wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2026 – 02:47 AM UTC

PDB ID	:	7JQM / pdb_00007jqm
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with Bac7-002, mRNA, and deacylated P-site tRNA at 3.05A resolution
Authors	:	Mardirossian, M.; Sola, R.; Beckert, B.; Valencic, E.; Collis, D.W.P.; Borisek, J.; Armas, F.; Di Stasi, A.; Buchmann, J.; Syroegin, E.A.; Polikanov, Y.S.; Magistrato, A.; Hilpert, K.; Wilson, D.N.; Scocchi, M.
Deposited on	:	2020-08-11
Resolution	:	3.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

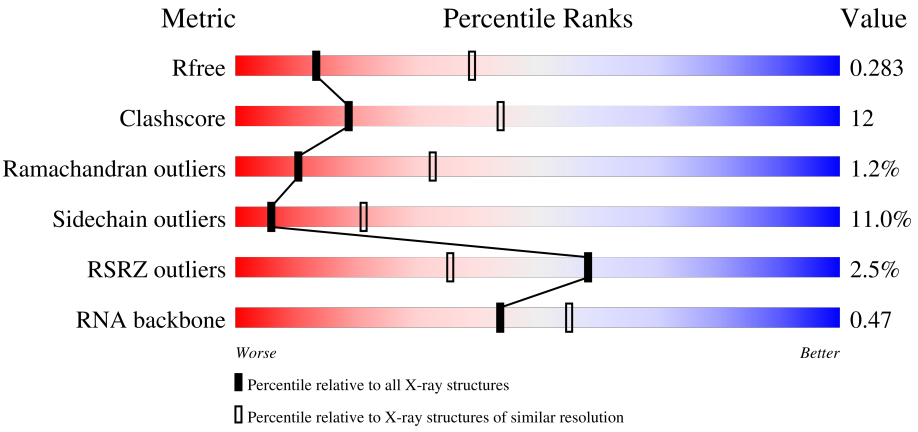
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 53% 37% 8%
1	2A	2915	% 46% 41% 9%
2	1B	121	64% 29% 7%

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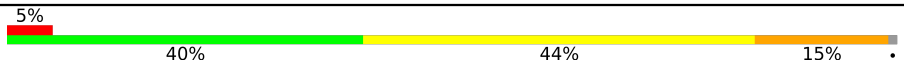
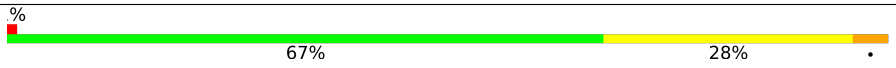
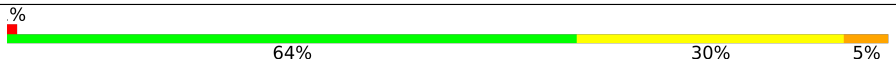
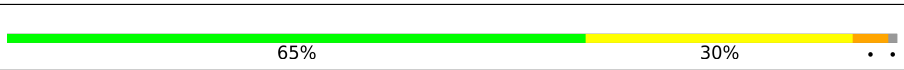
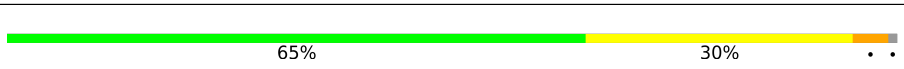
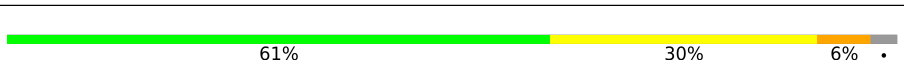
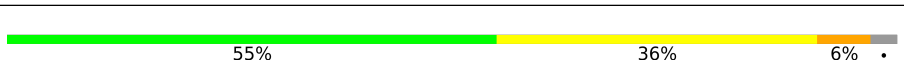
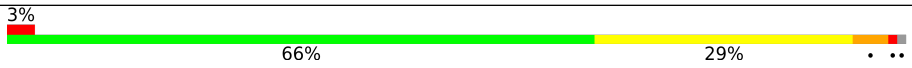
Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
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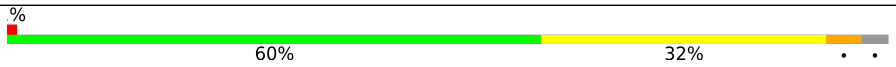
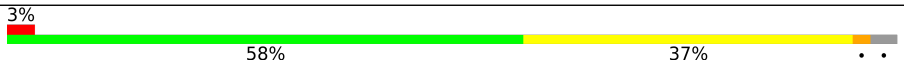
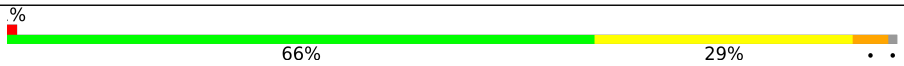
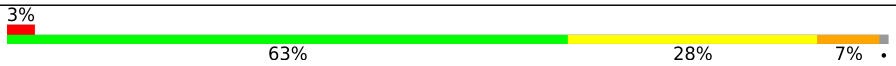
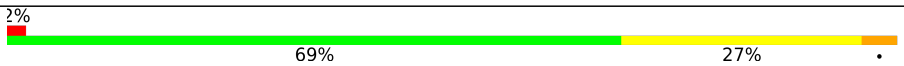
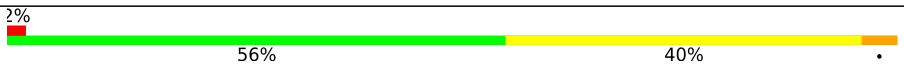
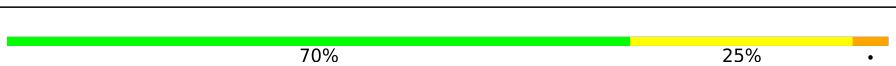
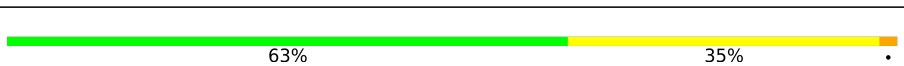
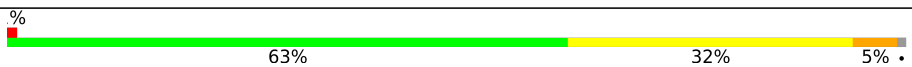
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
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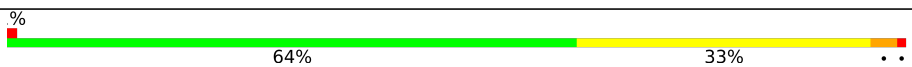
12	1Q	141	
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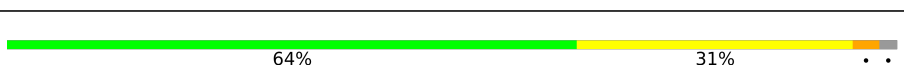
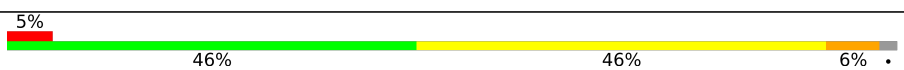
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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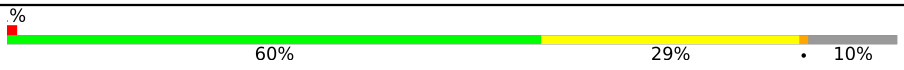
Mol	Chain	Length	Quality of chain
15	1T	146	
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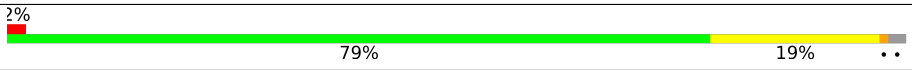
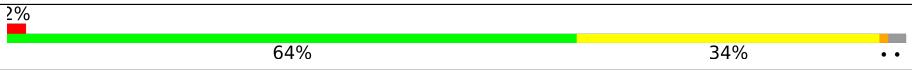
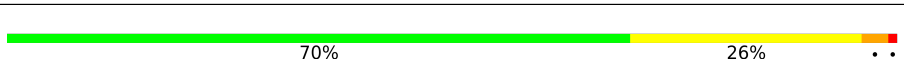
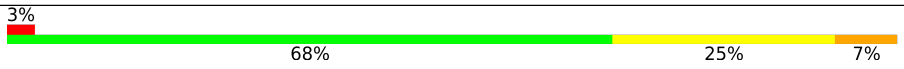
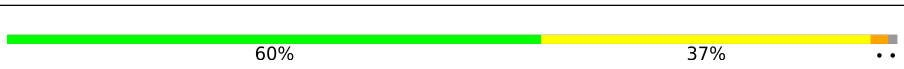
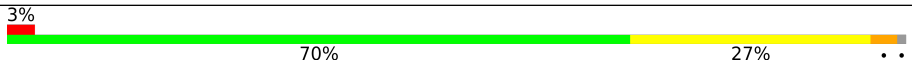
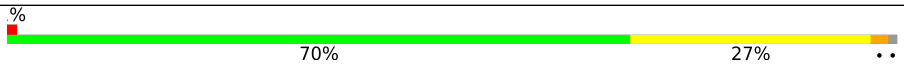
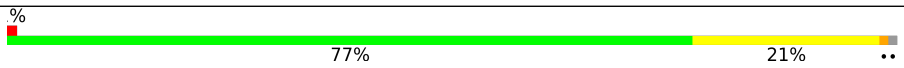
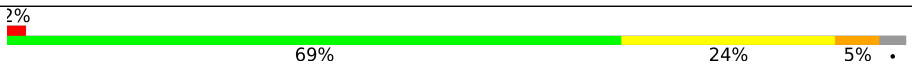
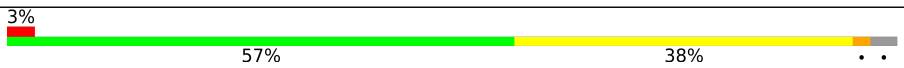
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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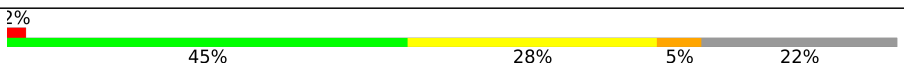
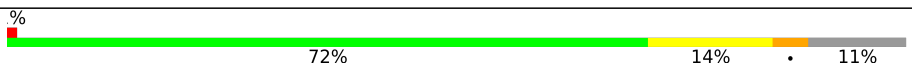
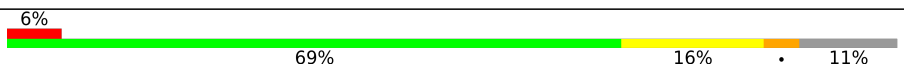
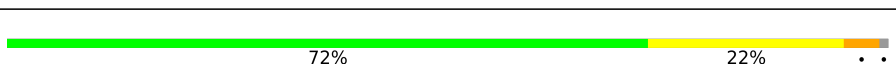
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
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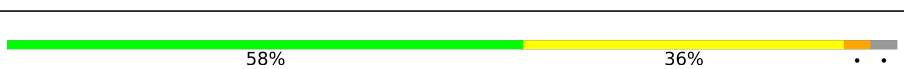
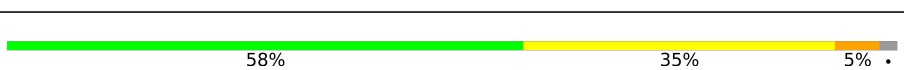
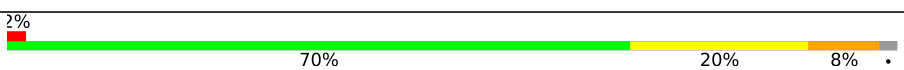
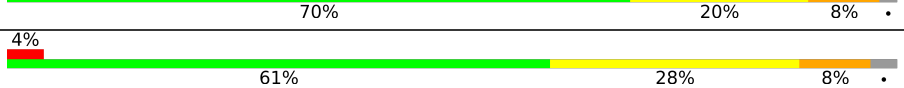
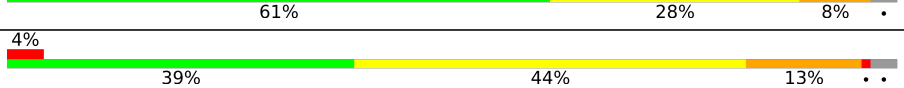
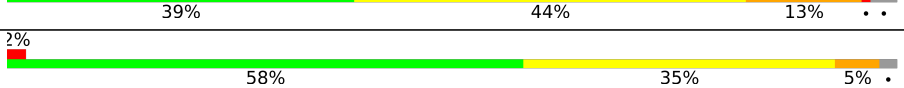
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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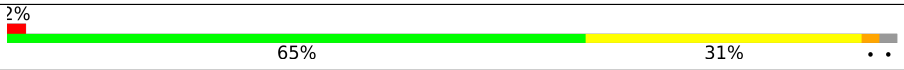
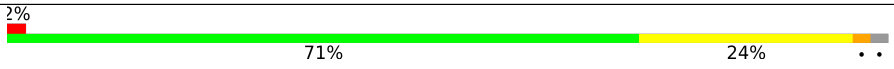
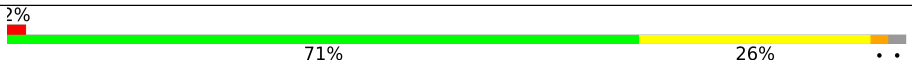
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
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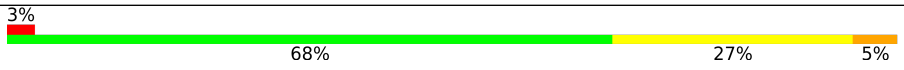
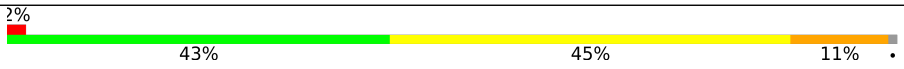
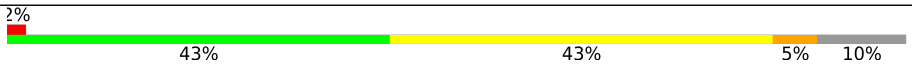
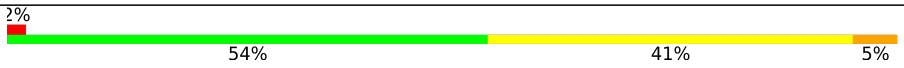
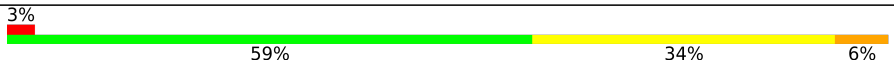
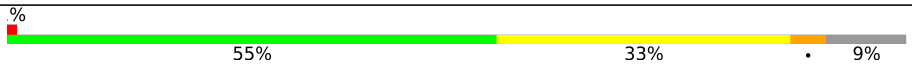
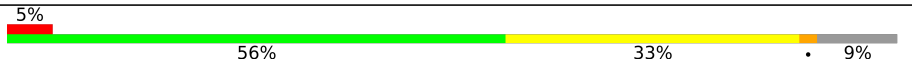
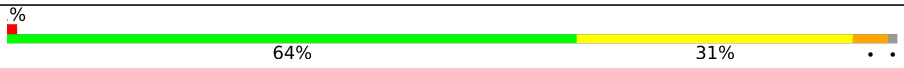
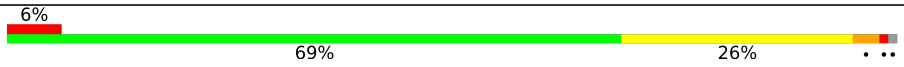
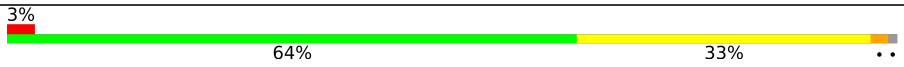
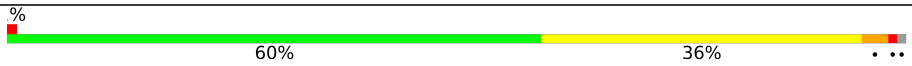
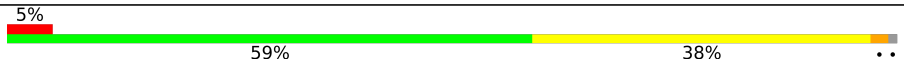
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

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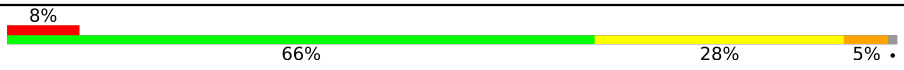
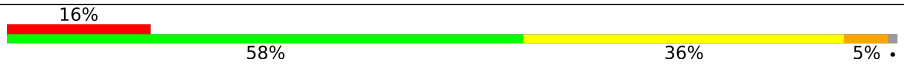
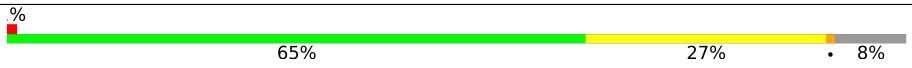
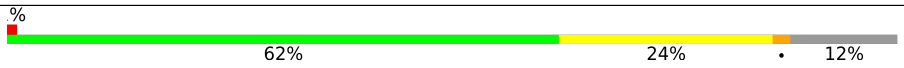
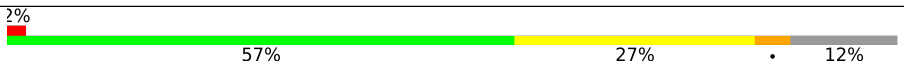
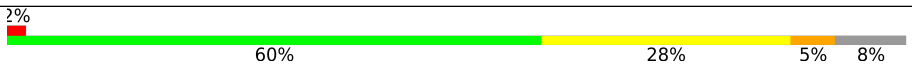
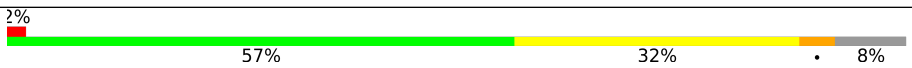
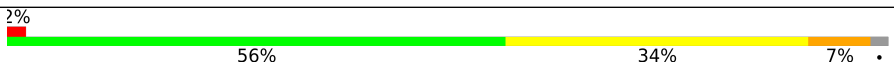
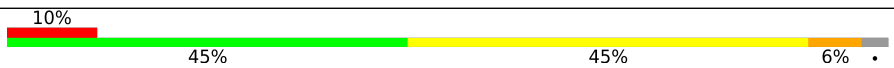
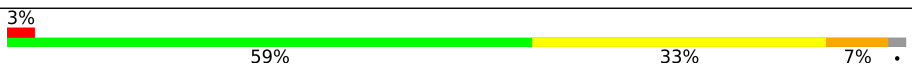
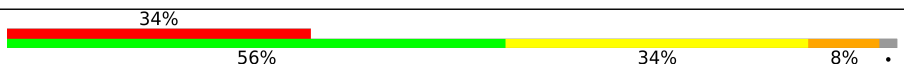
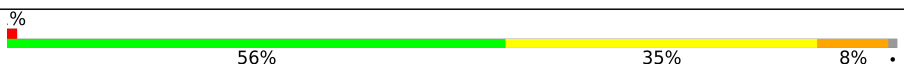
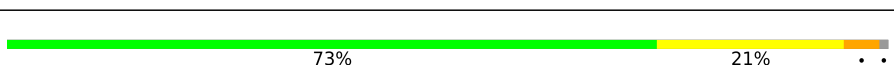
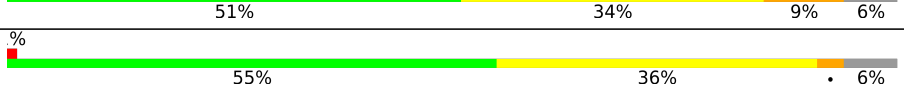
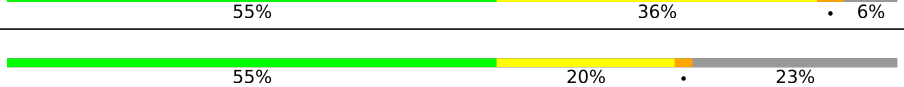
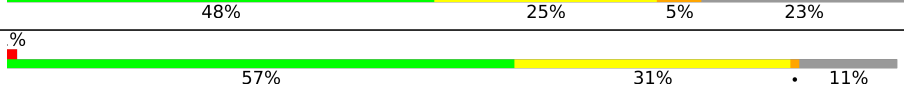
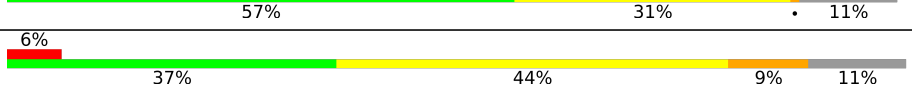
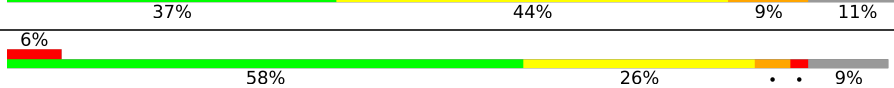
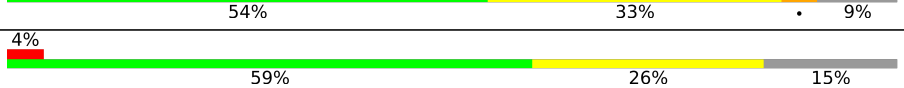
Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	22% 41% 37% 15%
53	1v	24	21% 25% 12% 17% 46%
53	2v	24	38% 25% 17% 12% 46%
54	1x	77	% 53% 38% 8%
54	2x	77	52% 36% 10%
55	1z	16	12% 50% 44% 6%
55	2z	16	19% 81% 12% 6%

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	3388	-	-	-	X
56	MG	1a	1744	-	-	-	X
56	MG	1a	1759	-	-	-	X
56	MG	2a	3082	-	-	-	X
56	MG	2a	3119	-	-	-	X
56	MG	2a	3145	-	-	-	X
58	SF4	1d	302	-	-	X	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 290774 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	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 277	C 125	N 51	O 88	P 13	0	0	0
53	2v	13	Total 277	C 125	N 51	O 88	P 13	0	0	0

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0
54	2x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0

- Molecule 55 is a protein called Bac7-002.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	16	Total 147	C 93	N 38	O 16	0	0	0
55	2z	16	Total 141	C 90	N 35	O 16	0	0	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	848	Total 848	Mg 848	0	0
56	1B	25	Total 25	Mg 25	0	0
56	1D	8	Total 8	Mg 8	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1F	12	Total 12	Mg 12	0	0
56	1G	4	Total 4	Mg 4	0	0
56	1H	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	1N	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	1	Total Mg 1 1	0	0
56	1P	5	Total Mg 5 5	0	0
56	1Q	4	Total Mg 4 4	0	0
56	1R	6	Total Mg 6 6	0	0
56	1S	1	Total Mg 1 1	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	6	Total Mg 6 6	0	0
56	1V	5	Total Mg 5 5	0	0
56	1W	6	Total Mg 6 6	0	0
56	1X	3	Total Mg 3 3	0	0
56	1Y	1	Total Mg 1 1	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	5	Total Mg 5 5	0	0
56	11	2	Total Mg 2 2	0	0
56	12	2	Total Mg 2 2	0	0
56	13	3	Total Mg 3 3	0	0
56	14	1	Total Mg 1 1	0	0
56	15	5	Total Mg 5 5	0	0
56	17	6	Total Mg 6 6	0	0
56	18	4	Total Mg 4 4	0	0
56	19	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	167	Total Mg 167 167	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1h	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	1s	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1x	10	Total Mg 10 10	0	0
56	1z	1	Total Mg 1 1	0	0
56	2A	625	Total Mg 625 625	0	0
56	2B	12	Total Mg 12 12	0	0
56	2D	2	Total Mg 2 2	0	0
56	2E	5	Total Mg 5 5	0	0
56	2F	4	Total Mg 4 4	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	3	Total Mg 3 3	0	0
56	2Q	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2R	1	Total Mg 1 1	0	0
56	2T	2	Total Mg 2 2	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	1	Total Mg 1 1	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	1	Total Mg 1 1	0	0
56	21	1	Total Mg 1 1	0	0
56	23	2	Total Mg 2 2	0	0
56	25	2	Total Mg 2 2	0	0
56	26	1	Total Mg 1 1	0	0
56	27	2	Total Mg 2 2	0	0
56	28	3	Total Mg 3 3	0	0
56	2a	145	Total Mg 145 145	0	0
56	2d	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	2	Total Mg 2 2	0	0
56	2q	2	Total Mg 2 2	0	0
56	2r	1	Total Mg 1 1	0	0

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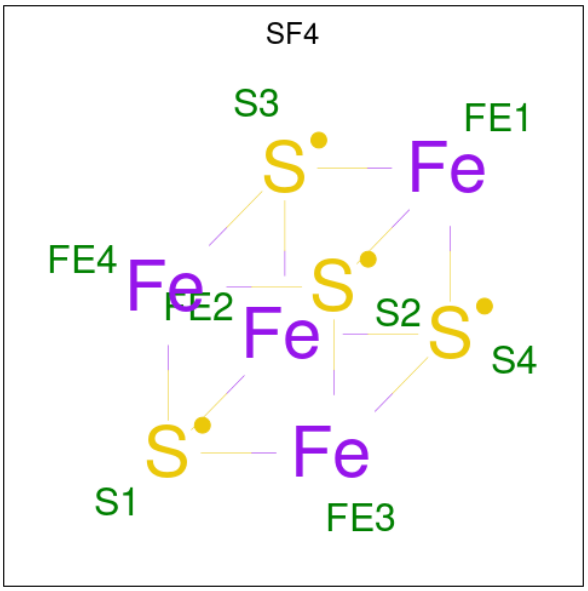
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2t	1	Total Mg 1 1	0	0
56	2v	2	Total Mg 2 2	0	0
56	2x	3	Total Mg 3 3	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1222	Total O 1222 1222	0	0
60	1B	27	Total O 27 27	0	0
60	1D	21	Total O 21 21	0	0
60	1E	11	Total O 11 11	0	0
60	1F	9	Total O 9 9	0	0
60	1N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1O	1	Total O 1 1	0	0
60	1P	14	Total O 14 14	0	0
60	1Q	2	Total O 2 2	0	0
60	1R	3	Total O 3 3	0	0
60	1S	2	Total O 2 2	0	0
60	1T	4	Total O 4 4	0	0
60	1U	4	Total O 4 4	0	0
60	1V	4	Total O 4 4	0	0
60	1W	3	Total O 3 3	0	0
60	10	2	Total O 2 2	0	0
60	11	2	Total O 2 2	0	0
60	12	2	Total O 2 2	0	0
60	13	2	Total O 2 2	0	0
60	18	2	Total O 2 2	0	0
60	1a	26	Total O 26 26	0	0
60	1d	1	Total O 1 1	0	0
60	1z	1	Total O 1 1	0	0
60	2A	416	Total O 416 416	0	0
60	2B	3	Total O 3 3	0	0
60	2D	12	Total O 12 12	0	0
60	2E	4	Total O 4 4	0	0

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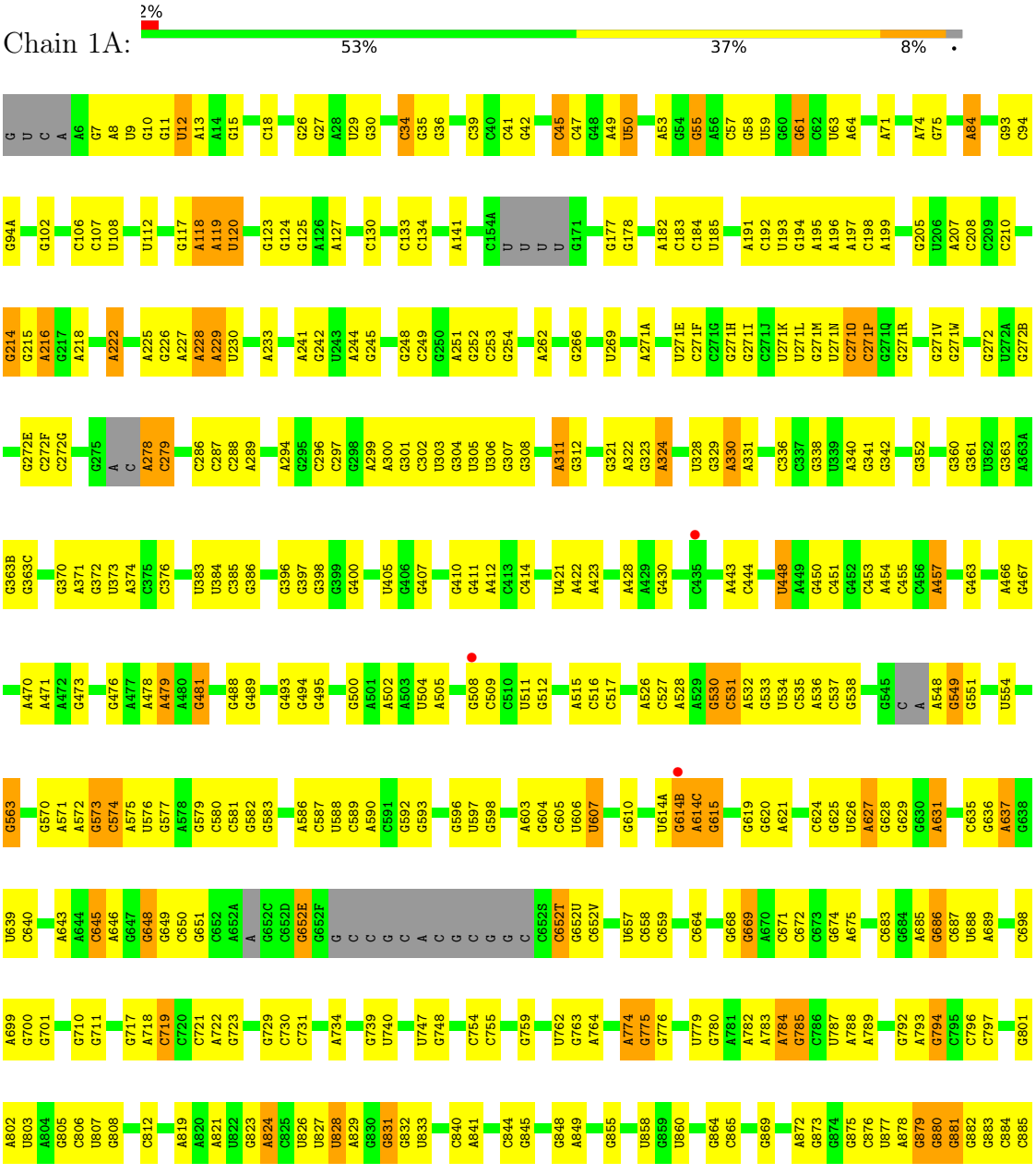
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2F	6	Total O 6 6	0	0
60	2I	1	Total O 1 1	0	0
60	2O	3	Total O 3 3	0	0
60	2P	4	Total O 4 4	0	0
60	2Q	1	Total O 1 1	0	0
60	2R	1	Total O 1 1	0	0
60	2T	1	Total O 1 1	0	0
60	2V	1	Total O 1 1	0	0
60	2W	2	Total O 2 2	0	0
60	20	1	Total O 1 1	0	0
60	21	2	Total O 2 2	0	0
60	28	2	Total O 2 2	0	0
60	2a	17	Total O 17 17	0	0
60	2l	1	Total O 1 1	0	0
60	2n	1	Total O 1 1	0	0
60	2t	1	Total O 1 1	0	0
60	2x	1	Total O 1 1	0	0

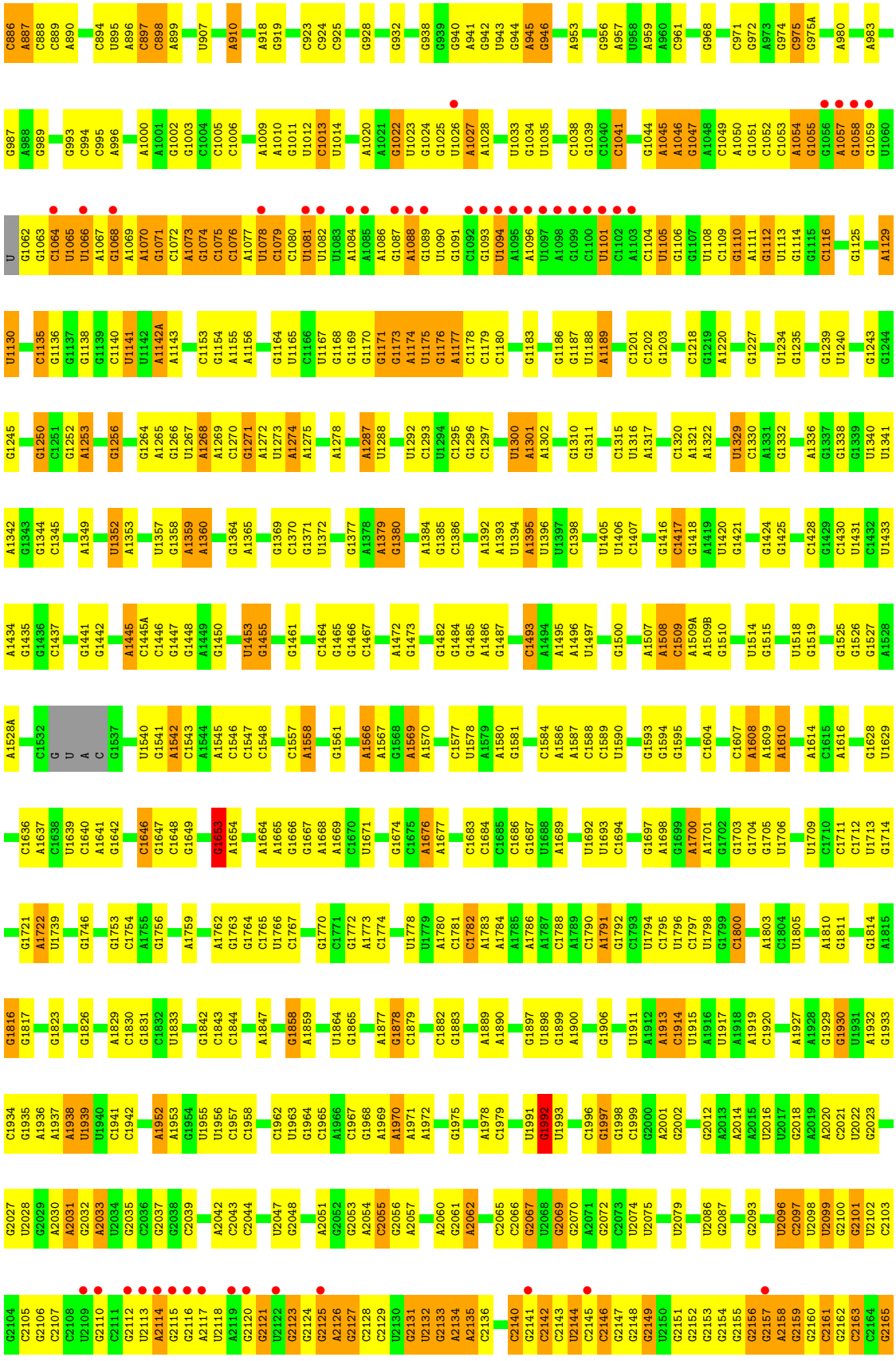
3 Residue-property plots (i)

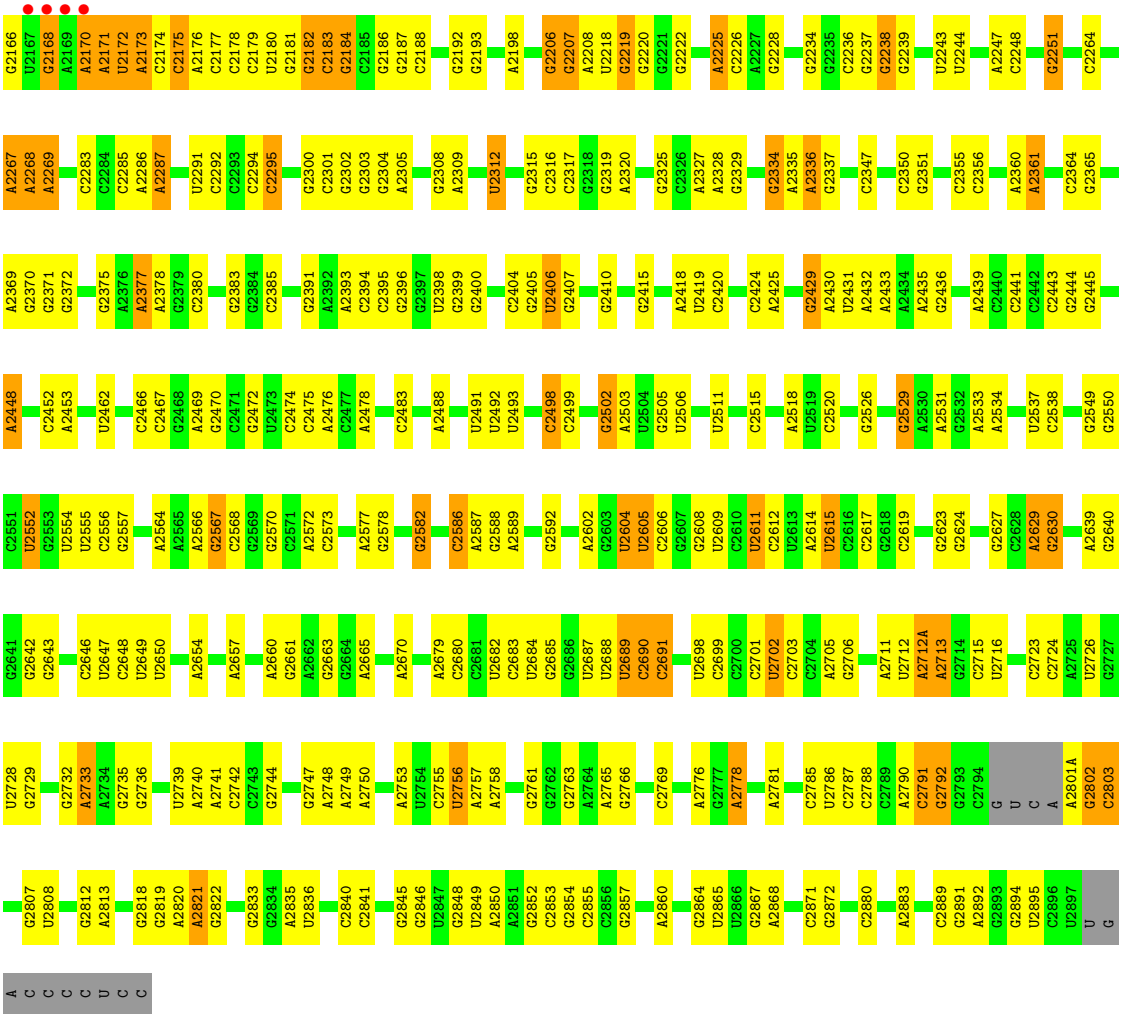
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

Chain 1A:

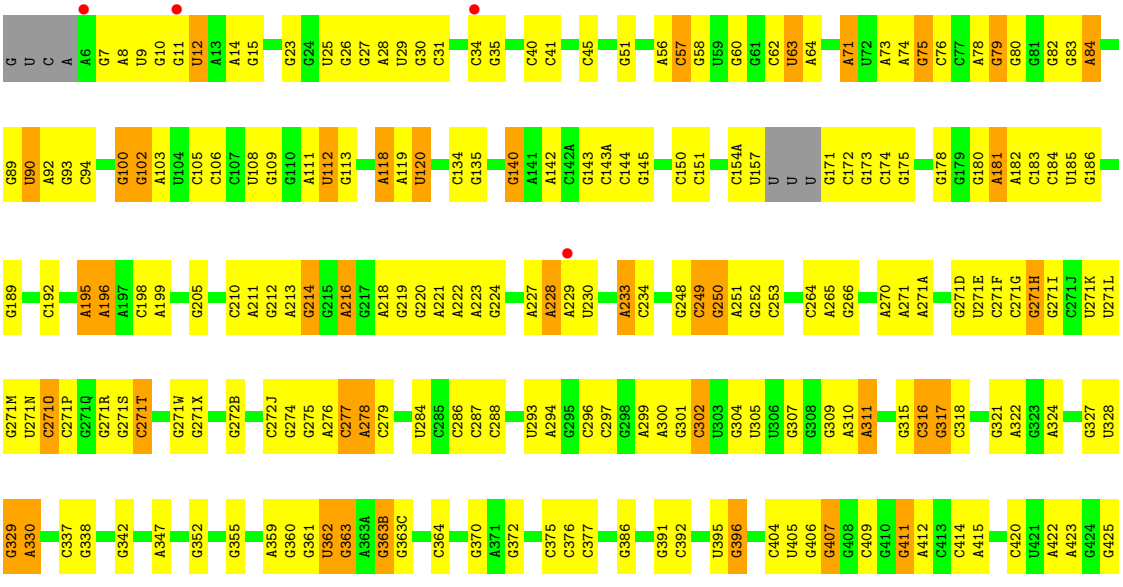


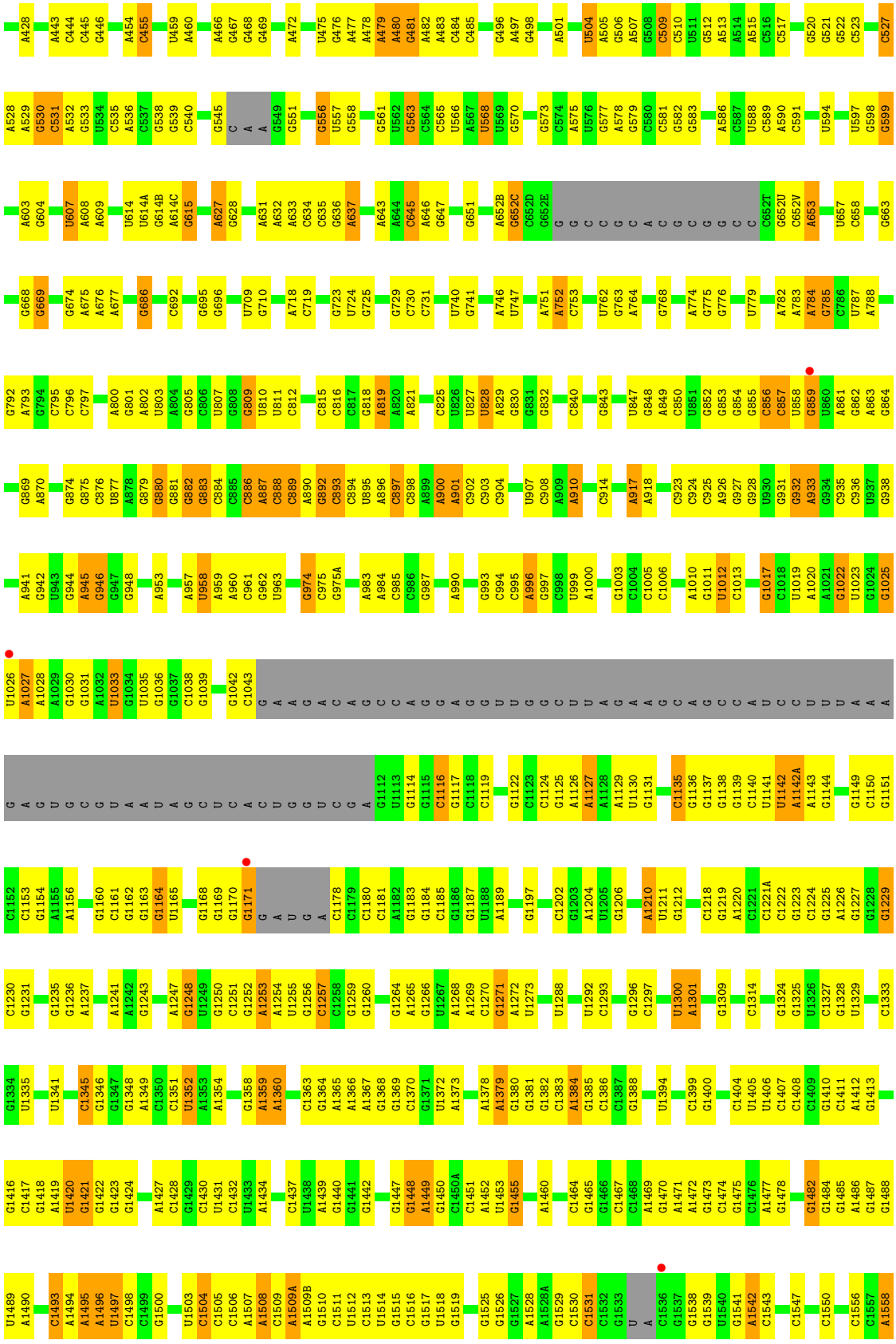


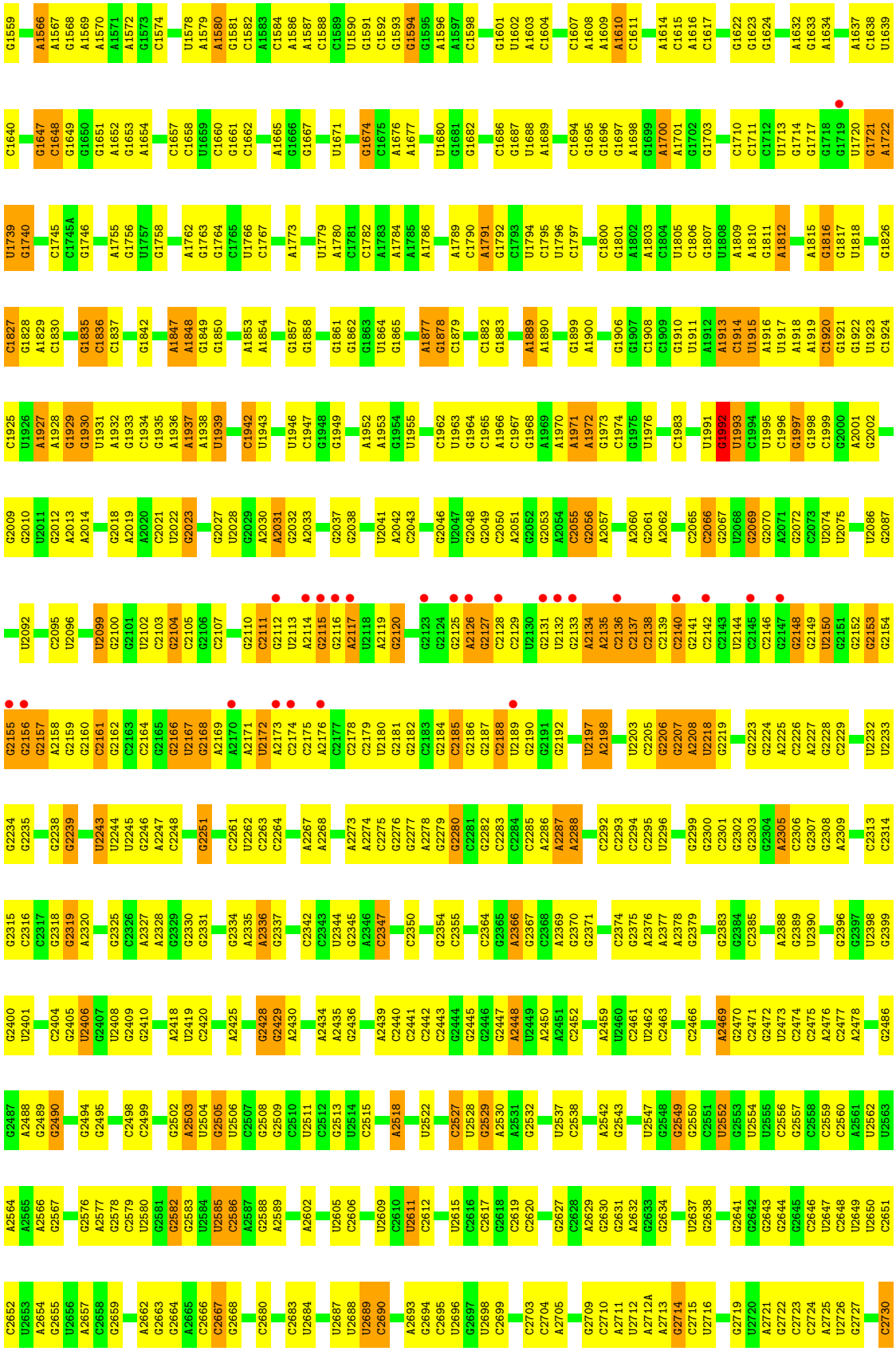


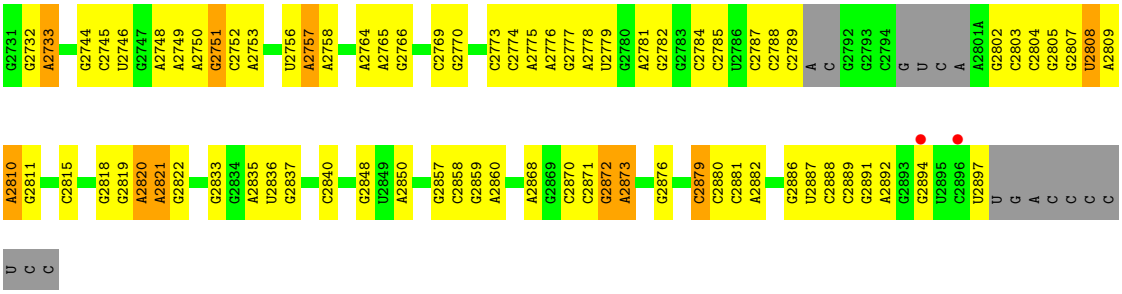
• Molecule 1: 23S Ribosomal RNA

Chain 2A:



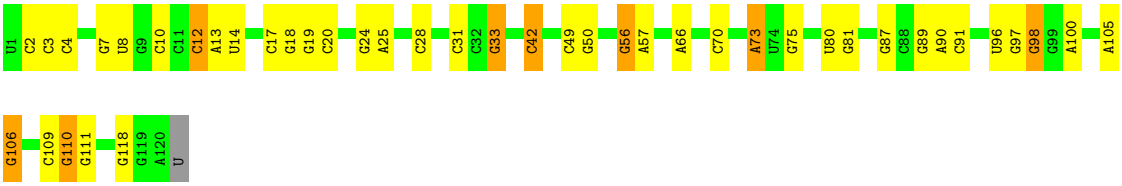






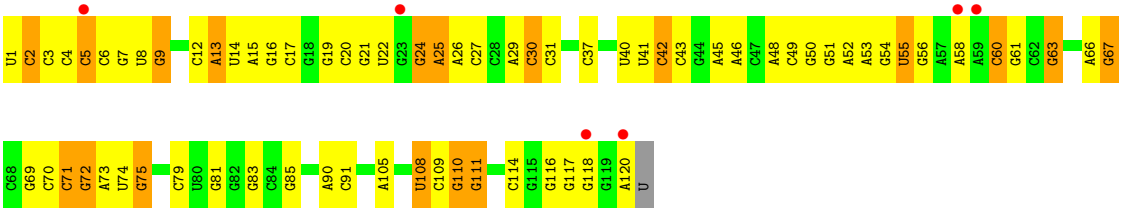
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



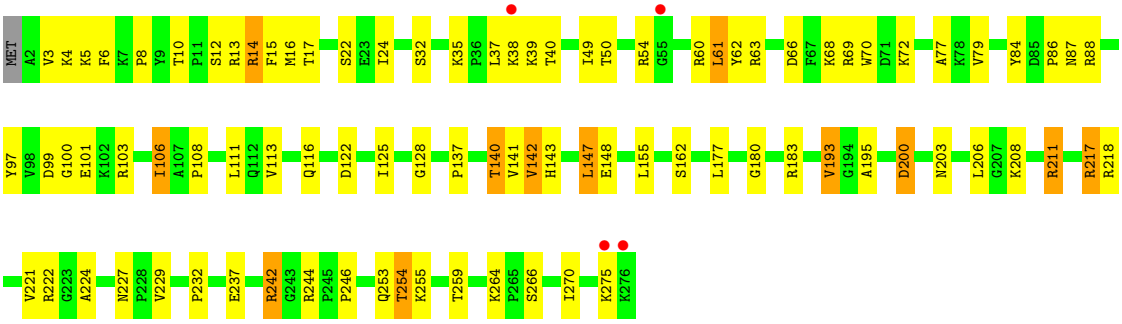
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



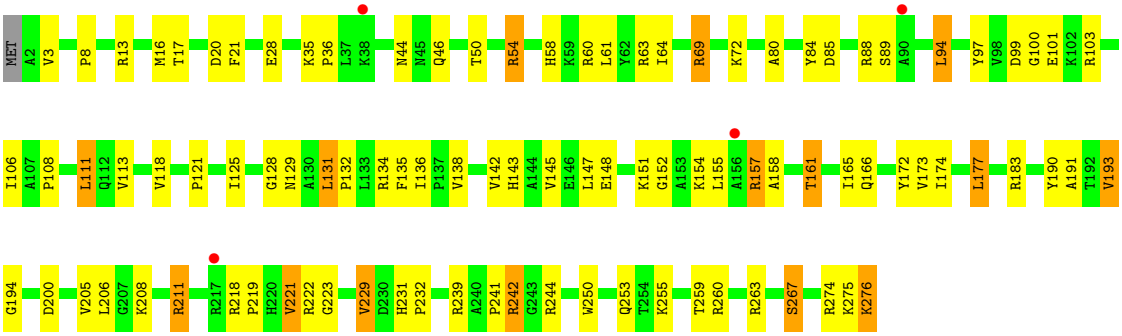
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



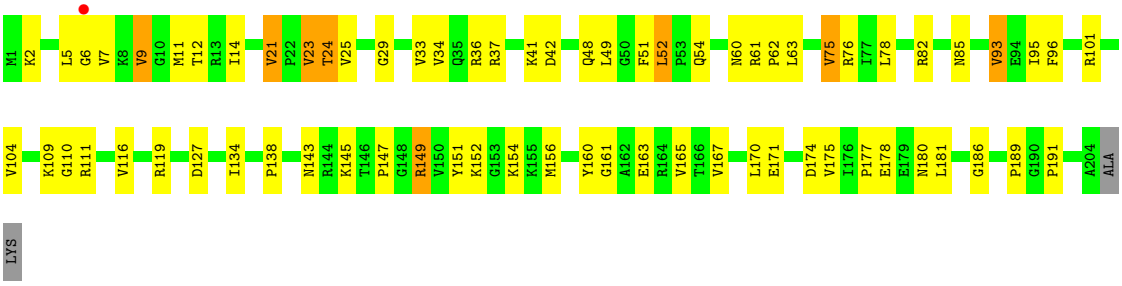
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



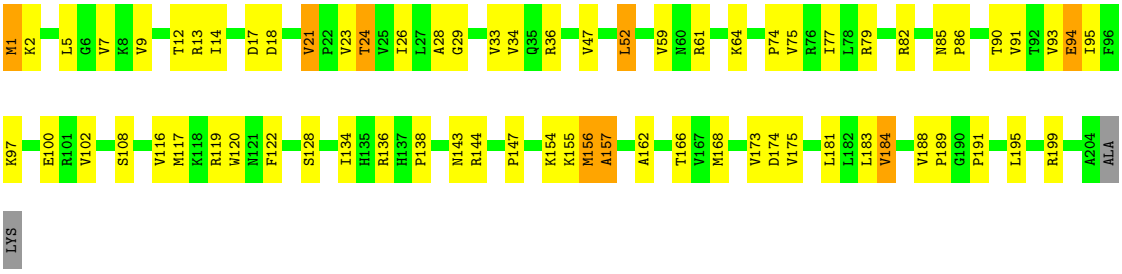
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



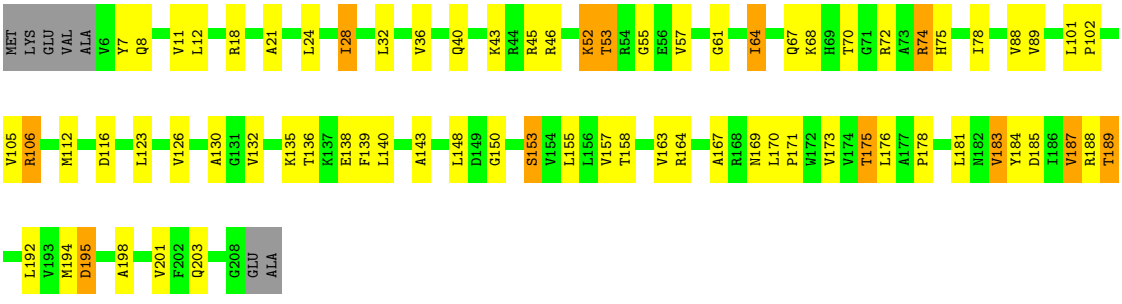
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



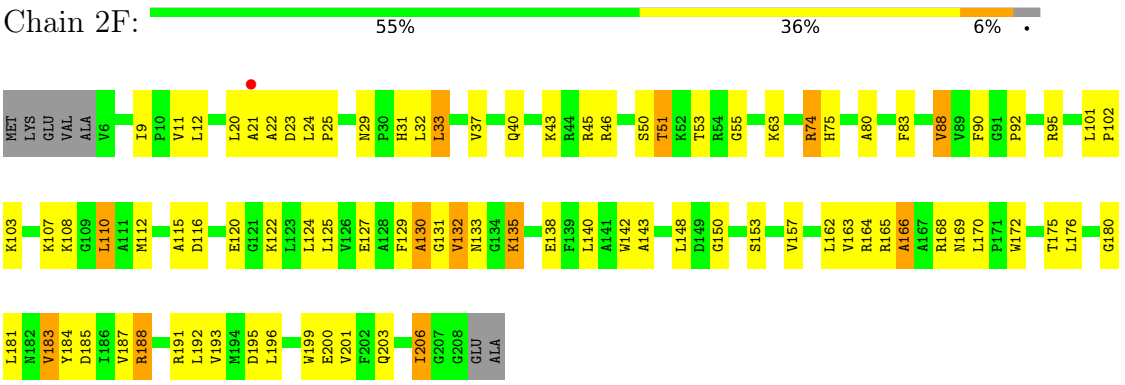
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



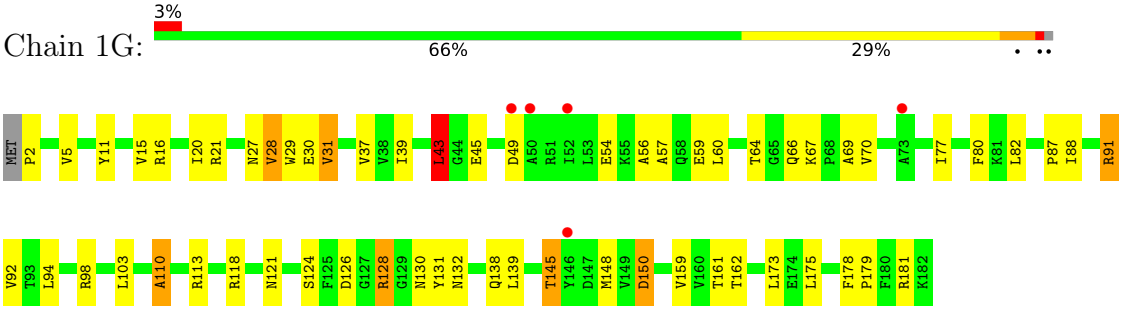
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



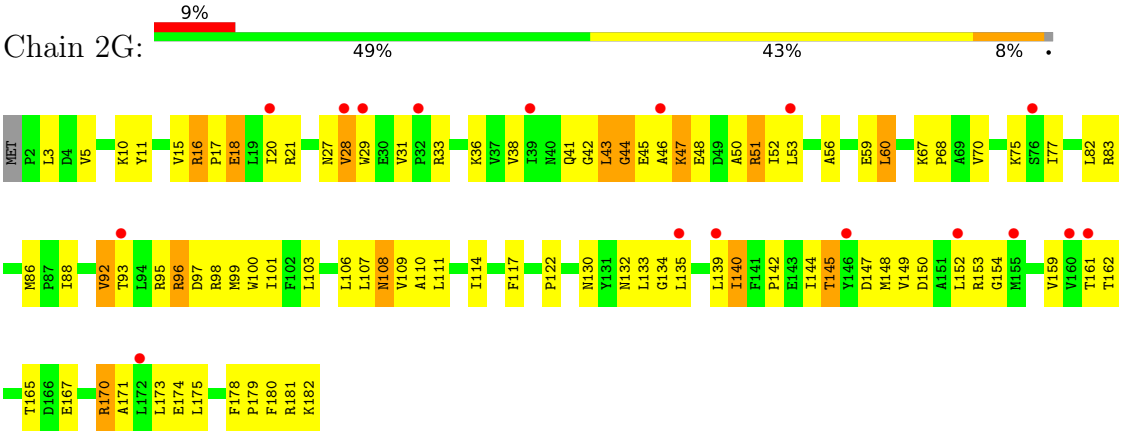
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



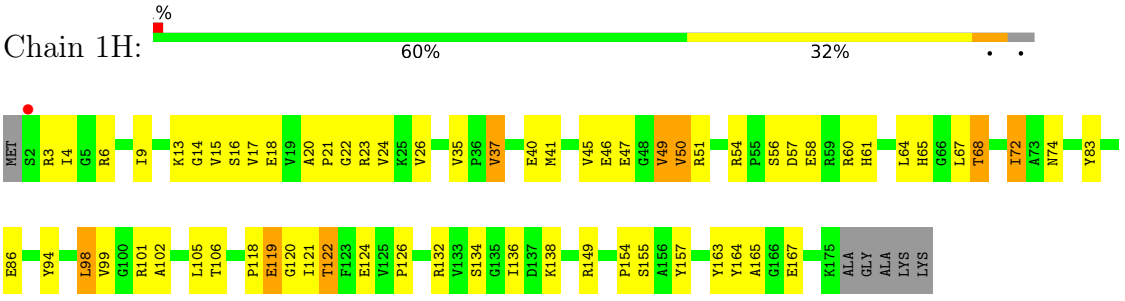
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



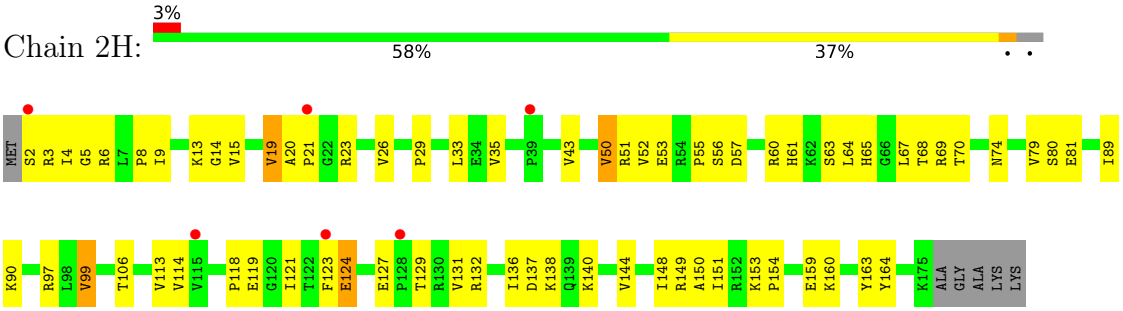
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



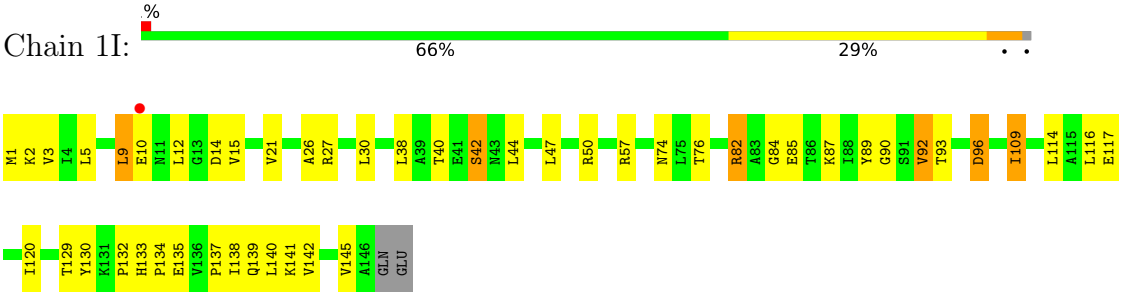
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



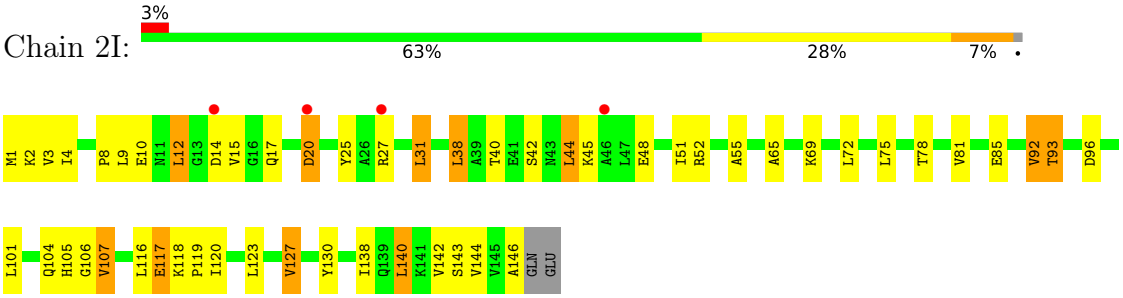
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



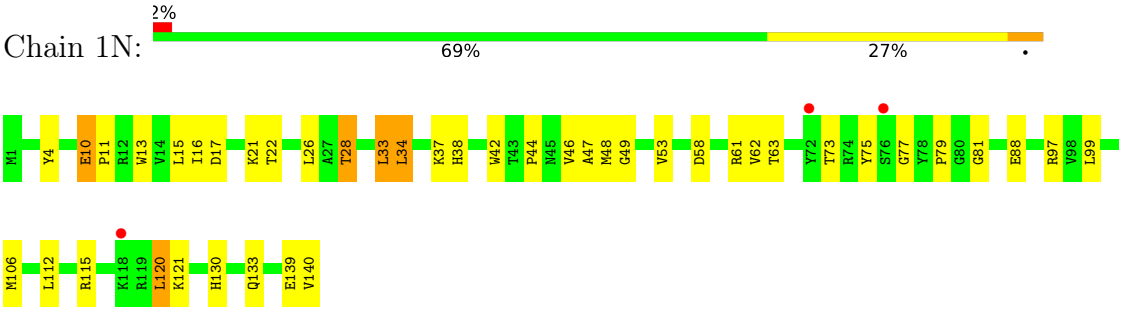
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



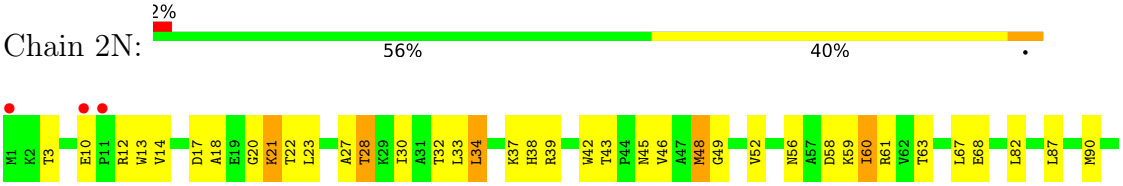
• Molecule 9: 50S ribosomal protein L13

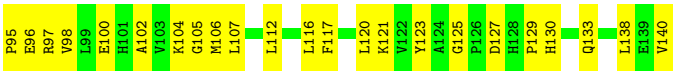
Chain 1N:



• Molecule 9: 50S ribosomal protein L13

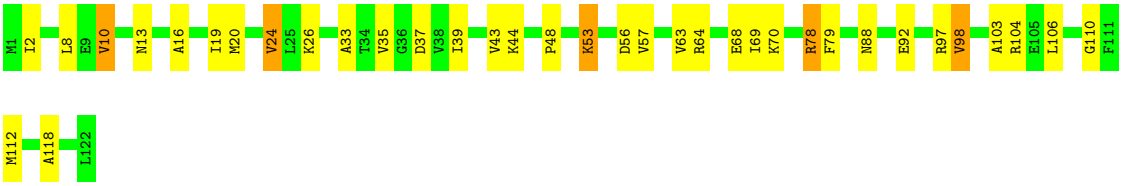
Chain 2N:





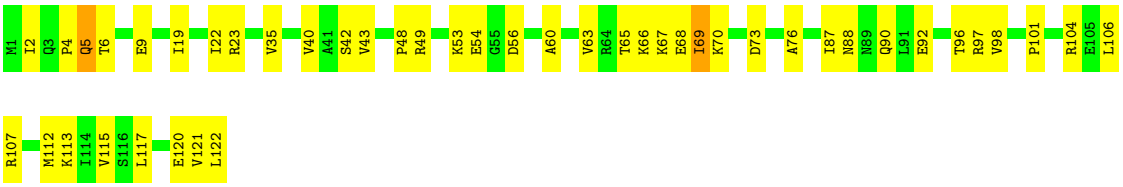
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



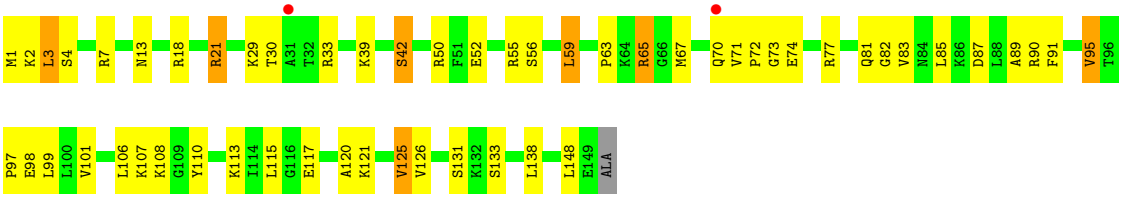
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



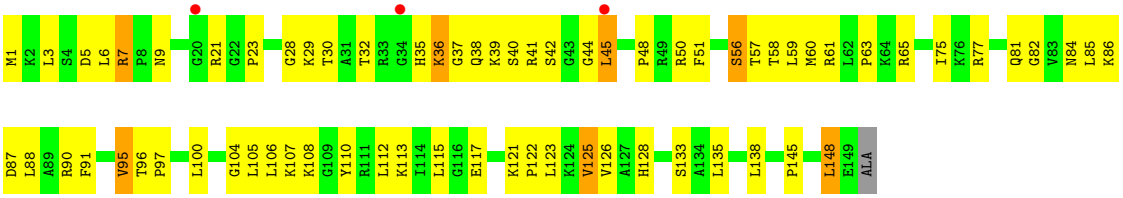
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



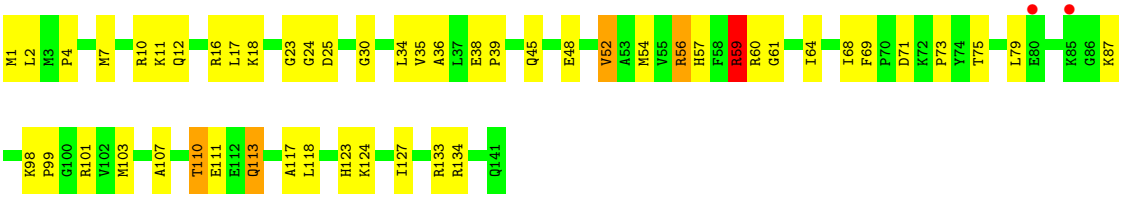
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



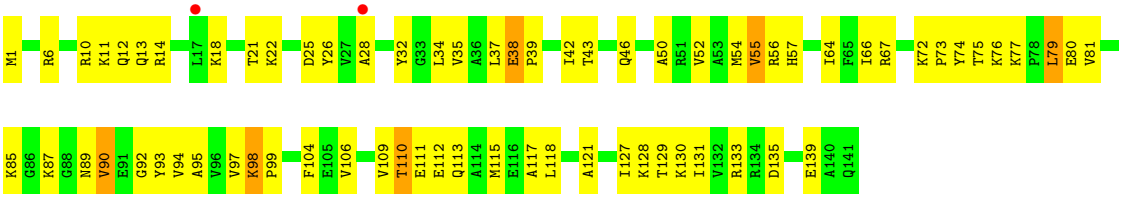
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



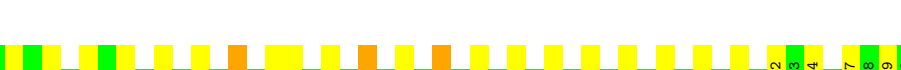
• Molecule 12: 50S ribosomal protein L16

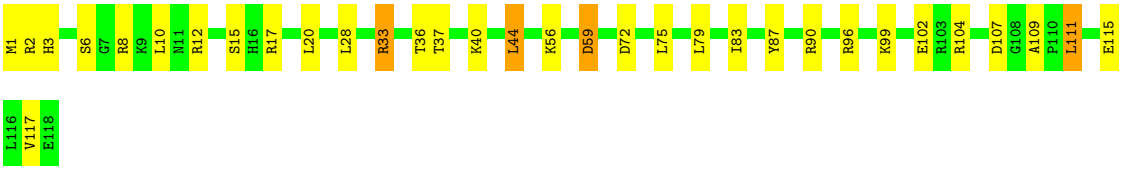
Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

Chain 1R:



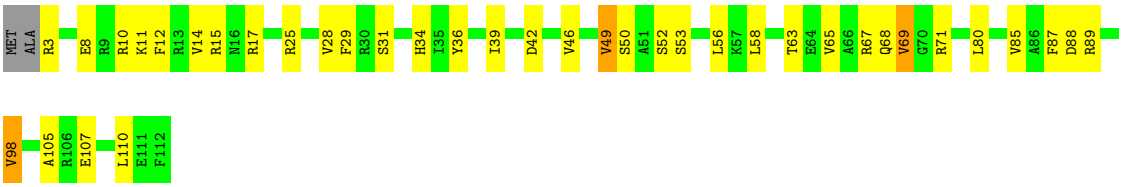


• Molecule 13: 50S ribosomal protein L17

Chain 2R:

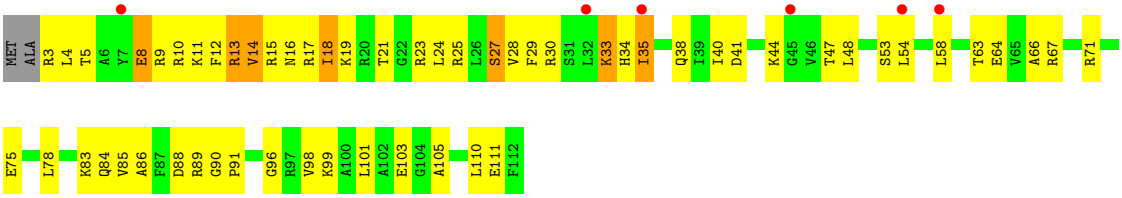
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



• Molecule 14: 50S ribosomal protein L18

Chain 2S:

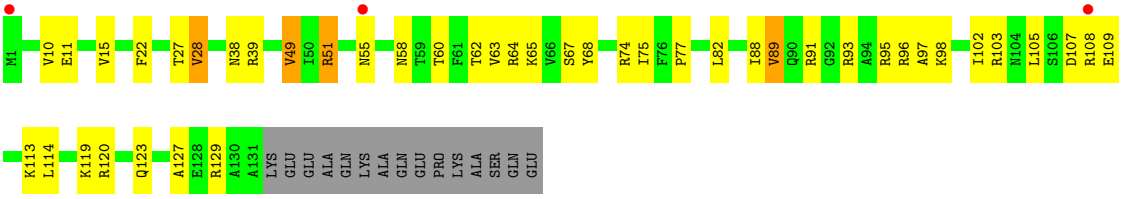


• Molecule 15: 50S ribosomal protein L19

Chain 1T:

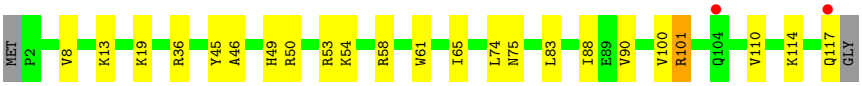
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



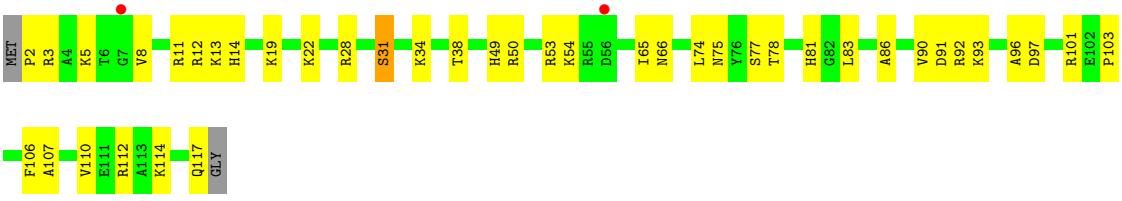
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



• Molecule 16: 50S ribosomal protein L20

Chain 2U:

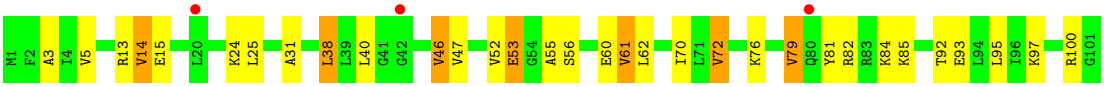


• Molecule 17: 50S ribosomal protein L21

Chain 1V:

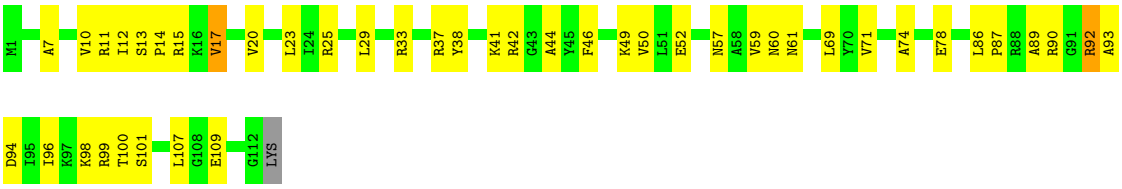
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



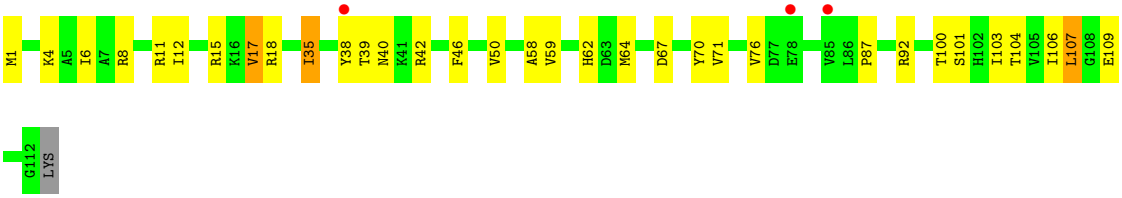
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



• Molecule 18: 50S ribosomal protein L22

Chain 2W:



• Molecule 19: 50S ribosomal protein L23

Chain 1X:

• Molecule 19: 50S ribosomal protein L23

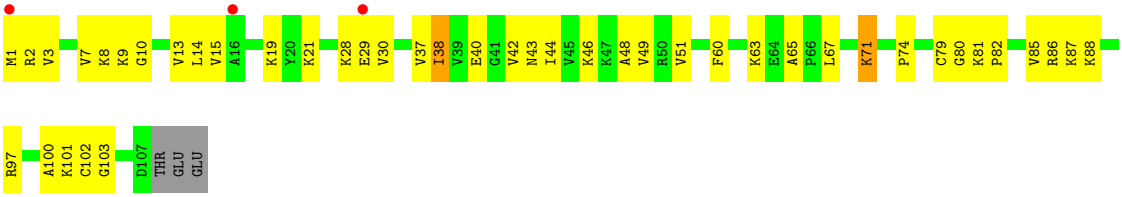
Chain 2X:

• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

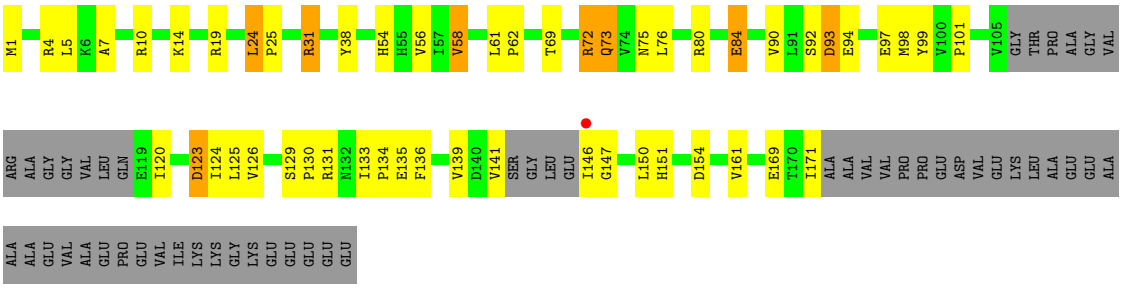
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



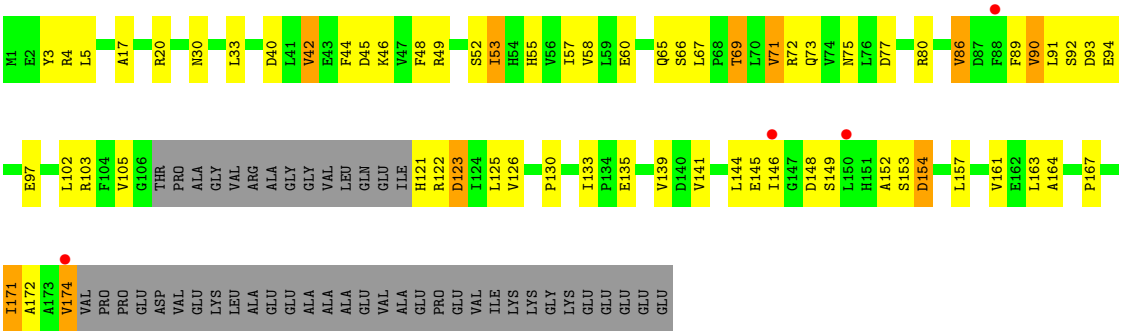
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

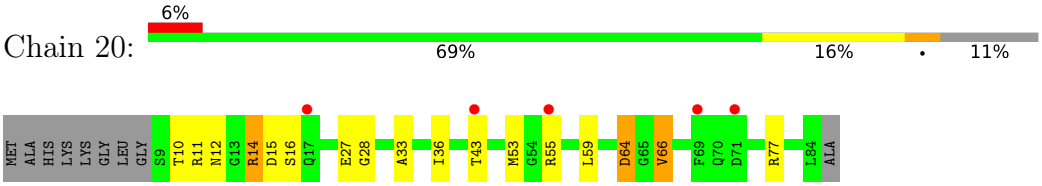


• Molecule 22: 50S ribosomal protein L27

Chain 10:

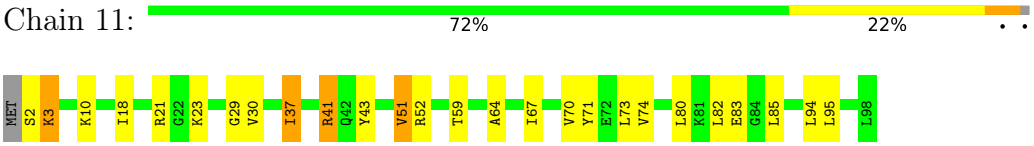
• Molecule 22: 50S ribosomal protein L27

Chain 20:



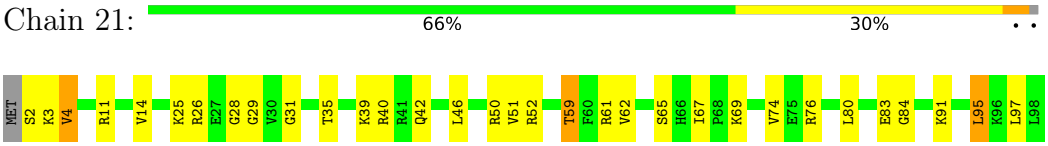
• Molecule 23: 50S ribosomal protein L28

Chain 11:



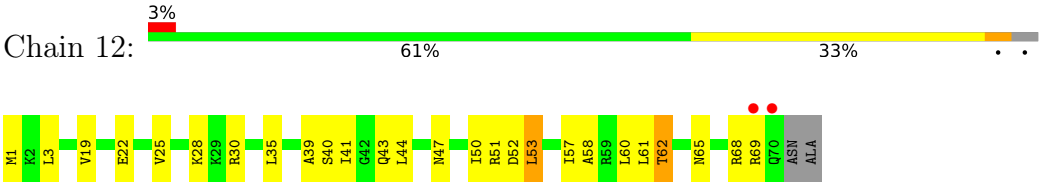
• Molecule 23: 50S ribosomal protein L28

Chain 21:



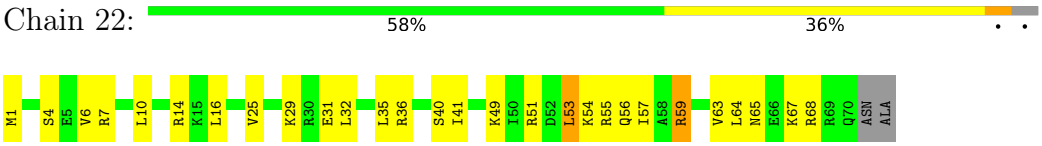
• Molecule 24: 50S ribosomal protein L29

Chain 12:



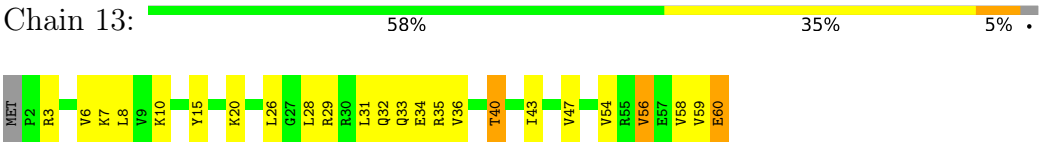
• Molecule 24: 50S ribosomal protein L29

Chain 22:



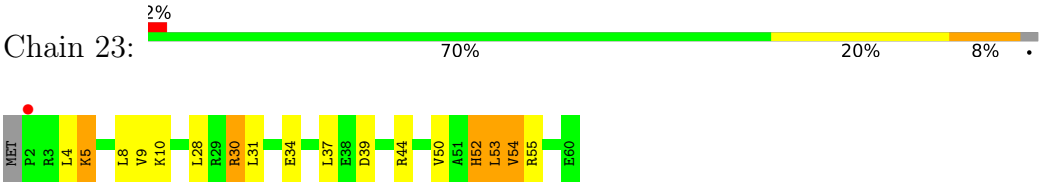
• Molecule 25: 50S ribosomal protein L30

Chain 13:



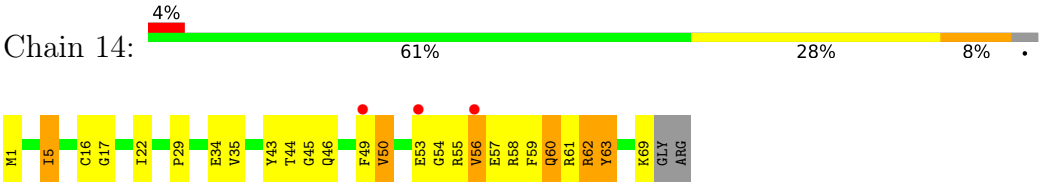
• Molecule 25: 50S ribosomal protein L30

Chain 23:



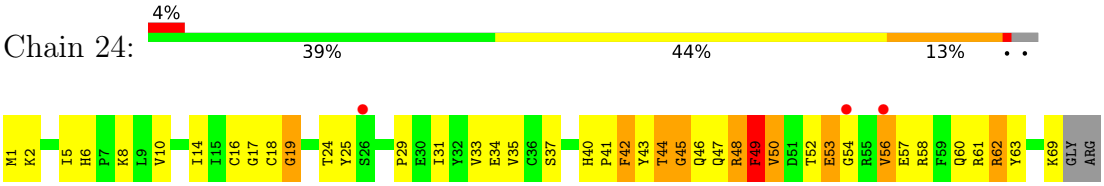
• Molecule 26: 50S ribosomal protein L31

Chain 14:



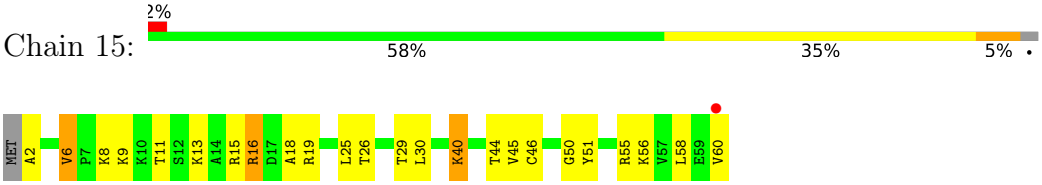
• Molecule 26: 50S ribosomal protein L31

Chain 24:



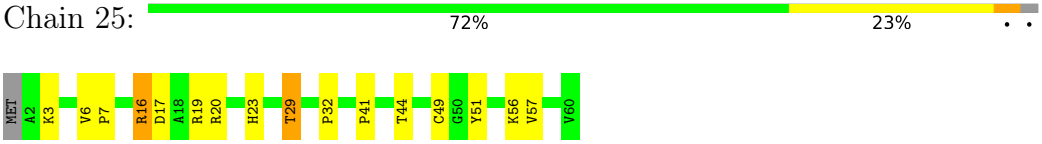
• Molecule 27: 50S ribosomal protein L32

Chain 15:



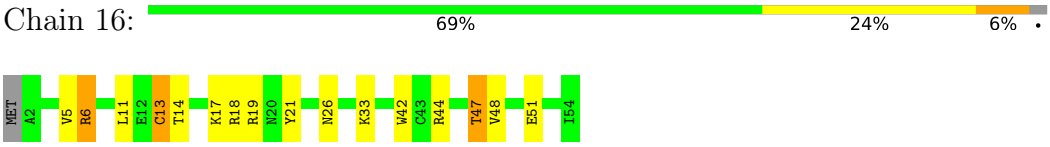
• Molecule 27: 50S ribosomal protein L32

Chain 25:



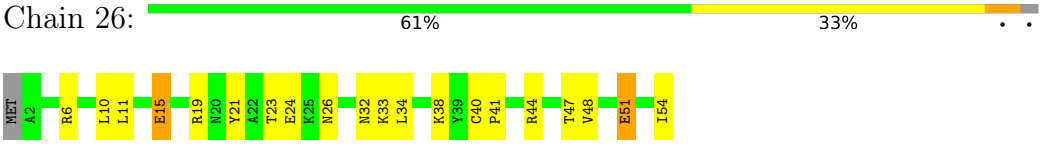
• Molecule 28: 50S ribosomal protein L33

Chain 16:



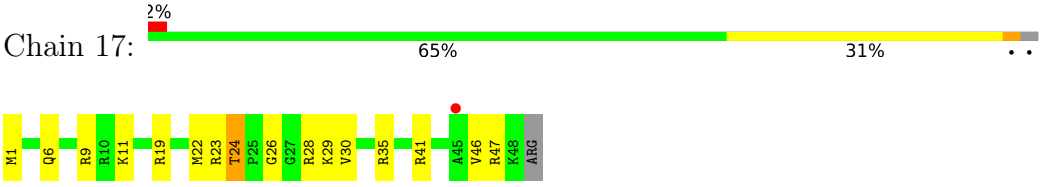
• Molecule 28: 50S ribosomal protein L33

Chain 26:



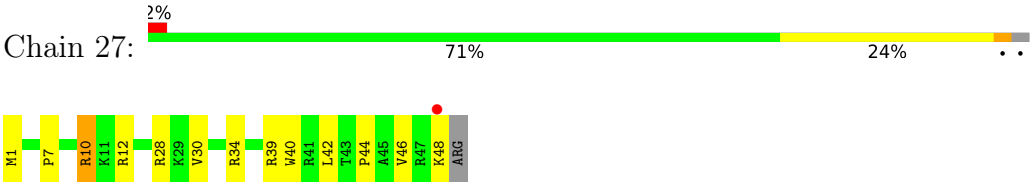
• Molecule 29: 50S ribosomal protein L34

Chain 17:



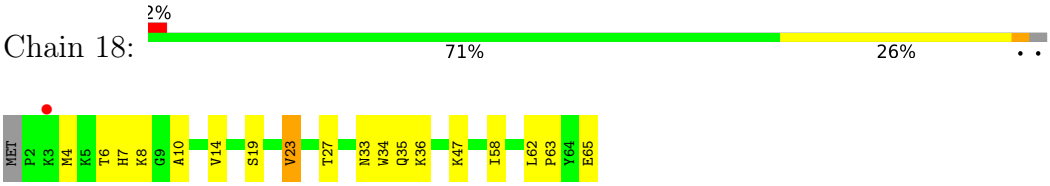
• Molecule 29: 50S ribosomal protein L34

Chain 27:



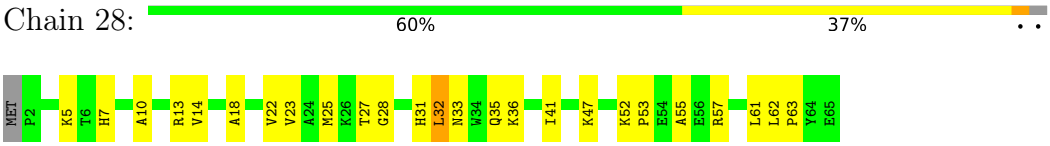
• Molecule 30: 50S ribosomal protein L35

Chain 18:



• Molecule 30: 50S ribosomal protein L35

Chain 28:

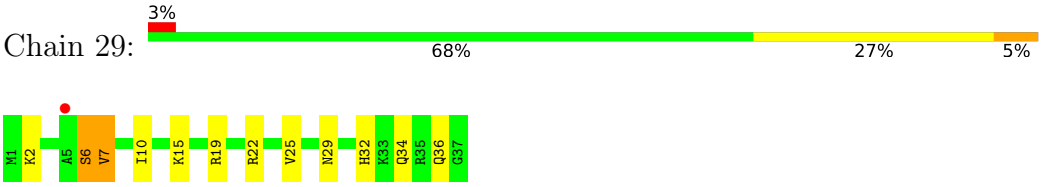


• Molecule 31: 50S ribosomal protein L36

Chain 19:

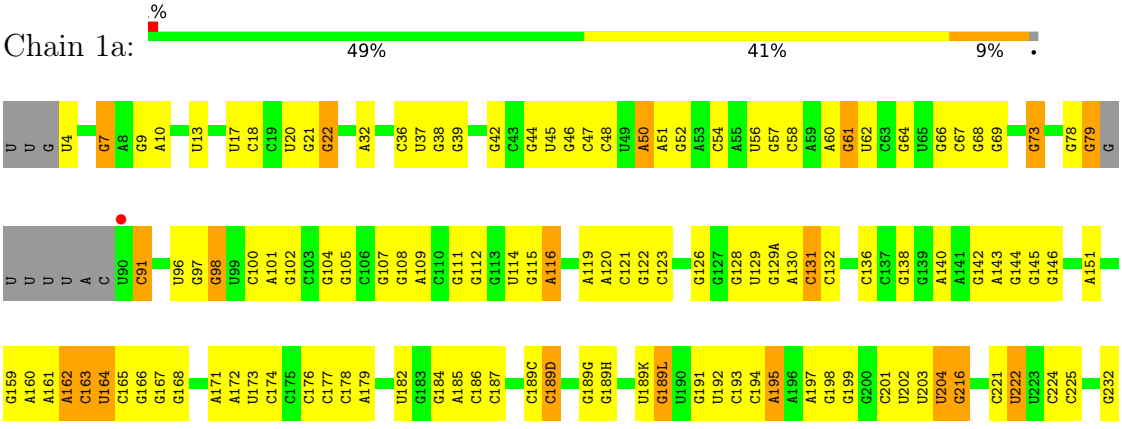
• Molecule 31: 50S ribosomal protein L36

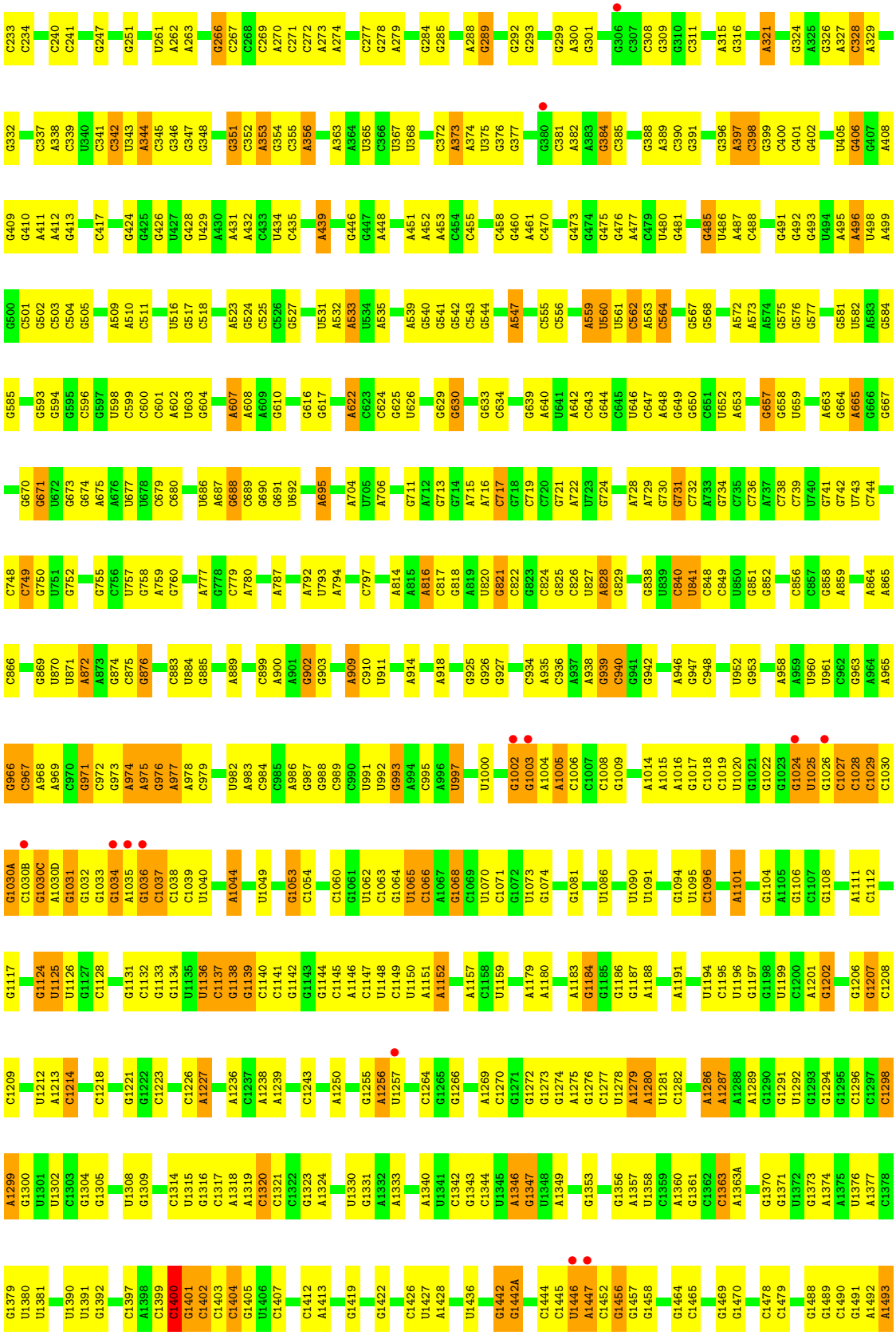
Chain 29:



• Molecule 32: 16S Ribosomal RNA

Chain 1a:




C233 C234 C240 C241 G247 G251 U261 A262 A263 G266 C267 C268 C269 A270 C271 C272 A273 A274 C277 G278 A279 G284 G285 A288 G289 G292 G293 G299 A300 G301 G306 C307 C308 G309 G310 C311 A315 G316 A321 G324 A325 G326 A327 C328 A329
G332 C337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 G351 C352 A353 G354 C355 A356 A363 A364 U365 C366 U367 U368 C372 A373 A374 U375 G376 G377 G380 C381 A382 A383 G384 C385 G388 A389 C390 G391 G396 A397 C398 G399 C400 C401 G402 U405 G406 G407 A408
G409 G410 A411 A412 G413 C417 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 A439 G446 G447 A448 A451 A452 A453 C454 C455 C458 G460 A461 C470 G473 G474 G475 G476 A477 C479 U480 G481 G485 U486 A487 C488 G491 G492 G493 U494 A495 A496 U498 A499
G500 C501 G502 C503 C504 G505 A509 A510 C511 U516 G517 C518 A523 G524 C525 C526 G527 U531 A532 A533 U534 A535 G539 G540 G541 G542 C543 G544 A547 C555 C556 A559 U560 U561 C562 A563 C564 G567 G568 A572 A573 A574 G575 G576 G577 G581 U582 A583 G584
G585 G593 G594 G595 C596 G597 U598 C599 C600 C601 A602 U603 G604 A607 A608 A609 G610 G616 G617 A622 C623 C624 G625 U626 G629 G630 G633 C634 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G657 G658 U659 A663 G664 A665 G666 G667
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C866 G869 U870 U871 A872 A873 G874 C875 G876 C883 U884 G885 A889 C899 A900 A901 G902 G903 A909 C910 U911 A914 A918 G925 G926 G927 C934 A935 C936 A937 A938 G939 C940 G941 G942 A946 G947 C948 U952 G953 A958 A959 U960 U961 C962 G963 A964 A965
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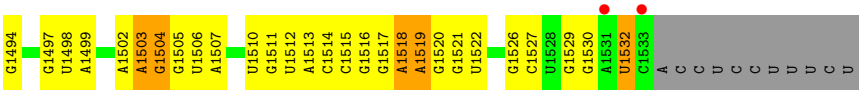
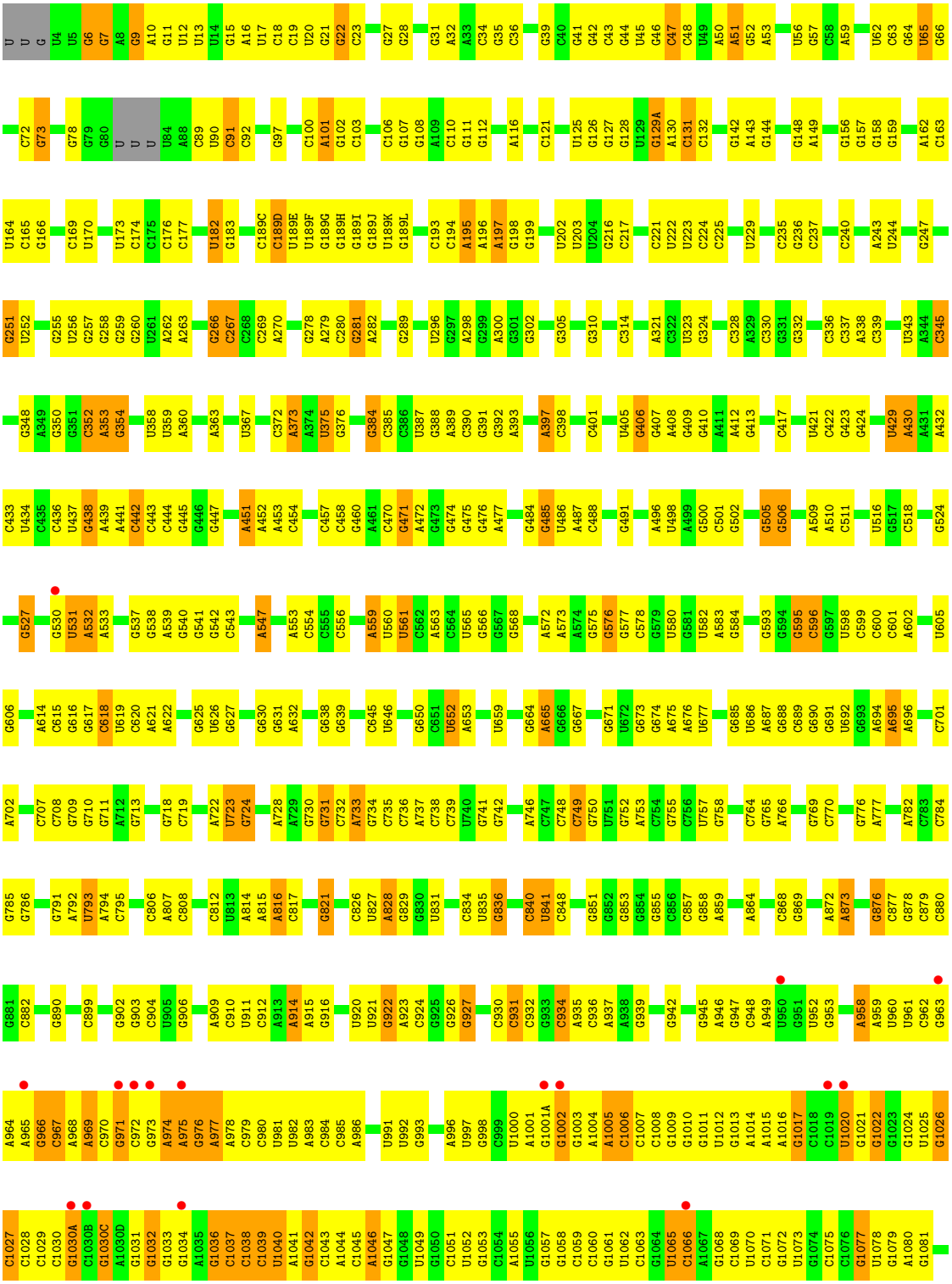
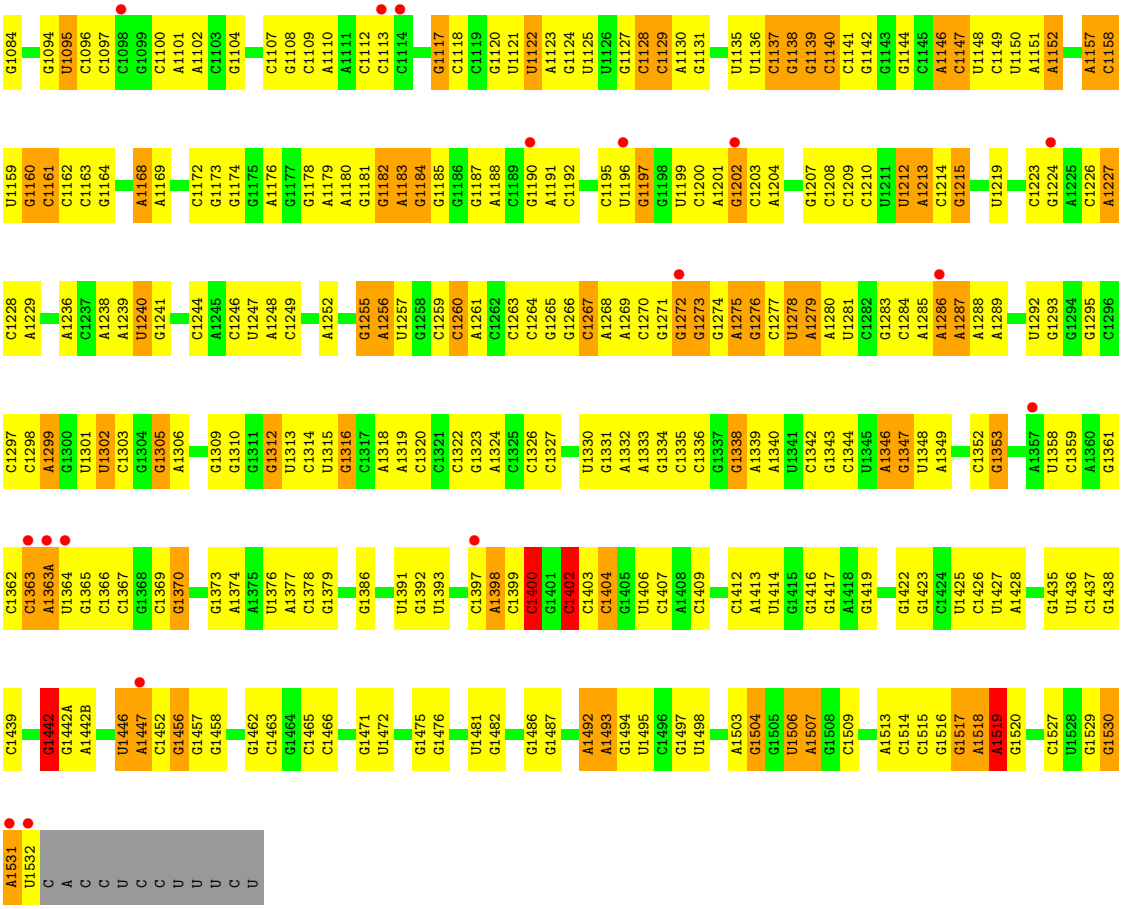
G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1044 U1049 G1053 C1054 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 G1081 U1086 U1090 U1091 G1094 U1095 C1096 A1101 G1104 A1105 G1106 C1107 G1108 A1111 C1112
G1117 G1124 U1125 U1126 G1127 C1128 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 A1157 C1158 U1159 A1179 A1180 A1183 G1184 G1185 G1186 G1187 A1188 A1191 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 G1206 G1207 C1208
C1209 U1212 A1213 C1214 C1218 G1221 G1222 C1223 C1226 A1227 A1236 C1237 A1238 A1239 C1243 A1250 G1255 A1256 U1257 C1264 G1265 G1266 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298
A1299 G1300 U1301 U1302 C1303 G1304 G1305 U1308 G1309 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 U1330 G1331 A1332 A1333 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 G1353 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1363 A1363A G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378
G1379 U1380 U1381 U1390 U1391 G1392 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 C1412 A1413 G1419 G1422 C1426 U1427 A1428 U1436 G1442 G1442A C1444 C1445 U1446 A1447 C1452 G1456 G1457 G1458 G1464 C1465 G1469 G1470 C1478 C1479 G1488 G1489 C1490 G1491 A1492 A1493



• Molecule 32: 16S Ribosomal RNA

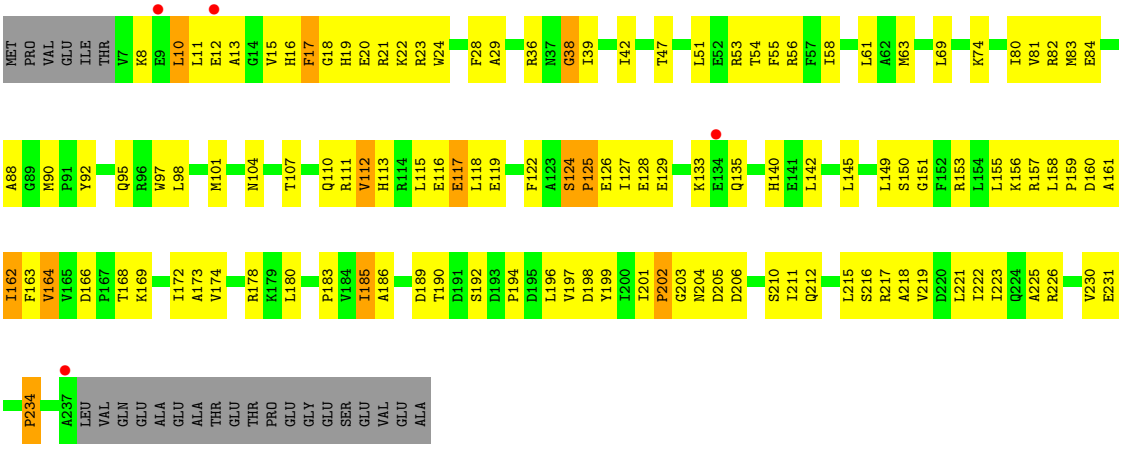
Chain 2a:





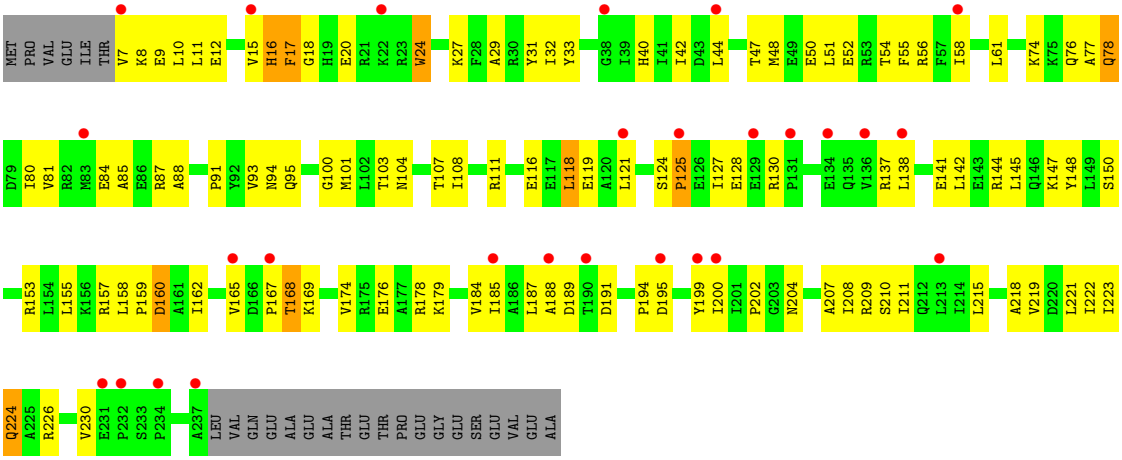
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



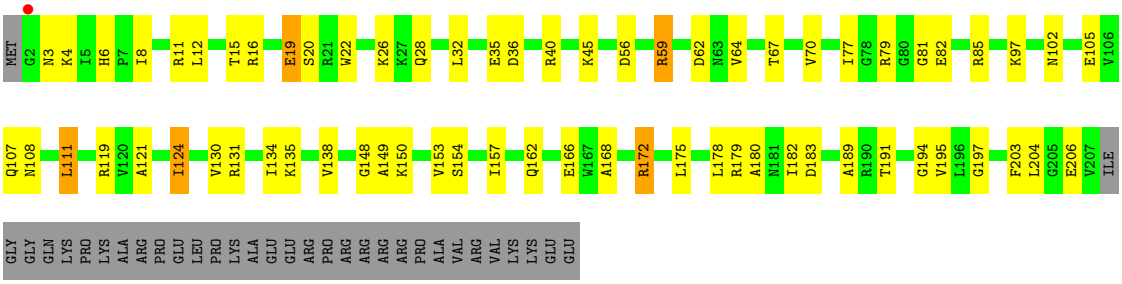
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



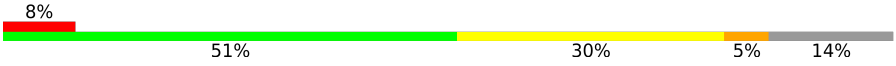
• Molecule 34: 30S ribosomal protein S3

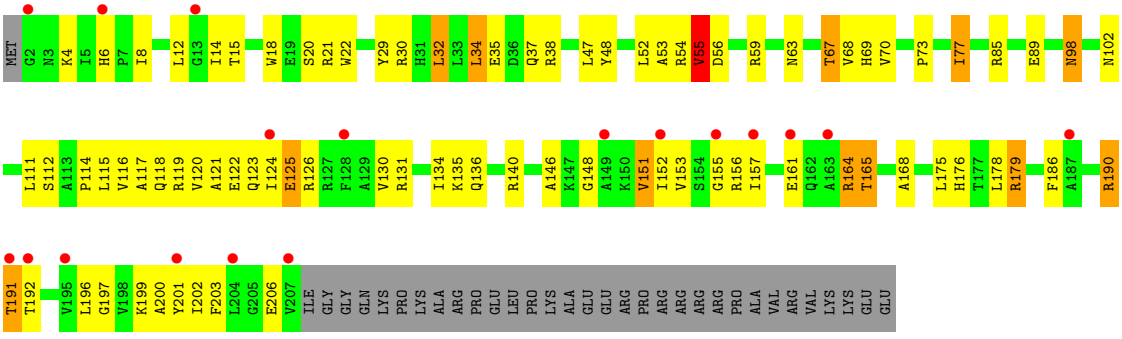
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

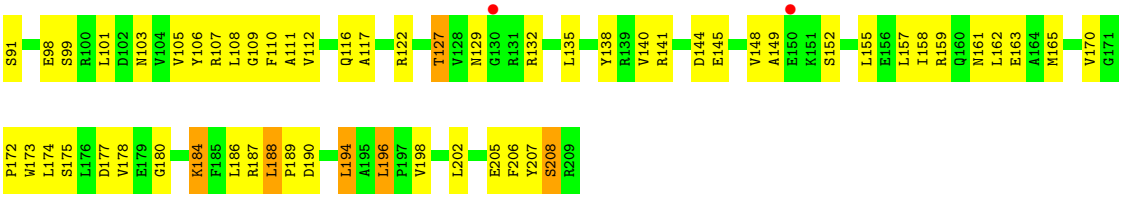
Chain 2c:





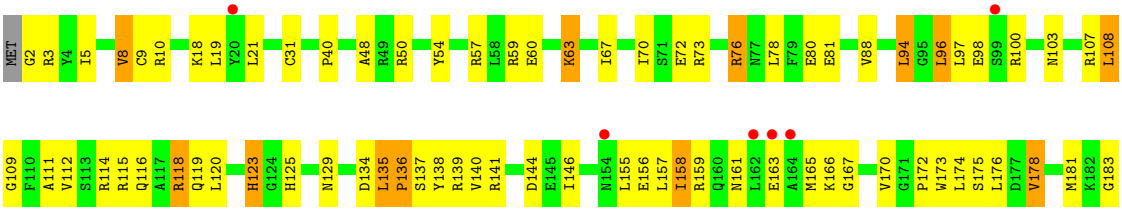
• Molecule 35: 30S ribosomal protein S4

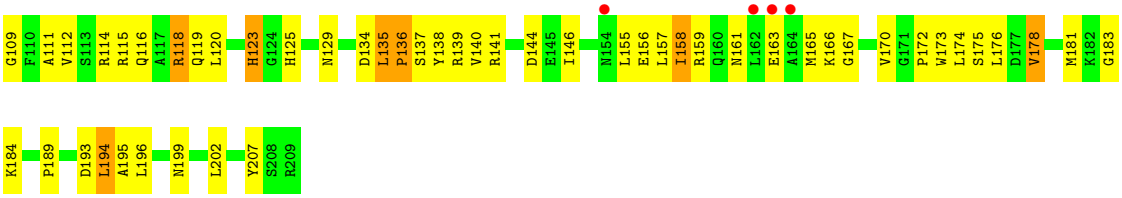
Chain 1d:



• Molecule 35: 30S ribosomal protein S4

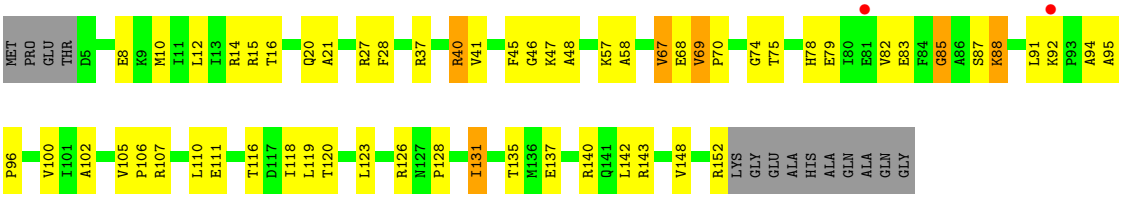
Chain 2d:





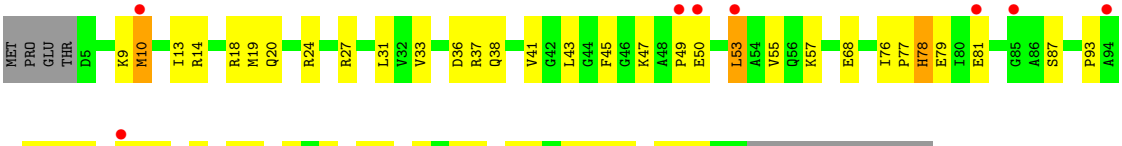
• Molecule 36: 30S ribosomal protein S5

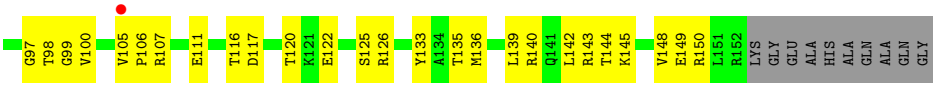
Chain 1e:



• Molecule 36: 30S ribosomal protein S5

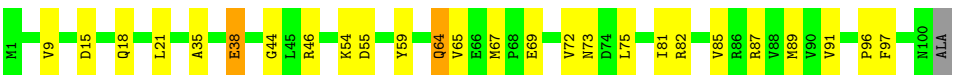
Chain 2e:





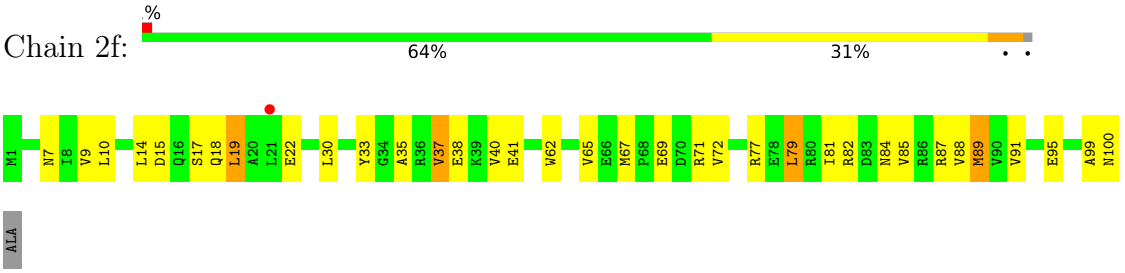
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



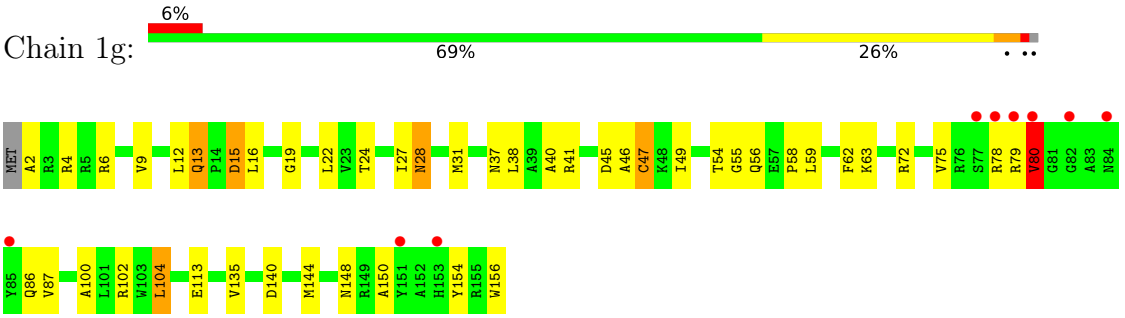
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



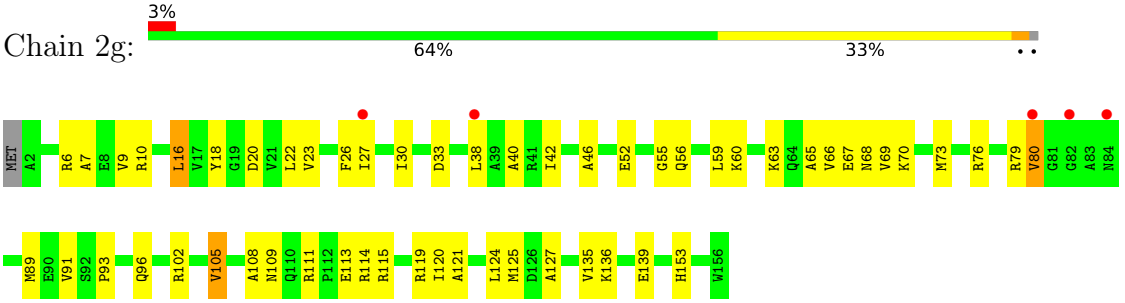
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



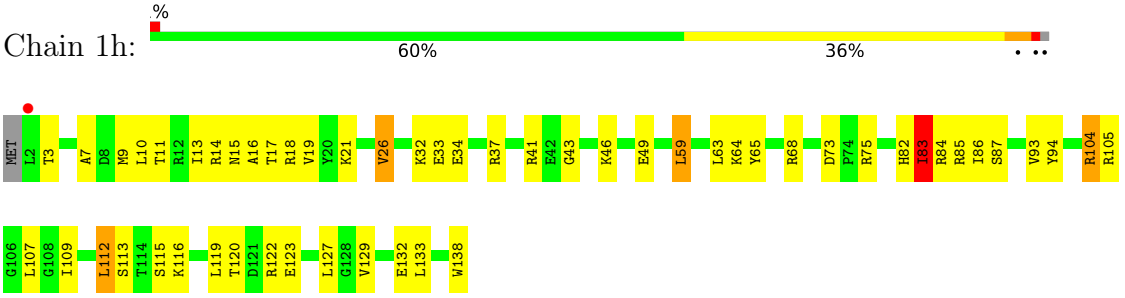
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



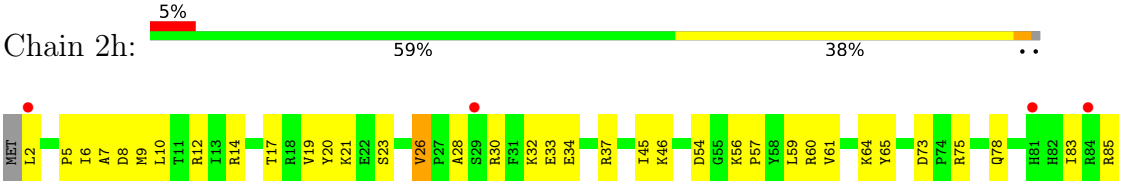
• Molecule 39: 30S ribosomal protein S8

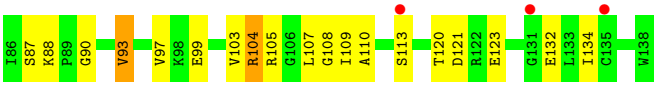
Chain 1h:



• Molecule 39: 30S ribosomal protein S8

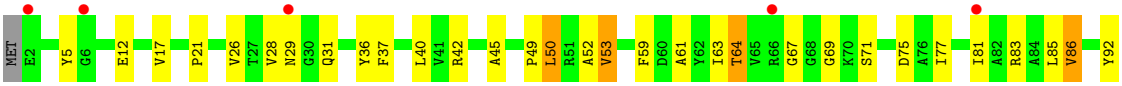
Chain 2h:

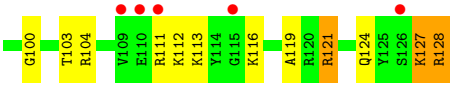




• Molecule 40: 30S ribosomal protein S9

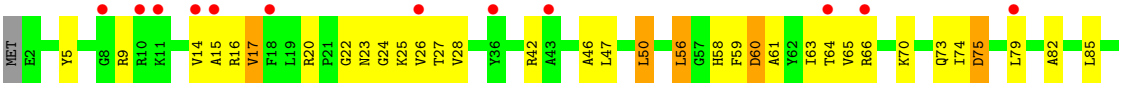
Chain 1i:

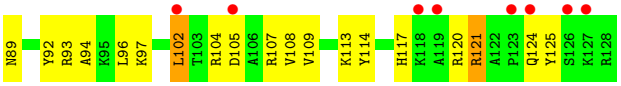




• Molecule 40: 30S ribosomal protein S9

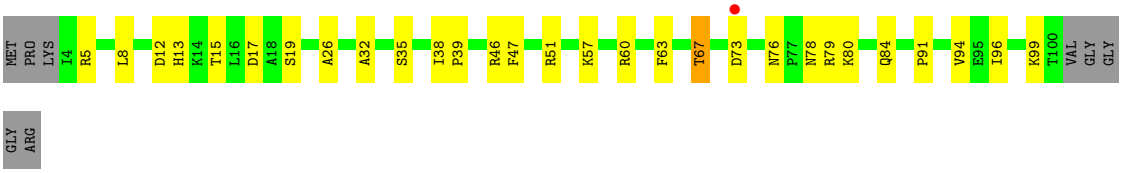
Chain 2i:





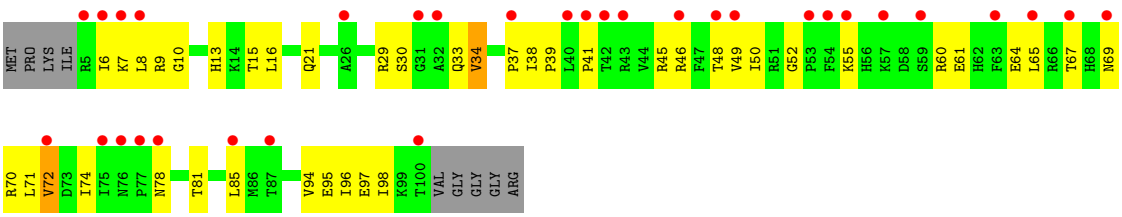
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



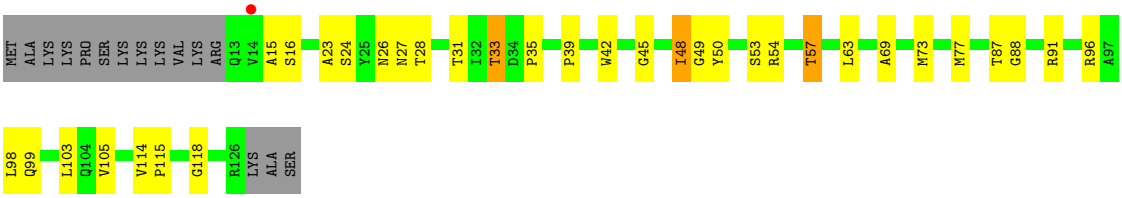
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



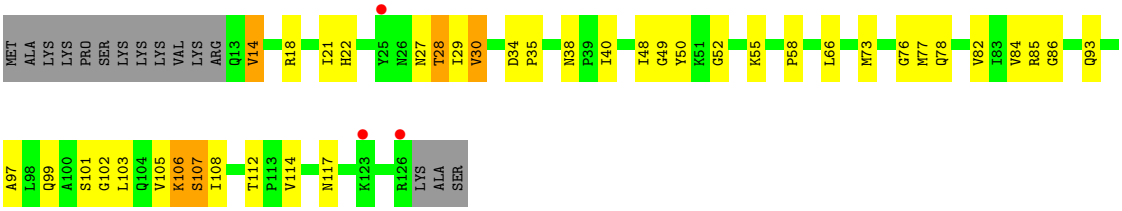
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



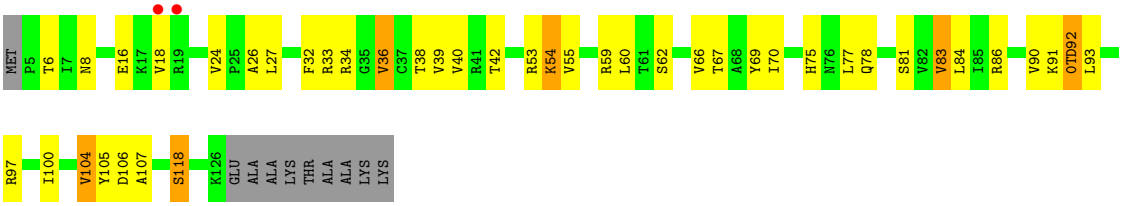
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



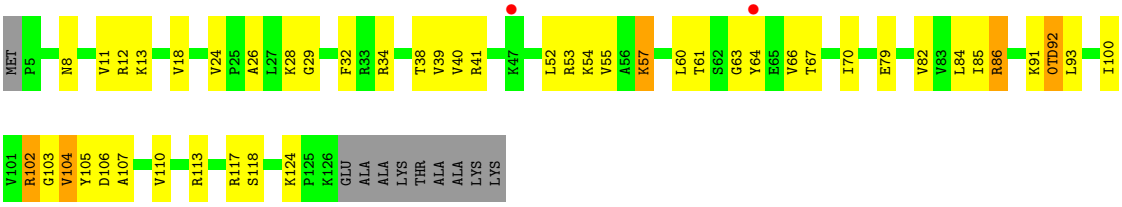
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



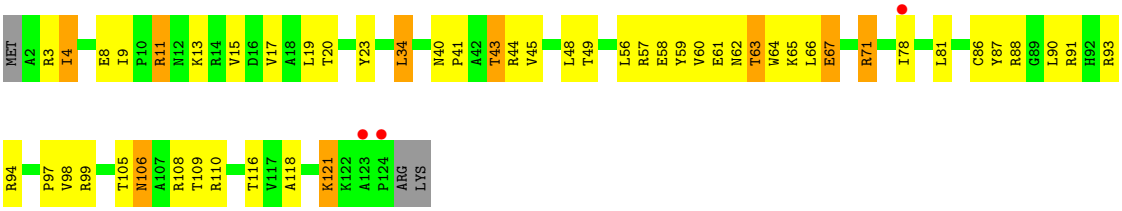
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



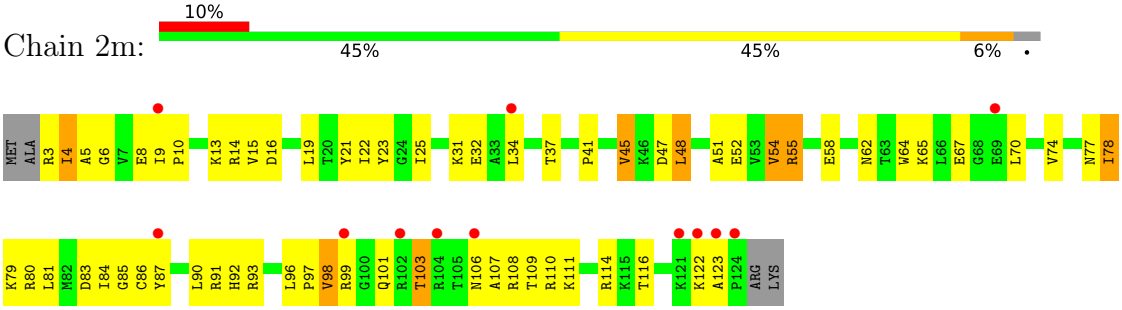
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



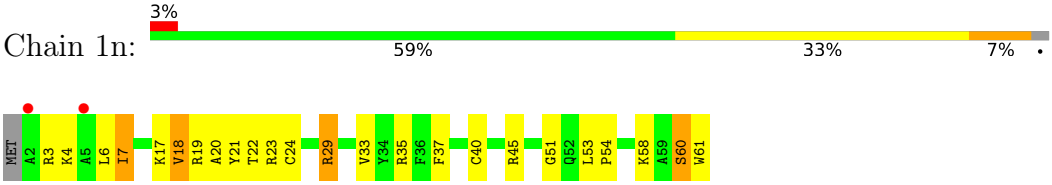
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



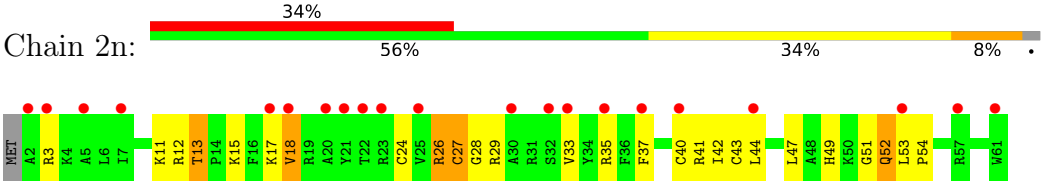
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



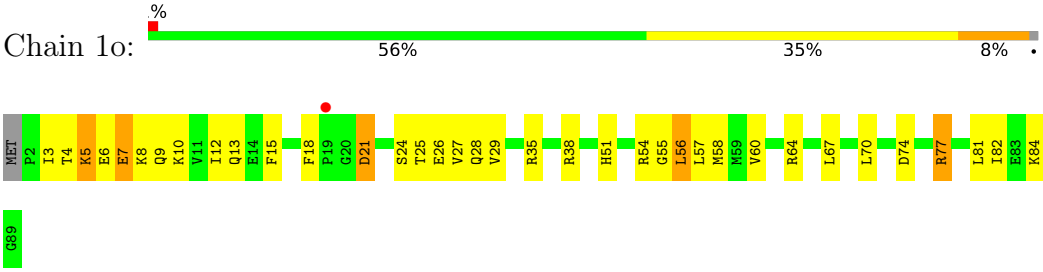
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



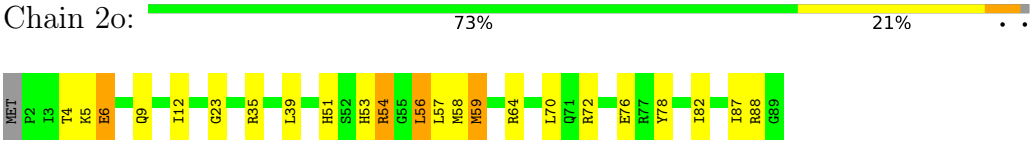
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



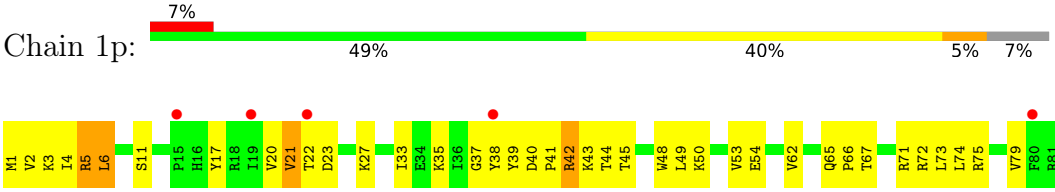
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



• Molecule 47: 30S ribosomal protein S16

Chain 1p:

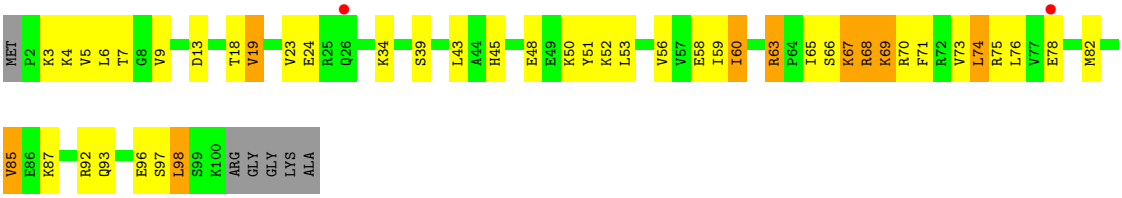


• Molecule 47: 30S ribosomal protein S16

Chain 2p:

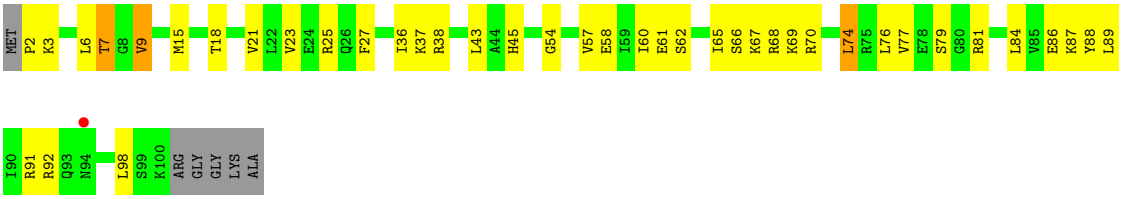
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



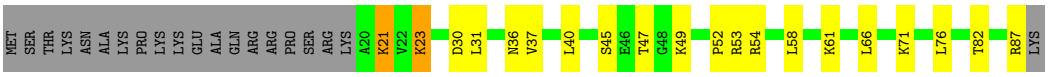
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



• Molecule 49: 30S ribosomal protein S18

Chain 1r:

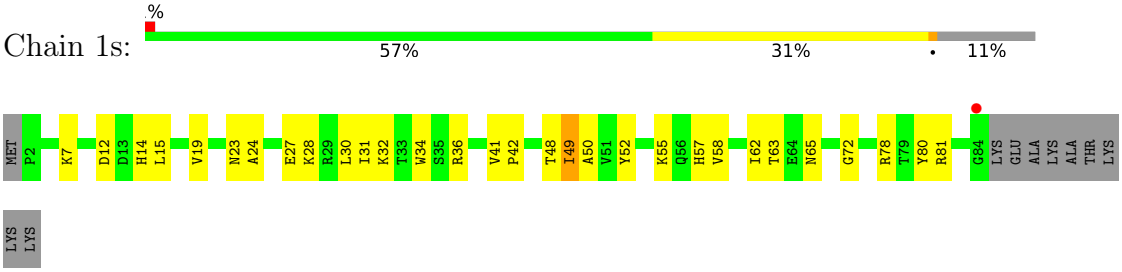


• Molecule 49: 30S ribosomal protein S18

Chain 2r:

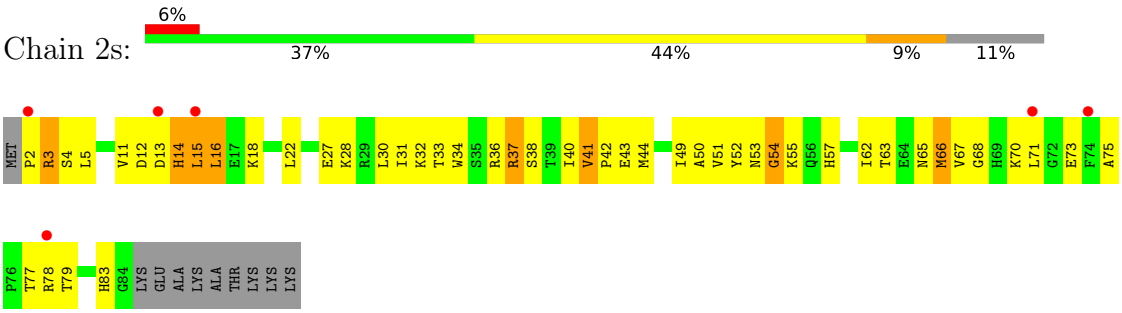
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



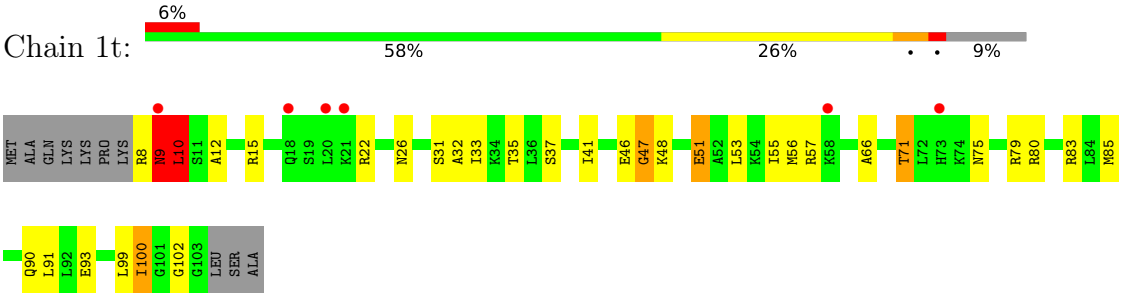
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



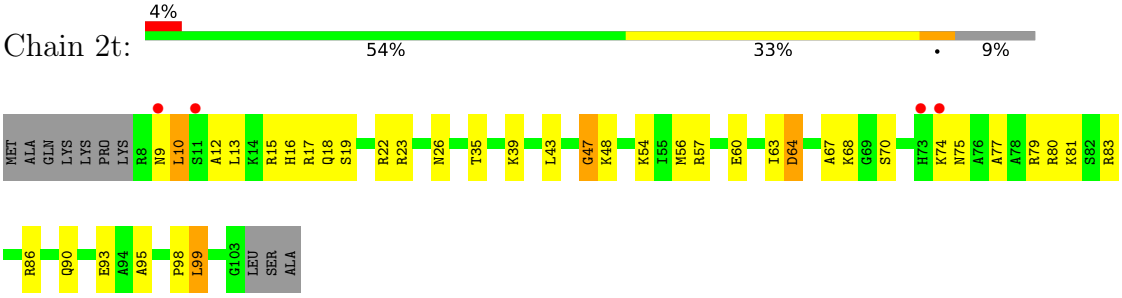
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



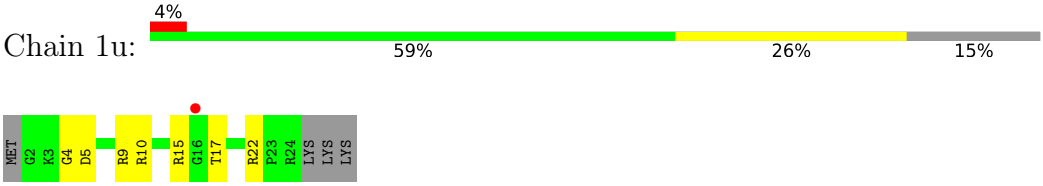
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



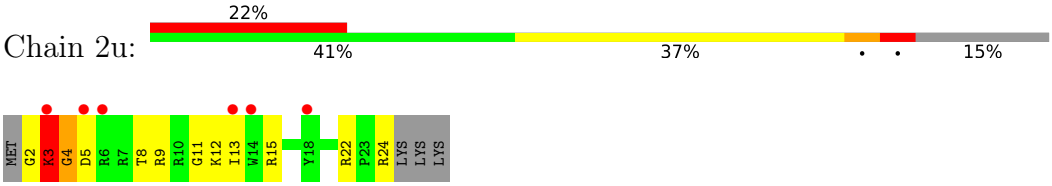
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



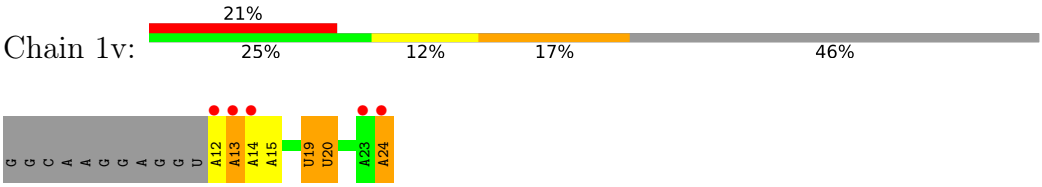
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



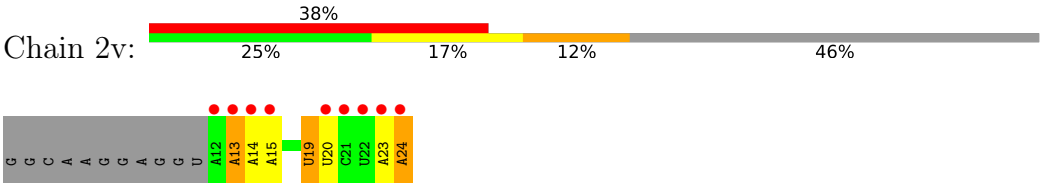
• Molecule 53: mRNA

Chain 1v:



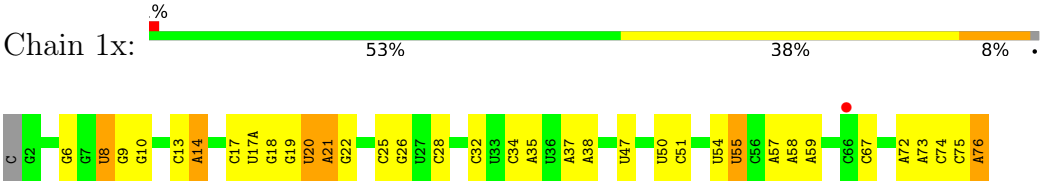
• Molecule 53: mRNA

Chain 2v:



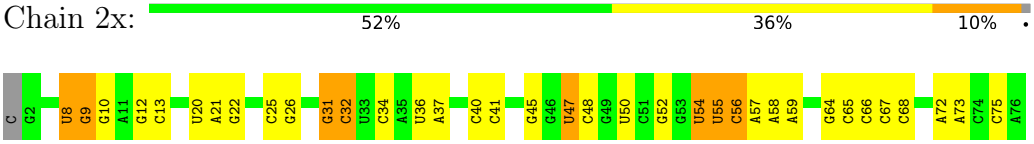
• Molecule 54: P-site tRNA

Chain 1x:



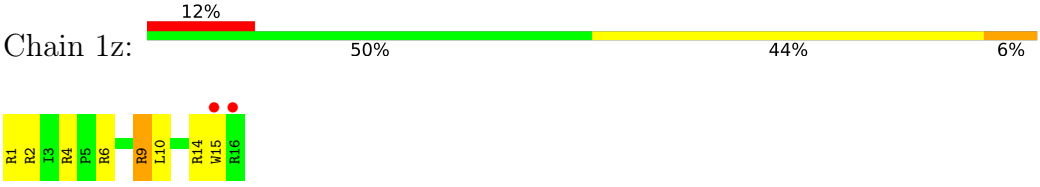
• Molecule 54: P-site tRNA

Chain 2x:



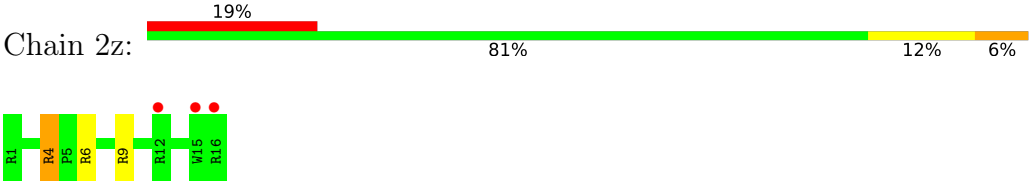
• Molecule 55: Bac7-002

Chain 1z:



• Molecule 55: Bac7-002

Chain 2z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.64Å 447.57Å 619.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.79 – 3.05 151.79 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.7 (151.79-3.05) 98.7 (151.79-3.05)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.227 , 0.283 0.226 , 0.283	Depositor DCC
R_{free} test set	53845 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	290774	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 7MG, UR3, M2G, 2MG, 5MU, OMG, 0TD, 4SU, MG, 2MU, 2MA, MA6, K, SF4, 4OC, PSU, ZN, 5MC

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	0.26	0/69009	0.43	2/107712 (0.0%)
1	2A	0.22	0/67293	0.40	1/105034 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.21	0/2879	0.41	0/4487
3	1D	0.26	0/2186	0.50	0/2944
3	2D	0.23	0/2186	0.48	0/2944
4	1E	0.25	0/1592	0.48	0/2149
4	2E	0.22	0/1592	0.44	0/2149
5	1F	0.25	0/1619	0.47	0/2193
5	2F	0.23	0/1615	0.47	0/2188
6	1G	0.22	0/1448	0.49	0/1957
6	2G	0.21	0/1453	0.44	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.20	0/1356	0.39	0/1834
8	1I	0.20	0/1112	0.40	0/1514
8	2I	0.18	0/1079	0.42	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.24	0/943	0.47	0/1269
10	2O	0.21	0/943	0.48	0/1269
11	1P	0.25	0/1152	0.48	0/1533
11	2P	0.22	0/1152	0.52	0/1533
12	1Q	0.25	0/1143	0.51	0/1527
12	2Q	0.21	0/1143	0.46	0/1527
13	1R	0.23	0/982	0.46	0/1312
13	2R	0.22	0/982	0.44	0/1312
14	1S	0.21	0/883	0.46	0/1176
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.21	0/1097	0.47	0/1468
16	1U	0.26	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.20	0/977	0.43	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.19	0/782	0.38	0/1049
18	1W	0.25	0/897	0.41	0/1205
18	2W	0.21	0/897	0.46	0/1205
19	1X	0.25	0/764	0.45	0/1025
19	2X	0.19	0/764	0.41	0/1025
20	1Y	0.21	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.44	0/1095
21	1Z	0.22	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.45	0/1763
22	10	0.25	0/612	0.51	0/816
22	20	0.22	0/612	0.47	0/816
23	11	0.25	0/762	0.44	0/1014
23	21	0.22	0/762	0.43	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.21	0/590	0.43	1/781 (0.1%)
25	13	0.23	0/474	0.46	0/635
25	23	0.20	0/469	0.44	0/630
26	14	0.25	0/565	0.53	0/761
26	24	0.26	0/545	0.62	0/737
27	15	0.26	0/469	0.46	0/635
27	25	0.24	0/469	0.46	0/635
28	16	0.25	0/460	0.52	0/613
28	26	0.21	0/456	0.42	0/608
29	17	0.28	0/426	0.50	0/561
29	27	0.26	0/426	0.47	0/561
30	18	0.26	0/525	0.44	0/691
30	28	0.22	0/525	0.43	0/691
31	19	0.27	0/310	0.44	0/407
31	29	0.21	0/310	0.46	0/407
32	1a	0.20	1/35795 (0.0%)	0.39	0/55864
32	2a	0.20	0/35886	0.39	1/56005 (0.0%)
33	1b	0.26	0/1881	0.53	3/2542 (0.1%)
33	2b	0.25	0/1860	0.50	0/2518
34	1c	0.20	0/1572	0.41	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.21	0/1685	0.46	0/2262
35	2d	0.21	0/1704	0.45	0/2284
36	1e	0.21	0/1145	0.45	0/1543
36	2e	0.23	0/1149	0.47	0/1548
37	1f	0.22	0/823	0.41	0/1115
37	2f	0.21	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1250	0.40	0/1679
38	2g	0.21	0/1254	0.45	0/1683
39	1h	0.20	0/1108	0.44	0/1494
39	2h	0.21	0/1108	0.45	0/1494
40	1i	0.19	0/1002	0.47	1/1346 (0.1%)
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.20	0/722	0.45	0/982
41	2j	0.25	0/727	0.46	0/988
42	1k	0.19	0/844	0.47	0/1145
42	2k	0.18	0/848	0.34	0/1149
43	1l	0.23	0/937	0.45	0/1260
43	2l	0.21	0/937	0.46	0/1260
44	1m	0.22	0/969	0.46	0/1302
44	2m	0.24	0/961	0.53	0/1291
45	1n	0.22	0/501	0.42	0/664
45	2n	0.23	0/501	0.43	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.19	0/739	0.42	0/985
47	1p	0.21	0/697	0.49	0/939
47	2p	0.20	0/693	0.43	0/935
48	1q	0.21	0/836	0.44	0/1117
48	2q	0.19	0/836	0.42	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.20	0/560	0.44	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.23	0/661	0.57	0/893
51	1t	0.20	0/730	0.52	0/965
51	2t	0.21	0/729	0.45	0/965
52	1u	0.21	0/203	0.50	0/266
52	2u	0.22	0/203	0.50	0/266
53	1v	0.23	0/310	0.37	0/480
53	2v	0.27	0/310	0.37	0/480
54	1x	0.27	0/1725	0.44	0/2689
54	2x	0.25	1/1725 (0.1%)	0.41	0/2689
55	1z	0.29	0/153	0.66	0/207
55	2z	0.29	0/147	0.49	0/200
All	All	0.23	2/310535 (0.0%)	0.42	9/464519 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	1Q	0	1
51	1t	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	8	4SU	O3'-P	5.28	1.61	1.56
32	1a	1498	UR3	O3'-P	5.07	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1b	38	GLY	N-CA-C	-5.57	107.28	115.30
33	1b	128	GLU	CA-C-N	5.50	132.05	121.54
33	1b	128	GLU	C-N-CA	5.50	132.05	121.54
1	1A	1992	G	C2'-C3'-O3'	5.34	117.52	109.50
1	2A	1992	G	C2'-C3'-O3'	5.34	117.50	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	59	ARG	Peptide
51	1t	9	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31189	917	0
1	2A	60322	0	30423	1007	0
2	1B	2577	0	1305	36	0
2	2B	2575	0	1303	54	0
3	1D	2136	0	2217	65	0
3	2D	2136	0	2218	69	0
4	1E	1559	0	1618	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	45	0
5	1F	1584	0	1625	58	0
5	2F	1580	0	1619	65	0
6	1G	1423	0	1436	38	0
6	2G	1428	0	1438	68	0
7	1H	1330	0	1407	44	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	35	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	30	0
9	2N	1117	0	1184	41	0
10	1O	933	0	996	26	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	44	0
11	2P	1135	0	1212	51	0
12	1Q	1122	0	1179	32	0
12	2Q	1122	0	1179	46	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	20	0
14	2S	870	0	923	44	0
15	1T	1091	0	1151	28	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1018	18	0
16	2U	959	0	1019	31	0
17	1V	771	0	829	17	0
17	2V	771	0	829	20	0
18	1W	886	0	940	35	0
18	2W	886	0	940	20	0
19	1X	750	0	814	19	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	28	0
21	2Z	1271	0	1273	47	0
22	10	604	0	619	13	0
22	20	604	0	619	12	0
23	11	755	0	826	19	0
23	21	755	0	826	24	0
24	12	588	0	643	13	0
24	22	588	0	643	21	0
25	13	469	0	518	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	12	0
26	14	552	0	533	15	0
26	24	532	0	503	35	0
27	15	455	0	465	18	0
27	25	455	0	465	15	0
28	16	453	0	473	9	0
28	26	449	0	469	13	0
29	17	418	0	467	12	0
29	27	418	0	467	13	0
30	18	517	0	582	15	0
30	28	517	0	582	20	0
31	19	307	0	335	12	0
31	29	307	0	335	12	0
32	1a	32246	0	16295	536	0
32	2a	32327	0	16338	639	0
33	1b	1846	0	1867	80	0
33	2b	1825	0	1828	79	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	63	0
35	1d	1655	0	1672	75	0
35	2d	1674	0	1714	72	0
36	1e	1129	0	1185	34	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	17	0
37	2f	816	0	808	22	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	38	0
40	1i	983	0	986	32	0
40	2i	978	0	966	36	0
41	1j	709	0	650	23	0
41	2j	714	0	672	32	0
42	1k	829	0	825	24	0
42	2k	833	0	836	23	0
43	1l	932	0	981	22	0
43	2l	932	0	981	30	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	55	0
45	1n	492	0	529	22	0
45	2n	492	0	529	23	0
46	1o	728	0	760	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	16	0
47	1p	681	0	697	23	0
47	2p	677	0	686	30	0
48	1q	823	0	891	35	0
48	2q	823	0	891	31	0
49	1r	555	0	618	15	0
49	2r	555	0	618	19	0
50	1s	652	0	662	19	0
50	2s	646	0	644	39	0
51	1t	728	0	798	26	0
51	2t	727	0	796	26	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	277	0	140	9	0
53	2v	277	0	140	5	0
54	1x	1625	0	829	21	0
54	2x	1625	0	828	23	0
55	1z	147	0	162	8	0
55	2z	141	0	151	2	0
56	10	5	0	0	0	0
56	11	2	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	5	0	0	0	0
56	17	6	0	0	0	0
56	18	4	0	0	0	0
56	19	1	0	0	0	0
56	1A	848	0	0	0	0
56	1B	25	0	0	0	0
56	1D	8	0	0	0	0
56	1E	8	0	0	0	0
56	1F	12	0	0	0	0
56	1G	4	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	3	0	0	0	0
56	1O	1	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	4	0	0	0	0
56	1R	6	0	0	0	0
56	1S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	5	0	0	0	0
56	1W	6	0	0	0	0
56	1X	3	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	167	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1s	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	10	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	2	0	0	0	0
56	25	2	0	0	0	0
56	26	1	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	2A	625	0	0	0	0
56	2B	12	0	0	0	0
56	2D	2	0	0	0	0
56	2E	5	0	0	0	0
56	2F	4	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	3	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	1	0	0	0	0
56	2T	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	145	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	2	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2x	3	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	3	0
58	2d	8	0	0	0	0
59	2x	1	0	0	0	0
60	10	2	0	0	1	0
60	11	2	0	0	0	0
60	12	2	0	0	0	0
60	13	2	0	0	0	0
60	18	2	0	0	0	0
60	1A	1222	0	0	109	0
60	1B	27	0	0	3	0
60	1D	21	0	0	1	0
60	1E	11	0	0	1	0
60	1F	9	0	0	1	0
60	1N	1	0	0	0	0
60	1O	1	0	0	0	0
60	1P	14	0	0	1	0
60	1Q	2	0	0	0	0
60	1R	3	0	0	0	0
60	1S	2	0	0	0	0
60	1T	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1U	4	0	0	0	0
60	1V	4	0	0	0	0
60	1W	3	0	0	1	0
60	1a	26	0	0	4	0
60	1d	1	0	0	0	0
60	1z	1	0	0	0	0
60	20	1	0	0	0	0
60	21	2	0	0	0	0
60	28	2	0	0	0	0
60	2A	416	0	0	59	0
60	2B	3	0	0	0	0
60	2D	12	0	0	1	0
60	2E	4	0	0	0	0
60	2F	6	0	0	0	0
60	2I	1	0	0	0	0
60	2O	3	0	0	0	0
60	2P	4	0	0	1	0
60	2Q	1	0	0	0	0
60	2R	1	0	0	0	0
60	2T	1	0	0	0	0
60	2V	1	0	0	0	0
60	2W	2	0	0	0	0
60	2a	17	0	0	0	0
60	2l	1	0	0	0	0
60	2n	1	0	0	0	0
60	2t	1	0	0	0	0
60	2x	1	0	0	1	0
All	All	290774	0	193677	5438	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 5438 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	1.41	1.19
32:1a:987:G:H1	32:1a:1218:C:N4	1.56	1.02
1:2A:2137:C:N4	1:2A:2154:G:H1	1.54	1.02
1:1A:2124:G:H1	1:1A:2174:C:N4	1.57	1.01
1:2A:2137:C:H42	1:2A:2154:G:H1	1.03	0.99

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%)	252 (92%)	21 (8%)	0	100 100
3	2D	273/276 (99%)	245 (90%)	28 (10%)	0	100 100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24 52
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	12 37
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24 52
5	2F	201/210 (96%)	181 (90%)	17 (8%)	3 (2%)	8 28
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11 34
6	2G	179/182 (98%)	153 (86%)	22 (12%)	4 (2%)	5 20
7	1H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	21 48
7	2H	172/180 (96%)	145 (84%)	25 (14%)	2 (1%)	10 32
8	1I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9 29
8	2I	144/148 (97%)	131 (91%)	10 (7%)	3 (2%)	5 21
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100 100
9	2N	138/140 (99%)	123 (89%)	15 (11%)	0	100 100
10	1O	120/122 (98%)	108 (90%)	12 (10%)	0	100 100
10	2O	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	7 25
11	1P	147/150 (98%)	132 (90%)	15 (10%)	0	100 100
11	2P	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	6 21
12	1Q	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5 20
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100 100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
13	2R	116/118 (98%)	104 (90%)	12 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	95 (88%)	12 (11%)	1 (1%)	14 39
15	1T	129/146 (88%)	117 (91%)	12 (9%)	0	100 100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 37
17	2V	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	6 21
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100 100
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5 20
19	2X	93/96 (97%)	78 (84%)	15 (16%)	0	100 100
20	1Y	105/110 (96%)	92 (88%)	11 (10%)	2 (2%)	6 23
20	2Y	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	6 23
21	1Z	148/206 (72%)	128 (86%)	17 (12%)	3 (2%)	6 21
21	2Z	156/206 (76%)	130 (83%)	25 (16%)	1 (1%)	21 48
22	10	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
22	20	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	9 29
23	11	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	11 34
23	21	95/98 (97%)	87 (92%)	8 (8%)	0	100 100
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100 100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	50 (88%)	7 (12%)	0	100 100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1 3
26	24	67/71 (94%)	48 (72%)	14 (21%)	5 (8%)	1 3
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6 24
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100 100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100 100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5 20
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	193 (84%)	25 (11%)	11 (5%)	2 9
33	2b	229/256 (90%)	185 (81%)	38 (17%)	6 (3%)	4 17
34	1c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	24 52
34	2c	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	24 52
35	1d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24 52
35	2d	206/209 (99%)	178 (86%)	24 (12%)	4 (2%)	6 23
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	9 29
36	2e	146/162 (90%)	127 (87%)	17 (12%)	2 (1%)	9 29
37	1f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	12 37
37	2f	98/101 (97%)	88 (90%)	9 (9%)	1 (1%)	12 37
38	1g	153/156 (98%)	138 (90%)	10 (6%)	5 (3%)	3 13
38	2g	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4 17
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18 45
39	2h	135/138 (98%)	120 (89%)	15 (11%)	0	100 100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100 100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100 100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3 14
41	2j	94/105 (90%)	88 (94%)	5 (5%)	1 (1%)	11 34
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14 39
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	4 16
43	1l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	7 25
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	7 25
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	7 25
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	4 17
45	1n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7 25
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	1o	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	5 19
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100 100
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100 100
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9 31
48	1q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	5 21
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4 17
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10 32
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5 21
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3 14
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
52	2u	21/27 (78%)	15 (71%)	4 (19%)	2 (10%)	0 2
55	1z	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1 4
55	2z	14/16 (88%)	13 (93%)	1 (7%)	0	100 100
All	All	11384/12160 (94%)	10190 (90%)	1061 (9%)	133 (1%)	10 32

5 of 133 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
12	1Q	24	GLY
12	1Q	60	ARG

5.3.2 Protein sidechains (i)

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%)	191 (89%)	24 (11%)	6 20
3	2D	215/218 (99%)	185 (86%)	30 (14%)	3 13
4	1E	164/166 (99%)	142 (87%)	22 (13%)	4 14
4	2E	164/166 (99%)	143 (87%)	21 (13%)	4 15
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5 18
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5 20
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7 26
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2 9
7	1H	144/148 (97%)	125 (87%)	19 (13%)	4 14
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14 38
8	1I	113/124 (91%)	100 (88%)	13 (12%)	5 19
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2 8
9	1N	118/119 (99%)	104 (88%)	14 (12%)	5 18
9	2N	118/119 (99%)	101 (86%)	17 (14%)	3 12
10	1O	100/100 (100%)	93 (93%)	7 (7%)	14 38
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28 56
11	1P	115/116 (99%)	99 (86%)	16 (14%)	3 13
11	2P	115/116 (99%)	99 (86%)	16 (14%)	3 13
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9 29
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4 14
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 29
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36 62
14	1S	86/88 (98%)	72 (84%)	14 (16%)	2 9
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2 7
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14 38
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8 26
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20 46
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34 60
17	1V	80/82 (98%)	71 (89%)	9 (11%)	5 20
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3 13
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19 45
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28 56
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 56
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5 18
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8 27
21	1Z	135/179 (75%)	118 (87%)	17 (13%)	4 16
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4 16
22	10	61/67 (91%)	55 (90%)	6 (10%)	7 26
22	20	61/67 (91%)	56 (92%)	5 (8%)	10 32
23	11	80/83 (96%)	72 (90%)	8 (10%)	7 25
23	21	80/83 (96%)	73 (91%)	7 (9%)	9 30
24	12	65/67 (97%)	57 (88%)	8 (12%)	4 16
24	22	65/67 (97%)	61 (94%)	4 (6%)	16 42
25	13	51/52 (98%)	43 (84%)	8 (16%)	2 10
25	23	50/52 (96%)	45 (90%)	5 (10%)	7 25
26	14	59/63 (94%)	51 (86%)	8 (14%)	3 13
26	24	53/63 (84%)	42 (79%)	11 (21%)	1 4
27	15	50/52 (96%)	44 (88%)	6 (12%)	5 17
27	25	50/52 (96%)	46 (92%)	4 (8%)	11 33
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 18
28	26	50/52 (96%)	44 (88%)	6 (12%)	5 17
29	17	41/42 (98%)	36 (88%)	5 (12%)	5 17
29	27	41/42 (98%)	38 (93%)	3 (7%)	13 36
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 57
30	28	54/55 (98%)	51 (94%)	3 (6%)	19 45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 62
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 30
33	1b	192/220 (87%)	172 (90%)	20 (10%)	7 23
33	2b	187/220 (85%)	169 (90%)	18 (10%)	8 26
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4 16
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3 12
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8 28
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5 19
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4 14
37	1f	84/90 (93%)	77 (92%)	7 (8%)	10 32
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10 32
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5 18
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6 22
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4 16
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9 30
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6 21
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3 12
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12 35
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3 12
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17 42
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10 31
43	1l	96/108 (89%)	83 (86%)	13 (14%)	4 14
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5 19
44	1m	93/101 (92%)	78 (84%)	15 (16%)	2 9
44	2m	92/101 (91%)	79 (86%)	13 (14%)	3 12
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3 12
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5 17
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9 29
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 29
47	1p	69/74 (93%)	55 (80%)	14 (20%)	1 4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2 9
48	1q	94/97 (97%)	80 (85%)	14 (15%)	3 11
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13 36
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 31
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5 18
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18 44
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	1t	70/82 (85%)	60 (86%)	10 (14%)	3 12
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18 45
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 45
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2 8
55	1z	15/16 (94%)	14 (93%)	1 (7%)	15 39
55	2z	14/16 (88%)	13 (93%)	1 (7%)	13 37
All	All	9324/10096 (92%)	8296 (89%)	1028 (11%)	6 21

5 of 1028 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	2i	121	ARG
43	2l	105	TYR
40	2i	117	HIS
38	1g	140	ASP
38	1g	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	118	GLN
35	2d	123	HIS
50	2s	14	HIS
35	1d	160	GLN
35	1d	123	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	473 (16%)	26 (0%)
1	2A	2791/2915 (95%)	507 (18%)	22 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1497/1521 (98%)	262 (17%)	0
32	2a	1501/1521 (98%)	307 (20%)	0
53	1v	12/24 (50%)	5 (41%)	0
53	2v	12/24 (50%)	5 (41%)	0
54	1x	75/77 (97%)	9 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2x	75/77 (97%)	11 (14%)	0
All	All	9063/9316 (97%)	1622 (17%)	48 (0%)

5 of 1622 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	50	U

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	266	G
1	2A	856	C
1	2A	271(K)	U
1	2A	479	A
1	2A	900	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	1A	1942	1	19,22,23	1.61	3 (15%)	26,32,35	1.18	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.16	3 (11%)
32	UR3	2a	1498	56,32	19,22,23	1.09	2 (10%)	26,32,35	1.68	4 (15%)
54	PSU	2x	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.18	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
32	5MC	2a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.12	3 (11%)
1	2MA	2A	2503	1,56	22,25,26	1.52	4 (18%)	32,37,40	2.41	7 (21%)
1	PSU	1A	2605	1,56	18,21,22	1.36	3 (16%)	21,30,33	2.00	5 (23%)
32	M2G	2a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.93	6 (18%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.09	6 (18%)
1	5MU	2A	1939	1	19,22,23	1.38	6 (31%)	27,32,35	2.30	6 (22%)
32	MA6	2a	1519	32	23,26,27	1.58	4 (17%)	33,38,41	2.27	11 (33%)
32	5MC	1a	967	32	19,22,23	1.54	3 (15%)	26,32,35	1.03	2 (7%)
32	7MG	1a	527	56,32	23,26,27	1.41	4 (17%)	27,39,42	2.59	7 (25%)
1	5MC	2A	1962	1,56	19,22,23	1.63	3 (15%)	26,32,35	1.19	3 (11%)
54	5MU	2x	54	54	19,22,23	1.33	5 (26%)	27,32,35	2.20	7 (25%)
54	4SU	2x	8	54	18,21,22	1.94	5 (27%)	25,30,33	1.66	7 (28%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.12	3 (12%)
1	2MU	2A	2552	1,56	19,22,24	1.17	1 (5%)	25,31,36	1.99	6 (24%)
1	OMG	1A	2251	1,54,56	23,26,27	1.24	3 (13%)	32,38,41	2.08	6 (18%)
32	MA6	1a	1519	32	23,26,27	1.55	4 (17%)	33,38,41	2.36	12 (36%)
32	5MC	2a	1400	32	19,22,23	1.84	3 (15%)	26,32,35	1.32	3 (11%)
54	5MC	1x	32	54	19,22,23	1.76	3 (15%)	26,32,35	1.19	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.81	0	25,32,35	1.06	2 (8%)
32	MA6	2a	1518	32	23,26,27	1.53	5 (21%)	33,38,41	2.30	14 (42%)
54	5MC	2x	32	54	19,22,23	1.53	2 (10%)	26,32,35	1.15	3 (11%)
32	MA6	1a	1518	32	23,26,27	1.56	4 (17%)	33,38,41	2.34	14 (42%)
1	2MA	1A	2503	1,56	22,25,26	1.43	5 (22%)	32,37,40	2.35	9 (28%)
1	4OC	2A	1920	1	19,22,24	0.79	0	25,31,35	0.92	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
32	PSU	1a	516	56,32	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	27,32,35	2.16	7 (25%)
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.21	3 (11%)
32	PSU	2a	516	56,32	18,21,22	1.35	3 (16%)	21,30,33	1.99	5 (23%)
54	PSU	1x	55	54,56	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
32	7MG	2a	527	32	23,26,27	1.38	4 (17%)	27,39,42	2.50	6 (22%)
43	0TD	1l	92	43	8,9,10	4.61	1 (12%)	6,11,13	2.22	3 (50%)
1	OMG	2A	2251	1,54,56	23,26,27	1.23	3 (13%)	32,38,41	1.93	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	4OC	1A	1920	1	19,22,24	0.83	1 (5%)	25,31,35	1.07	2 (8%)
54	5MU	1x	54	54	19,22,23	1.42	5 (26%)	27,32,35	1.96	6 (22%)
43	0TD	2l	92	43	8,9,10	4.65	1 (12%)	6,11,13	1.95	2 (33%)
1	5MU	1A	1939	1,56	19,22,23	1.48	5 (26%)	27,32,35	2.02	7 (25%)
1	5MC	2A	1942	1	19,22,23	1.71	3 (15%)	26,32,35	1.15	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.81	4 (15%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	3 (14%)
54	4SU	1x	8	54	18,21,22	2.05	4 (22%)	25,30,33	1.35	5 (20%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.57	2 (10%)	26,32,35	1.07	2 (7%)
1	5MU	2A	1915	1,56	19,22,23	1.50	6 (31%)	27,32,35	2.06	6 (22%)
1	5MC	1A	1962	1,56	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.16	8 (24%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.10	5 (23%)
1	2MU	1A	2552	1,56	19,22,24	1.21	2 (10%)	25,31,36	2.04	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	56,32	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	0/7/25/26	0/3/3/3
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1962	1,56	-	1/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	2MU	2A	2552	1,56	-	1/9/27/28	0/2/2/2
1	OMG	1A	2251	1,54,56	-	0/9/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
1	2MA	1A	2503	1,56	-	2/7/25/26	0/3/3/3
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	56,32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54,56	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
1	OMG	2A	2251	1,54,56	-	0/9/27/28	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	4/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.67	1.69	1.82
43	2l	92	0TD	CB-SB	-12.66	1.69	1.82
32	2a	1400	5MC	C5-C4	6.75	1.49	1.44
54	1x	32	5MC	C5-C4	6.39	1.49	1.44
32	2a	967	5MC	C5-C4	6.37	1.48	1.44

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2503	2MA	C5-C4-N3	-9.08	117.62	127.18
32	1a	527	7MG	N9-C4-N3	8.95	138.57	125.46
32	2a	527	7MG	N9-C4-N3	8.40	137.77	125.46
1	1A	2503	2MA	C5-C4-N3	-8.13	118.62	127.18
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

34 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2x	55	PSU	1	0
32	1a	1400	5MC	1	0
32	2a	967	5MC	3	0
1	2A	2503	2MA	1	0
1	1A	2605	PSU	1	0
32	2a	966	M2G	1	0
32	1a	1207	2MG	3	0
1	2A	1939	5MU	1	0
32	2a	1519	MA6	4	0
32	1a	967	5MC	1	0
54	2x	54	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2x	8	4SU	1	0
32	1a	1402	4OC	4	0
1	2A	2552	2MU	2	0
1	1A	2251	OMG	1	0
32	1a	1519	MA6	1	0
32	2a	1400	5MC	1	0
32	2a	1402	4OC	1	0
32	2a	1518	MA6	5	0
54	2x	32	5MC	1	0
32	1a	1518	MA6	1	0
1	2A	1920	4OC	1	0
32	1a	966	M2G	1	0
32	2a	1404	5MC	1	0
54	1x	55	PSU	1	0
43	1l	92	0TD	1	0
1	2A	2251	OMG	1	0
43	2l	92	0TD	1	0
1	1A	1939	5MU	1	0
1	2A	1942	5MC	1	0
54	1x	8	4SU	3	0
32	1a	1404	5MC	2	0
1	2A	1915	5MU	1	0
1	1A	2552	2MU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2024 ligands modelled in this entry, 2022 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	$\#\|Z\|>2$

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1d	302	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.34	50 (1%) 69 46	26, 42, 92, 108	0
1	2A	2789/2915 (95%)	-0.05	35 (1%) 75 53	35, 59, 90, 106	0
2	1B	120/121 (99%)	-0.47	0 100 100	36, 51, 67, 83	0
2	2B	120/121 (99%)	0.62	6 (5%) 34 17	64, 81, 90, 98	0
3	1D	275/276 (99%)	0.03	4 (1%) 72 50	29, 41, 54, 77	0
3	2D	275/276 (99%)	0.30	4 (1%) 72 50	35, 50, 62, 71	0
4	1E	204/206 (99%)	-0.00	1 (0%) 87 72	26, 45, 60, 73	0
4	2E	204/206 (99%)	0.05	0 100 100	37, 57, 67, 77	0
5	1F	203/210 (96%)	-0.10	0 100 100	28, 47, 65, 79	0
5	2F	203/210 (96%)	0.16	1 (0%) 87 72	37, 65, 77, 81	0
6	1G	181/182 (99%)	0.33	5 (2%) 55 32	42, 58, 70, 83	0
6	2G	181/182 (99%)	0.97	17 (9%) 14 7	69, 79, 86, 92	0
7	1H	174/180 (96%)	0.01	1 (0%) 85 69	45, 55, 66, 74	0
7	2H	174/180 (96%)	0.68	6 (3%) 48 27	64, 79, 87, 97	0
8	1I	146/148 (98%)	0.36	1 (0%) 84 66	45, 69, 78, 82	0
8	2I	146/148 (98%)	0.54	4 (2%) 56 33	57, 72, 81, 87	0
9	1N	140/140 (100%)	0.06	3 (2%) 63 40	34, 45, 62, 72	0
9	2N	140/140 (100%)	0.37	3 (2%) 63 40	46, 63, 76, 84	0
10	1O	122/122 (100%)	-0.16	0 100 100	34, 44, 58, 64	0
10	2O	122/122 (100%)	0.17	0 100 100	45, 56, 69, 74	0
11	1P	149/150 (99%)	0.16	2 (1%) 75 53	28, 49, 67, 86	0
11	2P	149/150 (99%)	0.31	3 (2%) 65 42	43, 66, 81, 84	0
12	1Q	141/141 (100%)	-0.07	2 (1%) 73 51	32, 46, 58, 67	0
12	2Q	141/141 (100%)	0.46	2 (1%) 73 51	47, 63, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.10	0 100 100	34, 41, 55, 63	0
13	2R	118/118 (100%)	0.18	1 (0%) 82 63	40, 53, 61, 67	0
14	1S	110/112 (98%)	0.08	0 100 100	42, 51, 60, 66	0
14	2S	110/112 (98%)	0.95	6 (5%) 30 16	63, 73, 82, 85	0
15	1T	131/146 (89%)	-0.01	1 (0%) 82 63	34, 48, 68, 83	0
15	2T	131/146 (89%)	0.35	3 (2%) 61 38	48, 58, 75, 85	0
16	1U	116/118 (98%)	0.01	2 (1%) 69 46	31, 41, 53, 66	0
16	2U	116/118 (98%)	0.35	2 (1%) 69 46	43, 60, 74, 81	0
17	1V	101/101 (100%)	-0.10	0 100 100	32, 47, 60, 73	0
17	2V	101/101 (100%)	0.37	3 (2%) 52 30	43, 68, 77, 81	0
18	1W	112/113 (99%)	-0.11	0 100 100	32, 40, 55, 76	0
18	2W	112/113 (99%)	0.19	3 (2%) 56 33	42, 52, 64, 87	0
19	1X	95/96 (98%)	-0.05	1 (1%) 78 57	32, 41, 58, 70	0
19	2X	95/96 (98%)	0.50	1 (1%) 78 57	53, 63, 74, 84	0
20	1Y	107/110 (97%)	0.01	2 (1%) 66 43	38, 52, 68, 73	0
20	2Y	107/110 (97%)	0.46	3 (2%) 55 32	58, 69, 78, 83	0
21	1Z	154/206 (74%)	0.04	1 (0%) 85 69	46, 62, 77, 80	0
21	2Z	160/206 (77%)	0.54	4 (2%) 58 35	66, 77, 85, 90	0
22	10	76/85 (89%)	-0.01	1 (1%) 75 53	33, 43, 55, 63	0
22	20	76/85 (89%)	0.61	5 (6%) 24 12	46, 63, 71, 80	0
23	11	97/98 (98%)	0.05	0 100 100	33, 46, 65, 71	0
23	21	97/98 (98%)	0.36	0 100 100	43, 55, 72, 76	0
24	12	70/72 (97%)	0.04	2 (2%) 53 31	38, 50, 60, 72	0
24	22	70/72 (97%)	0.31	0 100 100	61, 70, 75, 79	0
25	13	59/60 (98%)	0.00	0 100 100	31, 43, 61, 80	0
25	23	59/60 (98%)	0.23	1 (1%) 69 46	51, 65, 74, 82	0
26	14	69/71 (97%)	0.41	3 (4%) 40 21	55, 69, 83, 89	0
26	24	69/71 (97%)	0.71	3 (4%) 40 21	76, 85, 91, 95	0
27	15	59/60 (98%)	-0.10	1 (1%) 69 46	28, 40, 54, 66	0
27	25	59/60 (98%)	0.03	0 100 100	40, 52, 63, 72	0
28	16	53/54 (98%)	-0.32	0 100 100	36, 42, 54, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.27	0 100 100	52, 60, 66, 77	0
29	17	48/49 (97%)	-0.03	1 (2%) 63 40	29, 36, 58, 63	0
29	27	48/49 (97%)	0.18	1 (2%) 63 40	37, 45, 66, 74	0
30	18	64/65 (98%)	0.12	1 (1%) 70 47	29, 39, 48, 57	0
30	28	64/65 (98%)	0.38	0 100 100	49, 55, 63, 68	0
31	19	37/37 (100%)	-0.02	0 100 100	39, 46, 60, 66	0
31	29	37/37 (100%)	0.59	1 (2%) 56 33	60, 67, 74, 75	0
32	1a	1488/1521 (97%)	-0.04	16 (1%) 78 57	39, 65, 89, 105	0
32	2a	1491/1521 (98%)	0.37	33 (2%) 62 39	49, 75, 93, 105	0
33	1b	231/256 (90%)	0.38	4 (1%) 69 46	62, 75, 84, 94	0
33	2b	231/256 (90%)	0.92	27 (11%) 9 5	68, 81, 88, 95	0
34	1c	206/239 (86%)	0.07	1 (0%) 87 72	52, 67, 76, 83	0
34	2c	206/239 (86%)	0.80	18 (8%) 16 9	69, 81, 86, 92	0
35	1d	208/209 (99%)	0.29	4 (1%) 66 43	54, 67, 76, 80	0
35	2d	208/209 (99%)	0.74	6 (2%) 53 31	59, 72, 81, 86	0
36	1e	148/162 (91%)	0.31	2 (1%) 73 51	51, 63, 72, 77	0
36	2e	148/162 (91%)	0.68	8 (5%) 31 16	62, 73, 80, 85	0
37	1f	100/101 (99%)	-0.07	0 100 100	53, 62, 73, 74	0
37	2f	100/101 (99%)	0.12	1 (1%) 79 59	58, 70, 77, 81	0
38	1g	155/156 (99%)	0.30	9 (5%) 29 15	56, 66, 78, 86	0
38	2g	155/156 (99%)	0.42	5 (3%) 50 28	67, 77, 83, 88	0
39	1h	137/138 (99%)	0.22	1 (0%) 84 66	57, 66, 73, 79	0
39	2h	137/138 (99%)	0.71	7 (5%) 33 17	61, 72, 79, 80	0
40	1i	127/128 (99%)	0.72	10 (7%) 18 9	51, 71, 80, 85	0
40	2i	127/128 (99%)	1.17	20 (15%) 5 2	72, 82, 87, 91	0
41	1j	97/105 (92%)	0.49	1 (1%) 79 59	59, 72, 82, 85	0
41	2j	96/105 (91%)	1.62	32 (33%) 1 0	71, 83, 89, 92	0
42	1k	114/129 (88%)	0.09	1 (0%) 81 61	48, 65, 75, 81	0
42	2k	114/129 (88%)	0.52	3 (2%) 57 34	61, 70, 77, 86	0
43	1l	121/132 (91%)	0.05	2 (1%) 69 46	43, 56, 67, 75	0
43	2l	121/132 (91%)	0.54	2 (1%) 69 46	55, 65, 73, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.48	3 (2%) 59 37	54, 66, 77, 95	0
44	2m	122/126 (96%)	1.07	12 (9%) 13 6	71, 81, 86, 93	0
45	1n	60/61 (98%)	0.48	2 (3%) 49 28	52, 62, 69, 72	0
45	2n	60/61 (98%)	1.65	21 (35%) 1 0	72, 81, 86, 88	0
46	1o	88/89 (98%)	0.16	1 (1%) 78 57	48, 63, 75, 81	0
46	2o	88/89 (98%)	0.55	0 100 100	61, 71, 78, 85	0
47	1p	82/88 (93%)	0.94	6 (7%) 21 10	58, 66, 76, 86	0
47	2p	82/88 (93%)	0.86	2 (2%) 59 37	54, 68, 76, 82	0
48	1q	99/105 (94%)	0.46	2 (2%) 65 42	53, 65, 74, 77	0
48	2q	99/105 (94%)	0.47	1 (1%) 79 59	60, 68, 75, 80	0
49	1r	68/88 (77%)	-0.04	0 100 100	57, 65, 74, 80	0
49	2r	68/88 (77%)	0.27	0 100 100	61, 69, 78, 81	0
50	1s	83/93 (89%)	0.35	1 (1%) 76 55	57, 66, 77, 82	0
50	2s	83/93 (89%)	0.99	6 (7%) 21 11	75, 82, 89, 93	0
51	1t	96/106 (90%)	0.62	6 (6%) 26 13	58, 68, 79, 83	0
51	2t	96/106 (90%)	0.44	4 (4%) 40 21	56, 68, 79, 82	0
52	1u	23/27 (85%)	0.69	1 (4%) 40 21	59, 64, 69, 71	0
52	2u	23/27 (85%)	1.41	6 (26%) 1 1	72, 78, 83, 88	0
53	1v	13/24 (54%)	1.70	5 (38%) 1 0	52, 88, 95, 95	0
53	2v	13/24 (54%)	2.38	9 (69%) 0 0	65, 95, 100, 102	0
54	1x	72/77 (93%)	-0.12	1 (1%) 73 51	37, 63, 80, 94	0
54	2x	72/77 (93%)	0.08	0 100 100	51, 77, 89, 94	0
55	1z	16/16 (100%)	0.52	2 (12%) 8 4	37, 43, 62, 75	0
55	2z	16/16 (100%)	0.89	3 (18%) 3 2	48, 52, 72, 77	0
All	All	20628/21476 (96%)	0.17	510 (2%) 58 35	26, 62, 86, 108	0

The worst 5 of 510 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	7.4
44	2m	123	ALA	6.0
44	1m	123	ALA	5.8
1	2A	2133	G	5.4
53	1v	24	A	5.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	2x	55	20/21	0.71	0.14	75,83,93,101	0
54	5MU	2x	54	21/22	0.81	0.12	79,82,89,97	0
54	4SU	2x	8	20/21	0.81	0.11	77,86,93,93	0
32	2MG	2a	1207	24/25	0.84	0.11	76,83,88,95	0
1	5MU	2A	1915	21/22	0.84	0.09	74,78,84,97	0
32	5MC	2a	967	21/22	0.85	0.16	67,72,81,85	0
32	5MC	2a	1400	21/22	0.86	0.16	56,70,78,81	0
54	5MC	2x	32	21/22	0.88	0.13	68,74,76,78	0
1	PSU	2A	1911	20/21	0.88	0.12	64,69,77,77	0
32	M2G	2a	966	25/26	0.88	0.15	64,71,81,85	0
32	PSU	2a	516	20/21	0.89	0.09	66,74,81,82	0
54	5MU	1x	54	21/22	0.89	0.10	60,66,70,74	0
54	PSU	1x	55	20/21	0.89	0.09	62,65,72,76	0
32	4OC	2a	1402	22/23	0.90	0.12	64,69,76,79	0
43	0TD	2l	92	10/11	0.90	0.12	57,62,66,79	0
32	7MG	2a	527	24/25	0.90	0.14	65,69,75,76	0
32	2MG	1a	1207	24/25	0.91	0.09	54,66,75,81	0
1	PSU	2A	1917	20/21	0.91	0.08	58,69,74,76	0
1	5MC	2A	1942	21/22	0.91	0.10	49,62,66,67	0
54	4SU	1x	8	20/21	0.92	0.08	60,67,74,76	0
1	PSU	1A	1917	20/21	0.92	0.08	55,61,66,68	0
32	5MC	2a	1404	21/22	0.92	0.12	56,64,71,74	0
1	5MU	1A	1915	21/22	0.92	0.08	52,64,73,80	0
1	4OC	2A	1920	21/23	0.93	0.12	55,64,71,78	0
32	7MG	1a	527	24/25	0.93	0.11	40,50,56,60	0
32	4OC	1a	1402	22/23	0.93	0.12	48,54,61,63	0
1	5MC	2A	1962	21/22	0.94	0.10	45,55,59,64	0
1	5MC	1A	1942	21/22	0.94	0.09	39,45,50,58	0
32	MA6	2a	1518	24/25	0.94	0.11	53,63,68,75	0
32	PSU	1a	516	20/21	0.94	0.08	54,64,68,71	0
32	5MC	1a	1404	21/22	0.94	0.12	40,50,54,56	0
1	PSU	1A	1911	20/21	0.94	0.08	46,57,61,64	0
54	5MC	1x	32	21/22	0.94	0.10	47,53,58,64	0
32	M2G	1a	966	25/26	0.94	0.11	54,58,61,66	0
32	MA6	2a	1519	24/25	0.95	0.13	54,61,67,73	0
43	0TD	1l	92	10/11	0.95	0.08	53,56,59,62	0
32	5MC	1a	1400	21/22	0.95	0.11	49,55,62,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	967	21/22	0.95	0.11	55,63,65,65	0
32	UR3	2a	1498	21/22	0.95	0.11	46,54,62,69	0
1	4OC	1A	1920	21/23	0.95	0.10	39,52,55,65	0
1	5MU	2A	1939	21/22	0.96	0.09	32,48,52,55	0
1	OMG	1A	2251	24/25	0.96	0.10	26,37,40,44	0
32	5MC	1a	1407	21/22	0.96	0.08	39,45,49,51	0
1	OMG	2A	2251	24/25	0.96	0.09	35,44,49,50	0
1	2MA	2A	2503	23/24	0.96	0.10	39,46,49,52	0
1	2MU	2A	2552	21/23	0.96	0.10	33,42,49,52	0
32	MA6	1a	1519	24/25	0.96	0.10	44,52,54,55	0
32	5MC	2a	1407	21/22	0.96	0.07	49,61,69,71	0
1	2MU	1A	2552	21/23	0.97	0.07	26,37,42,48	0
1	PSU	1A	2605	20/21	0.97	0.07	28,36,41,42	0
1	5MC	1A	1962	21/22	0.97	0.07	35,44,48,50	0
1	PSU	2A	2605	20/21	0.97	0.07	35,42,46,46	0
32	UR3	1a	1498	21/22	0.97	0.08	42,49,56,60	0
32	MA6	1a	1518	24/25	0.97	0.10	34,49,55,55	0
1	5MU	1A	1939	21/22	0.97	0.08	28,36,41,43	0
1	2MA	1A	2503	23/24	0.98	0.07	24,32,35,41	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3483	1/1	0.44	0.22	73,73,73,73	0
56	MG	1A	3176	1/1	0.56	0.37	69,69,69,69	0
56	MG	2A	3351	1/1	0.63	0.17	59,59,59,59	0
56	MG	1A	3512	1/1	0.63	0.14	50,50,50,50	0
56	MG	2A	3197	1/1	0.64	0.24	73,73,73,73	0
56	MG	2a	3112	1/1	0.65	0.25	64,64,64,64	0
56	MG	1A	3837	1/1	0.66	0.29	64,64,64,64	0
56	MG	1a	1697	1/1	0.66	0.29	72,72,72,72	0
56	MG	1A	3802	1/1	0.69	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	105	1/1	0.69	0.21	60,60,60,60	0
56	MG	1A	3399	1/1	0.69	0.17	70,70,70,70	0
56	MG	2a	3055	1/1	0.70	0.22	61,61,61,61	0
56	MG	1a	1681	1/1	0.70	0.19	55,55,55,55	0
56	MG	2A	3550	1/1	0.71	0.19	61,61,61,61	0
56	MG	1a	1717	1/1	0.72	0.23	67,67,67,67	0
56	MG	2a	3061	1/1	0.72	0.27	51,51,51,51	0
56	MG	1A	3480	1/1	0.72	0.19	28,28,28,28	0
56	MG	2a	3140	1/1	0.72	0.25	64,64,64,64	0
56	MG	1a	1686	1/1	0.73	0.33	64,64,64,64	0
56	MG	1a	1723	1/1	0.74	0.24	57,57,57,57	0
56	MG	1A	3388	1/1	0.74	0.70	35,35,35,35	0
56	MG	2A	3506	1/1	0.74	0.23	68,68,68,68	0
56	MG	1A	3575	1/1	0.74	0.20	72,72,72,72	0
56	MG	1A	3179	1/1	0.75	0.26	59,59,59,59	0
56	MG	2A	3407	1/1	0.75	0.15	75,75,75,75	0
56	MG	1A	3461	1/1	0.75	0.27	52,52,52,52	0
56	MG	2a	3145	1/1	0.75	0.43	66,66,66,66	0
56	MG	2v	101	1/1	0.75	0.15	77,77,77,77	0
56	MG	2A	3312	1/1	0.76	0.09	53,53,53,53	0
56	MG	1a	1763	1/1	0.76	0.23	59,59,59,59	0
56	MG	1A	3763	1/1	0.76	0.20	68,68,68,68	0
56	MG	1A	3408	1/1	0.76	0.33	65,65,65,65	0
56	MG	1a	1759	1/1	0.77	0.41	65,65,65,65	0
56	MG	2A	3585	1/1	0.77	0.17	66,66,66,66	0
56	MG	2a	3003	1/1	0.77	0.29	61,61,61,61	0
56	MG	1A	3347	1/1	0.77	0.17	62,62,62,62	0
56	MG	2A	3395	1/1	0.77	0.27	52,52,52,52	0
56	MG	2a	3082	1/1	0.77	0.43	61,61,61,61	0
56	MG	1A	3712	1/1	0.77	0.33	43,43,43,43	0
56	MG	2A	3409	1/1	0.77	0.35	60,60,60,60	0
56	MG	1a	1744	1/1	0.77	0.48	58,58,58,58	0
56	MG	2A	3206	1/1	0.77	0.20	52,52,52,52	0
56	MG	2A	3082	1/1	0.78	0.29	52,52,52,52	0
56	MG	2A	3090	1/1	0.78	0.35	72,72,72,72	0
56	MG	1B	219	1/1	0.78	0.19	66,66,66,66	0
56	MG	1A	3284	1/1	0.78	0.17	51,51,51,51	0
56	MG	2F	302	1/1	0.78	0.15	45,45,45,45	0
56	MG	2Z	301	1/1	0.78	0.15	60,60,60,60	0
56	MG	1a	1756	1/1	0.78	0.35	54,54,54,54	0
56	MG	2A	3317	1/1	0.78	0.17	59,59,59,59	0
56	MG	2A	3326	1/1	0.78	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3081	1/1	0.78	0.24	55,55,55,55	0
56	MG	1A	3687	1/1	0.78	0.20	58,58,58,58	0
56	MG	2a	3105	1/1	0.78	0.31	53,53,53,53	0
56	MG	1A	3383	1/1	0.78	0.27	69,69,69,69	0
56	MG	2a	3123	1/1	0.78	0.24	62,62,62,62	0
56	MG	1B	213	1/1	0.78	0.25	58,58,58,58	0
56	MG	2A	3054	1/1	0.78	0.20	51,51,51,51	0
56	MG	2A	3413	1/1	0.78	0.18	57,57,57,57	0
56	MG	1A	3553	1/1	0.79	0.17	65,65,65,65	0
56	MG	2a	3025	1/1	0.79	0.11	73,73,73,73	0
56	MG	2a	3053	1/1	0.79	0.20	67,67,67,67	0
56	MG	2A	3344	1/1	0.79	0.18	66,66,66,66	0
56	MG	2a	3059	1/1	0.79	0.24	58,58,58,58	0
56	MG	2A	3421	1/1	0.79	0.27	54,54,54,54	0
56	MG	1A	3696	1/1	0.79	0.10	67,67,67,67	0
56	MG	2A	3368	1/1	0.79	0.30	70,70,70,70	0
56	MG	2A	3375	1/1	0.79	0.12	51,51,51,51	0
56	MG	2A	3391	1/1	0.79	0.13	94,94,94,94	0
56	MG	2a	3117	1/1	0.79	0.18	50,50,50,50	0
56	MG	2a	3122	1/1	0.79	0.26	65,65,65,65	0
56	MG	2A	3602	1/1	0.79	0.20	55,55,55,55	0
56	MG	1a	1612	1/1	0.79	0.24	45,45,45,45	0
56	MG	2N	201	1/1	0.79	0.08	49,49,49,49	0
56	MG	1A	3151	1/1	0.79	0.28	72,72,72,72	0
56	MG	1a	1659	1/1	0.80	0.25	64,64,64,64	0
56	MG	1A	3083	1/1	0.80	0.25	52,52,52,52	0
56	MG	1U	205	1/1	0.80	0.15	39,39,39,39	0
56	MG	2A	3471	1/1	0.80	0.12	54,54,54,54	0
56	MG	1A	3241	1/1	0.80	0.11	54,54,54,54	0
56	MG	2A	3492	1/1	0.80	0.25	69,69,69,69	0
56	MG	2a	3009	1/1	0.80	0.11	49,49,49,49	0
56	MG	2a	3119	1/1	0.80	0.51	76,76,76,76	0
56	MG	2A	3401	1/1	0.80	0.37	53,53,53,53	0
56	MG	2a	3029	1/1	0.80	0.19	47,47,47,47	0
56	MG	2a	3033	1/1	0.80	0.22	57,57,57,57	0
56	MG	2A	3217	1/1	0.80	0.26	48,48,48,48	0
56	MG	2A	3552	1/1	0.80	0.14	60,60,60,60	0
56	MG	2A	3416	1/1	0.81	0.18	63,63,63,63	0
56	MG	1A	3501	1/1	0.81	0.11	58,58,58,58	0
56	MG	2A	3429	1/1	0.81	0.42	59,59,59,59	0
56	MG	1A	3737	1/1	0.81	0.09	47,47,47,47	0
56	MG	1A	3594	1/1	0.81	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3767	1/1	0.81	0.16	51,51,51,51	0
56	MG	1A	3784	1/1	0.81	0.24	60,60,60,60	0
56	MG	2A	3357	1/1	0.81	0.32	54,54,54,54	0
56	MG	1A	3648	1/1	0.81	0.29	62,62,62,62	0
56	MG	2A	3566	1/1	0.81	0.19	62,62,62,62	0
56	MG	2A	3077	1/1	0.81	0.25	54,54,54,54	0
56	MG	1A	3187	1/1	0.81	0.13	49,49,49,49	0
56	MG	2B	205	1/1	0.81	0.22	79,79,79,79	0
56	MG	1A	3844	1/1	0.81	0.20	50,50,50,50	0
56	MG	2A	3143	1/1	0.81	0.22	56,56,56,56	0
56	MG	1A	3373	1/1	0.81	0.16	47,47,47,47	0
56	MG	1a	1724	1/1	0.81	0.26	52,52,52,52	0
56	MG	1a	1725	1/1	0.81	0.20	67,67,67,67	0
56	MG	1A	3254	1/1	0.82	0.18	64,64,64,64	0
56	MG	1a	1753	1/1	0.82	0.32	59,59,59,59	0
56	MG	1a	1691	1/1	0.82	0.25	42,42,42,42	0
56	MG	2A	3537	1/1	0.82	0.20	57,57,57,57	0
56	MG	2A	3210	1/1	0.82	0.11	76,76,76,76	0
56	MG	1A	3259	1/1	0.82	0.16	60,60,60,60	0
56	MG	2A	3560	1/1	0.82	0.20	75,75,75,75	0
56	MG	2A	3406	1/1	0.82	0.22	50,50,50,50	0
56	MG	1A	3660	1/1	0.82	0.14	63,63,63,63	0
56	MG	2a	3094	1/1	0.82	0.24	57,57,57,57	0
56	MG	1a	1621	1/1	0.82	0.25	51,51,51,51	0
56	MG	2a	3111	1/1	0.82	0.24	66,66,66,66	0
56	MG	1A	3667	1/1	0.82	0.13	33,33,33,33	0
56	MG	1A	3113	1/1	0.82	0.30	58,58,58,58	0
56	MG	1a	1728	1/1	0.82	0.27	63,63,63,63	0
56	MG	2A	3356	1/1	0.82	0.23	61,61,61,61	0
56	MG	2A	3450	1/1	0.82	0.19	41,41,41,41	0
56	MG	2a	3127	1/1	0.82	0.20	65,65,65,65	0
56	MG	2a	3139	1/1	0.82	0.19	54,54,54,54	0
56	MG	2a	3006	1/1	0.82	0.32	63,63,63,63	0
56	MG	2a	3142	1/1	0.82	0.27	49,49,49,49	0
56	MG	1a	1742	1/1	0.82	0.26	60,60,60,60	0
56	MG	2a	3018	1/1	0.82	0.22	59,59,59,59	0
56	MG	1A	3715	1/1	0.83	0.15	53,53,53,53	0
56	MG	1A	3302	1/1	0.83	0.23	55,55,55,55	0
56	MG	2a	3012	1/1	0.83	0.24	52,52,52,52	0
56	MG	2A	3102	1/1	0.83	0.21	50,50,50,50	0
56	MG	1A	3081	1/1	0.83	0.15	57,57,57,57	0
56	MG	1E	306	1/1	0.83	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	201	1/1	0.83	0.12	40,40,40,40	0
56	MG	2A	3207	1/1	0.83	0.09	55,55,55,55	0
56	MG	1A	3407	1/1	0.83	0.56	103,103,103,103	0
56	MG	1a	1606	1/1	0.83	0.14	54,54,54,54	0
56	MG	2A	3289	1/1	0.83	0.21	45,45,45,45	0
56	MG	1A	3230	1/1	0.83	0.12	49,49,49,49	0
56	MG	2A	3313	1/1	0.83	0.15	51,51,51,51	0
56	MG	2a	3085	1/1	0.83	0.33	52,52,52,52	0
56	MG	1a	1618	1/1	0.83	0.25	61,61,61,61	0
56	MG	1a	1752	1/1	0.83	0.17	60,60,60,60	0
56	MG	1A	3430	1/1	0.83	0.25	64,64,64,64	0
56	MG	1a	1628	1/1	0.83	0.18	43,43,43,43	0
56	MG	1a	1634	1/1	0.83	0.18	49,49,49,49	0
56	MG	1a	1644	1/1	0.83	0.23	54,54,54,54	0
56	MG	2A	3359	1/1	0.83	0.25	52,52,52,52	0
56	MG	1A	3826	1/1	0.83	0.15	51,51,51,51	0
56	MG	2A	3016	1/1	0.83	0.42	65,65,65,65	0
56	MG	2a	3136	1/1	0.83	0.15	62,62,62,62	0
56	MG	2A	3376	1/1	0.83	0.14	52,52,52,52	0
56	MG	1A	3827	1/1	0.83	0.16	51,51,51,51	0
56	MG	2T	201	1/1	0.83	0.10	33,33,33,33	0
56	MG	2A	3394	1/1	0.83	0.16	60,60,60,60	0
56	MG	1A	3002	1/1	0.83	0.15	56,56,56,56	0
56	MG	2v	102	1/1	0.83	0.51	57,57,57,57	0
56	MG	2x	102	1/1	0.83	0.17	47,47,47,47	0
56	MG	2A	3521	1/1	0.84	0.19	60,60,60,60	0
56	MG	1A	3738	1/1	0.84	0.11	44,44,44,44	0
56	MG	1A	3212	1/1	0.84	0.18	45,45,45,45	0
56	MG	1A	3221	1/1	0.84	0.15	36,36,36,36	0
56	MG	2a	3078	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3842	1/1	0.84	0.23	42,42,42,42	0
56	MG	1A	3679	1/1	0.84	0.15	52,52,52,52	0
56	MG	2A	3037	1/1	0.84	0.20	50,50,50,50	0
56	MG	2a	3093	1/1	0.84	0.13	50,50,50,50	0
56	MG	2A	3291	1/1	0.84	0.28	43,43,43,43	0
56	MG	2a	3097	1/1	0.84	0.21	68,68,68,68	0
56	MG	1A	3785	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3060	1/1	0.84	0.27	62,62,62,62	0
56	MG	2A	3069	1/1	0.84	0.25	53,53,53,53	0
56	MG	1B	218	1/1	0.84	0.26	52,52,52,52	0
56	MG	2A	3419	1/1	0.84	0.26	30,30,30,30	0
56	MG	2A	3329	1/1	0.84	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3786	1/1	0.84	0.14	58,58,58,58	0
56	MG	2a	3008	1/1	0.84	0.09	46,46,46,46	0
56	MG	1A	3795	1/1	0.84	0.11	39,39,39,39	0
56	MG	2a	3138	1/1	0.84	0.27	67,67,67,67	0
56	MG	1F	306	1/1	0.84	0.09	47,47,47,47	0
56	MG	2a	3016	1/1	0.84	0.19	76,76,76,76	0
56	MG	2A	3135	1/1	0.84	0.13	52,52,52,52	0
56	MG	1A	3269	1/1	0.84	0.08	34,34,34,34	0
56	MG	2A	3174	1/1	0.84	0.17	49,49,49,49	0
56	MG	2A	3516	1/1	0.84	0.18	67,67,67,67	0
56	MG	2a	3046	1/1	0.84	0.22	49,49,49,49	0
56	MG	2A	3545	1/1	0.85	0.28	53,53,53,53	0
56	MG	2A	3215	1/1	0.85	0.25	60,60,60,60	0
56	MG	2A	3384	1/1	0.85	0.25	45,45,45,45	0
56	MG	1a	1605	1/1	0.85	0.15	54,54,54,54	0
56	MG	2a	3064	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3282	1/1	0.85	0.26	58,58,58,58	0
56	MG	1a	1737	1/1	0.85	0.18	41,41,41,41	0
56	MG	2A	3597	1/1	0.85	0.18	49,49,49,49	0
56	MG	1a	1740	1/1	0.85	0.28	35,35,35,35	0
56	MG	2a	3086	1/1	0.85	0.17	69,69,69,69	0
56	MG	2A	3620	1/1	0.85	0.25	61,61,61,61	0
56	MG	1A	3339	1/1	0.85	0.14	55,55,55,55	0
56	MG	2B	209	1/1	0.85	0.27	50,50,50,50	0
56	MG	2a	3103	1/1	0.85	0.20	65,65,65,65	0
56	MG	1A	3500	1/1	0.85	0.15	59,59,59,59	0
56	MG	2a	3106	1/1	0.85	0.24	60,60,60,60	0
56	MG	1A	3289	1/1	0.85	0.14	46,46,46,46	0
56	MG	2A	3325	1/1	0.85	0.14	52,52,52,52	0
56	MG	1a	1692	1/1	0.85	0.31	43,43,43,43	0
56	MG	28	103	1/1	0.85	0.25	60,60,60,60	0
56	MG	1A	3389	1/1	0.85	0.12	50,50,50,50	0
56	MG	2A	3343	1/1	0.85	0.18	69,69,69,69	0
56	MG	1a	1757	1/1	0.85	0.25	51,51,51,51	0
56	MG	1A	3437	1/1	0.85	0.25	53,53,53,53	0
56	MG	2A	3355	1/1	0.85	0.12	61,61,61,61	0
56	MG	1A	3072	1/1	0.85	0.29	52,52,52,52	0
56	MG	1a	1767	1/1	0.85	0.19	47,47,47,47	0
56	MG	1a	1637	1/1	0.85	0.21	46,46,46,46	0
56	MG	2A	3010	1/1	0.85	0.14	56,56,56,56	0
56	MG	2A	3370	1/1	0.85	0.32	51,51,51,51	0
56	MG	17	3106	1/1	0.85	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3049	1/1	0.85	0.20	54,54,54,54	0
56	MG	2A	3399	1/1	0.86	0.23	47,47,47,47	0
56	MG	1A	3337	1/1	0.86	0.14	31,31,31,31	0
56	MG	2A	3212	1/1	0.86	0.20	62,62,62,62	0
56	MG	2a	3023	1/1	0.86	0.17	59,59,59,59	0
56	MG	1A	3404	1/1	0.86	0.18	52,52,52,52	0
56	MG	1A	3184	1/1	0.86	0.10	46,46,46,46	0
56	MG	2A	3260	1/1	0.86	0.19	53,53,53,53	0
56	MG	1T	201	1/1	0.86	0.15	44,44,44,44	0
56	MG	2a	3048	1/1	0.86	0.18	61,61,61,61	0
56	MG	2A	3005	1/1	0.86	0.21	42,42,42,42	0
56	MG	2a	3051	1/1	0.86	0.17	56,56,56,56	0
56	MG	1A	3150	1/1	0.86	0.12	35,35,35,35	0
56	MG	1a	1709	1/1	0.86	0.19	36,36,36,36	0
56	MG	2A	3435	1/1	0.86	0.35	49,49,49,49	0
56	MG	2A	3034	1/1	0.86	0.10	34,34,34,34	0
56	MG	1X	103	1/1	0.86	0.11	40,40,40,40	0
56	MG	2a	3065	1/1	0.86	0.24	56,56,56,56	0
56	MG	2a	3072	1/1	0.86	0.33	55,55,55,55	0
56	MG	2A	3051	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3825	1/1	0.86	0.15	46,46,46,46	0
56	MG	1A	3276	1/1	0.86	0.13	45,45,45,45	0
56	MG	2A	3333	1/1	0.86	0.33	51,51,51,51	0
56	MG	2A	3334	1/1	0.86	0.13	51,51,51,51	0
56	MG	2a	3091	1/1	0.86	0.15	43,43,43,43	0
56	MG	2A	3340	1/1	0.86	0.22	60,60,60,60	0
56	MG	2A	3341	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3063	1/1	0.86	0.14	46,46,46,46	0
56	MG	1A	3233	1/1	0.86	0.14	62,62,62,62	0
56	MG	1A	3627	1/1	0.86	0.11	36,36,36,36	0
56	MG	1a	1735	1/1	0.86	0.26	57,57,57,57	0
56	MG	1A	3841	1/1	0.86	0.17	57,57,57,57	0
56	MG	1A	3646	1/1	0.86	0.09	56,56,56,56	0
56	MG	1A	3739	1/1	0.86	0.19	66,66,66,66	0
56	MG	2A	3606	1/1	0.86	0.10	54,54,54,54	0
56	MG	2A	3364	1/1	0.86	0.24	53,53,53,53	0
56	MG	2A	3366	1/1	0.86	0.17	53,53,53,53	0
56	MG	1A	3074	1/1	0.86	0.13	55,55,55,55	0
56	MG	2a	3131	1/1	0.86	0.33	60,60,60,60	0
56	MG	2a	3132	1/1	0.86	0.39	55,55,55,55	0
56	MG	2A	3152	1/1	0.86	0.18	64,64,64,64	0
56	MG	1A	3214	1/1	0.86	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3179	1/1	0.86	0.29	54,54,54,54	0
56	MG	2A	3377	1/1	0.86	0.15	47,47,47,47	0
56	MG	2A	3185	1/1	0.86	0.14	49,49,49,49	0
56	MG	2A	3386	1/1	0.86	0.39	63,63,63,63	0
56	MG	1A	3666	1/1	0.86	0.14	48,48,48,48	0
56	MG	1B	221	1/1	0.86	0.10	63,63,63,63	0
56	MG	1a	1672	1/1	0.86	0.17	49,49,49,49	0
56	MG	1a	1665	1/1	0.87	0.23	40,40,40,40	0
56	MG	1A	3445	1/1	0.87	0.21	46,46,46,46	0
56	MG	1a	1675	1/1	0.87	0.33	53,53,53,53	0
56	MG	1A	3460	1/1	0.87	0.26	49,49,49,49	0
56	MG	1A	3120	1/1	0.87	0.11	46,46,46,46	0
56	MG	2a	3007	1/1	0.87	0.20	50,50,50,50	0
56	MG	1A	3469	1/1	0.87	0.22	48,48,48,48	0
56	MG	1A	3692	1/1	0.87	0.13	48,48,48,48	0
56	MG	2A	3096	1/1	0.87	0.19	49,49,49,49	0
56	MG	1a	1694	1/1	0.87	0.20	35,35,35,35	0
56	MG	1A	3024	1/1	0.87	0.16	76,76,76,76	0
56	MG	1a	1701	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3148	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3706	1/1	0.87	0.13	41,41,41,41	0
56	MG	2A	3165	1/1	0.87	0.15	44,44,44,44	0
56	MG	2A	3173	1/1	0.87	0.09	47,47,47,47	0
56	MG	2a	3047	1/1	0.87	0.09	67,67,67,67	0
56	MG	2A	3397	1/1	0.87	0.18	69,69,69,69	0
56	MG	1a	1715	1/1	0.87	0.15	42,42,42,42	0
56	MG	1A	3270	1/1	0.87	0.15	50,50,50,50	0
56	MG	1B	222	1/1	0.87	0.11	47,47,47,47	0
56	MG	1A	3274	1/1	0.87	0.21	52,52,52,52	0
56	MG	2a	3057	1/1	0.87	0.33	59,59,59,59	0
56	MG	2A	3201	1/1	0.87	0.14	46,46,46,46	0
56	MG	1E	307	1/1	0.87	0.17	38,38,38,38	0
56	MG	1A	3716	1/1	0.87	0.21	53,53,53,53	0
56	MG	1A	3728	1/1	0.87	0.12	58,58,58,58	0
56	MG	2a	3067	1/1	0.87	0.15	58,58,58,58	0
56	MG	1A	3503	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3094	1/1	0.87	0.15	42,42,42,42	0
56	MG	1W	204	1/1	0.87	0.26	53,53,53,53	0
56	MG	1A	3530	1/1	0.87	0.12	34,34,34,34	0
56	MG	2a	3084	1/1	0.87	0.29	67,67,67,67	0
56	MG	2A	3267	1/1	0.87	0.28	51,51,51,51	0
56	MG	2A	3270	1/1	0.87	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3090	1/1	0.87	0.36	52,52,52,52	0
56	MG	1a	1748	1/1	0.87	0.23	49,49,49,49	0
56	MG	2a	3092	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3495	1/1	0.87	0.30	44,44,44,44	0
56	MG	2A	3283	1/1	0.87	0.44	47,47,47,47	0
56	MG	1A	3239	1/1	0.87	0.19	53,53,53,53	0
56	MG	1a	1603	1/1	0.87	0.19	59,59,59,59	0
56	MG	2A	3305	1/1	0.87	0.32	43,43,43,43	0
56	MG	1A	3175	1/1	0.87	0.30	58,58,58,58	0
56	MG	2a	3108	1/1	0.87	0.21	48,48,48,48	0
56	MG	1A	3585	1/1	0.87	0.11	50,50,50,50	0
56	MG	1A	3296	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3244	1/1	0.87	0.08	49,49,49,49	0
56	MG	1a	1765	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3570	1/1	0.87	0.16	79,79,79,79	0
56	MG	2A	3573	1/1	0.87	0.10	55,55,55,55	0
56	MG	1A	3638	1/1	0.87	0.19	64,64,64,64	0
56	MG	2A	3587	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3591	1/1	0.87	0.14	36,36,36,36	0
56	MG	1a	1627	1/1	0.87	0.34	60,60,60,60	0
56	MG	1x	110	1/1	0.87	0.09	53,53,53,53	0
56	MG	1A	3308	1/1	0.87	0.17	47,47,47,47	0
56	MG	1A	3821	1/1	0.87	0.30	54,54,54,54	0
56	MG	1A	3324	1/1	0.87	0.11	56,56,56,56	0
56	MG	2a	3144	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3017	1/1	0.87	0.14	37,37,37,37	0
56	MG	2q	201	1/1	0.87	0.10	54,54,54,54	0
56	MG	2B	210	1/1	0.87	0.20	58,58,58,58	0
56	MG	1a	1657	1/1	0.87	0.34	58,58,58,58	0
56	MG	1A	3662	1/1	0.87	0.19	61,61,61,61	0
56	MG	1A	3215	1/1	0.88	0.28	49,49,49,49	0
56	MG	2A	3563	1/1	0.88	0.18	59,59,59,59	0
56	MG	2A	3565	1/1	0.88	0.07	44,44,44,44	0
56	MG	2A	3223	1/1	0.88	0.14	37,37,37,37	0
56	MG	1a	1602	1/1	0.88	0.16	51,51,51,51	0
56	MG	2A	3261	1/1	0.88	0.38	53,53,53,53	0
56	MG	1A	3774	1/1	0.88	0.16	80,80,80,80	0
56	MG	1a	1750	1/1	0.88	0.27	52,52,52,52	0
56	MG	2A	3590	1/1	0.88	0.18	49,49,49,49	0
56	MG	2A	3274	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3276	1/1	0.88	0.21	39,39,39,39	0
56	MG	2A	3601	1/1	0.88	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1751	1/1	0.88	0.44	60,60,60,60	0
56	MG	2A	3603	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3643	1/1	0.88	0.11	34,34,34,34	0
56	MG	2A	3610	1/1	0.88	0.21	46,46,46,46	0
56	MG	2A	3612	1/1	0.88	0.09	42,42,42,42	0
56	MG	1A	3475	1/1	0.88	0.13	29,29,29,29	0
56	MG	1A	3477	1/1	0.88	0.14	35,35,35,35	0
56	MG	1a	1615	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3659	1/1	0.88	0.23	56,56,56,56	0
56	MG	2B	211	1/1	0.88	0.25	54,54,54,54	0
56	MG	2F	301	1/1	0.88	0.08	44,44,44,44	0
56	MG	1A	3216	1/1	0.88	0.19	58,58,58,58	0
56	MG	1A	3497	1/1	0.88	0.12	45,45,45,45	0
56	MG	2O	201	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3318	1/1	0.88	0.17	51,51,51,51	0
56	MG	1A	3406	1/1	0.88	0.17	57,57,57,57	0
56	MG	26	101	1/1	0.88	0.12	56,56,56,56	0
56	MG	1n	102	1/1	0.88	0.16	47,47,47,47	0
56	MG	1A	3342	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3332	1/1	0.88	0.15	56,56,56,56	0
56	MG	1x	106	1/1	0.88	0.09	72,72,72,72	0
56	MG	1A	3078	1/1	0.88	0.15	43,43,43,43	0
56	MG	2A	3339	1/1	0.88	0.25	63,63,63,63	0
56	MG	1A	3830	1/1	0.88	0.13	52,52,52,52	0
56	MG	2a	3013	1/1	0.88	0.23	56,56,56,56	0
56	MG	1a	1650	1/1	0.88	0.23	45,45,45,45	0
56	MG	2a	3017	1/1	0.88	0.13	50,50,50,50	0
56	MG	1a	1654	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3021	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3345	1/1	0.88	0.25	56,56,56,56	0
56	MG	1A	3426	1/1	0.88	0.35	29,29,29,29	0
56	MG	2A	3036	1/1	0.88	0.12	55,55,55,55	0
56	MG	2a	3040	1/1	0.88	0.14	50,50,50,50	0
56	MG	1A	3691	1/1	0.88	0.14	46,46,46,46	0
56	MG	1a	1662	1/1	0.88	0.14	37,37,37,37	0
56	MG	1A	3371	1/1	0.88	0.31	47,47,47,47	0
56	MG	1A	3536	1/1	0.88	0.22	63,63,63,63	0
56	MG	2A	3365	1/1	0.88	0.16	69,69,69,69	0
56	MG	2A	3062	1/1	0.88	0.13	47,47,47,47	0
56	MG	2a	3054	1/1	0.88	0.20	63,63,63,63	0
56	MG	1B	212	1/1	0.88	0.32	51,51,51,51	0
56	MG	1A	3540	1/1	0.88	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	215	1/1	0.88	0.27	44,44,44,44	0
56	MG	1A	3545	1/1	0.88	0.13	48,48,48,48	0
56	MG	2a	3063	1/1	0.88	0.33	64,64,64,64	0
56	MG	1A	3222	1/1	0.88	0.11	40,40,40,40	0
56	MG	1A	3439	1/1	0.88	0.38	50,50,50,50	0
56	MG	1a	1695	1/1	0.88	0.16	59,59,59,59	0
56	MG	2A	3388	1/1	0.88	0.20	67,67,67,67	0
56	MG	2A	3389	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3126	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3130	1/1	0.88	0.06	29,29,29,29	0
56	MG	1A	3209	1/1	0.88	0.29	40,40,40,40	0
56	MG	2A	3139	1/1	0.88	0.07	30,30,30,30	0
56	MG	1B	224	1/1	0.88	0.10	42,42,42,42	0
56	MG	2A	3147	1/1	0.88	0.17	59,59,59,59	0
56	MG	1a	1705	1/1	0.88	0.23	52,52,52,52	0
56	MG	1A	3734	1/1	0.88	0.13	45,45,45,45	0
56	MG	2A	3153	1/1	0.88	0.13	49,49,49,49	0
56	MG	2A	3155	1/1	0.88	0.38	61,61,61,61	0
56	MG	1A	3152	1/1	0.88	0.23	47,47,47,47	0
56	MG	2a	3100	1/1	0.88	0.16	35,35,35,35	0
56	MG	2a	3102	1/1	0.88	0.17	53,53,53,53	0
56	MG	1A	3618	1/1	0.88	0.15	23,23,23,23	0
56	MG	1a	1719	1/1	0.88	0.40	53,53,53,53	0
56	MG	2A	3177	1/1	0.88	0.09	53,53,53,53	0
56	MG	2a	3107	1/1	0.88	0.34	36,36,36,36	0
56	MG	2A	3432	1/1	0.88	0.24	30,30,30,30	0
56	MG	1A	3115	1/1	0.88	0.09	31,31,31,31	0
56	MG	2A	3443	1/1	0.88	0.22	39,39,39,39	0
56	MG	2a	3115	1/1	0.88	0.31	58,58,58,58	0
56	MG	2A	3184	1/1	0.88	0.10	67,67,67,67	0
56	MG	2a	3118	1/1	0.88	0.28	61,61,61,61	0
56	MG	2A	3464	1/1	0.88	0.10	39,39,39,39	0
56	MG	1N	203	1/1	0.88	0.07	31,31,31,31	0
56	MG	2A	3187	1/1	0.88	0.17	56,56,56,56	0
56	MG	2a	3126	1/1	0.88	0.28	66,66,66,66	0
56	MG	1Q	202	1/1	0.88	0.07	40,40,40,40	0
56	MG	1A	3741	1/1	0.88	0.32	42,42,42,42	0
56	MG	1a	1732	1/1	0.88	0.19	42,42,42,42	0
56	MG	2A	3512	1/1	0.88	0.10	39,39,39,39	0
56	MG	2A	3515	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3753	1/1	0.88	0.12	31,31,31,31	0
56	MG	2A	3208	1/1	0.88	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3523	1/1	0.88	0.13	62,62,62,62	0
56	MG	1A	3633	1/1	0.88	0.08	34,34,34,34	0
56	MG	2A	3211	1/1	0.88	0.09	51,51,51,51	0
56	MG	1a	1739	1/1	0.88	0.14	48,48,48,48	0
56	MG	2t	201	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	3765	1/1	0.88	0.12	45,45,45,45	0
56	MG	2A	3554	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3557	1/1	0.88	0.17	47,47,47,47	0
56	MG	2A	3089	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3346	1/1	0.89	0.23	45,45,45,45	0
56	MG	1A	3295	1/1	0.89	0.19	45,45,45,45	0
56	MG	1A	3393	1/1	0.89	0.15	40,40,40,40	0
56	MG	1A	3543	1/1	0.89	0.14	29,29,29,29	0
56	MG	2A	3109	1/1	0.89	0.27	53,53,53,53	0
56	MG	1a	1706	1/1	0.89	0.13	48,48,48,48	0
56	MG	2A	3128	1/1	0.89	0.09	47,47,47,47	0
56	MG	1A	3735	1/1	0.89	0.10	56,56,56,56	0
56	MG	1N	201	1/1	0.89	0.17	45,45,45,45	0
56	MG	1a	1716	1/1	0.89	0.33	43,43,43,43	0
56	MG	1A	3395	1/1	0.89	0.16	45,45,45,45	0
56	MG	1A	3197	1/1	0.89	0.09	43,43,43,43	0
56	MG	1Q	204	1/1	0.89	0.13	41,41,41,41	0
56	MG	1A	3297	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3245	1/1	0.89	0.11	41,41,41,41	0
56	MG	1A	3591	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3156	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3307	1/1	0.89	0.12	52,52,52,52	0
56	MG	2A	3167	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3170	1/1	0.89	0.21	46,46,46,46	0
56	MG	1A	3597	1/1	0.89	0.09	34,34,34,34	0
56	MG	1A	3599	1/1	0.89	0.12	59,59,59,59	0
56	MG	2a	3043	1/1	0.89	0.20	64,64,64,64	0
56	MG	2a	3044	1/1	0.89	0.16	67,67,67,67	0
56	MG	1A	3040	1/1	0.89	0.18	49,49,49,49	0
56	MG	1A	3413	1/1	0.89	0.10	38,38,38,38	0
56	MG	1A	3309	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3311	1/1	0.89	0.20	60,60,60,60	0
56	MG	1A	3318	1/1	0.89	0.12	38,38,38,38	0
56	MG	2A	3190	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3033	1/1	0.89	0.12	43,43,43,43	0
56	MG	2A	3199	1/1	0.89	0.21	46,46,46,46	0
56	MG	2a	3056	1/1	0.89	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3819	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3426	1/1	0.89	0.45	45,45,45,45	0
56	MG	2A	3203	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3326	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3649	1/1	0.89	0.07	36,36,36,36	0
56	MG	2A	3438	1/1	0.89	0.18	30,30,30,30	0
56	MG	1A	3084	1/1	0.89	0.11	48,48,48,48	0
56	MG	2a	3069	1/1	0.89	0.19	53,53,53,53	0
56	MG	2A	3447	1/1	0.89	0.17	47,47,47,47	0
56	MG	1A	3234	1/1	0.89	0.13	44,44,44,44	0
56	MG	1A	3271	1/1	0.89	0.22	47,47,47,47	0
56	MG	1a	1647	1/1	0.89	0.09	49,49,49,49	0
56	MG	1a	1648	1/1	0.89	0.15	52,52,52,52	0
56	MG	2A	3484	1/1	0.89	0.10	44,44,44,44	0
56	MG	1A	3832	1/1	0.89	0.17	54,54,54,54	0
56	MG	1a	1652	1/1	0.89	0.23	51,51,51,51	0
56	MG	2A	3236	1/1	0.89	0.20	46,46,46,46	0
56	MG	2A	3245	1/1	0.89	0.17	46,46,46,46	0
56	MG	2A	3249	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3254	1/1	0.89	0.16	40,40,40,40	0
56	MG	1A	3664	1/1	0.89	0.12	58,58,58,58	0
56	MG	1a	1655	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3265	1/1	0.89	0.19	53,53,53,53	0
56	MG	1A	3345	1/1	0.89	0.16	50,50,50,50	0
56	MG	2a	3104	1/1	0.89	0.27	45,45,45,45	0
56	MG	1A	3273	1/1	0.89	0.13	59,59,59,59	0
56	MG	2A	3009	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1660	1/1	0.89	0.09	48,48,48,48	0
56	MG	2A	3012	1/1	0.89	0.21	47,47,47,47	0
56	MG	1A	3479	1/1	0.89	0.07	41,41,41,41	0
56	MG	2A	3019	1/1	0.89	0.18	51,51,51,51	0
56	MG	2a	3113	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3352	1/1	0.89	0.20	48,48,48,48	0
56	MG	2A	3023	1/1	0.89	0.15	45,45,45,45	0
56	MG	2A	3567	1/1	0.89	0.25	51,51,51,51	0
56	MG	2A	3024	1/1	0.89	0.24	49,49,49,49	0
56	MG	2a	3120	1/1	0.89	0.21	37,37,37,37	0
56	MG	2A	3025	1/1	0.89	0.10	53,53,53,53	0
56	MG	1a	1666	1/1	0.89	0.24	31,31,31,31	0
56	MG	1a	1669	1/1	0.89	0.18	38,38,38,38	0
56	MG	1A	3368	1/1	0.89	0.12	51,51,51,51	0
56	MG	1A	3117	1/1	0.89	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3328	1/1	0.89	0.24	57,57,57,57	0
56	MG	1A	3240	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3057	1/1	0.89	0.15	44,44,44,44	0
56	MG	1A	3705	1/1	0.89	0.09	45,45,45,45	0
56	MG	1a	1688	1/1	0.89	0.24	61,61,61,61	0
56	MG	2A	3336	1/1	0.89	0.09	64,64,64,64	0
56	MG	2A	3337	1/1	0.89	0.14	56,56,56,56	0
56	MG	1A	3380	1/1	0.89	0.09	53,53,53,53	0
56	MG	1A	3158	1/1	0.89	0.35	36,36,36,36	0
56	MG	2B	208	1/1	0.89	0.08	68,68,68,68	0
56	MG	2A	3070	1/1	0.89	0.15	42,42,42,42	0
56	MG	1A	3243	1/1	0.89	0.22	46,46,46,46	0
56	MG	1E	305	1/1	0.89	0.16	52,52,52,52	0
56	MG	2x	103	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3360	1/1	0.90	0.19	29,29,29,29	0
56	MG	2A	3071	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3613	1/1	0.90	0.25	53,53,53,53	0
56	MG	1A	3257	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3622	1/1	0.90	0.18	55,55,55,55	0
56	MG	2B	202	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3335	1/1	0.90	0.11	58,58,58,58	0
56	MG	2B	207	1/1	0.90	0.09	57,57,57,57	0
56	MG	1A	3605	1/1	0.90	0.11	29,29,29,29	0
56	MG	2A	3087	1/1	0.90	0.26	53,53,53,53	0
56	MG	1A	3746	1/1	0.90	0.17	48,48,48,48	0
56	MG	1a	1713	1/1	0.90	0.20	50,50,50,50	0
56	MG	1A	3752	1/1	0.90	0.11	73,73,73,73	0
56	MG	1A	3614	1/1	0.90	0.10	47,47,47,47	0
56	MG	1V	201	1/1	0.90	0.07	38,38,38,38	0
56	MG	2A	3118	1/1	0.90	0.15	42,42,42,42	0
56	MG	2A	3121	1/1	0.90	0.16	47,47,47,47	0
56	MG	1A	3754	1/1	0.90	0.10	61,61,61,61	0
56	MG	23	102	1/1	0.90	0.08	50,50,50,50	0
56	MG	1A	3617	1/1	0.90	0.15	48,48,48,48	0
56	MG	11	102	1/1	0.90	0.17	37,37,37,37	0
56	MG	17	3101	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	3004	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3136	1/1	0.90	0.12	24,24,24,24	0
56	MG	1A	3455	1/1	0.90	0.20	50,50,50,50	0
56	MG	1a	1730	1/1	0.90	0.20	67,67,67,67	0
56	MG	2A	3146	1/1	0.90	0.07	42,42,42,42	0
56	MG	2A	3367	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	18	103	1/1	0.90	0.25	62,62,62,62	0
56	MG	1a	1734	1/1	0.90	0.27	45,45,45,45	0
56	MG	2A	3373	1/1	0.90	0.14	34,34,34,34	0
56	MG	2A	3150	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3228	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3007	1/1	0.90	0.17	54,54,54,54	0
56	MG	1A	3377	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3098	1/1	0.90	0.12	54,54,54,54	0
56	MG	2a	3035	1/1	0.90	0.21	61,61,61,61	0
56	MG	2A	3387	1/1	0.90	0.09	38,38,38,38	0
56	MG	2A	3158	1/1	0.90	0.06	50,50,50,50	0
56	MG	1A	3203	1/1	0.90	0.22	41,41,41,41	0
56	MG	1a	1613	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3392	1/1	0.90	0.12	31,31,31,31	0
56	MG	1A	3313	1/1	0.90	0.20	34,34,34,34	0
56	MG	2A	3172	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3043	1/1	0.90	0.20	45,45,45,45	0
56	MG	1A	3813	1/1	0.90	0.09	36,36,36,36	0
56	MG	1a	1625	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3125	1/1	0.90	0.21	49,49,49,49	0
56	MG	2A	3183	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	1755	1/1	0.90	0.30	46,46,46,46	0
56	MG	1A	3172	1/1	0.90	0.09	52,52,52,52	0
56	MG	1A	3335	1/1	0.90	0.07	44,44,44,44	0
56	MG	1a	1758	1/1	0.90	0.34	49,49,49,49	0
56	MG	2A	3195	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3425	1/1	0.90	0.31	41,41,41,41	0
56	MG	2a	3066	1/1	0.90	0.22	48,48,48,48	0
56	MG	1A	3502	1/1	0.90	0.22	30,30,30,30	0
56	MG	1a	1642	1/1	0.90	0.26	41,41,41,41	0
56	MG	1A	3401	1/1	0.90	0.20	55,55,55,55	0
56	MG	2a	3073	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3829	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3437	1/1	0.90	0.21	33,33,33,33	0
56	MG	1e	201	1/1	0.90	0.09	73,73,73,73	0
56	MG	1f	201	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3506	1/1	0.90	0.10	41,41,41,41	0
56	MG	2A	3449	1/1	0.90	0.22	61,61,61,61	0
56	MG	2a	3087	1/1	0.90	0.20	67,67,67,67	0
56	MG	1x	103	1/1	0.90	0.21	55,55,55,55	0
56	MG	1A	3670	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3673	1/1	0.90	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3127	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3002	1/1	0.90	0.20	47,47,47,47	0
56	MG	1A	3129	1/1	0.90	0.07	45,45,45,45	0
56	MG	2a	3099	1/1	0.90	0.23	45,45,45,45	0
56	MG	2A	3232	1/1	0.90	0.28	63,63,63,63	0
56	MG	1A	3690	1/1	0.90	0.23	58,58,58,58	0
56	MG	1A	3845	1/1	0.90	0.33	47,47,47,47	0
56	MG	1A	3848	1/1	0.90	0.21	46,46,46,46	0
56	MG	1A	3341	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3291	1/1	0.90	0.19	33,33,33,33	0
56	MG	2A	3020	1/1	0.90	0.23	40,40,40,40	0
56	MG	2A	3535	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3694	1/1	0.90	0.13	40,40,40,40	0
56	MG	2A	3543	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	3143	1/1	0.90	0.08	41,41,41,41	0
56	MG	2A	3546	1/1	0.90	0.19	59,59,59,59	0
56	MG	2a	3116	1/1	0.90	0.23	51,51,51,51	0
56	MG	1A	3252	1/1	0.90	0.24	58,58,58,58	0
56	MG	1a	1673	1/1	0.90	0.29	47,47,47,47	0
56	MG	1A	3349	1/1	0.90	0.15	46,46,46,46	0
56	MG	1a	1678	1/1	0.90	0.06	45,45,45,45	0
56	MG	1A	3557	1/1	0.90	0.19	43,43,43,43	0
56	MG	2A	3040	1/1	0.90	0.28	55,55,55,55	0
56	MG	2a	3125	1/1	0.90	0.33	46,46,46,46	0
56	MG	2A	3042	1/1	0.90	0.13	31,31,31,31	0
56	MG	2A	3293	1/1	0.90	0.30	34,34,34,34	0
56	MG	2A	3299	1/1	0.90	0.11	46,46,46,46	0
56	MG	2A	3043	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3308	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3574	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3584	1/1	0.90	0.13	78,78,78,78	0
56	MG	1A	3567	1/1	0.90	0.16	59,59,59,59	0
56	MG	1A	3432	1/1	0.90	0.22	40,40,40,40	0
56	MG	2A	3314	1/1	0.90	0.08	40,40,40,40	0
56	MG	1A	3582	1/1	0.90	0.08	72,72,72,72	0
56	MG	1A	3434	1/1	0.90	0.17	53,53,53,53	0
56	MG	2q	202	1/1	0.90	0.15	77,77,77,77	0
56	MG	2A	3598	1/1	0.90	0.14	49,49,49,49	0
56	MG	1A	3146	1/1	0.90	0.24	40,40,40,40	0
56	MG	1F	308	1/1	0.90	0.15	33,33,33,33	0
56	MG	2A	3065	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3438	1/1	0.90	0.39	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3358	1/1	0.91	0.19	54,54,54,54	0
56	MG	1A	3225	1/1	0.91	0.16	35,35,35,35	0
56	MG	1A	3363	1/1	0.91	0.10	28,28,28,28	0
56	MG	2A	3621	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3364	1/1	0.91	0.07	40,40,40,40	0
56	MG	1a	1619	1/1	0.91	0.28	53,53,53,53	0
56	MG	2B	203	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3835	1/1	0.91	0.17	48,48,48,48	0
56	MG	1a	1743	1/1	0.91	0.28	34,34,34,34	0
56	MG	1A	3583	1/1	0.91	0.18	63,63,63,63	0
56	MG	1a	1747	1/1	0.91	0.26	46,46,46,46	0
56	MG	1A	3700	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3353	1/1	0.91	0.14	30,30,30,30	0
56	MG	2E	303	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3704	1/1	0.91	0.08	45,45,45,45	0
56	MG	1a	1633	1/1	0.91	0.22	56,56,56,56	0
56	MG	1A	3124	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3196	1/1	0.91	0.14	44,44,44,44	0
56	MG	1a	1638	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3079	1/1	0.91	0.07	32,32,32,32	0
56	MG	1B	210	1/1	0.91	0.11	41,41,41,41	0
56	MG	1a	1645	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3160	1/1	0.91	0.15	56,56,56,56	0
56	MG	2a	3001	1/1	0.91	0.29	55,55,55,55	0
56	MG	1A	3714	1/1	0.91	0.18	51,51,51,51	0
56	MG	2A	3166	1/1	0.91	0.10	72,72,72,72	0
56	MG	2a	3005	1/1	0.91	0.12	52,52,52,52	0
56	MG	1a	1761	1/1	0.91	0.34	36,36,36,36	0
56	MG	1A	3595	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3312	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3378	1/1	0.91	0.26	57,57,57,57	0
56	MG	2A	3380	1/1	0.91	0.17	44,44,44,44	0
56	MG	1A	3126	1/1	0.91	0.25	48,48,48,48	0
56	MG	1A	3019	1/1	0.91	0.21	39,39,39,39	0
56	MG	1A	3160	1/1	0.91	0.09	34,34,34,34	0
56	MG	1h	201	1/1	0.91	0.20	54,54,54,54	0
56	MG	2a	3022	1/1	0.91	0.08	68,68,68,68	0
56	MG	2A	3180	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	3325	1/1	0.91	0.11	52,52,52,52	0
56	MG	1x	101	1/1	0.91	0.24	26,26,26,26	0
56	MG	1x	102	1/1	0.91	0.12	45,45,45,45	0
56	MG	1a	1658	1/1	0.91	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	104	1/1	0.91	0.20	58,58,58,58	0
56	MG	2A	3192	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3057	1/1	0.91	0.18	20,20,20,20	0
56	MG	2a	3045	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3277	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3740	1/1	0.91	0.19	49,49,49,49	0
56	MG	1a	1663	1/1	0.91	0.21	53,53,53,53	0
56	MG	2A	3411	1/1	0.91	0.26	46,46,46,46	0
56	MG	2A	3202	1/1	0.91	0.14	44,44,44,44	0
56	MG	1A	3396	1/1	0.91	0.22	43,43,43,43	0
56	MG	2A	3006	1/1	0.91	0.21	46,46,46,46	0
56	MG	1E	308	1/1	0.91	0.17	39,39,39,39	0
56	MG	1a	1667	1/1	0.91	0.28	49,49,49,49	0
56	MG	1A	3484	1/1	0.91	0.10	51,51,51,51	0
56	MG	2A	3428	1/1	0.91	0.20	50,50,50,50	0
56	MG	2a	3060	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3242	1/1	0.91	0.06	43,43,43,43	0
56	MG	2A	3431	1/1	0.91	0.25	44,44,44,44	0
56	MG	1G	201	1/1	0.91	0.15	32,32,32,32	0
56	MG	1A	3400	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3141	1/1	0.91	0.07	41,41,41,41	0
56	MG	2A	3219	1/1	0.91	0.18	47,47,47,47	0
56	MG	2A	3221	1/1	0.91	0.22	42,42,42,42	0
56	MG	1A	3142	1/1	0.91	0.20	29,29,29,29	0
56	MG	2A	3448	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3225	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3229	1/1	0.91	0.21	56,56,56,56	0
56	MG	2A	3460	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3076	1/1	0.91	0.13	46,46,46,46	0
56	MG	1A	3059	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3030	1/1	0.91	0.22	54,54,54,54	0
56	MG	1R	203	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3485	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3489	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3224	1/1	0.91	0.11	33,33,33,33	0
56	MG	2A	3259	1/1	0.91	0.07	40,40,40,40	0
56	MG	2A	3497	1/1	0.91	0.17	45,45,45,45	0
56	MG	2a	3096	1/1	0.91	0.30	58,58,58,58	0
56	MG	2A	3500	1/1	0.91	0.08	58,58,58,58	0
56	MG	1A	3301	1/1	0.91	0.34	33,33,33,33	0
56	MG	2A	3039	1/1	0.91	0.06	42,42,42,42	0
56	MG	2A	3263	1/1	0.91	0.52	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3414	1/1	0.91	0.20	40,40,40,40	0
56	MG	2A	3517	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3266	1/1	0.91	0.21	38,38,38,38	0
56	MG	1a	1696	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3526	1/1	0.91	0.19	61,61,61,61	0
56	MG	1W	201	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3273	1/1	0.91	0.32	47,47,47,47	0
56	MG	2A	3044	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	1698	1/1	0.91	0.24	42,42,42,42	0
56	MG	1A	3417	1/1	0.91	0.12	30,30,30,30	0
56	MG	1a	1703	1/1	0.91	0.21	48,48,48,48	0
56	MG	2A	3284	1/1	0.91	0.28	47,47,47,47	0
56	MG	1A	3792	1/1	0.91	0.10	25,25,25,25	0
56	MG	1Z	302	1/1	0.91	0.04	39,39,39,39	0
56	MG	10	104	1/1	0.91	0.42	42,42,42,42	0
56	MG	10	105	1/1	0.91	0.18	35,35,35,35	0
56	MG	2A	3303	1/1	0.91	0.15	48,48,48,48	0
56	MG	11	101	1/1	0.91	0.07	36,36,36,36	0
56	MG	1A	3669	1/1	0.91	0.15	38,38,38,38	0
56	MG	15	102	1/1	0.91	0.23	31,31,31,31	0
56	MG	1A	3420	1/1	0.91	0.24	41,41,41,41	0
56	MG	1a	1721	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3575	1/1	0.91	0.10	48,48,48,48	0
56	MG	2a	3137	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3315	1/1	0.91	0.22	51,51,51,51	0
56	MG	2A	3083	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3811	1/1	0.91	0.21	17,17,17,17	0
56	MG	1A	3423	1/1	0.91	0.25	24,24,24,24	0
56	MG	1A	3675	1/1	0.91	0.24	59,59,59,59	0
56	MG	2A	3595	1/1	0.91	0.19	52,52,52,52	0
56	MG	2d	301	1/1	0.91	0.31	58,58,58,58	0
56	MG	1A	3678	1/1	0.91	0.08	35,35,35,35	0
56	MG	2A	3097	1/1	0.91	0.18	54,54,54,54	0
56	MG	2r	101	1/1	0.91	0.24	65,65,65,65	0
56	MG	2A	3330	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3101	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3549	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3104	1/1	0.91	0.16	38,38,38,38	0
56	MG	1A	3256	1/1	0.91	0.11	49,49,49,49	0
56	MG	2A	3614	1/1	0.92	0.11	38,38,38,38	0
56	MG	2A	3164	1/1	0.92	0.07	35,35,35,35	0
56	MG	1n	101	1/1	0.92	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3457	1/1	0.92	0.37	45,45,45,45	0
56	MG	1O	201	1/1	0.92	0.17	43,43,43,43	0
56	MG	2A	3168	1/1	0.92	0.18	54,54,54,54	0
56	MG	1A	3574	1/1	0.92	0.11	61,61,61,61	0
56	MG	2A	3171	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3676	1/1	0.92	0.31	67,67,67,67	0
56	MG	1A	3459	1/1	0.92	0.23	25,25,25,25	0
56	MG	1a	1670	1/1	0.92	0.22	34,34,34,34	0
56	MG	1A	3794	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3080	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3681	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3685	1/1	0.92	0.07	56,56,56,56	0
56	MG	1a	1680	1/1	0.92	0.43	60,60,60,60	0
56	MG	1A	3159	1/1	0.92	0.14	37,37,37,37	0
56	MG	1a	1683	1/1	0.92	0.15	53,53,53,53	0
56	MG	2V	202	1/1	0.92	0.07	53,53,53,53	0
56	MG	2Y	201	1/1	0.92	0.22	41,41,41,41	0
56	MG	2A	3189	1/1	0.92	0.20	49,49,49,49	0
56	MG	1a	1684	1/1	0.92	0.09	51,51,51,51	0
56	MG	2A	3382	1/1	0.92	0.23	53,53,53,53	0
56	MG	27	101	1/1	0.92	0.13	44,44,44,44	0
56	MG	2A	3191	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3817	1/1	0.92	0.07	47,47,47,47	0
56	MG	2A	3193	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3131	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3196	1/1	0.92	0.10	53,53,53,53	0
56	MG	10	102	1/1	0.92	0.07	49,49,49,49	0
56	MG	10	103	1/1	0.92	0.33	58,58,58,58	0
56	MG	1A	3167	1/1	0.92	0.14	63,63,63,63	0
56	MG	1A	3824	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3396	1/1	0.92	0.23	52,52,52,52	0
56	MG	1A	3116	1/1	0.92	0.16	44,44,44,44	0
56	MG	2a	3015	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3028	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3315	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3402	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3404	1/1	0.92	0.25	38,38,38,38	0
56	MG	1A	3066	1/1	0.92	0.15	39,39,39,39	0
56	MG	2a	3024	1/1	0.92	0.28	59,59,59,59	0
56	MG	1A	3697	1/1	0.92	0.08	25,25,25,25	0
56	MG	17	3103	1/1	0.92	0.15	37,37,37,37	0
56	MG	2a	3031	1/1	0.92	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3032	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3366	1/1	0.92	0.13	46,46,46,46	0
56	MG	2a	3034	1/1	0.92	0.33	57,57,57,57	0
56	MG	18	102	1/1	0.92	0.26	42,42,42,42	0
56	MG	2a	3036	1/1	0.92	0.14	58,58,58,58	0
56	MG	2a	3038	1/1	0.92	0.21	52,52,52,52	0
56	MG	2A	3414	1/1	0.92	0.15	45,45,45,45	0
56	MG	1a	1708	1/1	0.92	0.31	42,42,42,42	0
56	MG	2A	3218	1/1	0.92	0.26	49,49,49,49	0
56	MG	1A	3703	1/1	0.92	0.11	52,52,52,52	0
56	MG	1a	1601	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3045	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3492	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3052	1/1	0.92	0.17	32,32,32,32	0
56	MG	1A	3609	1/1	0.92	0.08	37,37,37,37	0
56	MG	2a	3052	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3234	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3434	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3235	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	1604	1/1	0.92	0.16	49,49,49,49	0
56	MG	2A	3237	1/1	0.92	0.23	57,57,57,57	0
56	MG	2A	3442	1/1	0.92	0.29	54,54,54,54	0
56	MG	2A	3238	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3241	1/1	0.92	0.28	42,42,42,42	0
56	MG	2A	3242	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3495	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3061	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3252	1/1	0.92	0.26	38,38,38,38	0
56	MG	1A	3048	1/1	0.92	0.18	50,50,50,50	0
56	MG	1a	1722	1/1	0.92	0.39	49,49,49,49	0
56	MG	2A	3473	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3055	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	3076	1/1	0.92	0.38	48,48,48,48	0
56	MG	1A	3249	1/1	0.92	0.08	58,58,58,58	0
56	MG	2a	3079	1/1	0.92	0.28	52,52,52,52	0
56	MG	1A	3332	1/1	0.92	0.07	50,50,50,50	0
56	MG	1a	1727	1/1	0.92	0.37	54,54,54,54	0
56	MG	2A	3490	1/1	0.92	0.19	47,47,47,47	0
56	MG	1B	203	1/1	0.92	0.13	61,61,61,61	0
56	MG	2A	3493	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3080	1/1	0.92	0.14	44,44,44,44	0
56	MG	2a	3089	1/1	0.92	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3727	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3027	1/1	0.92	0.19	30,30,30,30	0
56	MG	2A	3505	1/1	0.92	0.18	59,59,59,59	0
56	MG	1a	1622	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3507	1/1	0.92	0.12	68,68,68,68	0
56	MG	1a	1624	1/1	0.92	0.27	60,60,60,60	0
56	MG	2A	3278	1/1	0.92	0.23	23,23,23,23	0
56	MG	2A	3281	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3013	1/1	0.92	0.17	34,34,34,34	0
56	MG	1A	3431	1/1	0.92	0.16	42,42,42,42	0
56	MG	1A	3385	1/1	0.92	0.20	38,38,38,38	0
56	MG	2A	3524	1/1	0.92	0.17	55,55,55,55	0
56	MG	2A	3099	1/1	0.92	0.21	44,44,44,44	0
56	MG	1a	1629	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3193	1/1	0.92	0.27	34,34,34,34	0
56	MG	1A	3654	1/1	0.92	0.09	42,42,42,42	0
56	MG	2a	3109	1/1	0.92	0.22	60,60,60,60	0
56	MG	2a	3110	1/1	0.92	0.17	60,60,60,60	0
56	MG	1a	1635	1/1	0.92	0.29	57,57,57,57	0
56	MG	2A	3112	1/1	0.92	0.26	51,51,51,51	0
56	MG	2A	3114	1/1	0.92	0.11	46,46,46,46	0
56	MG	2a	3114	1/1	0.92	0.23	59,59,59,59	0
56	MG	2A	3115	1/1	0.92	0.07	53,53,53,53	0
56	MG	1A	3656	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3340	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3123	1/1	0.92	0.13	51,51,51,51	0
56	MG	1a	1641	1/1	0.92	0.15	57,57,57,57	0
56	MG	1D	306	1/1	0.92	0.17	47,47,47,47	0
56	MG	2A	3319	1/1	0.92	0.35	51,51,51,51	0
56	MG	2A	3322	1/1	0.92	0.22	44,44,44,44	0
56	MG	2A	3568	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3323	1/1	0.92	0.11	50,50,50,50	0
56	MG	1D	308	1/1	0.92	0.18	41,41,41,41	0
56	MG	1E	303	1/1	0.92	0.17	33,33,33,33	0
56	MG	2A	3327	1/1	0.92	0.14	40,40,40,40	0
56	MG	2a	3135	1/1	0.92	0.19	64,64,64,64	0
56	MG	2A	3577	1/1	0.92	0.12	65,65,65,65	0
56	MG	1E	304	1/1	0.92	0.08	42,42,42,42	0
56	MG	1A	3390	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3142	1/1	0.92	0.16	44,44,44,44	0
56	MG	1A	3062	1/1	0.92	0.11	28,28,28,28	0
56	MG	1A	3663	1/1	0.92	0.50	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3232	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	3551	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3155	1/1	0.92	0.07	47,47,47,47	0
56	MG	2j	201	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3456	1/1	0.92	0.43	49,49,49,49	0
56	MG	1A	3772	1/1	0.92	0.09	59,59,59,59	0
56	MG	1I	201	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3563	1/1	0.92	0.19	57,57,57,57	0
56	MG	1l	202	1/1	0.92	0.20	53,53,53,53	0
56	MG	2A	3611	1/1	0.92	0.17	41,41,41,41	0
56	MG	1l	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3161	1/1	0.92	0.10	48,48,48,48	0
56	MG	2x	104	1/1	0.92	0.26	41,41,41,41	0
59	K	2x	101	1/1	0.92	0.19	78,78,78,78	0
56	MG	2A	3111	1/1	0.93	0.20	38,38,38,38	0
56	MG	1A	3330	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3052	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3605	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3200	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3607	1/1	0.93	0.23	49,49,49,49	0
56	MG	2A	3609	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3117	1/1	0.93	0.32	53,53,53,53	0
56	MG	1A	3604	1/1	0.93	0.15	51,51,51,51	0
56	MG	15	104	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3202	1/1	0.93	0.23	38,38,38,38	0
56	MG	2A	3124	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3619	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	3053	1/1	0.93	0.08	32,32,32,32	0
56	MG	17	3105	1/1	0.93	0.08	28,28,28,28	0
56	MG	1A	3206	1/1	0.93	0.16	32,32,32,32	0
56	MG	2A	3625	1/1	0.93	0.26	51,51,51,51	0
56	MG	2B	201	1/1	0.93	0.27	67,67,67,67	0
56	MG	2A	3131	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3001	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3265	1/1	0.93	0.11	45,45,45,45	0
56	MG	2B	206	1/1	0.93	0.28	64,64,64,64	0
56	MG	2A	3138	1/1	0.93	0.06	32,32,32,32	0
56	MG	1A	3623	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3211	1/1	0.93	0.33	38,38,38,38	0
56	MG	1A	3442	1/1	0.93	0.25	36,36,36,36	0
56	MG	1A	3038	1/1	0.93	0.29	43,43,43,43	0
56	MG	2E	301	1/1	0.93	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3213	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	3272	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3353	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3026	1/1	0.93	0.09	45,45,45,45	0
56	MG	1a	1614	1/1	0.93	0.19	52,52,52,52	0
56	MG	2Q	201	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3818	1/1	0.93	0.16	28,28,28,28	0
56	MG	2A	3361	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1616	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3653	1/1	0.93	0.33	43,43,43,43	0
56	MG	20	101	1/1	0.93	0.32	63,63,63,63	0
56	MG	1A	3041	1/1	0.93	0.09	38,38,38,38	0
56	MG	1a	1620	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3162	1/1	0.93	0.13	68,68,68,68	0
56	MG	27	102	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3014	1/1	0.93	0.07	24,24,24,24	0
56	MG	2A	3372	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3219	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3069	1/1	0.93	0.17	36,36,36,36	0
56	MG	1A	3661	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3286	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3169	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3478	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3831	1/1	0.93	0.18	71,71,71,71	0
56	MG	1a	1630	1/1	0.93	0.16	38,38,38,38	0
56	MG	1a	1632	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3369	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3165	1/1	0.93	0.12	29,29,29,29	0
56	MG	2A	3178	1/1	0.93	0.06	47,47,47,47	0
56	MG	2A	3390	1/1	0.93	0.17	46,46,46,46	0
56	MG	2a	3020	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3482	1/1	0.93	0.13	37,37,37,37	0
56	MG	1A	3090	1/1	0.93	0.07	27,27,27,27	0
56	MG	1A	3128	1/1	0.93	0.19	51,51,51,51	0
56	MG	1A	3173	1/1	0.93	0.12	52,52,52,52	0
56	MG	2a	3026	1/1	0.93	0.13	54,54,54,54	0
56	MG	2a	3028	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3382	1/1	0.93	0.27	57,57,57,57	0
56	MG	2A	3186	1/1	0.93	0.14	52,52,52,52	0
56	MG	1a	1643	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3498	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3677	1/1	0.93	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	209	1/1	0.93	0.07	48,48,48,48	0
56	MG	1x	109	1/1	0.93	0.23	60,60,60,60	0
56	MG	2a	3037	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3174	1/1	0.93	0.12	41,41,41,41	0
56	MG	2A	3408	1/1	0.93	0.32	43,43,43,43	0
56	MG	2a	3041	1/1	0.93	0.33	58,58,58,58	0
56	MG	1A	3299	1/1	0.93	0.12	31,31,31,31	0
56	MG	2A	3003	1/1	0.93	0.14	45,45,45,45	0
56	MG	1a	1651	1/1	0.93	0.18	44,44,44,44	0
56	MG	1A	3680	1/1	0.93	0.14	38,38,38,38	0
56	MG	1a	1653	1/1	0.93	0.18	42,42,42,42	0
56	MG	1A	3070	1/1	0.93	0.07	32,32,32,32	0
56	MG	2A	3420	1/1	0.93	0.28	42,42,42,42	0
56	MG	2a	3050	1/1	0.93	0.21	31,31,31,31	0
56	MG	1A	3130	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3204	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3014	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3504	1/1	0.93	0.11	49,49,49,49	0
56	MG	1B	220	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3303	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	3391	1/1	0.93	0.32	35,35,35,35	0
56	MG	1A	3029	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3235	1/1	0.93	0.05	15,15,15,15	0
56	MG	2A	3436	1/1	0.93	0.23	40,40,40,40	0
56	MG	2a	3062	1/1	0.93	0.22	62,62,62,62	0
56	MG	1A	3236	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3026	1/1	0.93	0.15	60,60,60,60	0
56	MG	2A	3441	1/1	0.93	0.26	21,21,21,21	0
56	MG	2A	3027	1/1	0.93	0.15	34,34,34,34	0
56	MG	1E	302	1/1	0.93	0.12	34,34,34,34	0
56	MG	2a	3068	1/1	0.93	0.25	48,48,48,48	0
56	MG	1A	3398	1/1	0.93	0.24	48,48,48,48	0
56	MG	1A	3180	1/1	0.93	0.10	38,38,38,38	0
56	MG	1A	3181	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3104	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3402	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3463	1/1	0.93	0.11	47,47,47,47	0
56	MG	2a	3080	1/1	0.93	0.26	37,37,37,37	0
56	MG	1A	3403	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3041	1/1	0.93	0.06	35,35,35,35	0
56	MG	1F	302	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3711	1/1	0.93	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3562	1/1	0.93	0.10	61,61,61,61	0
56	MG	1A	3713	1/1	0.93	0.13	51,51,51,51	0
56	MG	2a	3088	1/1	0.93	0.17	48,48,48,48	0
56	MG	2A	3486	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3243	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3048	1/1	0.93	0.28	58,58,58,58	0
56	MG	2A	3246	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3248	1/1	0.93	0.10	40,40,40,40	0
56	MG	1G	204	1/1	0.93	0.21	44,44,44,44	0
56	MG	2A	3250	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3498	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3251	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3107	1/1	0.93	0.12	29,29,29,29	0
56	MG	2A	3253	1/1	0.93	0.17	63,63,63,63	0
56	MG	2A	3053	1/1	0.93	0.31	53,53,53,53	0
56	MG	1A	3565	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3317	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3717	1/1	0.93	0.11	33,33,33,33	0
56	MG	2A	3262	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3518	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3719	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3522	1/1	0.93	0.09	41,41,41,41	0
56	MG	1Q	201	1/1	0.93	0.20	34,34,34,34	0
56	MG	1A	3725	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3572	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3067	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3189	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3538	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1699	1/1	0.93	0.23	27,27,27,27	0
56	MG	1A	3319	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3073	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3549	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3076	1/1	0.93	0.14	43,43,43,43	0
56	MG	1a	1702	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3411	1/1	0.93	0.44	54,54,54,54	0
56	MG	2A	3555	1/1	0.93	0.13	37,37,37,37	0
56	MG	1a	1704	1/1	0.93	0.28	41,41,41,41	0
56	MG	2a	3129	1/1	0.93	0.09	46,46,46,46	0
56	MG	2A	3558	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3285	1/1	0.93	0.22	36,36,36,36	0
56	MG	2A	3562	1/1	0.93	0.13	53,53,53,53	0
56	MG	2A	3286	1/1	0.93	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3320	1/1	0.93	0.25	59,59,59,59	0
56	MG	2A	3290	1/1	0.93	0.23	36,36,36,36	0
56	MG	2A	3084	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3110	1/1	0.93	0.15	42,42,42,42	0
56	MG	1W	203	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3589	1/1	0.93	0.09	67,67,67,67	0
56	MG	2A	3095	1/1	0.93	0.11	38,38,38,38	0
56	MG	1a	1711	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3144	1/1	0.93	0.05	34,34,34,34	0
56	MG	2k	201	1/1	0.93	0.08	63,63,63,63	0
56	MG	2l	201	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3578	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3592	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3593	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3747	1/1	0.93	0.13	65,65,65,65	0
56	MG	2A	3316	1/1	0.93	0.22	44,44,44,44	0
56	MG	2A	3103	1/1	0.93	0.30	57,57,57,57	0
56	MG	1A	3248	1/1	0.93	0.09	49,49,49,49	0
56	MG	2A	3596	1/1	0.93	0.26	50,50,50,50	0
56	MG	2A	3106	1/1	0.93	0.13	33,33,33,33	0
56	MG	1a	1720	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3600	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3452	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3183	1/1	0.94	0.21	55,55,55,55	0
56	MG	2A	3320	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3604	1/1	0.94	0.11	51,51,51,51	0
56	MG	13	102	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3287	1/1	0.94	0.19	44,44,44,44	0
56	MG	2A	3324	1/1	0.94	0.18	53,53,53,53	0
56	MG	1A	3773	1/1	0.94	0.09	69,69,69,69	0
56	MG	2A	3122	1/1	0.94	0.19	54,54,54,54	0
56	MG	15	105	1/1	0.94	0.18	37,37,37,37	0
56	MG	1a	1731	1/1	0.94	0.20	34,34,34,34	0
56	MG	2A	3125	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3231	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3331	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3777	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3129	1/1	0.94	0.06	42,42,42,42	0
56	MG	17	3104	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3778	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3132	1/1	0.94	0.25	58,58,58,58	0
56	MG	1A	3458	1/1	0.94	0.34	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	18	101	1/1	0.94	0.08	39,39,39,39	0
56	MG	2B	204	1/1	0.94	0.07	62,62,62,62	0
56	MG	1a	1741	1/1	0.94	0.31	46,46,46,46	0
56	MG	1A	3365	1/1	0.94	0.16	30,30,30,30	0
56	MG	2A	3141	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3148	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3119	1/1	0.94	0.08	44,44,44,44	0
56	MG	1a	1745	1/1	0.94	0.28	44,44,44,44	0
56	MG	1A	3793	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3463	1/1	0.94	0.07	44,44,44,44	0
56	MG	2E	302	1/1	0.94	0.16	29,29,29,29	0
56	MG	2A	3149	1/1	0.94	0.27	55,55,55,55	0
56	MG	2E	304	1/1	0.94	0.27	52,52,52,52	0
56	MG	1A	3089	1/1	0.94	0.39	51,51,51,51	0
56	MG	2A	3151	1/1	0.94	0.42	53,53,53,53	0
56	MG	2F	303	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3358	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3034	1/1	0.94	0.14	41,41,41,41	0
56	MG	2P	202	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3036	1/1	0.94	0.18	42,42,42,42	0
56	MG	2R	201	1/1	0.94	0.08	31,31,31,31	0
56	MG	2A	3362	1/1	0.94	0.19	30,30,30,30	0
56	MG	2T	202	1/1	0.94	0.22	50,50,50,50	0
56	MG	2A	3363	1/1	0.94	0.18	43,43,43,43	0
56	MG	2W	201	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3237	1/1	0.94	0.06	45,45,45,45	0
56	MG	1A	3814	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3816	1/1	0.94	0.10	55,55,55,55	0
56	MG	21	101	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3012	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3381	1/1	0.94	0.15	45,45,45,45	0
56	MG	1a	1617	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3163	1/1	0.94	0.24	30,30,30,30	0
56	MG	1A	3199	1/1	0.94	0.11	74,74,74,74	0
56	MG	1A	3305	1/1	0.94	0.08	32,32,32,32	0
56	MG	2a	3002	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3306	1/1	0.94	0.30	48,48,48,48	0
56	MG	1A	3387	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3101	1/1	0.94	0.09	36,36,36,36	0
56	MG	2A	3379	1/1	0.94	0.31	34,34,34,34	0
56	MG	1e	202	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3381	1/1	0.94	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3665	1/1	0.94	0.06	33,33,33,33	0
56	MG	2a	3010	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3102	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3385	1/1	0.94	0.18	53,53,53,53	0
56	MG	2a	3014	1/1	0.94	0.17	35,35,35,35	0
56	MG	1a	1626	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3161	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3204	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3175	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3205	1/1	0.94	0.18	27,27,27,27	0
56	MG	1v	101	1/1	0.94	0.30	41,41,41,41	0
56	MG	1A	3247	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3393	1/1	0.94	0.23	30,30,30,30	0
56	MG	1A	3836	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3181	1/1	0.94	0.04	57,57,57,57	0
56	MG	1A	3028	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3208	1/1	0.94	0.23	41,41,41,41	0
56	MG	2a	3030	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3250	1/1	0.94	0.20	30,30,30,30	0
56	MG	1A	3527	1/1	0.94	0.09	23,23,23,23	0
56	MG	1x	108	1/1	0.94	0.21	44,44,44,44	0
56	MG	2A	3403	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3188	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3009	1/1	0.94	0.16	33,33,33,33	0
56	MG	1a	1639	1/1	0.94	0.12	40,40,40,40	0
56	MG	1z	101	1/1	0.94	0.20	49,49,49,49	0
56	MG	2a	3039	1/1	0.94	0.12	58,58,58,58	0
56	MG	1a	1640	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3847	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3531	1/1	0.94	0.09	46,46,46,46	0
56	MG	1B	201	1/1	0.94	0.06	31,31,31,31	0
56	MG	1B	202	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3534	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3683	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3171	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3423	1/1	0.94	0.25	34,34,34,34	0
56	MG	1A	3032	1/1	0.94	0.23	44,44,44,44	0
56	MG	1A	3689	1/1	0.94	0.06	43,43,43,43	0
56	MG	2A	3205	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3137	1/1	0.94	0.11	33,33,33,33	0
56	MG	2A	3430	1/1	0.94	0.23	20,20,20,20	0
56	MG	1A	3138	1/1	0.94	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3547	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3433	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3260	1/1	0.94	0.21	48,48,48,48	0
56	MG	1A	3112	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3333	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3214	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3409	1/1	0.94	0.15	38,38,38,38	0
56	MG	2A	3216	1/1	0.94	0.19	41,41,41,41	0
56	MG	1A	3558	1/1	0.94	0.08	49,49,49,49	0
56	MG	1a	1661	1/1	0.94	0.05	45,45,45,45	0
56	MG	2A	3031	1/1	0.94	0.05	44,44,44,44	0
56	MG	1A	3561	1/1	0.94	0.08	26,26,26,26	0
56	MG	1A	3266	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3412	1/1	0.94	0.07	28,28,28,28	0
56	MG	2A	3451	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3455	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3227	1/1	0.94	0.11	28,28,28,28	0
56	MG	2A	3228	1/1	0.94	0.40	45,45,45,45	0
56	MG	1A	3710	1/1	0.94	0.06	50,50,50,50	0
56	MG	1A	3336	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3566	1/1	0.94	0.12	38,38,38,38	0
56	MG	2a	3083	1/1	0.94	0.24	40,40,40,40	0
56	MG	1A	3267	1/1	0.94	0.29	61,61,61,61	0
56	MG	1A	3570	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3338	1/1	0.94	0.13	39,39,39,39	0
56	MG	1a	1674	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3573	1/1	0.94	0.07	53,53,53,53	0
56	MG	1F	307	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3046	1/1	0.94	0.27	46,46,46,46	0
56	MG	1F	312	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3422	1/1	0.94	0.16	27,27,27,27	0
56	MG	1G	202	1/1	0.94	0.19	37,37,37,37	0
56	MG	1A	3218	1/1	0.94	0.14	39,39,39,39	0
56	MG	1a	1687	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3177	1/1	0.94	0.14	53,53,53,53	0
56	MG	2a	3098	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3584	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3731	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3066	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3513	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1693	1/1	0.94	0.23	34,34,34,34	0
56	MG	1A	3733	1/1	0.94	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3428	1/1	0.94	0.38	58,58,58,58	0
56	MG	1A	3178	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3344	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3082	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3018	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3078	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	3435	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3272	1/1	0.94	0.20	46,46,46,46	0
56	MG	1U	202	1/1	0.94	0.09	32,32,32,32	0
56	MG	1U	203	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3541	1/1	0.94	0.20	38,38,38,38	0
56	MG	2A	3275	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3049	1/1	0.94	0.27	47,47,47,47	0
56	MG	2A	3085	1/1	0.94	0.14	42,42,42,42	0
56	MG	2A	3280	1/1	0.94	0.17	49,49,49,49	0
56	MG	2a	3121	1/1	0.94	0.25	48,48,48,48	0
56	MG	2A	3086	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3551	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3744	1/1	0.94	0.11	22,22,22,22	0
56	MG	1V	204	1/1	0.94	0.06	44,44,44,44	0
56	MG	1a	1707	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3091	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3745	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3559	1/1	0.94	0.11	64,64,64,64	0
56	MG	2a	3133	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3351	1/1	0.94	0.15	49,49,49,49	0
56	MG	1a	1710	1/1	0.94	0.45	55,55,55,55	0
56	MG	2A	3098	1/1	0.94	0.26	35,35,35,35	0
56	MG	2A	3292	1/1	0.94	0.24	32,32,32,32	0
56	MG	1A	3226	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3297	1/1	0.94	0.29	57,57,57,57	0
56	MG	2a	3141	1/1	0.94	0.22	46,46,46,46	0
56	MG	1X	102	1/1	0.94	0.10	58,58,58,58	0
56	MG	2a	3143	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3301	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3572	1/1	0.94	0.11	56,56,56,56	0
56	MG	2A	3302	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3283	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3304	1/1	0.94	0.25	49,49,49,49	0
56	MG	1Y	201	1/1	0.94	0.05	61,61,61,61	0
56	MG	2l	202	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3307	1/1	0.94	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3182	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3310	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3311	1/1	0.94	0.26	54,54,54,54	0
56	MG	2A	3105	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3449	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3759	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3760	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3613	1/1	0.94	0.08	27,27,27,27	0
57	ZN	24	501	1/1	0.94	0.09	130,130,130,130	0
56	MG	2A	3113	1/1	0.94	0.19	68,68,68,68	0
56	MG	2A	3213	1/1	0.95	0.23	55,55,55,55	0
56	MG	14	101	1/1	0.95	0.28	56,56,56,56	0
56	MG	1A	3051	1/1	0.95	0.09	43,43,43,43	0
56	MG	2D	301	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3217	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3833	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3068	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3834	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3606	1/1	0.95	0.20	32,32,32,32	0
56	MG	1a	1714	1/1	0.95	0.22	32,32,32,32	0
56	MG	2A	3224	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3134	1/1	0.95	0.11	32,32,32,32	0
56	MG	2A	3226	1/1	0.95	0.19	27,27,27,27	0
56	MG	1A	3610	1/1	0.95	0.08	35,35,35,35	0
56	MG	2A	3400	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.11	36,36,36,36	0
56	MG	1a	1718	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3230	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3079	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3612	1/1	0.95	0.06	34,34,34,34	0
56	MG	2A	3081	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3424	1/1	0.95	0.17	31,31,31,31	0
56	MG	1A	3136	1/1	0.95	0.05	32,32,32,32	0
56	MG	1A	3327	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3720	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3328	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3726	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3417	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3418	1/1	0.95	0.19	37,37,37,37	0
56	MG	2A	3244	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3620	1/1	0.95	0.15	29,29,29,29	0
56	MG	1A	3220	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3422	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3247	1/1	0.95	0.25	50,50,50,50	0
56	MG	1a	1607	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3092	1/1	0.95	0.13	49,49,49,49	0
56	MG	1a	1609	1/1	0.95	0.21	41,41,41,41	0
56	MG	1a	1610	1/1	0.95	0.16	28,28,28,28	0
56	MG	1B	204	1/1	0.95	0.12	38,38,38,38	0
56	MG	1B	205	1/1	0.95	0.21	53,53,53,53	0
56	MG	1B	208	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3256	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3100	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	3624	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3293	1/1	0.95	0.12	41,41,41,41	0
56	MG	1B	211	1/1	0.95	0.27	39,39,39,39	0
56	MG	1A	3524	1/1	0.95	0.06	51,51,51,51	0
56	MG	2a	3021	1/1	0.95	0.10	68,68,68,68	0
56	MG	2A	3439	1/1	0.95	0.25	47,47,47,47	0
56	MG	2A	3440	1/1	0.95	0.28	38,38,38,38	0
56	MG	1A	3190	1/1	0.95	0.19	37,37,37,37	0
56	MG	1B	214	1/1	0.95	0.18	45,45,45,45	0
56	MG	2A	3108	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3639	1/1	0.95	0.08	67,67,67,67	0
56	MG	2A	3110	1/1	0.95	0.11	49,49,49,49	0
56	MG	1B	217	1/1	0.95	0.08	43,43,43,43	0
56	MG	1a	1623	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3010	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3436	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3095	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3279	1/1	0.95	0.26	27,27,27,27	0
56	MG	1A	3298	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3467	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3651	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3472	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3140	1/1	0.95	0.11	37,37,37,37	0
56	MG	1D	303	1/1	0.95	0.09	55,55,55,55	0
56	MG	2a	3042	1/1	0.95	0.12	51,51,51,51	0
56	MG	1D	305	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3541	1/1	0.95	0.09	30,30,30,30	0
56	MG	1A	3542	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3287	1/1	0.95	0.12	38,38,38,38	0
56	MG	1a	1762	1/1	0.95	0.12	50,50,50,50	0
56	MG	2A	3491	1/1	0.95	0.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1E	301	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3657	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3494	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3198	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	3443	1/1	0.95	0.22	33,33,33,33	0
56	MG	2A	3294	1/1	0.95	0.30	51,51,51,51	0
56	MG	2A	3295	1/1	0.95	0.25	38,38,38,38	0
56	MG	2A	3504	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3296	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3169	1/1	0.95	0.20	50,50,50,50	0
56	MG	2A	3133	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3508	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	3447	1/1	0.95	0.18	47,47,47,47	0
56	MG	1f	202	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3137	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3448	1/1	0.95	0.05	17,17,17,17	0
56	MG	1A	3394	1/1	0.95	0.25	42,42,42,42	0
56	MG	2A	3306	1/1	0.95	0.19	35,35,35,35	0
56	MG	1F	301	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3555	1/1	0.95	0.12	35,35,35,35	0
56	MG	2a	3070	1/1	0.95	0.26	43,43,43,43	0
56	MG	2a	3071	1/1	0.95	0.23	44,44,44,44	0
56	MG	1F	303	1/1	0.95	0.15	36,36,36,36	0
56	MG	2A	3144	1/1	0.95	0.14	35,35,35,35	0
56	MG	2a	3074	1/1	0.95	0.18	40,40,40,40	0
56	MG	1A	3096	1/1	0.95	0.08	41,41,41,41	0
56	MG	2a	3077	1/1	0.95	0.26	46,46,46,46	0
56	MG	2A	3530	1/1	0.95	0.06	39,39,39,39	0
56	MG	1a	1649	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3304	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3047	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3540	1/1	0.95	0.15	39,39,39,39	0
56	MG	1F	311	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3542	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3042	1/1	0.95	0.21	33,33,33,33	0
56	MG	2A	3544	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3071	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3779	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3548	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3780	1/1	0.95	0.14	64,64,64,64	0
56	MG	1A	3348	1/1	0.95	0.23	34,34,34,34	0
56	MG	1A	3103	1/1	0.95	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3056	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3553	1/1	0.95	0.11	62,62,62,62	0
56	MG	2a	3095	1/1	0.95	0.29	57,57,57,57	0
56	MG	1A	3789	1/1	0.95	0.11	29,29,29,29	0
56	MG	1A	3790	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3310	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3007	1/1	0.95	0.15	49,49,49,49	0
56	MG	1A	3464	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	3466	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3106	1/1	0.95	0.20	35,35,35,35	0
56	MG	1a	1668	1/1	0.95	0.21	31,31,31,31	0
56	MG	2A	3564	1/1	0.95	0.07	47,47,47,47	0
56	MG	1R	204	1/1	0.95	0.28	51,51,51,51	0
56	MG	2A	3018	1/1	0.95	0.05	44,44,44,44	0
56	MG	1R	206	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	3471	1/1	0.95	0.15	44,44,44,44	0
56	MG	1T	202	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3022	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3805	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3808	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3342	1/1	0.95	0.19	21,21,21,21	0
56	MG	1A	3579	1/1	0.95	0.06	41,41,41,41	0
56	MG	1a	1679	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3581	1/1	0.95	0.07	81,81,81,81	0
56	MG	1A	3472	1/1	0.95	0.12	27,27,27,27	0
56	MG	1V	203	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3348	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3182	1/1	0.95	0.24	58,58,58,58	0
56	MG	1a	1682	1/1	0.95	0.25	35,35,35,35	0
56	MG	2A	3593	1/1	0.95	0.19	45,45,45,45	0
56	MG	2A	3594	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3354	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3356	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3815	1/1	0.95	0.10	30,30,30,30	0
56	MG	1A	3005	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3086	1/1	0.95	0.11	33,33,33,33	0
56	MG	2A	3038	1/1	0.95	0.05	54,54,54,54	0
56	MG	2a	3134	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3360	1/1	0.95	0.15	32,32,32,32	0
56	MG	1W	205	1/1	0.95	0.07	38,38,38,38	0
56	MG	1X	101	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3410	1/1	0.95	0.29	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3314	1/1	0.95	0.26	38,38,38,38	0
56	MG	1A	3820	1/1	0.95	0.19	41,41,41,41	0
56	MG	1Z	301	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3153	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3047	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3369	1/1	0.95	0.17	58,58,58,58	0
56	MG	2A	3198	1/1	0.95	0.27	47,47,47,47	0
56	MG	2A	3371	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3615	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3618	1/1	0.95	0.09	54,54,54,54	0
56	MG	10	101	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3050	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3374	1/1	0.95	0.34	47,47,47,47	0
56	MG	1A	3822	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3050	1/1	0.95	0.28	49,49,49,49	0
56	MG	1A	3487	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3156	1/1	0.95	0.26	51,51,51,51	0
56	MG	2A	3056	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3494	1/1	0.95	0.07	24,24,24,24	0
56	MG	2A	3059	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3157	1/1	0.95	0.10	46,46,46,46	0
56	MG	12	101	1/1	0.95	0.05	37,37,37,37	0
56	MG	1A	3602	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3220	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	3075	1/1	0.96	0.14	28,28,28,28	0
56	MG	2A	3222	1/1	0.96	0.04	47,47,47,47	0
56	MG	1A	3645	1/1	0.96	0.08	50,50,50,50	0
56	MG	1V	202	1/1	0.96	0.33	34,34,34,34	0
56	MG	1A	3039	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3499	1/1	0.96	0.16	23,23,23,23	0
56	MG	2A	3398	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3343	1/1	0.96	0.12	34,34,34,34	0
56	MG	2B	212	1/1	0.96	0.19	49,49,49,49	0
56	MG	1A	3650	1/1	0.96	0.09	29,29,29,29	0
56	MG	2D	302	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3246	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3797	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3231	1/1	0.96	0.19	50,50,50,50	0
56	MG	1W	206	1/1	0.96	0.06	25,25,25,25	0
56	MG	2E	305	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3405	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3799	1/1	0.96	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3072	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3008	1/1	0.96	0.06	22,22,22,22	0
56	MG	2A	3074	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3346	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3412	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3239	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3240	1/1	0.96	0.30	41,41,41,41	0
56	MG	1A	3806	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3060	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3505	1/1	0.96	0.13	48,48,48,48	0
56	MG	1A	3061	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3300	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3516	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3517	1/1	0.96	0.05	43,43,43,43	0
56	MG	23	101	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3520	1/1	0.96	0.08	37,37,37,37	0
56	MG	25	101	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3419	1/1	0.96	0.18	18,18,18,18	0
56	MG	1A	3132	1/1	0.96	0.24	40,40,40,40	0
56	MG	2A	3427	1/1	0.96	0.33	42,42,42,42	0
56	MG	1A	3251	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3088	1/1	0.96	0.11	35,35,35,35	0
56	MG	12	102	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3133	1/1	0.96	0.03	31,31,31,31	0
56	MG	2A	3255	1/1	0.96	0.07	65,65,65,65	0
56	MG	13	103	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3257	1/1	0.96	0.34	51,51,51,51	0
56	MG	1A	3533	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3354	1/1	0.96	0.10	40,40,40,40	0
56	MG	15	103	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3672	1/1	0.96	0.17	46,46,46,46	0
56	MG	2a	3011	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3355	1/1	0.96	0.36	45,45,45,45	0
56	MG	2A	3264	1/1	0.96	0.19	47,47,47,47	0
56	MG	1a	1726	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3674	1/1	0.96	0.08	58,58,58,58	0
56	MG	17	3102	1/1	0.96	0.07	27,27,27,27	0
56	MG	2A	3445	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3446	1/1	0.96	0.11	35,35,35,35	0
56	MG	2a	3019	1/1	0.96	0.16	55,55,55,55	0
56	MG	2A	3269	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3253	1/1	0.96	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3429	1/1	0.96	0.20	31,31,31,31	0
56	MG	1A	3021	1/1	0.96	0.14	37,37,37,37	0
56	MG	1a	1733	1/1	0.96	0.20	25,25,25,25	0
56	MG	2A	3452	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3135	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3458	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3459	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3107	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3362	1/1	0.96	0.24	46,46,46,46	0
56	MG	1A	3433	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3191	1/1	0.96	0.19	41,41,41,41	0
56	MG	18	104	1/1	0.96	0.13	18,18,18,18	0
56	MG	1A	3682	1/1	0.96	0.05	39,39,39,39	0
56	MG	1A	3223	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3474	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3481	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3482	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3684	1/1	0.96	0.07	30,30,30,30	0
56	MG	1A	3840	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3116	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3552	1/1	0.96	0.06	14,14,14,14	0
56	MG	1a	1746	1/1	0.96	0.26	34,34,34,34	0
56	MG	2A	3119	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3686	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3843	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1749	1/1	0.96	0.24	31,31,31,31	0
56	MG	1A	3063	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3263	1/1	0.96	0.26	38,38,38,38	0
56	MG	2A	3496	1/1	0.96	0.14	41,41,41,41	0
56	MG	1a	1611	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3556	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3298	1/1	0.96	0.25	44,44,44,44	0
56	MG	1a	1754	1/1	0.96	0.24	49,49,49,49	0
56	MG	1A	3367	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3162	1/1	0.96	0.17	36,36,36,36	0
56	MG	2a	3058	1/1	0.96	0.35	53,53,53,53	0
56	MG	1A	3559	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3440	1/1	0.96	0.23	46,46,46,46	0
56	MG	2A	3510	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3134	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3441	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3514	1/1	0.96	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1760	1/1	0.96	0.25	37,37,37,37	0
56	MG	1A	3698	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3309	1/1	0.96	0.08	65,65,65,65	0
56	MG	1B	207	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3064	1/1	0.96	0.05	58,58,58,58	0
56	MG	1A	3166	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3444	1/1	0.96	0.06	33,33,33,33	0
56	MG	1d	301	1/1	0.96	0.29	57,57,57,57	0
56	MG	2A	3525	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3268	1/1	0.96	0.15	43,43,43,43	0
56	MG	2a	3075	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3527	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3145	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3533	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3534	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3375	1/1	0.96	0.24	44,44,44,44	0
56	MG	1A	3709	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3376	1/1	0.96	0.12	25,25,25,25	0
56	MG	1A	3229	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3450	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3379	1/1	0.96	0.18	38,38,38,38	0
56	MG	1A	3577	1/1	0.96	0.06	61,61,61,61	0
56	MG	1a	1631	1/1	0.96	0.17	56,56,56,56	0
56	MG	1s	101	1/1	0.96	0.21	55,55,55,55	0
56	MG	1A	3453	1/1	0.96	0.27	48,48,48,48	0
56	MG	1A	3454	1/1	0.96	0.18	56,56,56,56	0
56	MG	1A	3316	1/1	0.96	0.19	45,45,45,45	0
56	MG	1A	3035	1/1	0.96	0.06	33,33,33,33	0
56	MG	1D	302	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	3067	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3201	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3384	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3170	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3323	1/1	0.96	0.22	48,48,48,48	0
56	MG	1A	3030	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3045	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3465	1/1	0.96	0.07	26,26,26,26	0
56	MG	2A	3561	1/1	0.96	0.09	51,51,51,51	0
56	MG	1a	1646	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3092	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3278	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3603	1/1	0.96	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3470	1/1	0.96	0.17	40,40,40,40	0
56	MG	2A	3011	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3392	1/1	0.96	0.12	23,23,23,23	0
56	MG	2A	3349	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3350	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3282	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3352	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3329	1/1	0.96	0.22	34,34,34,34	0
56	MG	1F	304	1/1	0.96	0.16	38,38,38,38	0
56	MG	1F	305	1/1	0.96	0.13	40,40,40,40	0
56	MG	2A	3579	1/1	0.96	0.10	68,68,68,68	0
56	MG	2A	3580	1/1	0.96	0.06	31,31,31,31	0
56	MG	1a	1656	1/1	0.96	0.21	44,44,44,44	0
56	MG	2A	3583	1/1	0.96	0.12	63,63,63,63	0
56	MG	1A	3054	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3037	1/1	0.96	0.17	27,27,27,27	0
56	MG	2a	3124	1/1	0.96	0.25	56,56,56,56	0
56	MG	2A	3586	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3073	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3751	1/1	0.96	0.10	53,53,53,53	0
56	MG	2a	3128	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	3334	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3615	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3210	1/1	0.96	0.28	48,48,48,48	0
56	MG	1a	1664	1/1	0.96	0.08	31,31,31,31	0
56	MG	2A	3029	1/1	0.96	0.16	38,38,38,38	0
56	MG	1G	203	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3288	1/1	0.96	0.18	52,52,52,52	0
56	MG	2A	3599	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3485	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3761	1/1	0.96	0.06	48,48,48,48	0
56	MG	1A	3622	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3149	1/1	0.96	0.10	58,58,58,58	0
56	MG	1a	1671	1/1	0.96	0.26	34,34,34,34	0
56	MG	1A	3488	1/1	0.96	0.07	47,47,47,47	0
56	MG	1P	201	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3290	1/1	0.96	0.26	45,45,45,45	0
56	MG	1A	3628	1/1	0.96	0.06	68,68,68,68	0
56	MG	2f	201	1/1	0.96	0.06	54,54,54,54	0
56	MG	1Q	203	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3629	1/1	0.96	0.14	54,54,54,54	0
56	MG	2A	3046	1/1	0.96	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1R	202	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3776	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3630	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3383	1/1	0.96	0.19	25,25,25,25	0
56	MG	1A	3023	1/1	0.96	0.24	42,42,42,42	0
56	MG	1A	3292	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3496	1/1	0.96	0.09	58,58,58,58	0
56	MG	1U	201	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3624	1/1	0.96	0.04	34,34,34,34	0
56	MG	1A	3640	1/1	0.96	0.07	30,30,30,30	0
56	MG	1a	1689	1/1	0.96	0.32	48,48,48,48	0
56	MG	1A	3642	1/1	0.96	0.07	21,21,21,21	0
56	MG	1P	203	1/1	0.97	0.27	25,25,25,25	0
56	MG	1P	204	1/1	0.97	0.19	44,44,44,44	0
56	MG	1P	205	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3701	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3702	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3087	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3625	1/1	0.97	0.08	24,24,24,24	0
56	MG	1R	201	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3626	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3554	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3114	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3359	1/1	0.97	0.24	49,49,49,49	0
56	MG	1S	201	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3233	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3100	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3529	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3631	1/1	0.97	0.04	69,69,69,69	0
56	MG	2A	3531	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	3361	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3635	1/1	0.97	0.06	53,53,53,53	0
56	MG	1l	201	1/1	0.97	0.04	56,56,56,56	0
56	MG	2a	3027	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3637	1/1	0.97	0.12	58,58,58,58	0
56	MG	1U	204	1/1	0.97	0.11	43,43,43,43	0
56	MG	2A	3539	1/1	0.97	0.09	68,68,68,68	0
56	MG	1A	3088	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3022	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3489	1/1	0.97	0.10	19,19,19,19	0
56	MG	1A	3275	1/1	0.97	0.18	55,55,55,55	0
56	MG	1A	3723	1/1	0.97	0.13	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1V	205	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3120	1/1	0.97	0.11	39,39,39,39	0
56	MG	2A	3547	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3724	1/1	0.97	0.05	26,26,26,26	0
56	MG	1W	202	1/1	0.97	0.23	40,40,40,40	0
56	MG	1A	3564	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3644	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3168	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3185	1/1	0.97	0.19	34,34,34,34	0
56	MG	2A	3127	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3730	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3647	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3732	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3258	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3186	1/1	0.97	0.09	53,53,53,53	0
56	MG	1a	1676	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3568	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3569	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3846	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3279	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3405	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3280	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3013	1/1	0.97	0.12	24,24,24,24	0
56	MG	2A	3569	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3268	1/1	0.97	0.15	19,19,19,19	0
56	MG	1A	3370	1/1	0.97	0.05	39,39,39,39	0
56	MG	1a	1685	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3281	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3372	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3576	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3118	1/1	0.97	0.11	38,38,38,38	0
56	MG	1B	206	1/1	0.97	0.09	42,42,42,42	0
56	MG	1a	1690	1/1	0.97	0.23	35,35,35,35	0
56	MG	2A	3277	1/1	0.97	0.24	37,37,37,37	0
56	MG	13	101	1/1	0.97	0.05	42,42,42,42	0
56	MG	2A	3582	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3410	1/1	0.97	0.22	32,32,32,32	0
56	MG	1A	3188	1/1	0.97	0.17	29,29,29,29	0
56	MG	1A	3077	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3750	1/1	0.97	0.08	58,58,58,58	0
56	MG	15	101	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3588	1/1	0.97	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3285	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3154	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3507	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3587	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3157	1/1	0.97	0.07	57,57,57,57	0
56	MG	2A	3288	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3588	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3756	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3424	1/1	0.97	0.30	43,43,43,43	0
56	MG	1A	3510	1/1	0.97	0.11	33,33,33,33	0
56	MG	1B	216	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3668	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3378	1/1	0.97	0.08	29,29,29,29	0
56	MG	1A	3415	1/1	0.97	0.21	36,36,36,36	0
56	MG	1A	3671	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3003	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3768	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3418	1/1	0.97	0.13	28,28,28,28	0
56	MG	2A	3300	1/1	0.97	0.14	29,29,29,29	0
56	MG	1B	225	1/1	0.97	0.06	29,29,29,29	0
56	MG	1a	1712	1/1	0.97	0.28	40,40,40,40	0
56	MG	1D	301	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3522	1/1	0.97	0.08	26,26,26,26	0
56	MG	2a	3101	1/1	0.97	0.21	27,27,27,27	0
56	MG	2A	3049	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3616	1/1	0.97	0.21	25,25,25,25	0
56	MG	2A	3617	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3596	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3176	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3154	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3598	1/1	0.97	0.09	40,40,40,40	0
56	MG	2A	3444	1/1	0.97	0.27	34,34,34,34	0
56	MG	1D	307	1/1	0.97	0.07	46,46,46,46	0
56	MG	1a	1608	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3055	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3258	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3462	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3421	1/1	0.97	0.06	21,21,21,21	0
56	MG	1A	3781	1/1	0.97	0.05	39,39,39,39	0
56	MG	1A	3782	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3121	1/1	0.97	0.14	22,22,22,22	0
56	MG	2A	3457	1/1	0.97	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3194	1/1	0.97	0.10	52,52,52,52	0
56	MG	2A	3064	1/1	0.97	0.17	37,37,37,37	0
56	MG	2A	3321	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3461	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3462	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3238	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3788	1/1	0.97	0.11	33,33,33,33	0
56	MG	2A	3465	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3608	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3469	1/1	0.97	0.07	34,34,34,34	0
56	MG	2a	3130	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3539	1/1	0.97	0.07	32,32,32,32	0
56	MG	1A	3467	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3468	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3425	1/1	0.97	0.16	24,24,24,24	0
56	MG	2F	304	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3350	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3796	1/1	0.97	0.07	69,69,69,69	0
56	MG	1a	1738	1/1	0.97	0.28	46,46,46,46	0
56	MG	2A	3075	1/1	0.97	0.08	34,34,34,34	0
56	MG	2Q	202	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3105	1/1	0.97	0.32	35,35,35,35	0
56	MG	1F	310	1/1	0.97	0.12	31,31,31,31	0
56	MG	2A	3487	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3488	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3798	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3616	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3093	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3803	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3209	1/1	0.97	0.05	63,63,63,63	0
56	MG	1A	3804	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3695	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3548	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3015	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3809	1/1	0.97	0.06	46,46,46,46	0
56	MG	1a	1636	1/1	0.97	0.09	48,48,48,48	0
56	MG	28	102	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3503	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3347	1/1	0.97	0.34	28,28,28,28	0
56	MG	1N	202	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3810	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3085	1/1	0.97	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	ZN	2n	501	1/1	0.97	0.04	96,96,96,96	0
56	MG	1A	3006	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3397	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3576	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3147	1/1	0.98	0.10	48,48,48,48	0
56	MG	2A	3466	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3578	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3255	1/1	0.98	0.08	41,41,41,41	0
56	MG	2A	3470	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3801	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3581	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3044	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3159	1/1	0.98	0.06	44,44,44,44	0
56	MG	2A	3476	1/1	0.98	0.04	48,48,48,48	0
56	MG	2A	3478	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3523	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3099	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3525	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3807	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3586	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3721	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3722	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3526	1/1	0.98	0.06	16,16,16,16	0
56	MG	1A	3655	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3271	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3004	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3528	1/1	0.98	0.07	28,28,28,28	0
56	MG	1a	1677	1/1	0.98	0.20	30,30,30,30	0
56	MG	1a	1764	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3658	1/1	0.98	0.05	48,48,48,48	0
56	MG	1a	1766	1/1	0.98	0.04	32,32,32,32	0
56	MG	2A	3623	1/1	0.98	0.03	39,39,39,39	0
56	MG	1A	3590	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3729	1/1	0.98	0.05	52,52,52,52	0
56	MG	1F	309	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3502	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3011	1/1	0.98	0.17	31,31,31,31	0
56	MG	19	101	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3016	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3262	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3091	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3823	1/1	0.98	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3509	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3374	1/1	0.98	0.17	43,43,43,43	0
56	MG	2A	3511	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3537	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3538	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3264	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3828	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3481	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3600	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3020	1/1	0.98	0.07	19,19,19,19	0
56	MG	2A	3519	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3483	1/1	0.98	0.06	49,49,49,49	0
56	MG	1P	202	1/1	0.98	0.23	31,31,31,31	0
56	MG	2A	3194	1/1	0.98	0.19	43,43,43,43	0
56	MG	2A	3093	1/1	0.98	0.17	30,30,30,30	0
56	MG	2A	3094	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3025	1/1	0.98	0.07	48,48,48,48	0
56	MG	2P	201	1/1	0.98	0.14	47,47,47,47	0
56	MG	1x	107	1/1	0.98	0.26	48,48,48,48	0
56	MG	2P	203	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3544	1/1	0.98	0.08	30,30,30,30	0
56	MG	1a	1700	1/1	0.98	0.28	24,24,24,24	0
56	MG	1A	3031	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3748	1/1	0.98	0.04	77,77,77,77	0
56	MG	2A	3001	1/1	0.98	0.17	35,35,35,35	0
56	MG	2V	201	1/1	0.98	0.14	48,48,48,48	0
56	MG	1A	3486	1/1	0.98	0.09	34,34,34,34	0
56	MG	2A	3536	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3446	1/1	0.98	0.17	22,22,22,22	0
56	MG	2A	3004	1/1	0.98	0.26	48,48,48,48	0
56	MG	1A	3839	1/1	0.98	0.08	46,46,46,46	0
56	MG	1A	3122	1/1	0.98	0.11	27,27,27,27	0
56	MG	2A	3415	1/1	0.98	0.21	35,35,35,35	0
56	MG	1A	3611	1/1	0.98	0.05	42,42,42,42	0
56	MG	2A	3008	1/1	0.98	0.04	47,47,47,47	0
56	MG	25	102	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3550	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3294	1/1	0.98	0.04	27,27,27,27	0
56	MG	1R	205	1/1	0.98	0.15	29,29,29,29	0
56	MG	1A	3490	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3321	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3493	1/1	0.98	0.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3015	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	3322	1/1	0.98	0.14	38,38,38,38	0
56	MG	2A	3017	1/1	0.98	0.14	45,45,45,45	0
56	MG	1A	3451	1/1	0.98	0.16	20,20,20,20	0
56	MG	1A	3416	1/1	0.98	0.14	19,19,19,19	0
56	MG	1A	3621	1/1	0.98	0.04	16,16,16,16	0
56	MG	1A	3770	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3771	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3688	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3123	1/1	0.98	0.03	23,23,23,23	0
56	MG	1A	3058	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3775	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3560	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3108	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3068	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3111	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3357	1/1	0.98	0.12	26,26,26,26	0
56	MG	2A	3032	1/1	0.98	0.16	33,33,33,33	0
56	MG	2A	3338	1/1	0.98	0.19	45,45,45,45	0
56	MG	2A	3033	1/1	0.98	0.15	39,39,39,39	0
56	MG	1a	1729	1/1	0.98	0.25	38,38,38,38	0
56	MG	2A	3035	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3163	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3227	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3699	1/1	0.98	0.09	61,61,61,61	0
56	MG	1A	3164	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3331	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3207	1/1	0.98	0.12	26,26,26,26	0
56	MG	1a	1736	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3453	1/1	0.98	0.10	35,35,35,35	0
56	MG	2A	3454	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3509	1/1	0.98	0.05	45,45,45,45	0
56	MG	2A	3456	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3145	1/1	0.98	0.13	53,53,53,53	0
56	MG	1Z	303	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3791	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3097	1/1	0.98	0.13	38,38,38,38	0
56	MG	2A	3589	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3514	1/1	0.98	0.08	25,25,25,25	0
58	SF4	1d	302	8/8	0.98	0.04	57,68,71,74	0
58	SF4	2d	302	8/8	0.98	0.05	71,76,86,97	0
56	MG	1A	3708	1/1	0.98	0.05	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3707	1/1	0.99	0.08	48,48,48,48	0
56	MG	1A	3743	1/1	0.99	0.02	33,33,33,33	0
56	MG	1A	3192	1/1	0.99	0.05	44,44,44,44	0
56	MG	2A	3468	1/1	0.99	0.06	29,29,29,29	0
56	MG	1A	3787	1/1	0.99	0.04	42,42,42,42	0
56	MG	2A	3528	1/1	0.99	0.02	43,43,43,43	0
56	MG	1A	3065	1/1	0.99	0.04	33,33,33,33	0
56	MG	1D	304	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3619	1/1	0.99	0.03	39,39,39,39	0
56	MG	2A	3532	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3529	1/1	0.99	0.10	20,20,20,20	0
56	MG	1A	3511	1/1	0.99	0.03	36,36,36,36	0
56	MG	2A	3475	1/1	0.99	0.14	35,35,35,35	0
56	MG	1A	3749	1/1	0.99	0.06	78,78,78,78	0
56	MG	2A	3477	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3427	1/1	0.99	0.25	39,39,39,39	0
56	MG	2A	3479	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3480	1/1	0.99	0.08	36,36,36,36	0
56	MG	1A	3652	1/1	0.99	0.03	31,31,31,31	0
56	MG	1m	3001	1/1	0.99	0.11	51,51,51,51	0
56	MG	1A	3532	1/1	0.99	0.04	22,22,22,22	0
56	MG	1A	3513	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3608	1/1	0.99	0.10	37,37,37,37	0
56	MG	1A	3139	1/1	0.99	0.11	32,32,32,32	0
56	MG	28	101	1/1	0.99	0.33	50,50,50,50	0
56	MG	1A	3755	1/1	0.99	0.04	55,55,55,55	0
56	MG	1A	3601	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3758	1/1	0.99	0.03	26,26,26,26	0
56	MG	1U	206	1/1	0.99	0.23	37,37,37,37	0
56	MG	1A	3515	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3580	1/1	0.99	0.06	39,39,39,39	0
56	MG	1A	3386	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	3762	1/1	0.99	0.05	54,54,54,54	0
56	MG	2A	3140	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3491	1/1	0.99	0.04	25,25,25,25	0
56	MG	2A	3556	1/1	0.99	0.05	68,68,68,68	0
56	MG	1A	3764	1/1	0.99	0.04	62,62,62,62	0
56	MG	1A	3518	1/1	0.99	0.13	27,27,27,27	0
56	MG	1A	3766	1/1	0.99	0.03	57,57,57,57	0
56	MG	2A	3499	1/1	0.99	0.03	33,33,33,33	0
56	MG	1A	3632	1/1	0.99	0.05	36,36,36,36	0
56	MG	2A	3501	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3693	1/1	0.99	0.10	23,23,23,23	0
56	MG	1A	3812	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3769	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3607	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3634	1/1	0.99	0.07	40,40,40,40	0
56	MG	2A	3200	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3519	1/1	0.99	0.04	31,31,31,31	0
56	MG	1A	3636	1/1	0.99	0.03	29,29,29,29	0
56	MG	2A	3571	1/1	0.99	0.06	53,53,53,53	0
56	MG	1A	3195	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	3521	1/1	0.99	0.03	22,22,22,22	0
56	MG	2A	3058	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3261	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3109	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3641	1/1	0.99	0.07	23,23,23,23	0
56	MG	1A	3473	1/1	0.99	0.05	26,26,26,26	0
56	MG	1A	3546	1/1	0.99	0.06	12,12,12,12	0
57	ZN	14	102	1/1	0.99	0.04	88,88,88,88	0
57	ZN	15	106	1/1	0.99	0.03	44,44,44,44	0
57	ZN	1n	103	1/1	0.99	0.03	72,72,72,72	0
57	ZN	2Y	202	1/1	0.99	0.03	76,76,76,76	0
56	MG	1A	3474	1/1	0.99	0.06	33,33,33,33	0
57	ZN	25	103	1/1	0.99	0.03	51,51,51,51	0
57	ZN	26	102	1/1	0.99	0.06	64,64,64,64	0
57	ZN	29	501	1/1	0.99	0.04	67,67,67,67	0
56	MG	1A	3508	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3520	1/1	0.99	0.12	39,39,39,39	0
56	MG	1A	3783	1/1	0.99	0.10	32,32,32,32	0
56	MG	1B	223	1/1	0.99	0.04	34,34,34,34	0
57	ZN	16	501	1/1	1.00	0.02	45,45,45,45	0
57	ZN	19	102	1/1	1.00	0.01	42,42,42,42	0
56	MG	1A	3800	1/1	1.00	0.02	30,30,30,30	0
56	MG	1A	3718	1/1	1.00	0.02	17,17,17,17	0
56	MG	1A	3571	1/1	1.00	0.05	29,29,29,29	0
56	MG	1A	3736	1/1	1.00	0.02	35,35,35,35	0
56	MG	1A	3742	1/1	1.00	0.06	29,29,29,29	0
56	MG	1A	3535	1/1	1.00	0.04	20,20,20,20	0
56	MG	2A	3592	1/1	1.00	0.05	38,38,38,38	0
57	ZN	1Y	202	1/1	1.00	0.02	57,57,57,57	0
56	MG	1A	3476	1/1	1.00	0.06	33,33,33,33	0
56	MG	1A	3757	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.