105,105,105,105	0
56	MG	1A	3232	1/1	0.91	0.24	52,52,52,52	0
56	MG	2a	3001	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3333	1/1	0.91	0.30	73,73,73,73	0
56	MG	1A	3285	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	3328	1/1	0.91	0.34	94,94,94,94	0
56	MG	1a	3185	1/1	0.91	0.11	90,90,90,90	0
56	MG	1a	3021	1/1	0.91	0.24	102,102,102,102	0
56	MG	1A	3652	1/1	0.91	0.13	86,86,86,86	0
56	MG	1A	3010	1/1	0.91	0.64	65,65,65,65	0
56	MG	1a	3216	1/1	0.91	0.14	81,81,81,81	0
56	MG	2A	3268	1/1	0.91	0.06	82,82,82,82	0
56	MG	1A	3553	1/1	0.91	0.22	89,89,89,89	0
56	MG	2A	3168	1/1	0.91	0.30	98,98,98,98	0
56	MG	1A	3380	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3256	1/1	0.91	0.42	84,84,84,84	0
56	MG	1A	3119	1/1	0.91	0.23	107,107,107,107	0
56	MG	2A	3314	1/1	0.91	0.13	94,94,94,94	0
56	MG	1A	3294	1/1	0.91	0.38	87,87,87,87	0
56	MG	2a	3091	1/1	0.91	0.24	92,92,92,92	0
56	MG	2A	3284	1/1	0.91	0.09	79,79,79,79	0
56	MG	1a	3061	1/1	0.91	0.35	79,79,79,79	0
56	MG	1A	3033	1/1	0.91	0.31	86,86,86,86	0
56	MG	1A	3335	1/1	0.91	0.14	66,66,66,66	0
56	MG	1A	3426	1/1	0.91	0.25	72,72,72,72	0
56	MG	2A	3321	1/1	0.91	0.10	101,101,101,101	0
56	MG	1A	3478	1/1	0.91	0.30	83,83,83,83	0
56	MG	2A	3149	1/1	0.91	0.27	84,84,84,84	0
56	MG	2a	3145	1/1	0.91	0.20	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3178	1/1	0.91	0.43	82,82,82,82	0
56	MG	2A	3320	1/1	0.91	0.10	79,79,79,79	0
56	MG	2A	3036	1/1	0.91	0.94	87,87,87,87	0
56	MG	1A	3035	1/1	0.91	0.15	70,70,70,70	0
56	MG	2A	3169	1/1	0.91	0.26	79,79,79,79	0
56	MG	1a	3232	1/1	0.91	0.19	76,76,76,76	0
56	MG	1A	3357	1/1	0.91	0.32	76,76,76,76	0
56	MG	1A	3361	1/1	0.91	0.27	71,71,71,71	0
56	MG	2a	3095	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3388	1/1	0.91	0.34	69,69,69,69	0
56	MG	1A	3141	1/1	0.91	0.21	70,70,70,70	0
56	MG	1A	3243	1/1	0.91	0.12	81,81,81,81	0
56	MG	1A	3504	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3091	1/1	0.91	0.28	74,74,74,74	0
56	MG	1A	3460	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3559	1/1	0.91	0.10	115,115,115,115	0
56	MG	2a	3127	1/1	0.91	0.10	100,100,100,100	0
56	MG	2A	3170	1/1	0.91	0.20	95,95,95,95	0
56	MG	2A	3054	1/1	0.91	0.17	89,89,89,89	0
56	MG	2A	3257	1/1	0.91	0.26	76,76,76,76	0
56	MG	1A	3616	1/1	0.91	0.27	84,84,84,84	0
56	MG	1a	3025	1/1	0.91	0.09	85,85,85,85	0
56	MG	1a	3112	1/1	0.91	0.25	70,70,70,70	0
56	MG	1A	3454	1/1	0.91	0.20	66,66,66,66	0
56	MG	2A	3348	1/1	0.91	0.25	79,79,79,79	0
56	MG	1A	3350	1/1	0.91	0.13	76,76,76,76	0
56	MG	2A	3009	1/1	0.91	0.90	89,89,89,89	0
56	MG	2A	3210	1/1	0.91	0.12	75,75,75,75	0
56	MG	1A	3201	1/1	0.91	0.29	68,68,68,68	0
56	MG	1A	3470	1/1	0.91	0.31	100,100,100,100	0
56	MG	1A	3427	1/1	0.91	0.20	78,78,78,78	0
56	MG	1a	3098	1/1	0.91	0.35	87,87,87,87	0
56	MG	1A	3060	1/1	0.91	0.17	75,75,75,75	0
56	MG	2a	3023	1/1	0.91	0.47	80,80,80,80	0
56	MG	2A	3303	1/1	0.91	0.65	98,98,98,98	0
56	MG	1a	3202	1/1	0.91	0.22	89,89,89,89	0
56	MG	1A	3310	1/1	0.91	0.14	76,76,76,76	0
56	MG	1a	3015	1/1	0.91	0.39	90,90,90,90	0
56	MG	1a	3031	1/1	0.91	0.49	103,103,103,103	0
56	MG	1a	3186	1/1	0.91	0.19	85,85,85,85	0
56	MG	2a	3071	1/1	0.91	0.41	88,88,88,88	0
56	MG	1A	3290	1/1	0.92	0.35	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3187	1/1	0.92	0.14	81,81,81,81	0
56	MG	1a	3079	1/1	0.92	0.19	73,73,73,73	0
56	MG	2A	3164	1/1	0.92	0.16	82,82,82,82	0
56	MG	2a	3123	1/1	0.92	0.16	79,79,79,79	0
56	MG	1A	3275	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3551	1/1	0.92	0.24	97,97,97,97	0
56	MG	1A	3126	1/1	0.92	0.64	76,76,76,76	0
56	MG	2a	3086	1/1	0.92	0.14	87,87,87,87	0
56	MG	2a	3152	1/1	0.92	0.19	111,111,111,111	0
56	MG	1A	3642	1/1	0.92	0.29	74,74,74,74	0
56	MG	1A	3491	1/1	0.92	0.23	84,84,84,84	0
56	MG	1A	3313	1/1	0.92	0.29	72,72,72,72	0
56	MG	1A	3340	1/1	0.92	0.32	78,78,78,78	0
56	MG	1A	3171	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3449	1/1	0.92	0.27	76,76,76,76	0
56	MG	2A	3242	1/1	0.92	0.18	70,70,70,70	0
56	MG	2A	3180	1/1	0.92	0.15	74,74,74,74	0
56	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
56	MG	1a	3059	1/1	0.92	0.68	82,82,82,82	0
56	MG	1a	3091	1/1	0.92	0.57	83,83,83,83	0
56	MG	1A	3563	1/1	0.92	0.17	97,97,97,97	0
56	MG	2A	3020	1/1	0.92	0.29	69,69,69,69	0
56	MG	1A	3204	1/1	0.92	0.19	60,60,60,60	0
56	MG	1A	3211	1/1	0.92	0.30	88,88,88,88	0
56	MG	2a	3046	1/1	0.92	0.10	85,85,85,85	0
56	MG	1A	3110	1/1	0.92	0.67	82,82,82,82	0
56	MG	1A	3207	1/1	0.92	0.11	74,74,74,74	0
56	MG	1A	3618	1/1	0.92	0.19	98,98,98,98	0
56	MG	1a	3178	1/1	0.92	0.32	81,81,81,81	0
56	MG	1A	3409	1/1	0.92	0.33	70,70,70,70	0
56	MG	1a	3229	1/1	0.92	0.24	85,85,85,85	0
56	MG	2A	3044	1/1	0.92	0.22	78,78,78,78	0
56	MG	1a	3207	1/1	0.92	0.20	96,96,96,96	0
56	MG	1A	3055	1/1	0.92	0.22	79,79,79,79	0
56	MG	2A	3211	1/1	0.92	0.29	81,81,81,81	0
56	MG	2a	3033	1/1	0.92	0.13	86,86,86,86	0
56	MG	1A	3672	1/1	0.92	0.28	68,68,68,68	0
56	MG	1a	3034	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3495	1/1	0.92	0.23	66,66,66,66	0
56	MG	1A	3581	1/1	0.92	0.13	84,84,84,84	0
56	MG	2A	3116	1/1	0.92	0.35	91,91,91,91	0
56	MG	2A	3068	1/1	0.92	0.18	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3411	1/1	0.92	0.17	66,66,66,66	0
56	MG	2a	3156	1/1	0.92	0.08	104,104,104,104	0
56	MG	1A	3461	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3582	1/1	0.92	0.20	73,73,73,73	0
56	MG	2A	3182	1/1	0.92	0.23	81,81,81,81	0
56	MG	1A	3356	1/1	0.92	0.67	61,61,61,61	0
56	MG	1A	3274	1/1	0.92	0.24	78,78,78,78	0
56	MG	2A	3335	1/1	0.92	0.09	100,100,100,100	0
56	MG	1A	3550	1/1	0.92	0.31	101,101,101,101	0
56	MG	2A	3252	1/1	0.92	0.13	73,73,73,73	0
56	MG	1A	3599	1/1	0.92	0.30	100,100,100,100	0
56	MG	2A	3007	1/1	0.92	0.14	80,80,80,80	0
56	MG	2A	3229	1/1	0.92	0.18	90,90,90,90	0
56	MG	2a	3073	1/1	0.92	0.19	113,113,113,113	0
56	MG	1A	3488	1/1	0.92	0.16	80,80,80,80	0
56	MG	1a	3010	1/1	0.92	0.26	85,85,85,85	0
56	MG	1A	3466	1/1	0.92	0.16	92,92,92,92	0
56	MG	1A	3596	1/1	0.92	0.16	81,81,81,81	0
56	MG	1A	3329	1/1	0.92	0.20	77,77,77,77	0
56	MG	2A	3135	1/1	0.92	0.25	78,78,78,78	0
56	MG	1A	3389	1/1	0.92	0.49	75,75,75,75	0
56	MG	2A	3145	1/1	0.92	0.11	77,77,77,77	0
56	MG	2A	3043	1/1	0.92	0.21	82,82,82,82	0
56	MG	1A	3500	1/1	0.92	0.17	86,86,86,86	0
56	MG	1A	3283	1/1	0.92	0.25	58,58,58,58	0
56	MG	2A	3238	1/1	0.92	0.17	93,93,93,93	0
56	MG	2a	3039	1/1	0.92	0.13	89,89,89,89	0
56	MG	1a	3197	1/1	0.92	0.12	102,102,102,102	0
56	MG	1a	3022	1/1	0.92	0.21	89,89,89,89	0
56	MG	2A	3066	1/1	0.92	0.13	92,92,92,92	0
56	MG	2a	3113	1/1	0.92	0.08	111,111,111,111	0
56	MG	1a	3123	1/1	0.92	0.16	72,72,72,72	0
56	MG	1A	3187	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3325	1/1	0.92	0.19	69,69,69,69	0
56	MG	2A	3050	1/1	0.92	0.36	81,81,81,81	0
56	MG	2A	3081	1/1	0.92	0.10	79,79,79,79	0
56	MG	1a	3026	1/1	0.92	0.22	80,80,80,80	0
56	MG	1A	3124	1/1	0.92	0.79	86,86,86,86	0
56	MG	2A	3326	1/1	0.92	0.16	91,91,91,91	0
56	MG	1A	3384	1/1	0.92	0.46	75,75,75,75	0
56	MG	2A	3312	1/1	0.92	0.10	74,74,74,74	0
56	MG	2a	3119	1/1	0.92	0.12	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3026	1/1	0.92	0.15	90,90,90,90	0
56	MG	1A	3115	1/1	0.92	0.23	87,87,87,87	0
56	MG	1A	3638	1/1	0.92	0.13	80,80,80,80	0
56	MG	1a	3084	1/1	0.92	0.20	94,94,94,94	0
56	MG	1A	3143	1/1	0.92	0.32	84,84,84,84	0
56	MG	2A	3305	1/1	0.92	0.11	85,85,85,85	0
56	MG	2a	3075	1/1	0.92	0.30	98,98,98,98	0
56	MG	1A	3365	1/1	0.92	0.31	75,75,75,75	0
56	MG	2A	3046	1/1	0.92	0.13	68,68,68,68	0
56	MG	1a	3160	1/1	0.93	0.23	76,76,76,76	0
56	MG	1A	3038	1/1	0.93	0.16	74,74,74,74	0
56	MG	1a	3003	1/1	0.93	0.11	92,92,92,92	0
56	MG	1A	3233	1/1	0.93	0.09	58,58,58,58	0
56	MG	2a	3104	1/1	0.93	0.11	100,100,100,100	0
56	MG	2A	3202	1/1	0.93	0.32	88,88,88,88	0
56	MG	1A	3542	1/1	0.93	0.42	77,77,77,77	0
56	MG	1A	3158	1/1	0.93	0.19	67,67,67,67	0
56	MG	1A	3334	1/1	0.93	0.18	64,64,64,64	0
56	MG	1A	3223	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3271	1/1	0.93	0.18	83,83,83,83	0
56	MG	1A	3469	1/1	0.93	0.37	84,84,84,84	0
56	MG	1A	3235	1/1	0.93	0.13	73,73,73,73	0
56	MG	1a	3125	1/1	0.93	0.21	106,106,106,106	0
56	MG	1A	3047	1/1	0.93	0.99	68,68,68,68	0
56	MG	1a	3198	1/1	0.93	0.28	89,89,89,89	0
56	MG	2a	3025	1/1	0.93	0.08	86,86,86,86	0
56	MG	2A	3107	1/1	0.93	0.27	92,92,92,92	0
56	MG	1A	3640	1/1	0.93	0.26	81,81,81,81	0
56	MG	1A	3025	1/1	0.93	0.29	87,87,87,87	0
56	MG	1A	3537	1/1	0.93	1.62	113,113,113,113	0
56	MG	2A	3311	1/1	0.93	0.22	106,106,106,106	0
56	MG	1A	3438	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3137	1/1	0.93	0.28	91,91,91,91	0
56	MG	2A	3177	1/1	0.93	0.22	74,74,74,74	0
56	MG	2A	3341	1/1	0.93	0.15	94,94,94,94	0
56	MG	1A	3476	1/1	0.93	0.11	89,89,89,89	0
56	MG	1A	3029	1/1	0.93	0.21	65,65,65,65	0
56	MG	2A	3309	1/1	0.93	0.12	85,85,85,85	0
56	MG	1A	3355	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3081	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3273	1/1	0.93	0.23	62,62,62,62	0
56	MG	2a	3114	1/1	0.93	0.34	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3001	1/1	0.93	0.14	75,75,75,75	0
56	MG	1a	3159	1/1	0.93	0.28	72,72,72,72	0
56	MG	1A	3530	1/1	0.93	0.79	79,79,79,79	0
56	MG	1a	3132	1/1	0.93	0.12	101,101,101,101	0
56	MG	2A	3280	1/1	0.93	0.83	94,94,94,94	0
56	MG	1A	3523	1/1	0.93	0.11	96,96,96,96	0
56	MG	2A	3230	1/1	0.93	0.35	82,82,82,82	0
56	MG	1A	3413	1/1	0.93	0.24	71,71,71,71	0
56	MG	2A	3322	1/1	0.93	0.15	86,86,86,86	0
56	MG	2A	3133	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3037	1/1	0.93	0.26	75,75,75,75	0
56	MG	2A	3260	1/1	0.93	0.24	87,87,87,87	0
56	MG	2a	3084	1/1	0.93	0.14	78,78,78,78	0
56	MG	1A	3289	1/1	0.93	0.71	92,92,92,92	0
56	MG	1A	3331	1/1	0.93	0.12	75,75,75,75	0
56	MG	2a	3173	1/1	0.93	0.35	115,115,115,115	0
56	MG	1A	3512	1/1	0.93	0.29	82,82,82,82	0
56	MG	1a	3151	1/1	0.93	0.21	80,80,80,80	0
56	MG	1a	3206	1/1	0.93	0.10	89,89,89,89	0
56	MG	2A	3075	1/1	0.93	0.34	83,83,83,83	0
56	MG	1A	3255	1/1	0.93	0.26	59,59,59,59	0
56	MG	1A	3278	1/1	0.93	0.28	59,59,59,59	0
56	MG	1A	3414	1/1	0.93	0.36	82,82,82,82	0
56	MG	2A	3308	1/1	0.93	0.13	103,103,103,103	0
56	MG	1A	3074	1/1	0.93	0.14	81,81,81,81	0
56	MG	1A	3670	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3221	1/1	0.93	0.31	79,79,79,79	0
56	MG	1A	3120	1/1	0.93	0.23	111,111,111,111	0
56	MG	1A	3202	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3189	1/1	0.93	0.49	78,78,78,78	0
56	MG	1A	3592	1/1	0.93	0.25	84,84,84,84	0
56	MG	1A	3624	1/1	0.93	0.29	64,64,64,64	0
56	MG	1A	3229	1/1	0.93	0.21	74,74,74,74	0
56	MG	1a	3102	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	3312	1/1	0.93	0.30	62,62,62,62	0
56	MG	1a	3204	1/1	0.93	0.17	80,80,80,80	0
56	MG	2A	3219	1/1	0.93	0.13	80,80,80,80	0
56	MG	2a	3020	1/1	0.93	0.08	98,98,98,98	0
56	MG	2a	3008	1/1	0.93	0.10	85,85,85,85	0
56	MG	2a	3027	1/1	0.93	0.12	83,83,83,83	0
56	MG	1a	3141	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3285	1/1	0.93	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3166	1/1	0.93	0.33	77,77,77,77	0
56	MG	2A	3129	1/1	0.93	0.32	73,73,73,73	0
56	MG	1A	3241	1/1	0.93	0.32	68,68,68,68	0
56	MG	1a	3041	1/1	0.93	0.14	81,81,81,81	0
56	MG	2A	3208	1/1	0.93	0.12	71,71,71,71	0
56	MG	2a	3148	1/1	0.93	0.13	92,92,92,92	0
56	MG	1a	3196	1/1	0.93	0.15	85,85,85,85	0
56	MG	1a	3235	1/1	0.93	0.32	93,93,93,93	0
56	MG	1A	3496	1/1	0.93	0.24	72,72,72,72	0
56	MG	1A	3132	1/1	0.93	0.22	82,82,82,82	0
56	MG	2a	3137	1/1	0.94	0.09	81,81,81,81	0
56	MG	1A	3623	1/1	0.94	0.15	87,87,87,87	0
56	MG	1A	3305	1/1	0.94	0.20	65,65,65,65	0
56	MG	2A	3056	1/1	0.94	0.67	73,73,73,73	0
56	MG	1A	3264	1/1	0.94	0.43	67,67,67,67	0
56	MG	1A	3227	1/1	0.94	0.18	72,72,72,72	0
56	MG	1A	3603	1/1	0.94	0.21	67,67,67,67	0
56	MG	1a	3078	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	3134	1/1	0.94	0.30	63,63,63,63	0
56	MG	2a	3056	1/1	0.94	0.11	97,97,97,97	0
56	MG	2A	3251	1/1	0.94	0.13	73,73,73,73	0
56	MG	1A	3663	1/1	0.94	0.23	89,89,89,89	0
56	MG	1A	3668	1/1	0.94	0.11	82,82,82,82	0
56	MG	2a	3128	1/1	0.94	0.17	74,74,74,74	0
56	MG	1A	3224	1/1	0.94	0.22	65,65,65,65	0
56	MG	2A	3218	1/1	0.94	0.23	83,83,83,83	0
56	MG	2a	3136	1/1	0.94	0.27	85,85,85,85	0
56	MG	2A	3128	1/1	0.94	0.16	54,54,54,54	0
56	MG	2A	3045	1/1	0.94	0.21	76,76,76,76	0
56	MG	2a	3081	1/1	0.94	0.10	61,61,61,61	0
56	MG	2a	3153	1/1	0.94	0.13	106,106,106,106	0
56	MG	1A	3605	1/1	0.94	0.20	93,93,93,93	0
56	MG	2a	3013	1/1	0.94	0.28	85,85,85,85	0
56	MG	2A	3082	1/1	0.94	0.05	85,85,85,85	0
56	MG	1A	3650	1/1	0.94	1.24	90,90,90,90	0
56	MG	2a	3112	1/1	0.94	0.14	87,87,87,87	0
56	MG	1a	3006	1/1	0.94	0.21	90,90,90,90	0
56	MG	1A	3116	1/1	0.94	0.41	113,113,113,113	0
56	MG	2a	3132	1/1	0.94	0.20	83,83,83,83	0
56	MG	1A	3595	1/1	0.94	0.32	69,69,69,69	0
56	MG	1A	3039	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3370	1/1	0.94	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3234	1/1	0.94	0.18	85,85,85,85	0
56	MG	2A	3212	1/1	0.94	0.52	83,83,83,83	0
56	MG	1a	3218	1/1	0.94	0.21	80,80,80,80	0
56	MG	1A	3366	1/1	0.94	0.14	72,72,72,72	0
56	MG	2A	3108	1/1	0.94	0.25	72,72,72,72	0
56	MG	2a	3174	1/1	0.94	0.12	101,101,101,101	0
56	MG	1A	3017	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3574	1/1	0.94	0.23	77,77,77,77	0
56	MG	2A	3109	1/1	0.94	0.14	93,93,93,93	0
56	MG	1a	3193	1/1	0.94	0.24	88,88,88,88	0
56	MG	1A	3473	1/1	0.94	0.12	86,86,86,86	0
56	MG	1A	3422	1/1	0.94	0.32	67,67,67,67	0
56	MG	2a	3067	1/1	0.94	0.09	112,112,112,112	0
56	MG	2A	3185	1/1	0.94	0.32	76,76,76,76	0
56	MG	1A	3209	1/1	0.94	0.19	56,56,56,56	0
56	MG	2a	3182	1/1	0.94	0.17	106,106,106,106	0
56	MG	2A	3226	1/1	0.94	0.11	73,73,73,73	0
56	MG	1A	3578	1/1	0.94	0.12	86,86,86,86	0
56	MG	1A	3254	1/1	0.94	0.14	78,78,78,78	0
56	MG	1A	3659	1/1	0.94	0.18	80,80,80,80	0
56	MG	1A	3412	1/1	0.94	0.45	79,79,79,79	0
56	MG	1A	3088	1/1	0.94	0.18	71,71,71,71	0
56	MG	2A	3261	1/1	0.94	0.40	98,98,98,98	0
56	MG	2A	3095	1/1	0.94	0.43	89,89,89,89	0
56	MG	1a	3017	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3316	1/1	0.94	0.29	83,83,83,83	0
56	MG	2A	3171	1/1	0.94	0.19	86,86,86,86	0
56	MG	1A	3351	1/1	0.94	0.24	58,58,58,58	0
56	MG	1A	3220	1/1	0.94	0.18	71,71,71,71	0
56	MG	2A	3103	1/1	0.94	0.24	83,83,83,83	0
56	MG	1A	3332	1/1	0.94	0.24	77,77,77,77	0
56	MG	1A	3558	1/1	0.94	0.14	97,97,97,97	0
56	MG	2A	3346	1/1	0.94	0.27	78,78,78,78	0
56	MG	1A	3383	1/1	0.94	0.24	69,69,69,69	0
56	MG	1A	3576	1/1	0.94	0.14	76,76,76,76	0
56	MG	2A	3012	1/1	0.94	0.30	92,92,92,92	0
56	MG	2A	3304	1/1	0.94	0.46	92,92,92,92	0
56	MG	2a	3083	1/1	0.94	0.52	76,76,76,76	0
56	MG	1A	3387	1/1	0.94	0.17	80,80,80,80	0
56	MG	1a	3055	1/1	0.94	0.18	83,83,83,83	0
56	MG	2A	3220	1/1	0.94	0.33	74,74,74,74	0
56	MG	1A	3077	1/1	0.94	0.30	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3110	1/1	0.94	0.13	80,80,80,80	0
56	MG	2a	3109	1/1	0.94	0.11	82,82,82,82	0
56	MG	1A	3130	1/1	0.94	0.36	81,81,81,81	0
56	MG	1A	3561	1/1	0.94	0.17	64,64,64,64	0
56	MG	2A	3174	1/1	0.94	0.13	79,79,79,79	0
56	MG	1a	3137	1/1	0.94	0.10	79,79,79,79	0
56	MG	1a	3155	1/1	0.94	0.08	74,74,74,74	0
56	MG	1a	3199	1/1	0.94	0.31	93,93,93,93	0
56	MG	2A	3235	1/1	0.94	0.19	69,69,69,69	0
56	MG	1A	3266	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3337	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3644	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3586	1/1	0.94	0.32	71,71,71,71	0
56	MG	1A	3080	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3649	1/1	0.94	0.05	86,86,86,86	0
56	MG	2A	3233	1/1	0.94	0.25	71,71,71,71	0
56	MG	1A	3666	1/1	0.94	0.17	92,92,92,92	0
56	MG	2A	3113	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3381	1/1	0.94	0.27	68,68,68,68	0
56	MG	1A	3051	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3564	1/1	0.94	0.10	97,97,97,97	0
56	MG	2a	3131	1/1	0.94	0.13	84,84,84,84	0
56	MG	2A	3214	1/1	0.94	0.49	92,92,92,92	0
56	MG	1A	3152	1/1	0.94	0.67	84,84,84,84	0
56	MG	2a	3032	1/1	0.94	0.17	79,79,79,79	0
56	MG	1A	3677	1/1	0.94	0.23	55,55,55,55	0
56	MG	1A	3245	1/1	0.94	0.31	56,56,56,56	0
56	MG	2A	3088	1/1	0.94	0.17	77,77,77,77	0
56	MG	1A	3321	1/1	0.94	0.21	62,62,62,62	0
56	MG	2A	3289	1/1	0.94	0.07	102,102,102,102	0
56	MG	1A	3418	1/1	0.94	0.35	75,75,75,75	0
56	MG	1A	3593	1/1	0.94	0.17	65,65,65,65	0
56	MG	2A	3032	1/1	0.94	0.25	78,78,78,78	0
56	MG	1A	3326	1/1	0.94	0.20	83,83,83,83	0
56	MG	2a	3018	1/1	0.94	0.13	71,71,71,71	0
56	MG	1A	3610	1/1	0.94	0.21	79,79,79,79	0
56	MG	1a	3056	1/1	0.94	0.11	83,83,83,83	0
56	MG	1A	3079	1/1	0.94	0.12	96,96,96,96	0
56	MG	2A	3228	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3206	1/1	0.94	0.07	76,76,76,76	0
56	MG	2a	3111	1/1	0.94	0.13	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3656	1/1	0.94	0.20	70,70,70,70	0
56	MG	2A	3342	1/1	0.94	0.26	78,78,78,78	0
56	MG	1A	3404	1/1	0.95	0.16	62,62,62,62	0
56	MG	1a	3104	1/1	0.95	0.15	74,74,74,74	0
56	MG	1A	3669	1/1	0.95	0.19	79,79,79,79	0
56	MG	1A	3484	1/1	0.95	0.25	80,80,80,80	0
56	MG	1A	3342	1/1	0.95	0.20	64,64,64,64	0
56	MG	2A	3255	1/1	0.95	0.60	91,91,91,91	0
56	MG	1A	3230	1/1	0.95	0.20	72,72,72,72	0
56	MG	2A	3010	1/1	0.95	0.14	85,85,85,85	0
56	MG	1A	3386	1/1	0.95	0.49	68,68,68,68	0
56	MG	1A	3360	1/1	0.95	0.14	68,68,68,68	0
56	MG	2a	3019	1/1	0.95	0.13	95,95,95,95	0
56	MG	1A	3528	1/1	0.95	0.28	78,78,78,78	0
56	MG	1A	3675	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3382	1/1	0.95	0.23	60,60,60,60	0
56	MG	2A	3338	1/1	0.95	0.64	97,97,97,97	0
56	MG	1A	3182	1/1	0.95	0.69	72,72,72,72	0
56	MG	2A	3274	1/1	0.95	0.23	92,92,92,92	0
56	MG	1A	3083	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3540	1/1	0.95	0.10	94,94,94,94	0
56	MG	1a	3181	1/1	0.95	0.28	66,66,66,66	0
56	MG	2A	3125	1/1	0.95	0.28	88,88,88,88	0
56	MG	2A	3281	1/1	0.95	0.10	88,88,88,88	0
56	MG	1a	3157	1/1	0.95	0.45	89,89,89,89	0
56	MG	1A	3054	1/1	0.95	0.24	86,86,86,86	0
56	MG	2A	3049	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3522	1/1	0.95	0.10	69,69,69,69	0
56	MG	1A	3664	1/1	0.95	0.21	82,82,82,82	0
56	MG	2a	3147	1/1	0.95	0.36	89,89,89,89	0
56	MG	1a	3145	1/1	0.95	0.48	97,97,97,97	0
56	MG	1A	3373	1/1	0.95	0.35	54,54,54,54	0
56	MG	1a	3040	1/1	0.95	0.08	89,89,89,89	0
56	MG	2A	3016	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3501	1/1	0.95	0.28	71,71,71,71	0
56	MG	2a	3134	1/1	0.95	0.19	100,100,100,100	0
56	MG	1A	3402	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3236	1/1	0.95	0.29	60,60,60,60	0
56	MG	1a	3081	1/1	0.95	0.16	81,81,81,81	0
56	MG	1a	3164	1/1	0.95	0.73	81,81,81,81	0
56	MG	1a	3172	1/1	0.95	0.14	90,90,90,90	0
56	MG	2a	3135	1/1	0.95	0.14	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3122	1/1	0.95	0.09	114,114,114,114	0
56	MG	1A	3446	1/1	0.95	0.16	65,65,65,65	0
56	MG	2A	3262	1/1	0.95	0.66	84,84,84,84	0
56	MG	1A	3076	1/1	0.95	0.60	54,54,54,54	0
56	MG	1A	3403	1/1	0.95	0.36	59,59,59,59	0
56	MG	1A	3458	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3626	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3393	1/1	0.95	0.18	82,82,82,82	0
56	MG	1A	3487	1/1	0.95	0.11	81,81,81,81	0
56	MG	2a	3057	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3432	1/1	0.95	0.32	57,57,57,57	0
56	MG	1A	3570	1/1	0.95	0.32	99,99,99,99	0
56	MG	1a	3195	1/1	0.95	0.22	80,80,80,80	0
56	MG	1A	3031	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3349	1/1	0.95	0.26	81,81,81,81	0
56	MG	2A	3248	1/1	0.95	0.11	85,85,85,85	0
56	MG	1A	3536	1/1	0.95	0.22	74,74,74,74	0
56	MG	2A	3005	1/1	0.95	0.09	84,84,84,84	0
56	MG	1A	3462	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3018	1/1	0.95	0.56	84,84,84,84	0
56	MG	2A	3324	1/1	0.95	0.27	83,83,83,83	0
56	MG	1A	3309	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3631	1/1	0.95	0.08	82,82,82,82	0
56	MG	1A	3162	1/1	0.95	0.09	83,83,83,83	0
56	MG	1A	3602	1/1	0.95	0.22	67,67,67,67	0
56	MG	2a	3021	1/1	0.95	0.09	101,101,101,101	0
56	MG	2A	3347	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3108	1/1	0.95	0.43	84,84,84,84	0
56	MG	1A	3008	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3238	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3020	1/1	0.95	0.36	89,89,89,89	0
56	MG	2A	3183	1/1	0.95	0.15	80,80,80,80	0
56	MG	2a	3002	1/1	0.95	0.13	98,98,98,98	0
56	MG	2a	3030	1/1	0.95	0.12	77,77,77,77	0
56	MG	1a	3128	1/1	0.95	0.22	98,98,98,98	0
56	MG	1a	3114	1/1	0.95	0.09	86,86,86,86	0
56	MG	1A	3397	1/1	0.95	0.09	83,83,83,83	0
56	MG	2a	3068	1/1	0.95	0.16	83,83,83,83	0
56	MG	1A	3587	1/1	0.95	0.18	80,80,80,80	0
56	MG	2A	3015	1/1	0.95	0.53	84,84,84,84	0
56	MG	2A	3200	1/1	0.95	0.26	86,86,86,86	0
56	MG	2a	3172	1/1	0.95	0.38	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3228	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3260	1/1	0.95	0.26	62,62,62,62	0
56	MG	2A	3062	1/1	0.95	0.12	84,84,84,84	0
56	MG	1a	3212	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3341	1/1	0.95	0.21	70,70,70,70	0
56	MG	2A	3052	1/1	0.95	0.15	72,72,72,72	0
56	MG	1A	3302	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3109	1/1	0.95	0.16	78,78,78,78	0
56	MG	2A	3027	1/1	0.95	0.16	87,87,87,87	0
56	MG	1A	3349	1/1	0.95	0.25	72,72,72,72	0
56	MG	1A	3082	1/1	0.95	0.15	69,69,69,69	0
56	MG	1A	3225	1/1	0.95	0.38	65,65,65,65	0
56	MG	1A	3131	1/1	0.95	0.18	84,84,84,84	0
56	MG	1A	3395	1/1	0.95	0.14	72,72,72,72	0
56	MG	1A	3003	1/1	0.95	0.39	60,60,60,60	0
56	MG	1A	3546	1/1	0.95	0.21	69,69,69,69	0
56	MG	1A	3091	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3336	1/1	0.95	0.41	81,81,81,81	0
56	MG	1A	3369	1/1	0.95	0.31	86,86,86,86	0
56	MG	1A	3281	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3392	1/1	0.96	0.36	80,80,80,80	0
56	MG	1A	3514	1/1	0.96	0.12	94,94,94,94	0
56	MG	2A	3221	1/1	0.96	0.14	107,107,107,107	0
57	ZN	29	501	1/1	0.96	0.19	105,105,105,105	0
56	MG	1a	3096	1/1	0.96	0.10	95,95,95,95	0
56	MG	1a	3237	1/1	0.96	0.06	106,106,106,106	0
56	MG	1A	3430	1/1	0.96	0.24	61,61,61,61	0
56	MG	1A	3627	1/1	0.96	0.20	60,60,60,60	0
56	MG	2A	3096	1/1	0.96	0.17	90,90,90,90	0
56	MG	2a	3038	1/1	0.96	0.20	101,101,101,101	0
56	MG	2A	3029	1/1	0.96	0.21	94,94,94,94	0
56	MG	1A	3193	1/1	0.96	0.17	62,62,62,62	0
56	MG	2a	3016	1/1	0.96	0.29	91,91,91,91	0
56	MG	1A	3634	1/1	0.96	0.19	83,83,83,83	0
56	MG	1A	3641	1/1	0.96	0.17	68,68,68,68	0
56	MG	2a	3146	1/1	0.96	0.17	100,100,100,100	0
56	MG	1A	3172	1/1	0.96	0.26	94,94,94,94	0
56	MG	1A	3440	1/1	0.96	0.14	77,77,77,77	0
56	MG	1a	3100	1/1	0.96	0.13	78,78,78,78	0
56	MG	1A	3163	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3362	1/1	0.96	0.21	53,53,53,53	0
56	MG	2a	3171	1/1	0.96	0.07	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3270	1/1	0.96	0.11	80,80,80,80	0
56	MG	1a	3210	1/1	0.96	0.23	91,91,91,91	0
56	MG	2A	3272	1/1	0.96	0.15	89,89,89,89	0
56	MG	1A	3344	1/1	0.96	0.19	79,79,79,79	0
56	MG	1A	3027	1/1	0.96	1.18	68,68,68,68	0
56	MG	1A	3399	1/1	0.96	0.28	68,68,68,68	0
56	MG	1a	3074	1/1	0.96	0.12	88,88,88,88	0
56	MG	1A	3591	1/1	0.96	0.34	83,83,83,83	0
56	MG	1A	3538	1/1	0.96	0.09	87,87,87,87	0
56	MG	1a	3011	1/1	0.96	0.20	94,94,94,94	0
56	MG	1a	3130	1/1	0.96	0.27	99,99,99,99	0
56	MG	1A	3590	1/1	0.96	0.21	68,68,68,68	0
56	MG	1A	3170	1/1	0.96	0.30	99,99,99,99	0
56	MG	1A	3222	1/1	0.96	0.22	64,64,64,64	0
56	MG	1A	3348	1/1	0.96	0.34	74,74,74,74	0
56	MG	1A	3406	1/1	0.96	0.22	59,59,59,59	0
56	MG	2a	3133	1/1	0.96	0.23	92,92,92,92	0
56	MG	2A	3083	1/1	0.96	0.10	80,80,80,80	0
56	MG	2A	3340	1/1	0.96	0.19	67,67,67,67	0
56	MG	1A	3654	1/1	0.96	0.16	89,89,89,89	0
56	MG	2A	3236	1/1	0.96	0.18	69,69,69,69	0
56	MG	2A	3264	1/1	0.96	0.10	91,91,91,91	0
56	MG	1A	3037	1/1	0.96	0.18	83,83,83,83	0
56	MG	2A	3199	1/1	0.96	0.37	74,74,74,74	0
56	MG	1A	3317	1/1	0.96	0.30	56,56,56,56	0
56	MG	1A	3059	1/1	0.96	0.13	81,81,81,81	0
56	MG	1a	3225	1/1	0.96	0.57	85,85,85,85	0
56	MG	2A	3240	1/1	0.96	0.12	84,84,84,84	0
56	MG	2a	3181	1/1	0.96	0.17	90,90,90,90	0
56	MG	1A	3678	1/1	0.96	0.23	75,75,75,75	0
56	MG	1a	3161	1/1	0.96	0.10	82,82,82,82	0
56	MG	1a	3057	1/1	0.96	0.24	92,92,92,92	0
56	MG	2A	3279	1/1	0.96	0.25	70,70,70,70	0
56	MG	1a	3176	1/1	0.96	0.10	84,84,84,84	0
56	MG	2A	3299	1/1	0.96	0.48	66,66,66,66	0
56	MG	1A	3421	1/1	0.96	0.22	68,68,68,68	0
56	MG	1a	3168	1/1	0.96	0.14	111,111,111,111	0
56	MG	1A	3562	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3269	1/1	0.96	0.75	74,74,74,74	0
56	MG	2a	3035	1/1	0.96	0.15	94,94,94,94	0
56	MG	1A	3195	1/1	0.96	0.33	78,78,78,78	0
56	MG	1A	3282	1/1	0.96	0.29	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3117	1/1	0.96	0.10	98,98,98,98	0
56	MG	1a	3044	1/1	0.96	0.29	90,90,90,90	0
56	MG	2A	3014	1/1	0.96	0.38	72,72,72,72	0
56	MG	2a	3108	1/1	0.96	0.05	98,98,98,98	0
56	MG	1A	3467	1/1	0.96	0.11	73,73,73,73	0
56	MG	1a	3142	1/1	0.96	0.16	85,85,85,85	0
56	MG	1A	3539	1/1	0.96	0.33	85,85,85,85	0
56	MG	1A	3445	1/1	0.96	0.20	80,80,80,80	0
56	MG	1A	3226	1/1	0.96	0.22	62,62,62,62	0
56	MG	1A	3284	1/1	0.96	0.16	86,86,86,86	0
56	MG	1A	3597	1/1	0.96	0.16	87,87,87,87	0
56	MG	2A	3176	1/1	0.96	0.22	89,89,89,89	0
56	MG	2A	3161	1/1	0.96	0.11	69,69,69,69	0
56	MG	1A	3297	1/1	0.96	0.13	77,77,77,77	0
56	MG	2a	3052	1/1	0.96	0.09	95,95,95,95	0
56	MG	2A	3259	1/1	0.96	0.21	76,76,76,76	0
56	MG	1A	3480	1/1	0.96	0.27	104,104,104,104	0
56	MG	1A	3248	1/1	0.96	0.20	76,76,76,76	0
56	MG	1A	3450	1/1	0.96	0.38	76,76,76,76	0
56	MG	1A	3673	1/1	0.96	0.30	77,77,77,77	0
56	MG	1A	3398	1/1	0.96	0.14	67,67,67,67	0
56	MG	2A	3155	1/1	0.96	0.07	66,66,66,66	0
57	ZN	16	501	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3653	1/1	0.96	0.17	95,95,95,95	0
56	MG	2A	3307	1/1	0.96	0.17	79,79,79,79	0
56	MG	1A	3516	1/1	0.96	0.07	81,81,81,81	0
56	MG	1a	3023	1/1	0.96	0.23	87,87,87,87	0
56	MG	2A	3132	1/1	0.96	0.19	97,97,97,97	0
56	MG	2A	3329	1/1	0.96	0.29	100,100,100,100	0
56	MG	1a	3001	1/1	0.96	0.25	90,90,90,90	0
56	MG	1a	3087	1/1	0.96	0.13	100,100,100,100	0
56	MG	1A	3471	1/1	0.96	0.19	88,88,88,88	0
56	MG	2A	3006	1/1	0.96	0.24	71,71,71,71	0
56	MG	1a	3223	1/1	0.96	0.24	84,84,84,84	0
56	MG	1A	3269	1/1	0.96	0.15	69,69,69,69	0
56	MG	1A	3625	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3598	1/1	0.96	0.27	74,74,74,74	0
56	MG	2A	3325	1/1	0.96	0.20	91,91,91,91	0
56	MG	1A	3410	1/1	0.96	0.17	77,77,77,77	0
56	MG	2a	3094	1/1	0.96	0.29	89,89,89,89	0
56	MG	1a	3171	1/1	0.96	0.23	86,86,86,86	0
56	MG	1A	3535	1/1	0.96	0.34	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3630	1/1	0.96	0.17	77,77,77,77	0
56	MG	1a	3150	1/1	0.96	0.15	83,83,83,83	0
56	MG	2A	3189	1/1	0.96	0.23	89,89,89,89	0
56	MG	2a	3093	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3671	1/1	0.96	0.16	79,79,79,79	0
56	MG	1A	3298	1/1	0.96	0.42	83,83,83,83	0
56	MG	1A	3216	1/1	0.96	0.32	50,50,50,50	0
56	MG	1A	3378	1/1	0.96	0.43	73,73,73,73	0
56	MG	1a	3013	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3213	1/1	0.96	0.16	66,66,66,66	0
56	MG	1A	3315	1/1	0.96	0.12	57,57,57,57	0
56	MG	1a	3208	1/1	0.96	0.14	80,80,80,80	0
56	MG	1A	3228	1/1	0.96	0.17	59,59,59,59	0
56	MG	1A	3508	1/1	0.96	0.12	86,86,86,86	0
56	MG	1A	3090	1/1	0.96	0.50	84,84,84,84	0
56	MG	2A	3175	1/1	0.97	0.16	65,65,65,65	0
56	MG	1A	3215	1/1	0.97	0.15	49,49,49,49	0
56	MG	1a	3119	1/1	0.97	0.58	88,88,88,88	0
56	MG	1A	3071	1/1	0.97	0.21	74,74,74,74	0
56	MG	1A	3680	1/1	0.97	0.19	85,85,85,85	0
57	ZN	1n	501	1/1	0.97	0.20	105,105,105,105	0
56	MG	1A	3499	1/1	0.97	0.09	72,72,72,72	0
56	MG	2A	3021	1/1	0.97	0.43	98,98,98,98	0
56	MG	2A	3191	1/1	0.97	0.36	74,74,74,74	0
57	ZN	2n	501	1/1	0.97	0.10	117,117,117,117	0
56	MG	1A	3401	1/1	0.97	0.27	90,90,90,90	0
56	MG	2a	3149	1/1	0.97	0.09	74,74,74,74	0
56	MG	1A	3068	1/1	0.97	0.08	74,74,74,74	0
56	MG	2A	3002	1/1	0.97	0.22	81,81,81,81	0
56	MG	1a	3231	1/1	0.97	0.16	82,82,82,82	0
56	MG	1A	3606	1/1	0.97	0.47	71,71,71,71	0
56	MG	2A	3241	1/1	0.97	0.12	89,89,89,89	0
56	MG	1A	3619	1/1	0.97	0.15	86,86,86,86	0
56	MG	2A	3065	1/1	0.97	0.36	88,88,88,88	0
56	MG	1A	3643	1/1	0.97	0.13	86,86,86,86	0
56	MG	1A	3474	1/1	0.97	0.24	74,74,74,74	0
56	MG	1a	3131	1/1	0.97	0.25	107,107,107,107	0
56	MG	2A	3102	1/1	0.97	0.55	72,72,72,72	0
56	MG	2A	3291	1/1	0.97	0.10	87,87,87,87	0
56	MG	2a	3098	1/1	0.97	0.37	101,101,101,101	0
56	MG	2A	3093	1/1	0.97	0.16	71,71,71,71	0
56	MG	2A	3345	1/1	0.97	0.60	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3311	1/1	0.97	0.34	61,61,61,61	0
56	MG	1A	3628	1/1	0.97	0.16	56,56,56,56	0
56	MG	1A	3475	1/1	0.97	0.30	88,88,88,88	0
56	MG	2A	3063	1/1	0.97	0.07	67,67,67,67	0
56	MG	2a	3041	1/1	0.97	0.20	69,69,69,69	0
56	MG	1A	3296	1/1	0.97	0.12	76,76,76,76	0
56	MG	1A	3483	1/1	0.97	0.07	77,77,77,77	0
56	MG	1A	3061	1/1	0.97	0.21	77,77,77,77	0
56	MG	1A	3085	1/1	0.97	0.37	92,92,92,92	0
56	MG	1A	3611	1/1	0.97	0.30	75,75,75,75	0
56	MG	1a	3038	1/1	0.97	0.12	88,88,88,88	0
56	MG	1A	3292	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	3146	1/1	0.97	0.17	62,62,62,62	0
56	MG	1A	3526	1/1	0.97	0.12	76,76,76,76	0
56	MG	2A	3073	1/1	0.97	0.16	85,85,85,85	0
56	MG	2A	3172	1/1	0.97	0.23	80,80,80,80	0
56	MG	1a	3194	1/1	0.97	0.22	102,102,102,102	0
56	MG	2A	3350	1/1	0.97	0.33	70,70,70,70	0
56	MG	2A	3275	1/1	0.97	0.34	81,81,81,81	0
56	MG	1a	3054	1/1	0.97	0.21	85,85,85,85	0
56	MG	1a	3029	1/1	0.97	0.12	64,64,64,64	0
56	MG	2a	3022	1/1	0.97	0.15	83,83,83,83	0
56	MG	1A	3043	1/1	0.97	0.13	74,74,74,74	0
56	MG	2a	3044	1/1	0.97	0.29	86,86,86,86	0
56	MG	1A	3106	1/1	0.97	0.26	63,63,63,63	0
56	MG	1a	3183	1/1	0.97	0.34	78,78,78,78	0
56	MG	1A	3307	1/1	0.97	0.28	60,60,60,60	0
56	MG	1a	3138	1/1	0.97	0.20	91,91,91,91	0
56	MG	1A	3155	1/1	0.97	0.15	65,65,65,65	0
56	MG	1A	3464	1/1	0.97	0.15	73,73,73,73	0
56	MG	1A	3005	1/1	0.97	0.13	74,74,74,74	0
56	MG	1a	3148	1/1	0.97	0.21	112,112,112,112	0
56	MG	1A	3084	1/1	0.97	0.28	71,71,71,71	0
56	MG	1A	3093	1/1	0.97	0.15	73,73,73,73	0
56	MG	1A	3040	1/1	0.97	0.24	115,115,115,115	0
56	MG	2A	3117	1/1	0.97	0.17	83,83,83,83	0
56	MG	1A	3338	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3212	1/1	0.97	0.21	54,54,54,54	0
56	MG	1a	3135	1/1	0.97	0.10	82,82,82,82	0
56	MG	1a	3144	1/1	0.97	0.18	71,71,71,71	0
56	MG	1a	3002	1/1	0.97	0.12	83,83,83,83	0
56	MG	2A	3232	1/1	0.97	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3271	1/1	0.97	0.17	49,49,49,49	0
56	MG	2A	3085	1/1	0.97	0.66	101,101,101,101	0
56	MG	1A	3448	1/1	0.97	0.15	78,78,78,78	0
56	MG	1A	3594	1/1	0.97	0.17	77,77,77,77	0
56	MG	1A	3510	1/1	0.97	0.17	64,64,64,64	0
56	MG	2A	3319	1/1	0.97	0.14	78,78,78,78	0
56	MG	2A	3239	1/1	0.97	0.08	77,77,77,77	0
56	MG	1A	3660	1/1	0.97	0.25	65,65,65,65	0
56	MG	1A	3424	1/1	0.97	1.40	81,81,81,81	0
56	MG	2a	3103	1/1	0.97	0.27	73,73,73,73	0
56	MG	1a	3156	1/1	0.97	0.19	73,73,73,73	0
56	MG	2A	3276	1/1	0.97	0.12	82,82,82,82	0
56	MG	1A	3490	1/1	0.97	0.19	79,79,79,79	0
56	MG	2A	3292	1/1	0.97	0.08	91,91,91,91	0
56	MG	1A	3086	1/1	0.97	0.17	70,70,70,70	0
56	MG	2A	3023	1/1	0.97	0.07	71,71,71,71	0
56	MG	1A	3635	1/1	0.97	0.20	78,78,78,78	0
56	MG	1A	3217	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3492	1/1	0.97	0.12	77,77,77,77	0
56	MG	2A	3179	1/1	0.97	0.14	74,74,74,74	0
56	MG	1A	3463	1/1	0.97	0.29	75,75,75,75	0
56	MG	2a	3150	1/1	0.97	0.21	87,87,87,87	0
56	MG	1A	3276	1/1	0.98	0.24	64,64,64,64	0
56	MG	1a	3188	1/1	0.98	0.12	81,81,81,81	0
56	MG	1a	3088	1/1	0.98	0.18	96,96,96,96	0
56	MG	2A	3224	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3345	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3262	1/1	0.98	0.22	64,64,64,64	0
56	MG	2A	3069	1/1	0.98	0.15	82,82,82,82	0
56	MG	1A	3097	1/1	0.98	0.11	94,94,94,94	0
56	MG	1a	3075	1/1	0.98	0.24	72,72,72,72	0
56	MG	1A	3655	1/1	0.98	0.35	67,67,67,67	0
56	MG	1a	3076	1/1	0.98	0.21	58,58,58,58	0
56	MG	1A	3247	1/1	0.98	0.10	55,55,55,55	0
56	MG	2a	3065	1/1	0.98	0.17	83,83,83,83	0
56	MG	2A	3030	1/1	0.98	0.11	81,81,81,81	0
56	MG	1A	3069	1/1	0.98	0.90	67,67,67,67	0
56	MG	1A	3632	1/1	0.98	0.16	63,63,63,63	0
56	MG	2A	3267	1/1	0.98	0.21	93,93,93,93	0
56	MG	2A	3300	1/1	0.98	0.35	79,79,79,79	0
56	MG	2a	3045	1/1	0.98	0.08	102,102,102,102	0
56	MG	1A	3451	1/1	0.98	0.11	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3200	1/1	0.98	0.22	63,63,63,63	0
56	MG	1A	3046	1/1	0.98	0.09	54,54,54,54	0
56	MG	1A	3517	1/1	0.98	0.20	77,77,77,77	0
56	MG	1A	3435	1/1	0.98	0.17	59,59,59,59	0
56	MG	1A	3072	1/1	0.98	0.47	67,67,67,67	0
56	MG	1a	3200	1/1	0.98	0.17	83,83,83,83	0
56	MG	2a	3140	1/1	0.98	0.14	88,88,88,88	0
56	MG	1A	3667	1/1	0.98	0.45	68,68,68,68	0
56	MG	1A	3532	1/1	0.98	0.09	88,88,88,88	0
56	MG	1A	3456	1/1	0.98	0.25	96,96,96,96	0
56	MG	1A	3101	1/1	0.98	0.23	86,86,86,86	0
56	MG	2a	3165	1/1	0.98	0.08	116,116,116,116	0
56	MG	1a	3129	1/1	0.98	0.11	88,88,88,88	0
57	ZN	1Y	501	1/1	0.98	0.18	100,100,100,100	0
56	MG	2A	3339	1/1	0.98	0.14	92,92,92,92	0
56	MG	1A	3259	1/1	0.98	0.20	54,54,54,54	0
56	MG	1a	3080	1/1	0.98	0.17	88,88,88,88	0
56	MG	1A	3507	1/1	0.98	0.25	92,92,92,92	0
56	MG	1A	3477	1/1	0.98	0.15	56,56,56,56	0
56	MG	1a	3221	1/1	0.98	0.20	79,79,79,79	0
56	MG	1A	3509	1/1	0.98	0.28	75,75,75,75	0
56	MG	1A	3604	1/1	0.98	0.14	67,67,67,67	0
56	MG	2A	3120	1/1	0.98	0.13	94,94,94,94	0
56	MG	2A	3178	1/1	0.98	0.17	63,63,63,63	0
56	MG	2A	3059	1/1	0.98	0.12	93,93,93,93	0
56	MG	1A	3129	1/1	0.98	0.16	93,93,93,93	0
56	MG	1A	3502	1/1	0.98	0.27	61,61,61,61	0
56	MG	1A	3179	1/1	0.98	0.34	90,90,90,90	0
56	MG	2A	3306	1/1	0.98	0.19	74,74,74,74	0
56	MG	2A	3122	1/1	0.98	0.21	86,86,86,86	0
56	MG	1A	3646	1/1	0.98	0.31	92,92,92,92	0
56	MG	2A	3163	1/1	0.98	0.22	79,79,79,79	0
56	MG	1a	3219	1/1	0.98	0.20	74,74,74,74	0
56	MG	1a	3047	1/1	0.98	0.20	82,82,82,82	0
56	MG	1A	3482	1/1	0.98	0.22	75,75,75,75	0
56	MG	2A	3064	1/1	0.98	0.34	82,82,82,82	0
56	MG	1A	3314	1/1	0.98	0.29	54,54,54,54	0
56	MG	2A	3067	1/1	0.98	0.14	82,82,82,82	0
56	MG	2a	3125	1/1	0.98	0.14	75,75,75,75	0
56	MG	1A	3089	1/1	0.98	0.66	59,59,59,59	0
56	MG	2A	3167	1/1	0.98	0.12	87,87,87,87	0
56	MG	1a	3177	1/1	0.99	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3064	1/1	0.99	0.17	84,84,84,84	0
56	MG	1A	3107	1/1	0.99	0.27	81,81,81,81	0
56	MG	1A	3498	1/1	0.99	0.14	85,85,85,85	0
56	MG	2A	3288	1/1	0.99	0.19	71,71,71,71	0
57	ZN	19	501	1/1	0.99	0.25	77,77,77,77	0
56	MG	1A	3379	1/1	0.99	0.26	55,55,55,55	0
56	MG	1A	3102	1/1	0.99	0.12	78,78,78,78	0
56	MG	1A	3073	1/1	0.99	0.25	81,81,81,81	0
56	MG	1A	3111	1/1	0.99	0.10	83,83,83,83	0
56	MG	1A	3135	1/1	0.99	0.10	59,59,59,59	0
58	SF4	2d	501	8/8	0.99	0.18	95,106,118,119	0
56	MG	1A	3375	1/1	0.99	0.24	62,62,62,62	0
57	ZN	26	501	1/1	0.99	0.26	98,98,98,98	0
58	SF4	1d	501	8/8	0.99	0.23	76,91,99,101	0
56	MG	2A	3225	1/1	0.99	0.27	75,75,75,75	0
56	MG	1a	3086	1/1	0.99	0.33	76,76,76,76	0
56	MG	1A	3057	1/1	0.99	0.16	79,79,79,79	0
56	MG	2A	3250	1/1	0.99	0.24	65,65,65,65	0
57	ZN	25	501	1/1	0.99	0.23	97,97,97,97	0
57	ZN	15	501	1/1	0.99	0.21	87,87,87,87	0
56	MG	1A	3485	1/1	0.99	0.18	61,61,61,61	0
56	MG	1A	3013	1/1	0.99	0.25	69,69,69,69	0
56	MG	1a	3227	1/1	0.99	0.33	64,64,64,64	0
56	MG	1A	3028	1/1	0.99	0.23	68,68,68,68	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.