wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 08:18 PM EST

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

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

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

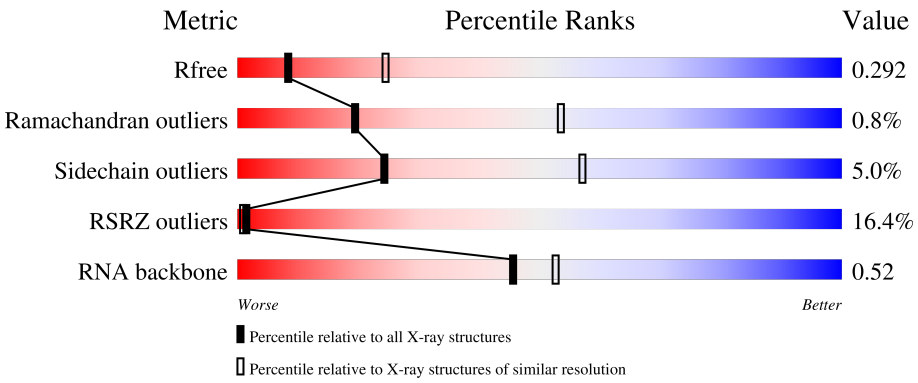
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	3%, 81%, 17%, ·
1	2A	2915	4%, 77%, 19%, ·
2	1B	121	87%, 12%, ·
2	2B	121	83%, 16%, ·
3	1D	276	48%, 96%, ·

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Mol	Chain	Length	Quality of chain
3	2D	276	41% 96%
4	1E	206	41% 95%
4	2E	206	30% 94% 5%
5	1F	210	25% 94%
5	2F	210	27% 90% 6%
6	1G	182	3% 96%
6	2G	182	5% 95% 5%
7	1H	180	% 92%
7	2H	180	34% 92%
8	1I	148	14% 93% 5%
8	2I	148	24% 93% 6%
9	1N	140	48% 95% 5%
9	2N	140	73% 94% 6%
10	1O	122	53% 95% 5%
10	2O	122	37% 96%
11	1P	150	27% 96%
11	2P	150	43% 95% 5%
12	1Q	141	25% 99%
12	2Q	141	28% 96%
13	1R	118	39% 93% 7%
13	2R	118	26% 93% 7%
14	1S	112	% 96%
14	2S	112	95%
15	1T	146	32% 87% 10%
15	2T	146	22% 86% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	47% 94%
16	2U	118	46% 94%
17	1V	101	23% 92% 8%
17	2V	101	26% 95% 5%
18	1W	113	29% 97%
18	2W	113	41% 96%
19	1X	96	18% 99%
19	2X	96	21% 96%
20	1Y	110	6% 86% 11%
20	2Y	110	42% 93% 5%
21	1Z	206	% 70% 25%
21	2Z	206	76% 22%
22	10	85	15% 98%
22	20	85	29% 95%
23	11	98	61% 96%
23	21	98	45% 97%
24	12	72	8% 94%
24	22	72	6% 96%
25	13	60	5% 95%
25	23	60	37% 97%
26	14	71	89%
26	24	71	% 89% 8%
27	15	60	32% 90% 8%
27	25	60	30% 93% 5%
28	16	54	11% 85% 13%

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Mol	Chain	Length	Quality of chain
28	26	54	17% 89% 9%
29	17	49	49% 90% 8%
29	27	49	59% 90% 8%
30	18	65	49% 94% 5%
30	28	65	63% 97%
31	19	37	32% 97%
31	29	37	57% 95% 5%
32	1a	1521	2% 79% 19%
32	2a	1521	2% 78% 20%
33	1b	256	6% 84% 6% 10%
33	2b	256	10% 83% 7% 10%
34	1c	239	20% 83% 14%
34	2c	239	27% 83% 14%
35	1d	209	11% 94%
35	2d	209	42% 93% 6%
36	1e	162	23% 87% 9%
36	2e	162	33% 86% 5% 9%
37	1f	101	13% 95%
37	2f	101	2% 95%
38	1g	156	22% 95%
38	2g	156	12% 96%
39	1h	138	20% 91% 9%
39	2h	138	35% 95%
40	1i	128	16% 94% 5%
40	2i	128	34% 90% 9%

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Mol	Chain	Length	Quality of chain
41	1j	105	17% 85% 8% 8%
41	2j	105	27% 84% 8% 9%
42	1k	129	70% 85% • 12%
42	2k	129	33% 84% 5% 12%
43	1l	132	15% 89% • 8%
43	2l	132	26% 87% 5% 8%
44	1m	126	10% 98% •
44	2m	126	18% 96% • •
45	1n	61	33% 89% 10% •
45	2n	61	67% 93% 5% •
46	1o	89	16% 94% • •
46	2o	89	21% 92% 7% •
47	1p	88	32% 86% 7% 7%
47	2p	88	32% 89% 5% 7%
48	1q	105	7% 92% • 6%
48	2q	105	49% 90% 5% 6%
49	1r	88	16% 74% • 23%
49	2r	88	11% 73% 5% 23%
50	1s	93	3% 88% • 11%
50	2s	93	6% 87% • 11%
51	1t	106	26% 87% • • 9%
51	2t	106	25% 87% • 9%
52	1u	27	7% 78% 7% 15%
52	2u	27	22% 85% 15%
53	1v	24	25% 42% 8% • 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	8% 21% 8% 67%
54	1w	76	28% 62% 28% 7%
54	1y	76	24% 51% 43%
54	2w	76	8% 61% 26% 9%
54	2y	76	12% 53% 41%
55	1x	77	4% 78% 19%
55	2x	77	3% 78% 19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3036	-	-	-	X
56	MG	1A	3098	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3114	-	-	-	X
56	MG	1A	3121	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3190	-	-	-	X
56	MG	1A	3318	-	-	-	X
56	MG	1A	3359	-	-	-	X
56	MG	1A	3368	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3433	-	-	-	X
56	MG	1A	3506	-	-	-	X
56	MG	1A	3513	-	-	-	X
56	MG	1a	3016	-	-	-	X
56	MG	1a	3037	-	-	-	X
56	MG	1a	3043	-	-	-	X
56	MG	1a	3053	-	-	-	X
56	MG	1a	3082	-	-	-	X
56	MG	1a	3092	-	-	-	X
56	MG	1a	3094	-	-	-	X

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

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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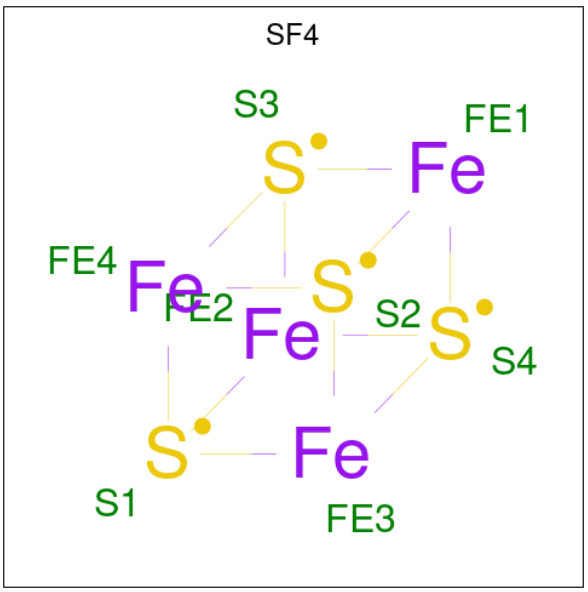
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is water.

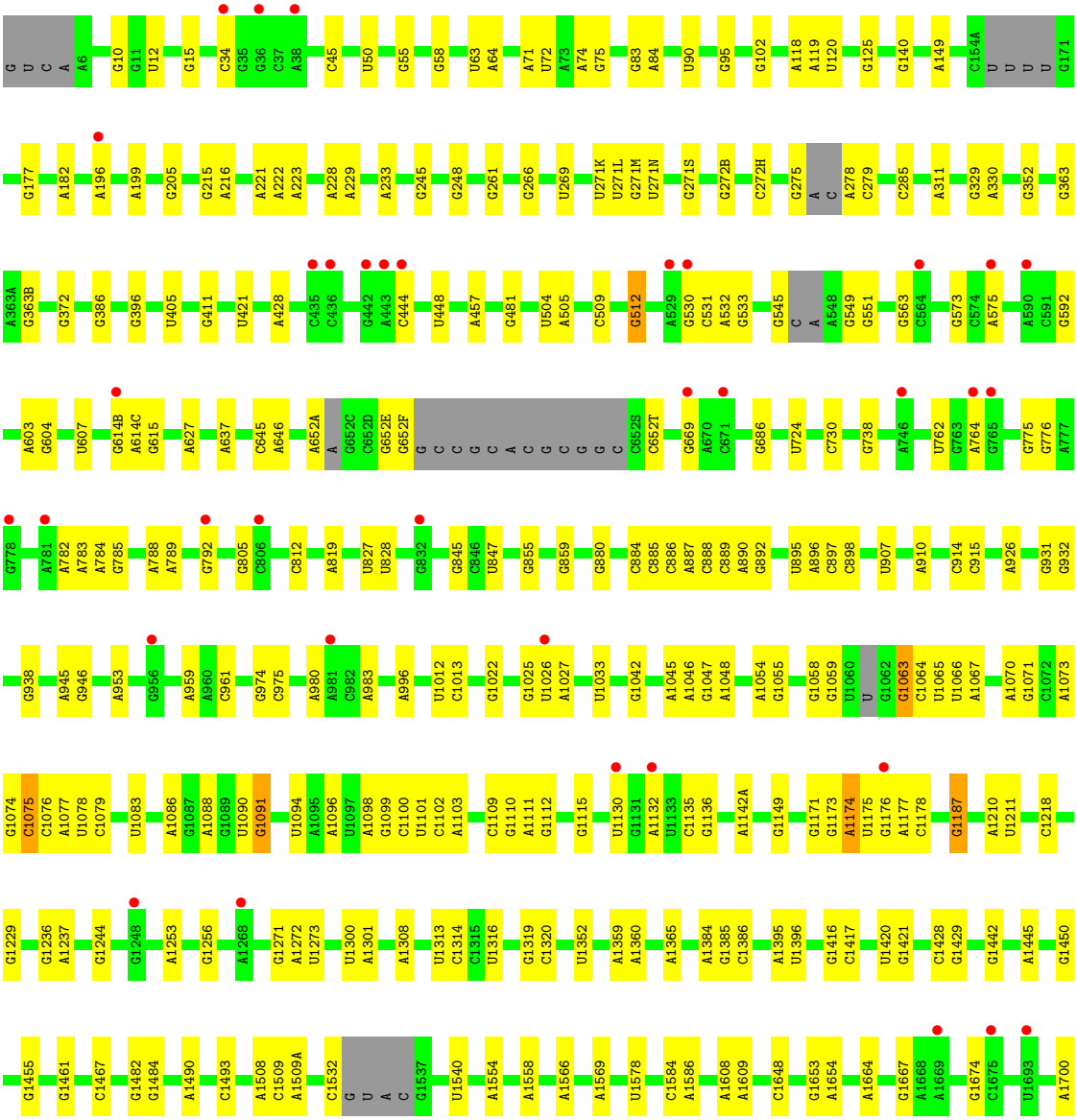
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
59	1A	585	585	585	0	0
			Total	O		
59	1a	181	181	181	0	0
			Total	O		
59	2A	234	234	234	0	0
			Total	O		
59	2a	167	167	167	0	0

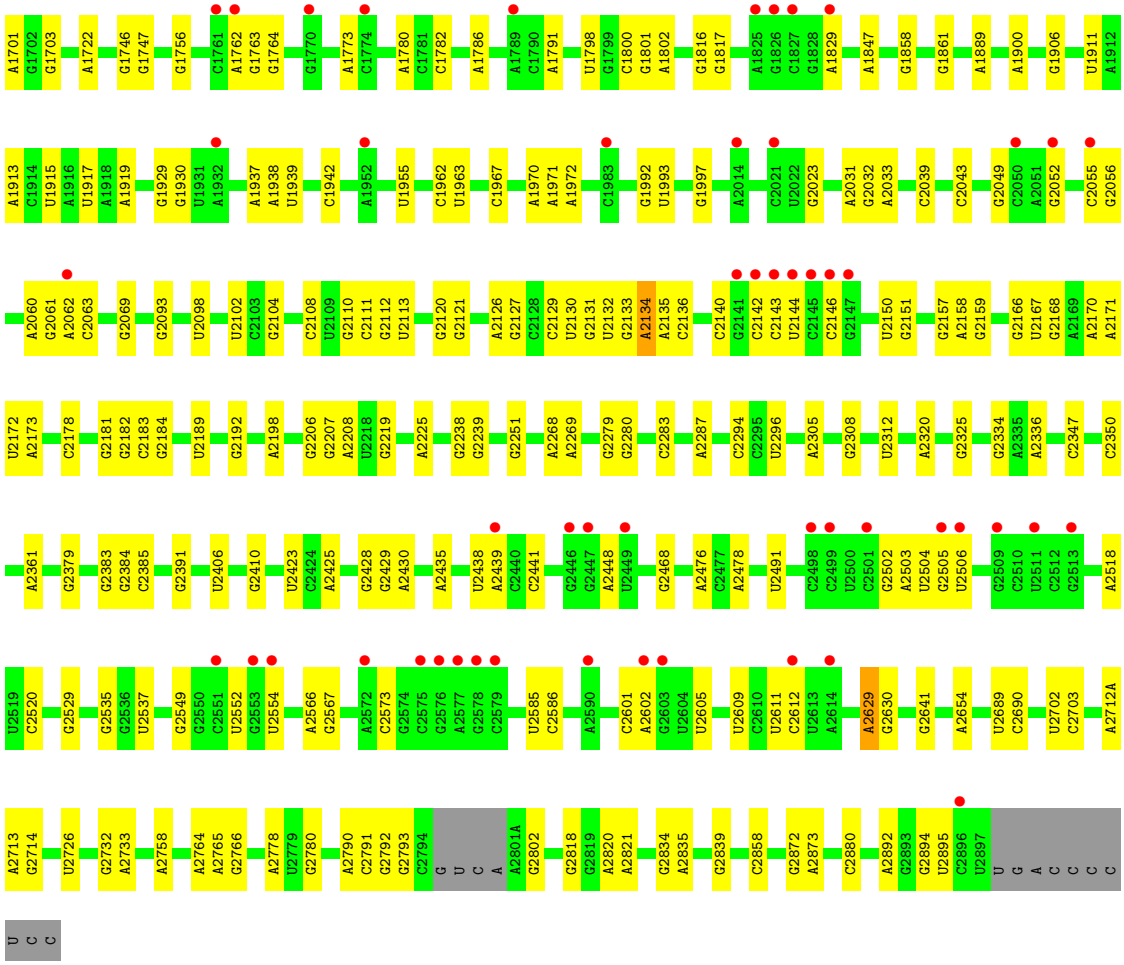
3 Residue-property plots (i)

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

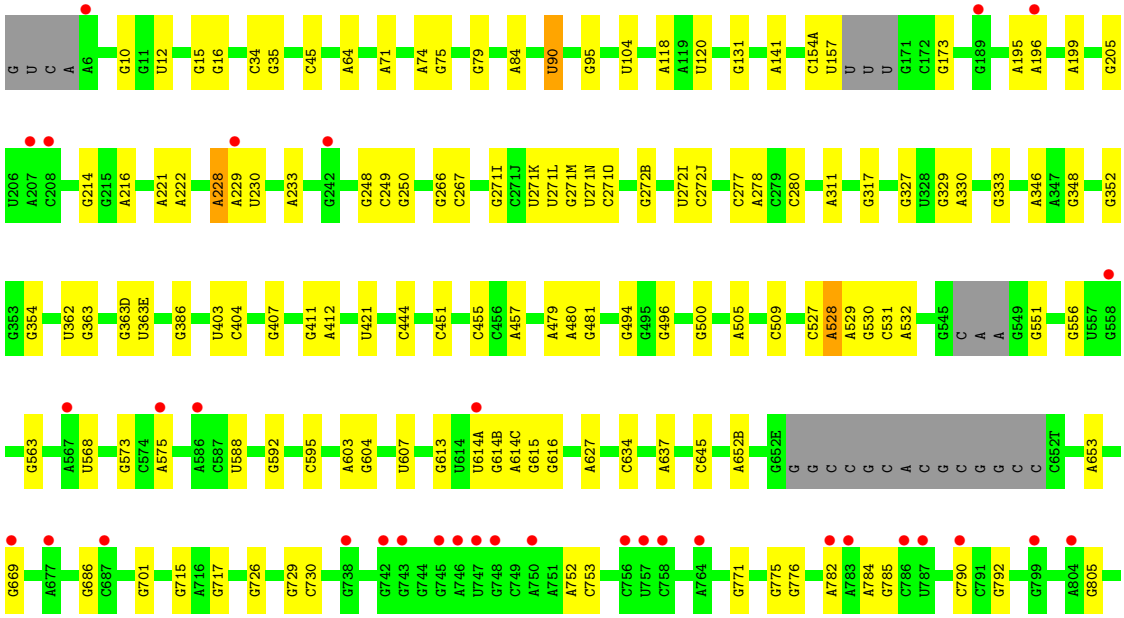
Chain 1A: 3% 81% 17%

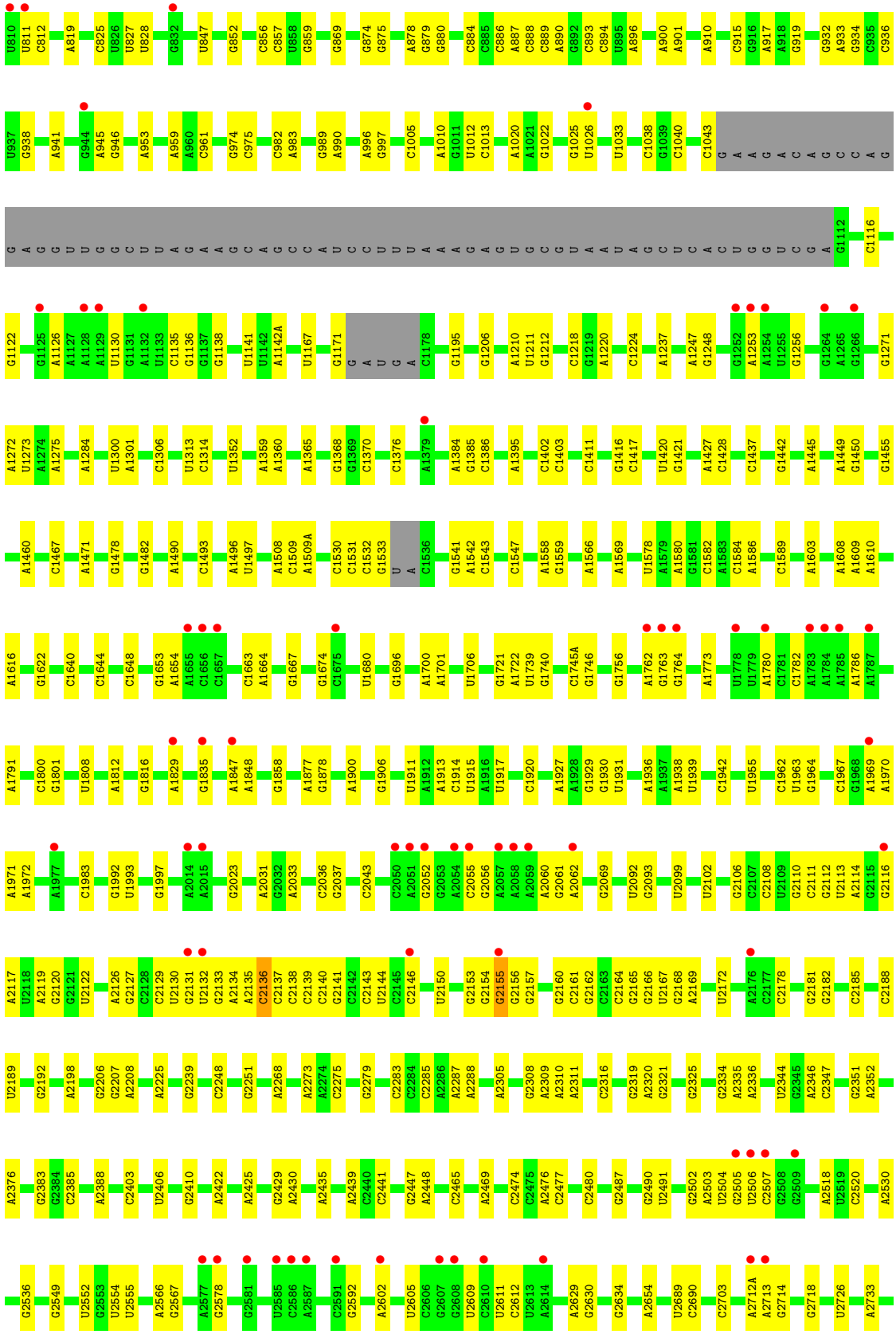


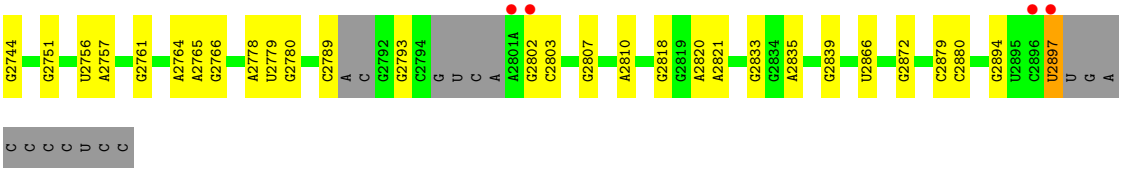


- Molecule 1: 23S Ribosomal RNA

Chain 2A:

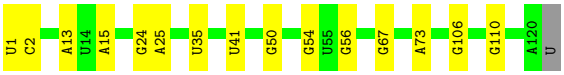



U810 U811 C812 A819 C825 U826 U827 U828 G832 U847 G852 C856 C857 U858 G859 G869 G874 G875 A878 G879 G880 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 A900 A901 A910 C915 G916 A917 A918 G919 G932 A933 G934 C935 C936
U937 G938 A941 G944 A945 G946 A953 A959 A960 C961 G974 C975 G982 A983 G989 A990 A996 G997 C1005 A1010 G1011 U1012 C1013 A1020 A1021 G1022 G1025 U1026 U1033 C1038 G1039 C1040 C1043 G A A G A C A G C C A G
G A G G U U G G C U U A G A A G C A G C C A U C C U U U U A A A G U G C G U A A U A G C U C A C U U G G U C G A G1112 C1116
G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 U1141 U1142 A1142A U1167 G1171 G A U G A C1178 G1195 G1206 A1210 U1211 G1212 C1218 G1219 A1220 C1224 A1237 A1247 G1248 G1252 A1253 A1254 U1255 G1256 G1264 A1265 G1266 G1271
A1272 U1273 A1274 A1275 A1284 U1300 A1301 C1306 U1313 C1314 U1352 A1359 A1360 A1365 G1368 G1369 C1370 C1376 A1379 A1384 G1385 C1386 A1395 C1402 C1403 C1411 G1416 C1417 U1420 G1421 A1427 C1428 C1437 G1442 A1445 A1449 G1450 G1455
A1460 C1467 A1471 G1478 G1482 A1490 C1493 A1496 U1497 A1508 C1509 A1509A C1530 C1531 C1532 G1533 U A C1536 G1541 A1542 C1543 C1547 A1558 G1559 A1566 A1569 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 C1589 A1603 A1608 A1609 A1610
A1616 G1622 C1640 C1644 C1648 G1653 A1654 A1655 C1656 C1657 C1663 A1664 G1667 G1674 C1675 U1680 G1696 A1700 A1701 U1706 G1721 A1722 U1739 G1740 C1745A G1746 G1756 A1762 G1763 G1764 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787
A1791 C1800 G1801 U1808 A1812 G1816 A1829 G1835 A1847 A1848 G1858 A1877 G1878 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920 A1927 A1928 G1929 G1930 U1931 A1936 A1937 A1938 U1939 C1942 U1955 C1962 U1963 G1964 C1967 G1968 A1969 A1970
A1971 A1972 A1977 C1983 G1992 U1993 G1997 A2014 A2015 G2023 A2031 G2032 A2033 C2036 G2037 C2043 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 G2069 U2092 G2093 U2099 U2102 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116
A2117 U2118 A2119 G2120 G2121 U2122 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 U2150 G2153 G2154 G2155 G2156 G2157 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 U2172 A2176 C2177 C2178 G2181 G2182 C2185 C2188
U2189 G2192 A2198 G2206 G2207 A2208 A2225 G2239 C2248 G2251 A2268 A2273 A2274 C2275 G2279 C2283 C2284 C2285 A2286 A2287 A2288 A2305 G2308 A2309 A2310 A2311 C2316 G2319 A2320 G2321 G2325 G2334 A2335 A2336 U2344 G2345 A2346 C2347 G2351 A2352
A2376 G2383 G2384 C2385 A2388 C2403 U2406 G2410 A2422 A2425 G2429 A2430 A2435 A2439 C2440 C2441 G2447 A2448 C2465 A2469 C2474 C2475 A2476 C2477 C2480 G2487 G2490 U2491 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 A2518 U2519 C2520 A2530
G2536 G2549 U2552 G2553 U2554 U2555 A2566 G2567 A2577 G2578 G2581 U2585 C2586 A2587 C2591 G2592 A2602 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 A2629 G2630 G2634 A2654 U2689 C2690 C2703 A2712A A2713 G2714 G2718 U2726 A2733



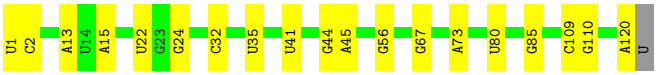
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



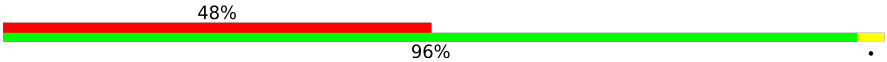
• Molecule 2: 5S Ribosomal RNA

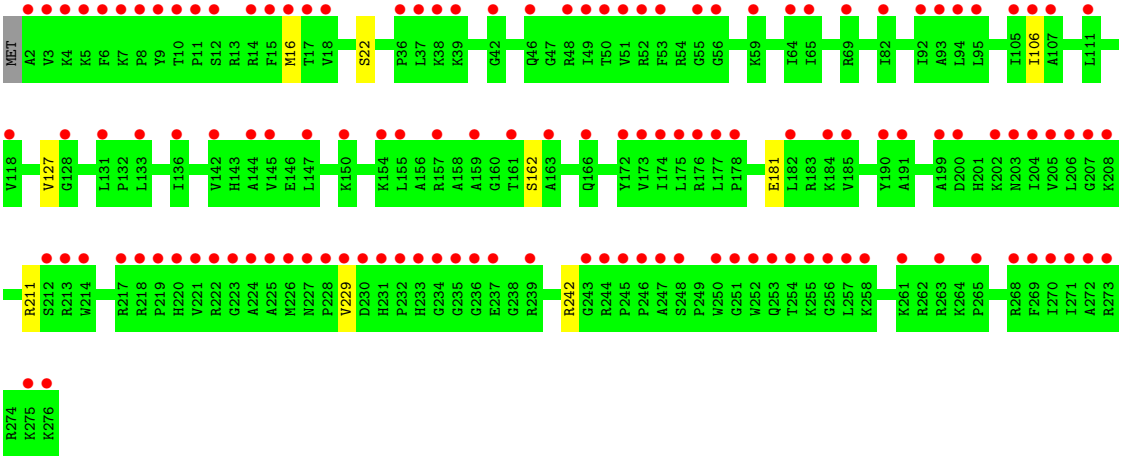
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

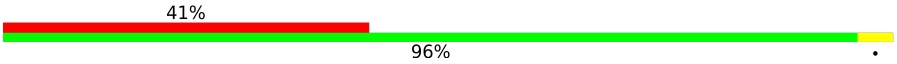
Chain 1D:

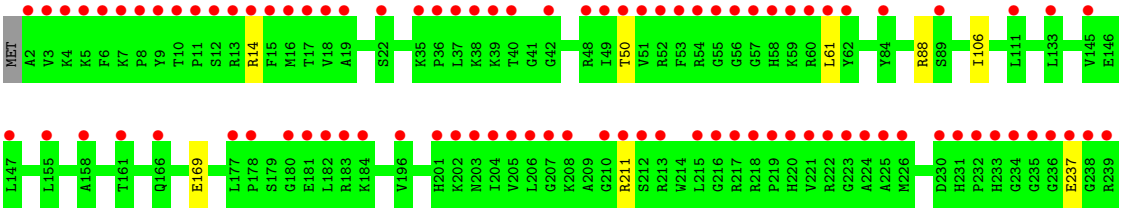


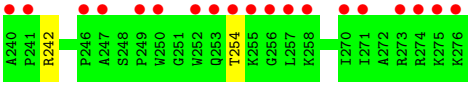


• Molecule 3: 50S ribosomal protein L2

Chain 2D:

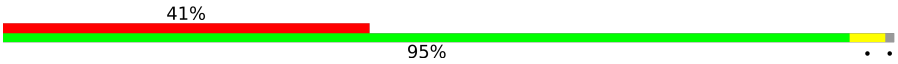


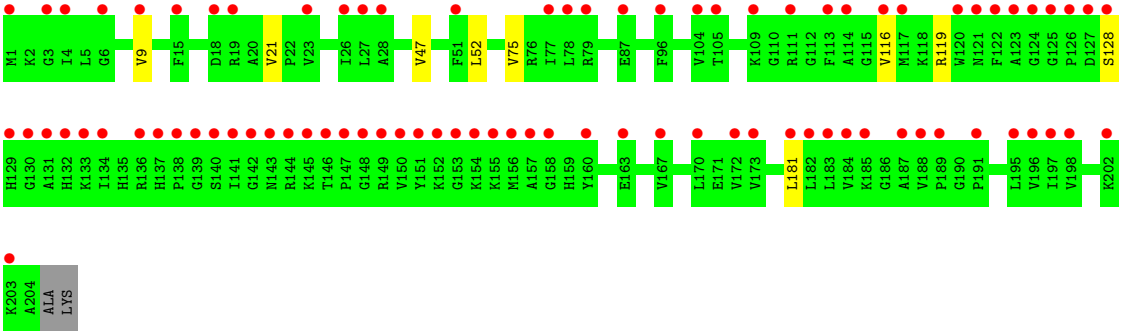




• Molecule 4: 50S ribosomal protein L3

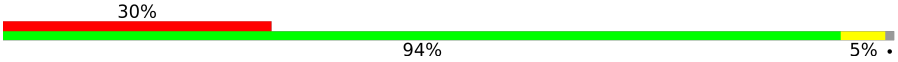
Chain 1E:

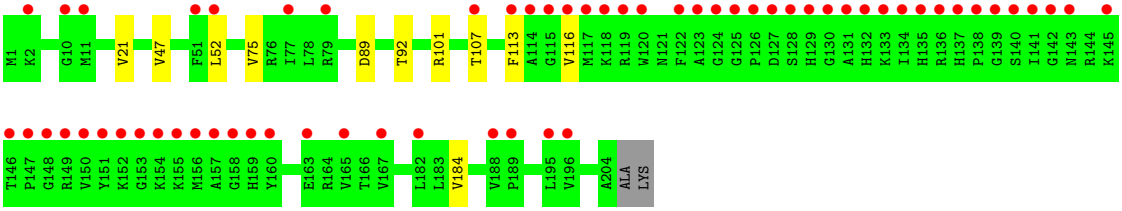




• Molecule 4: 50S ribosomal protein L3

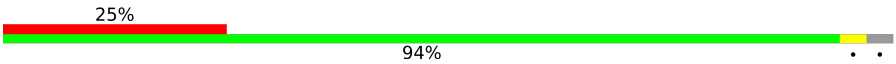
Chain 2E:

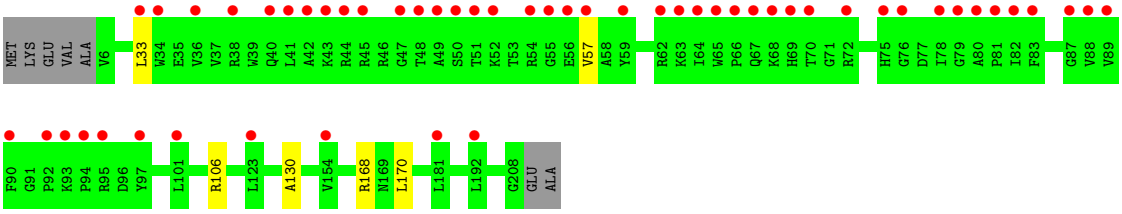




• Molecule 5: 50S ribosomal protein L4

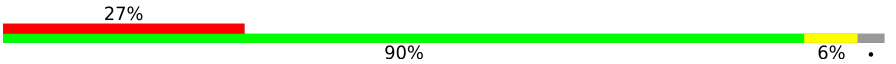
Chain 1F:

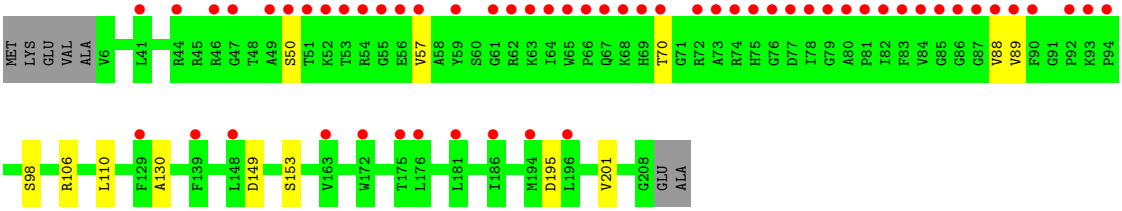




• Molecule 5: 50S ribosomal protein L4

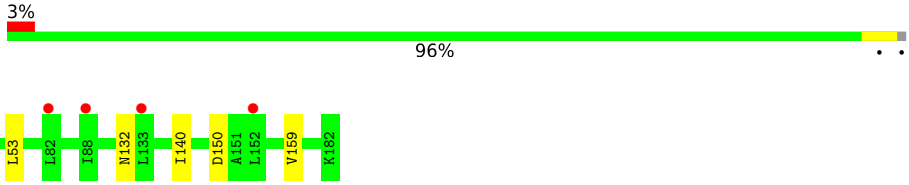
Chain 2F:





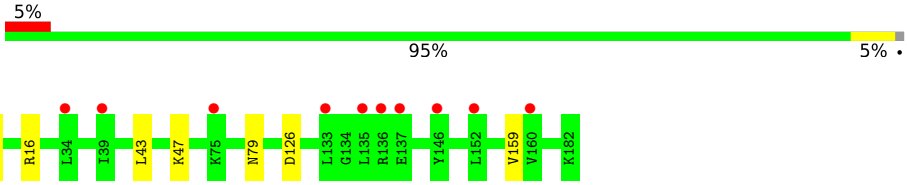
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



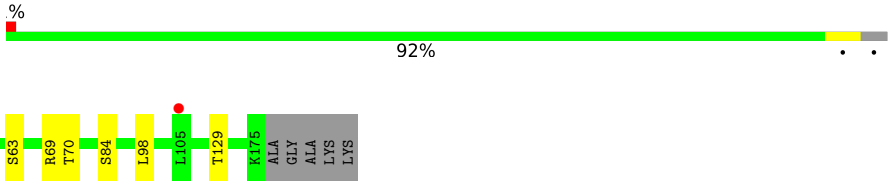
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



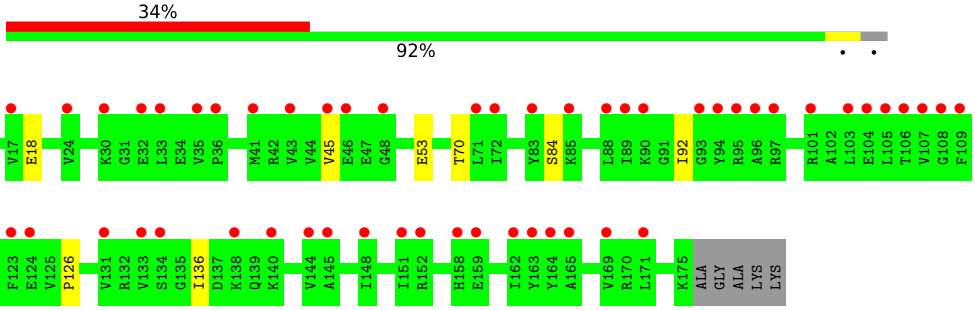
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



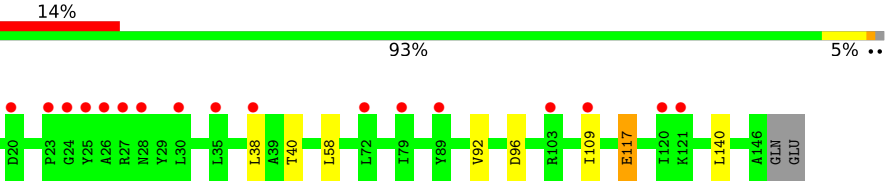
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



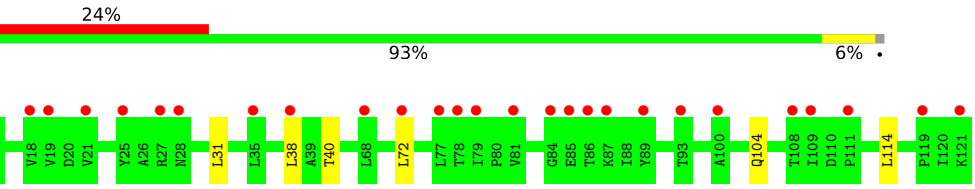
• Molecule 8: 50S ribosomal protein L9

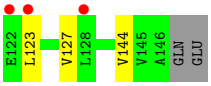
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

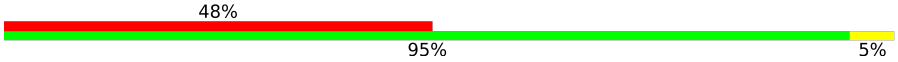
Chain 2I:

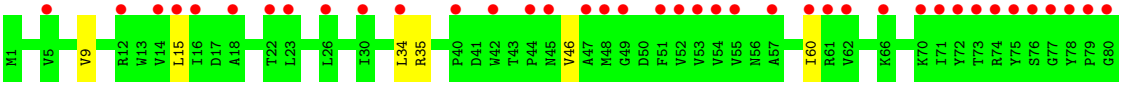


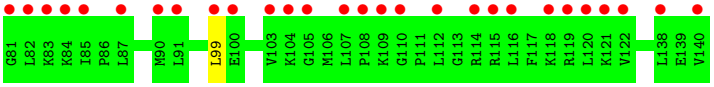


• Molecule 9: 50S ribosomal protein L13

Chain 1N:

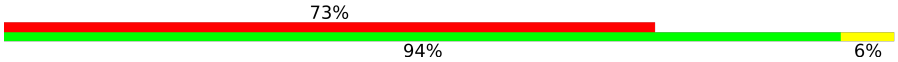


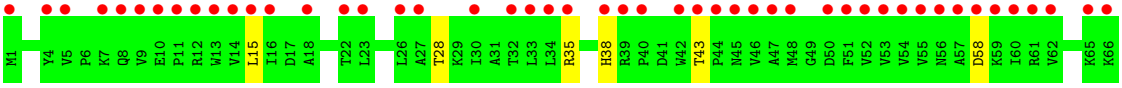


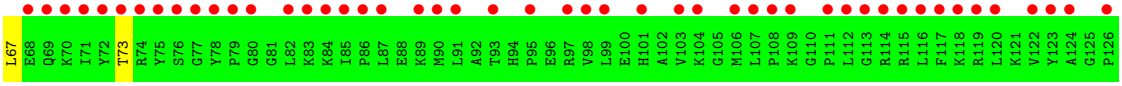


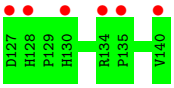
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



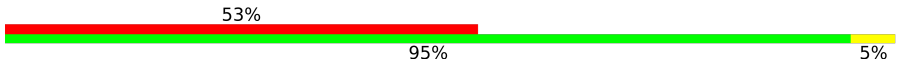


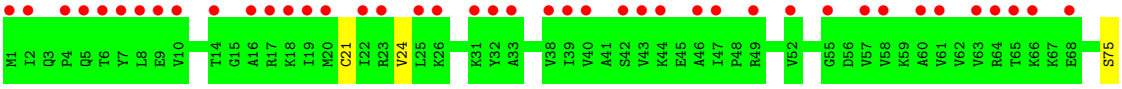


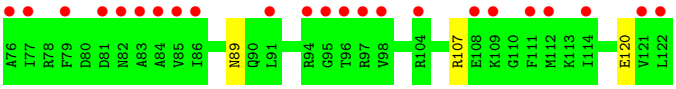


• Molecule 10: 50S ribosomal protein L14

Chain 1O:

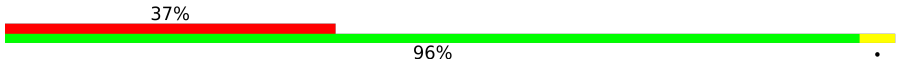


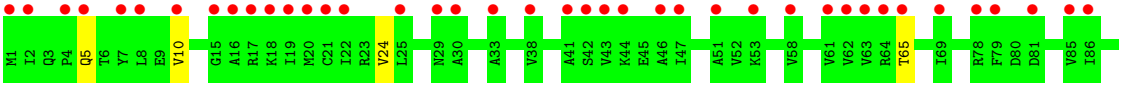


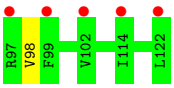


• Molecule 10: 50S ribosomal protein L14

Chain 2O:

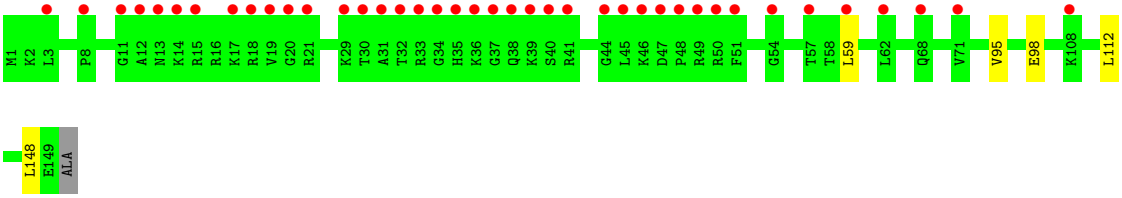






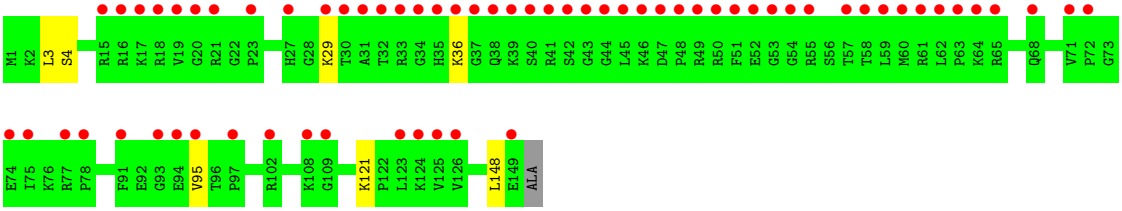
• Molecule 11: 50S ribosomal protein L15

Chain 1P: 27% 96%



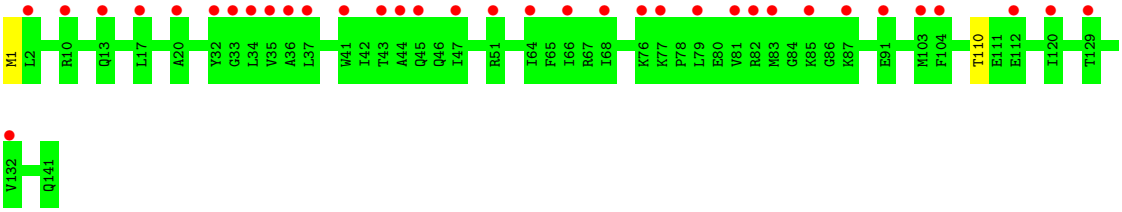
• Molecule 11: 50S ribosomal protein L15

Chain 2P: 43% 95% 5%



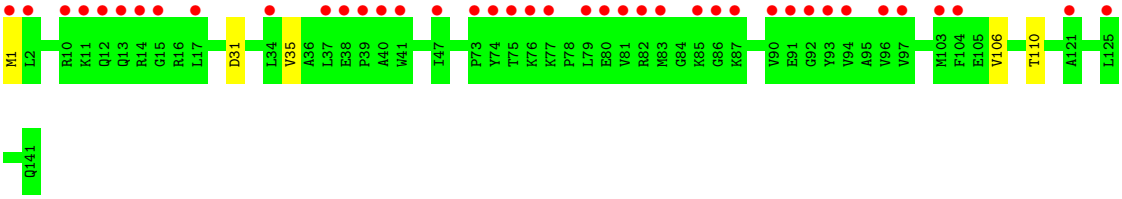
• Molecule 12: 50S ribosomal protein L16

Chain 1Q: 25% 99%



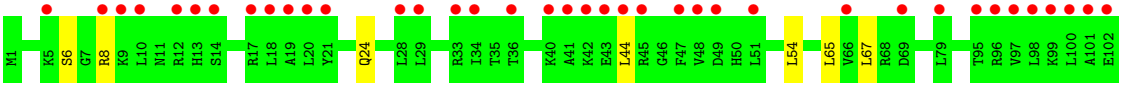
• Molecule 12: 50S ribosomal protein L16

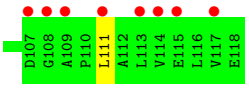
Chain 2Q: 28% 96%



• Molecule 13: 50S ribosomal protein L17

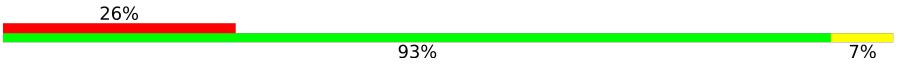
Chain 1R: 39% 93% 7%

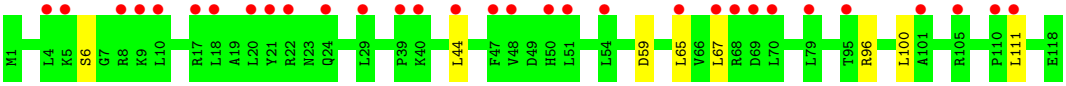




• Molecule 13: 50S ribosomal protein L17

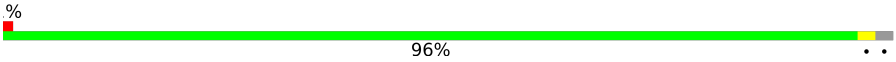
Chain 2R:





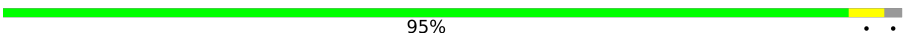
• Molecule 14: 50S ribosomal protein L18

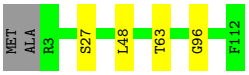
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

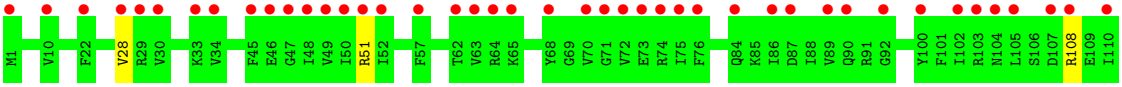
Chain 2S:

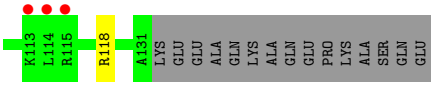




• Molecule 15: 50S ribosomal protein L19

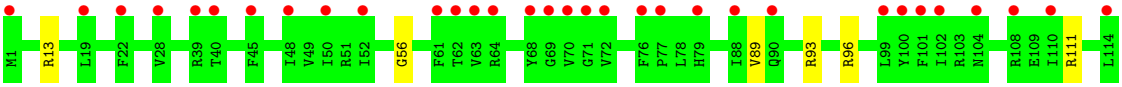
Chain 1T:

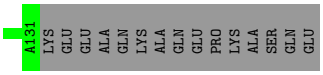




• Molecule 15: 50S ribosomal protein L19

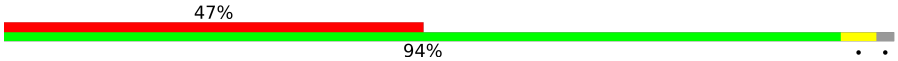
Chain 2T:

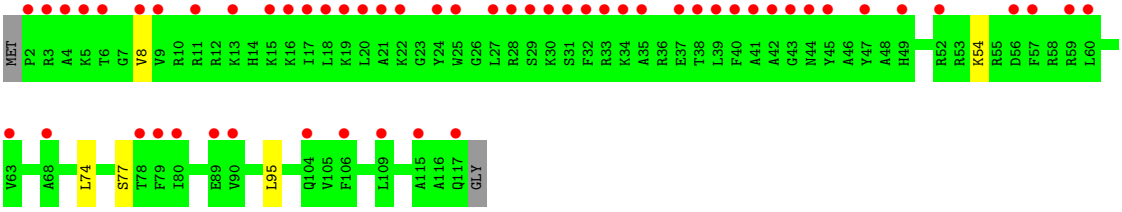




• Molecule 16: 50S ribosomal protein L20

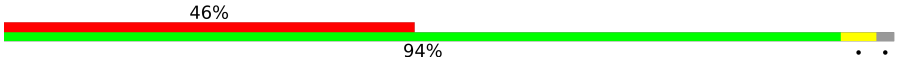
Chain 1U:





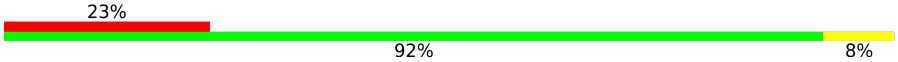
- Molecule 16: 50S ribosomal protein L20

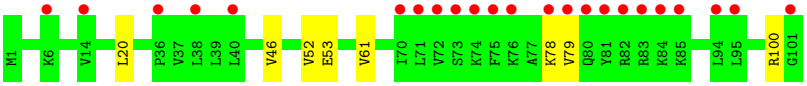
Chain 2U:



- Molecule 17: 50S ribosomal protein L21

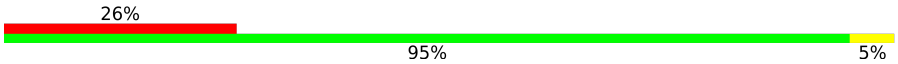
Chain 1V:

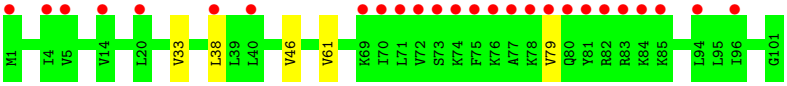




- Molecule 17: 50S ribosomal protein L21

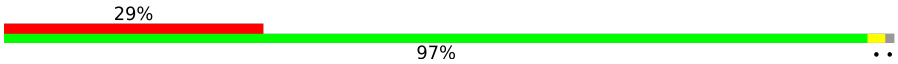
Chain 2V:

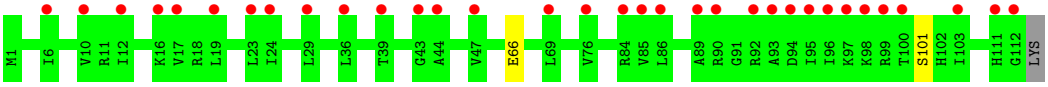




- Molecule 18: 50S ribosomal protein L22

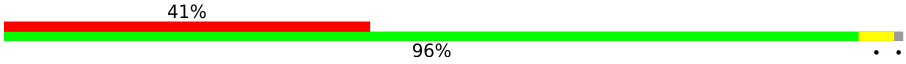
Chain 1W:

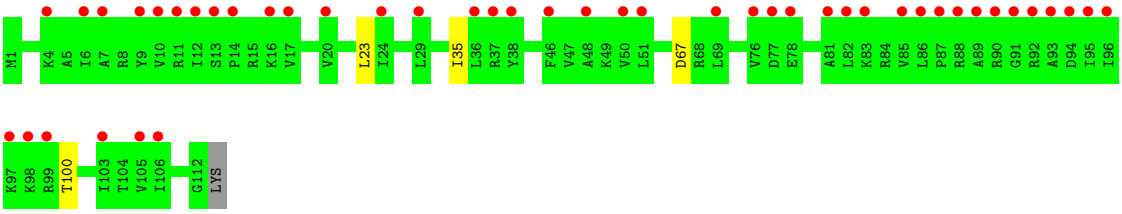




- Molecule 18: 50S ribosomal protein L22

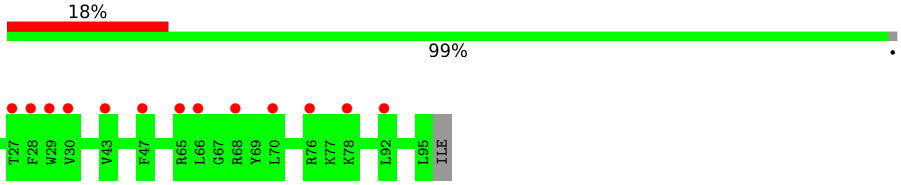
Chain 2W:





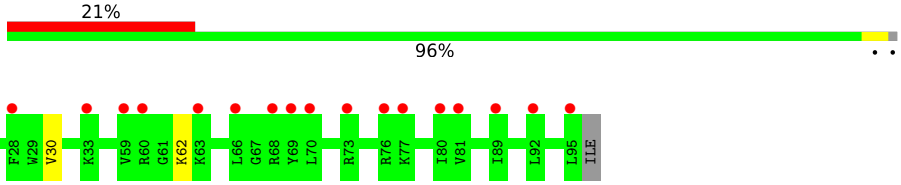
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



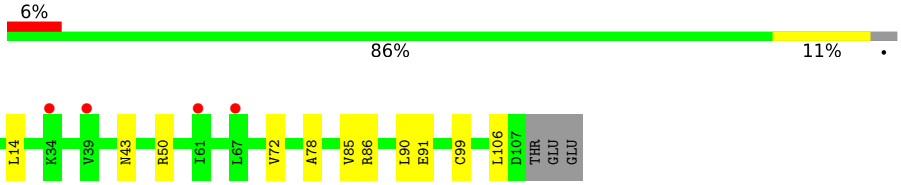
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



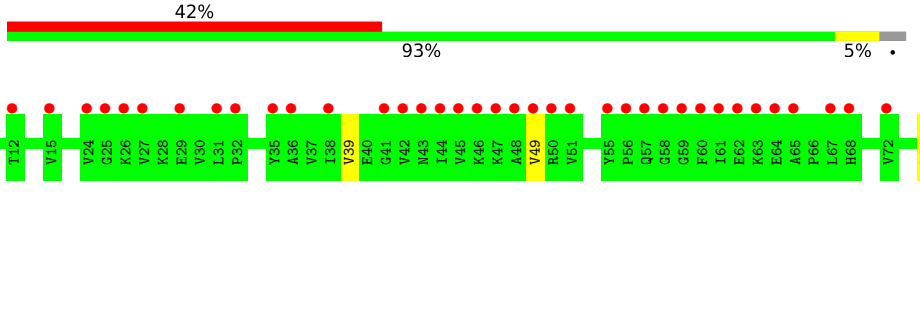
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



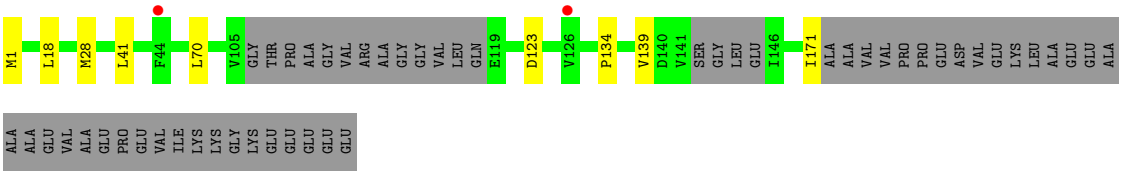
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

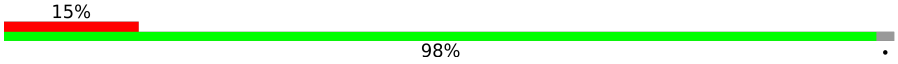


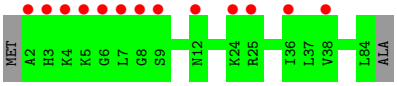
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

- Molecule 22: 50S ribosomal protein L27

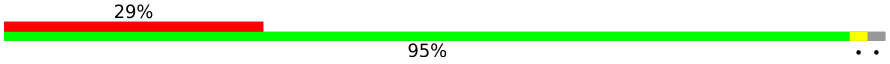
Chain 10:

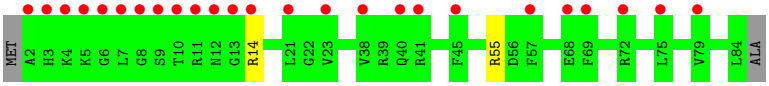




- Molecule 22: 50S ribosomal protein L27

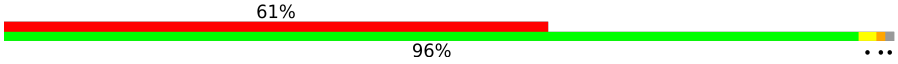
Chain 20:

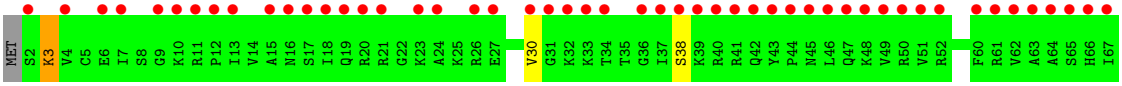


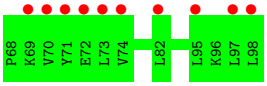


- Molecule 23: 50S ribosomal protein L28

Chain 11:

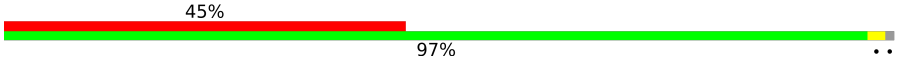


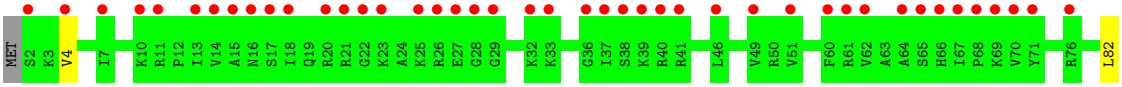




- Molecule 23: 50S ribosomal protein L28

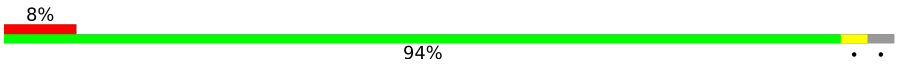
Chain 21:

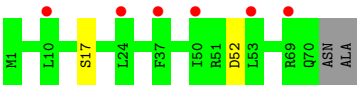




- Molecule 24: 50S ribosomal protein L29

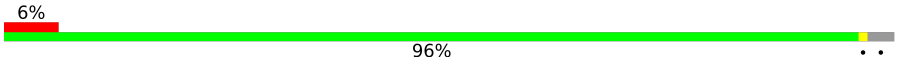
Chain 12:

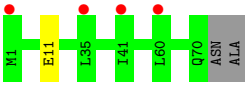




- Molecule 24: 50S ribosomal protein L29

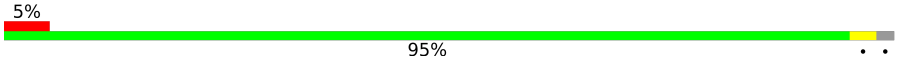
Chain 22:





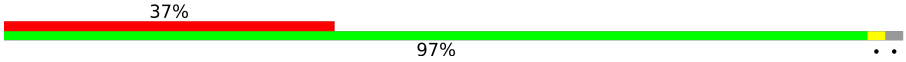
• Molecule 25: 50S ribosomal protein L30

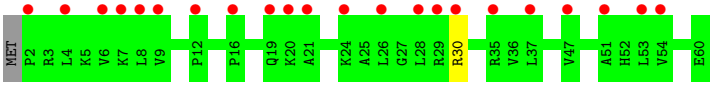
Chain 13:



• Molecule 25: 50S ribosomal protein L30

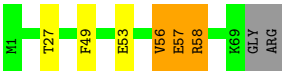
Chain 23:





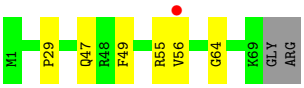
• Molecule 26: 50S ribosomal protein L31

Chain 14:



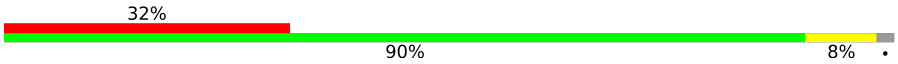
• Molecule 26: 50S ribosomal protein L31

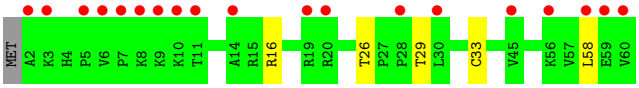
Chain 24:



• Molecule 27: 50S ribosomal protein L32

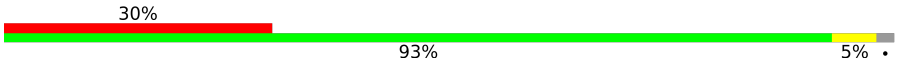
Chain 15:

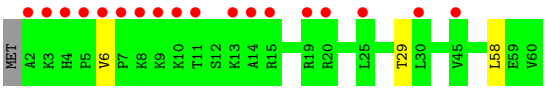




• Molecule 27: 50S ribosomal protein L32

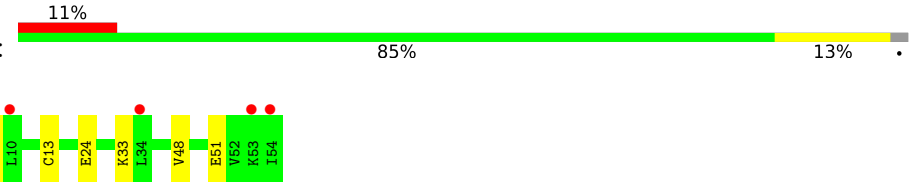
Chain 25:





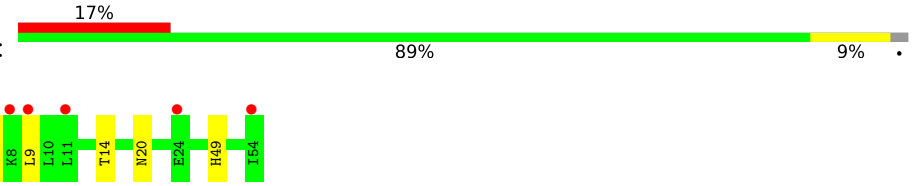
• Molecule 28: 50S ribosomal protein L33

Chain 16:



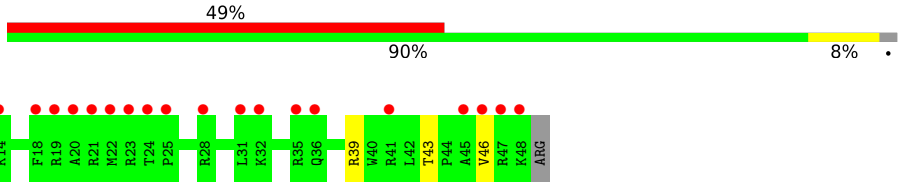
• Molecule 28: 50S ribosomal protein L33

Chain 26:



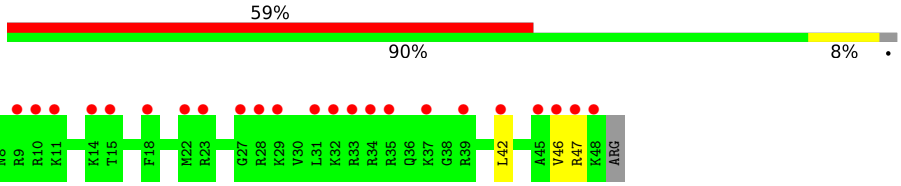
• Molecule 29: 50S ribosomal protein L34

Chain 17:



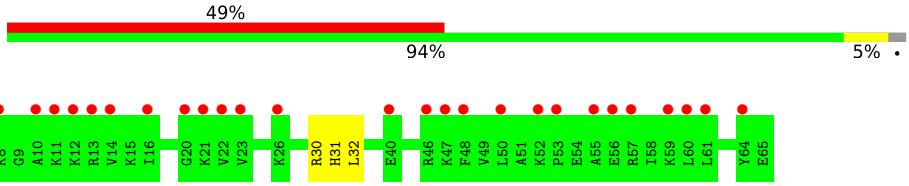
• Molecule 29: 50S ribosomal protein L34

Chain 27:



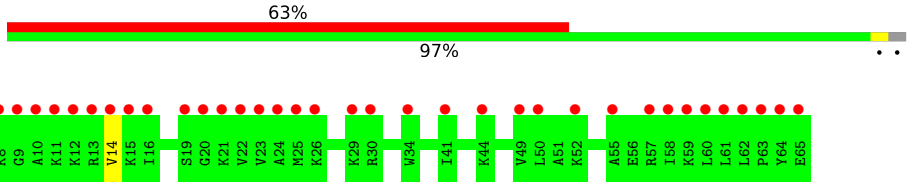
• Molecule 30: 50S ribosomal protein L35

Chain 18:



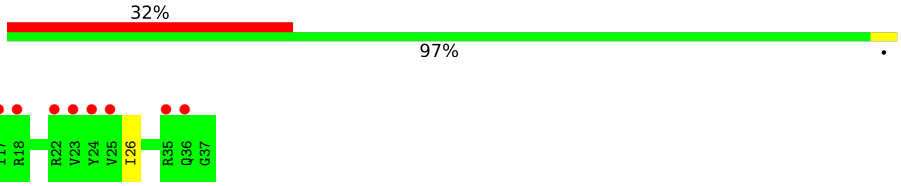
• Molecule 30: 50S ribosomal protein L35

Chain 28:



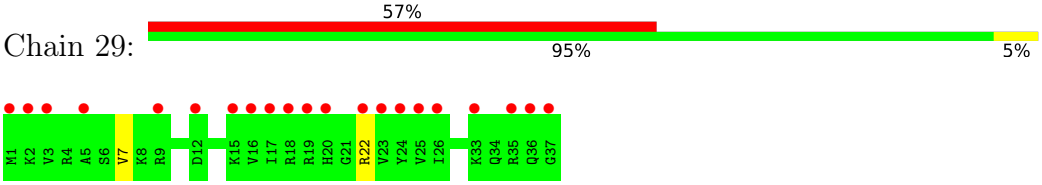
• Molecule 31: 50S ribosomal protein L36

Chain 19:



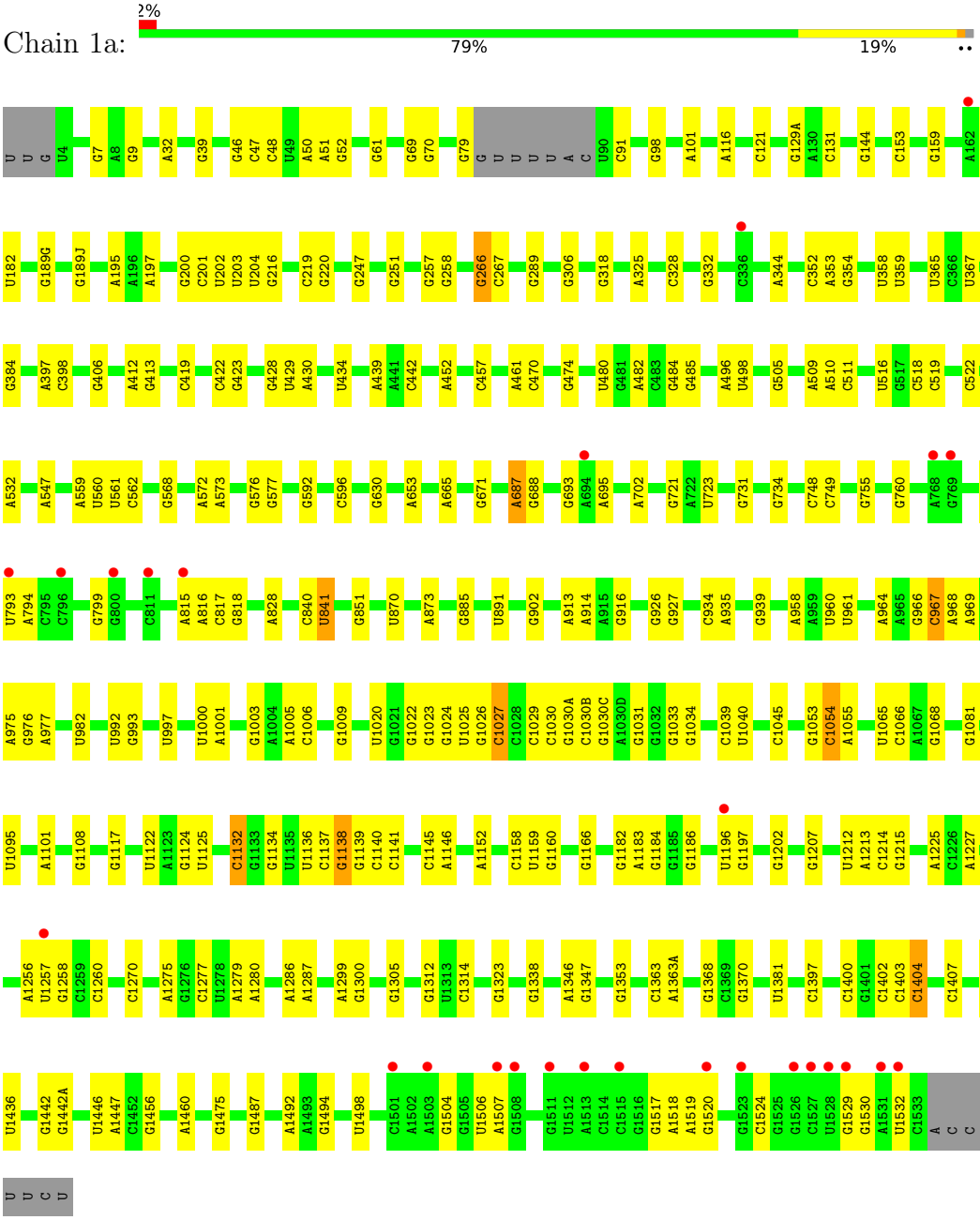
- Molecule 31: 50S ribosomal protein L36

Chain 29:



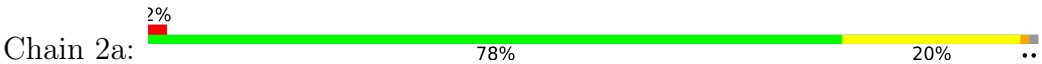
- Molecule 32: 16S Ribosomal RNA

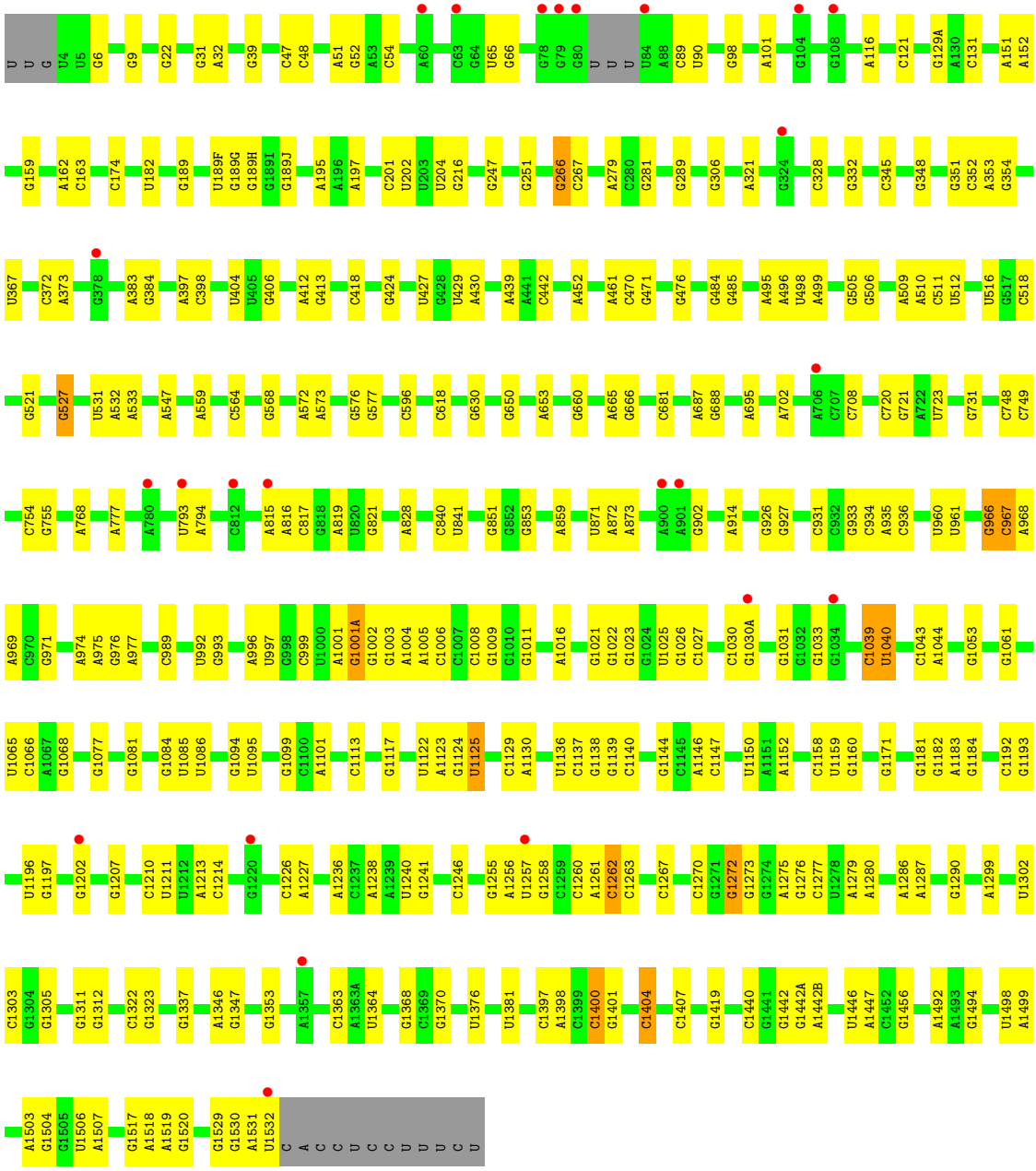
Chain 1a:



- Molecule 32: 16S Ribosomal RNA

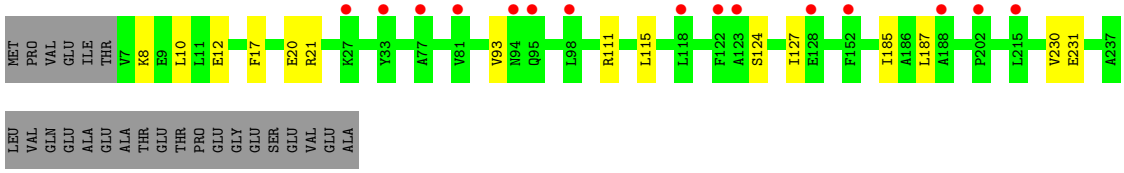
Chain 2a:





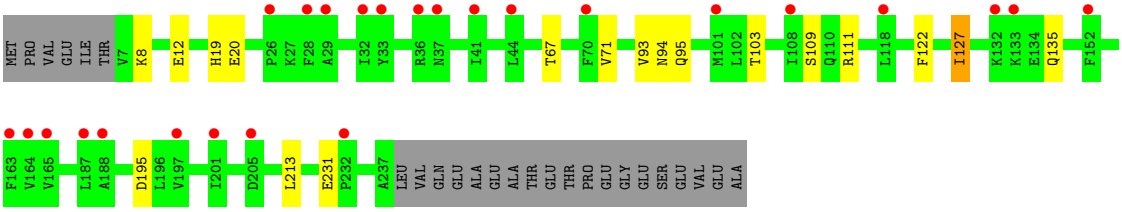
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



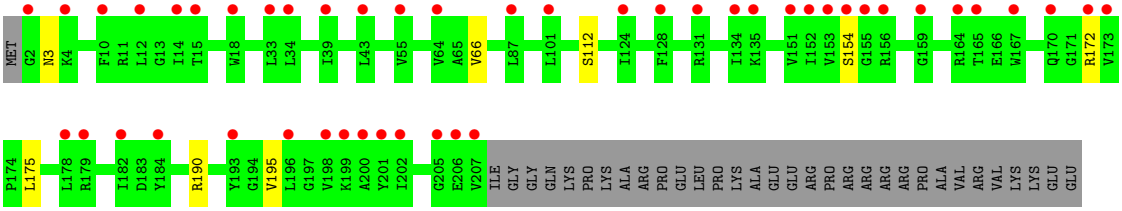
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



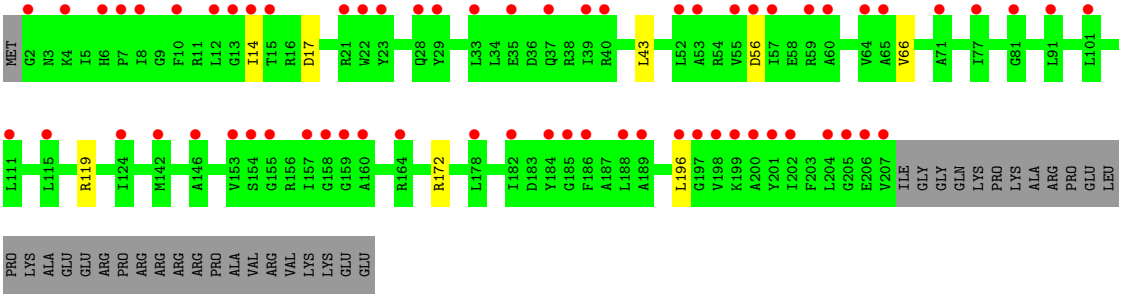
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



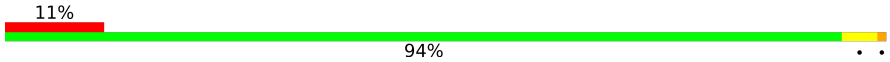
- Molecule 34: 30S ribosomal protein S3

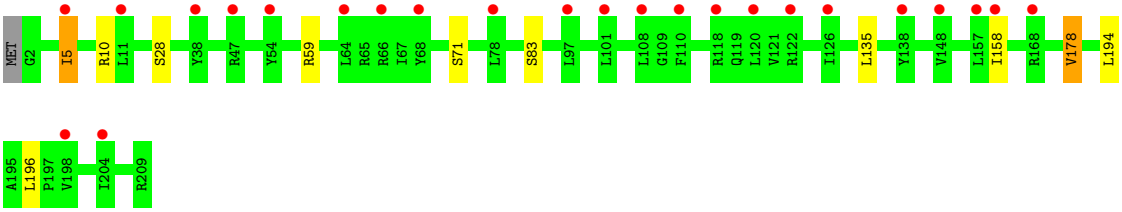
Chain 2c:



- Molecule 35: 30S ribosomal protein S4

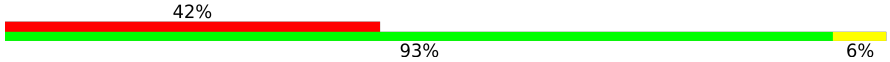
Chain 1d:

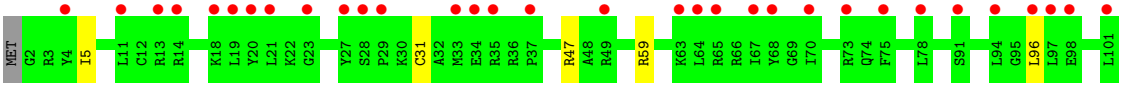


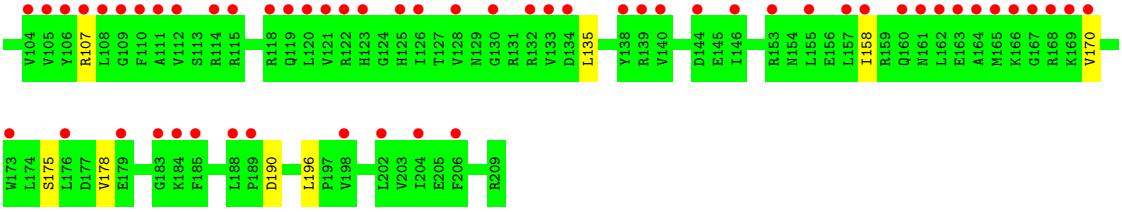


- Molecule 35: 30S ribosomal protein S4

Chain 2d:

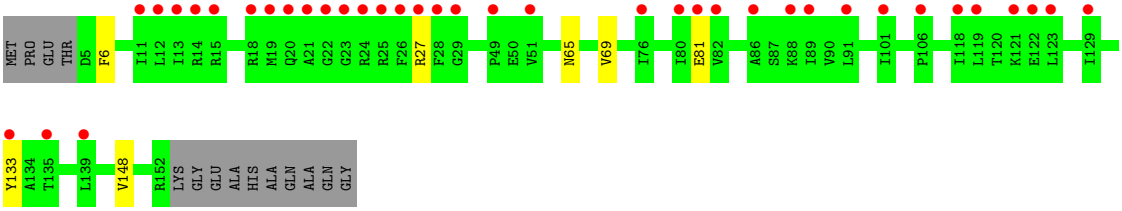






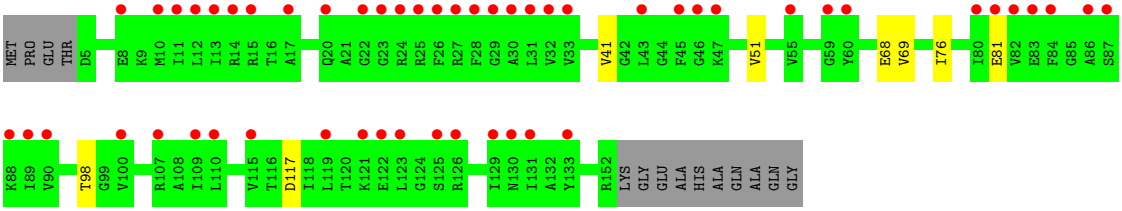
- Molecule 36: 30S ribosomal protein S5

Chain 1e:



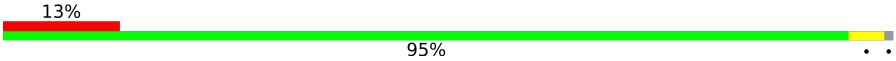
- Molecule 36: 30S ribosomal protein S5

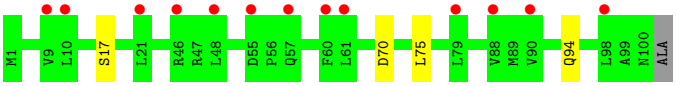
Chain 2e:



- Molecule 37: 30S ribosomal protein S6

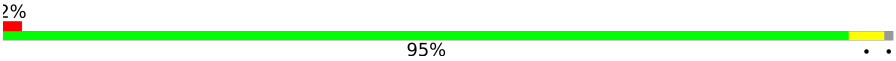
Chain 1f:





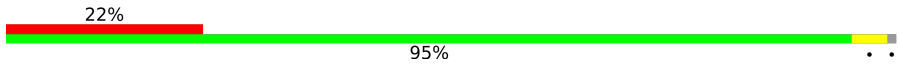
- Molecule 37: 30S ribosomal protein S6

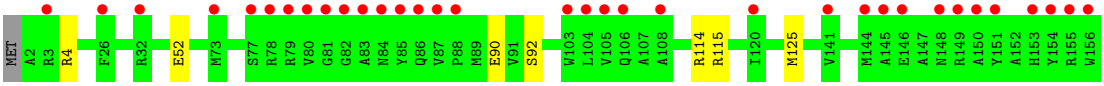
Chain 2f:



- Molecule 38: 30S ribosomal protein S7

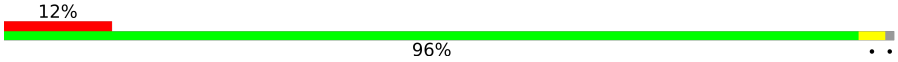
Chain 1g:

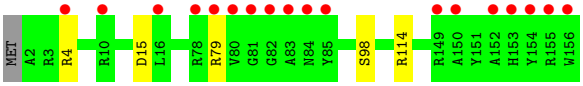




• Molecule 38: 30S ribosomal protein S7

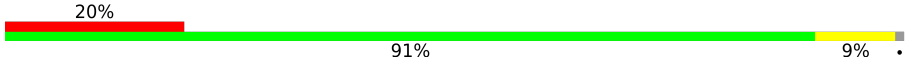
Chain 2g:

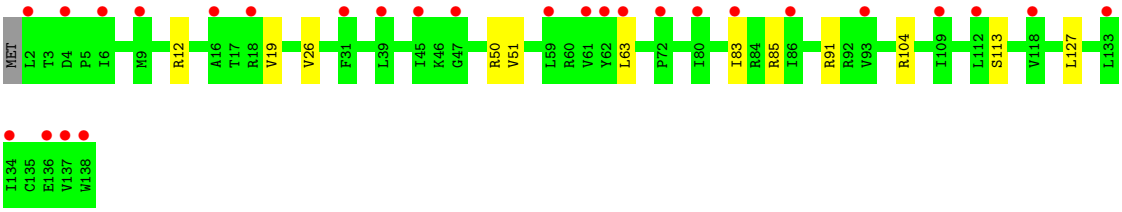




• Molecule 39: 30S ribosomal protein S8

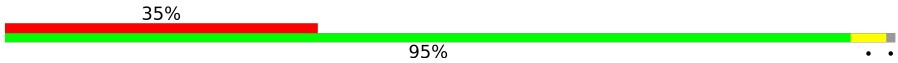
Chain 1h:

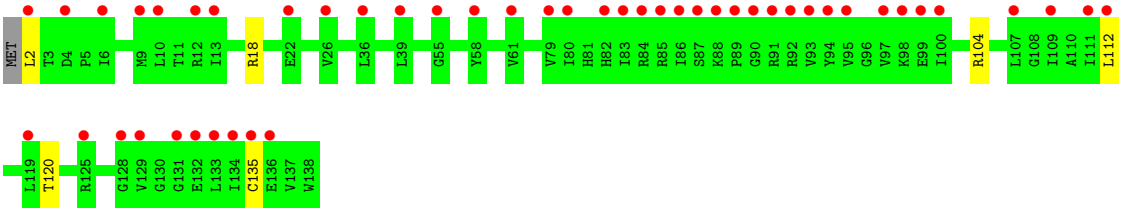




• Molecule 39: 30S ribosomal protein S8

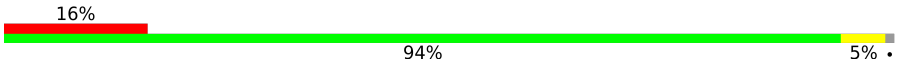
Chain 2h:

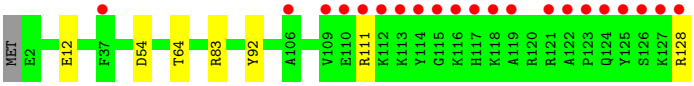




• Molecule 40: 30S ribosomal protein S9

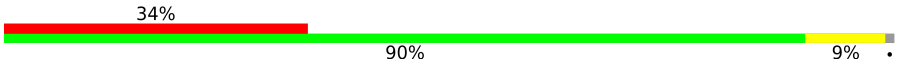
Chain 1i:

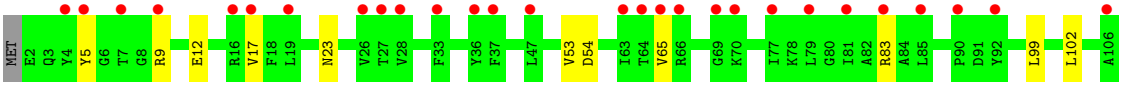


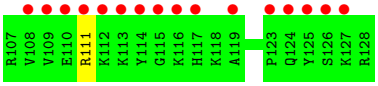


• Molecule 40: 30S ribosomal protein S9

Chain 2i:

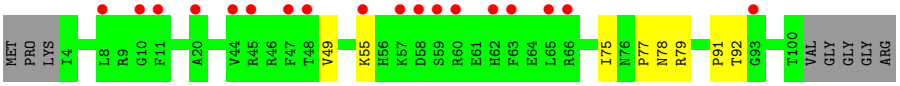






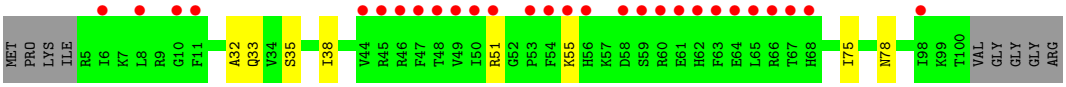
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



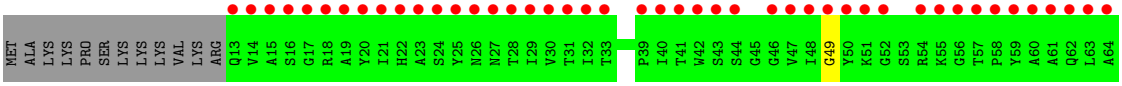
• Molecule 41: 30S ribosomal protein S10

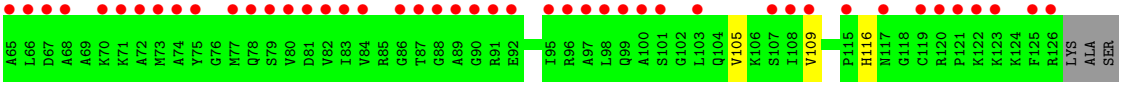
Chain 2j:



• Molecule 42: 30S ribosomal protein S11

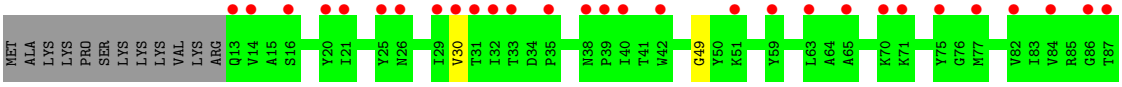
Chain 1k:

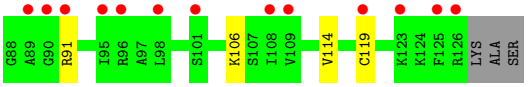




• Molecule 42: 30S ribosomal protein S11

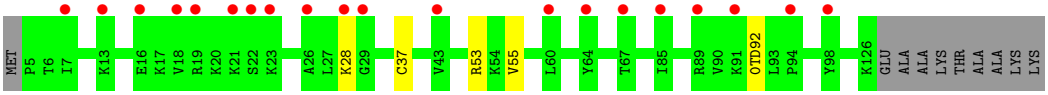
Chain 2k:





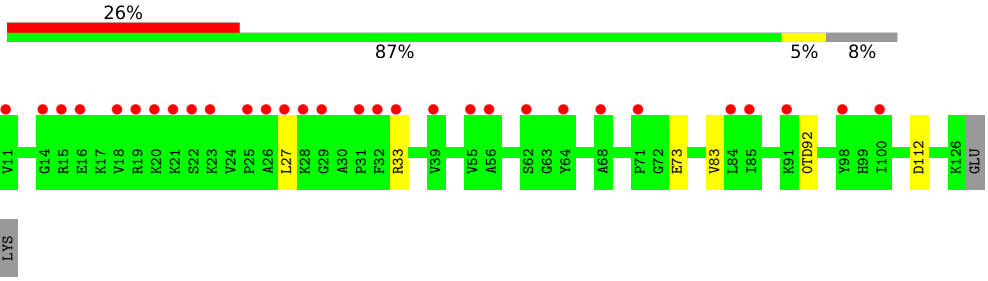
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



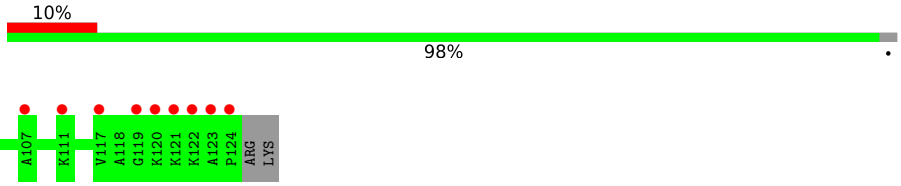
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



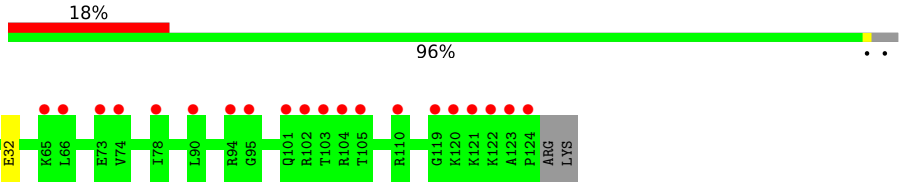
- Molecule 44: 30S ribosomal protein S13

Chain 1m:



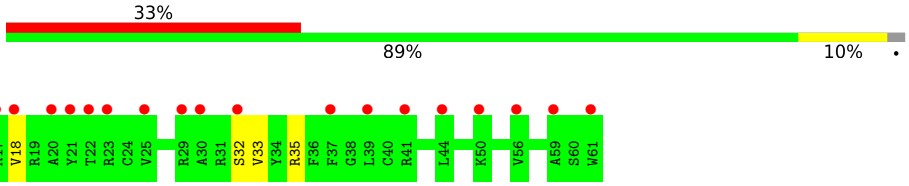
- Molecule 44: 30S ribosomal protein S13

Chain 2m:



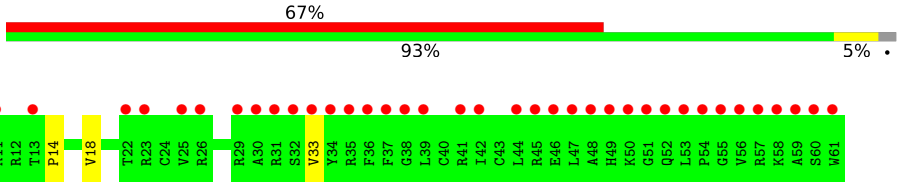
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



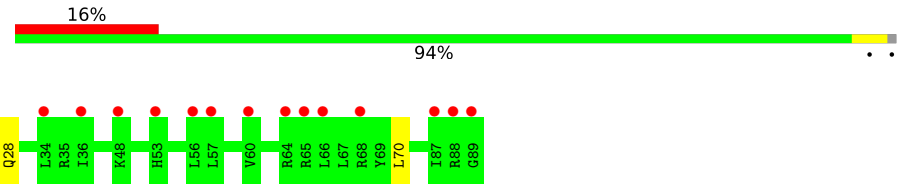
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



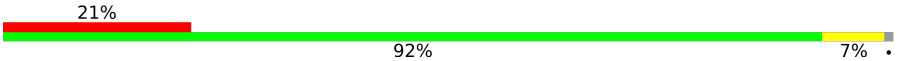
- Molecule 46: 30S ribosomal protein S15

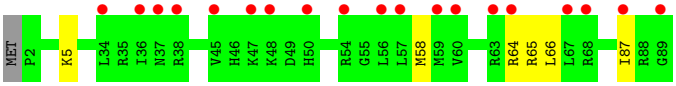
Chain 1o:



- Molecule 46: 30S ribosomal protein S15

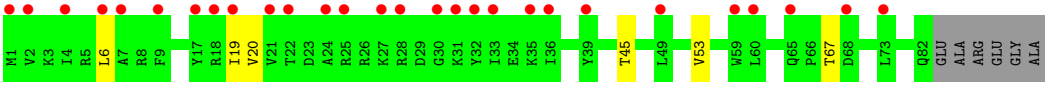
Chain 2o:





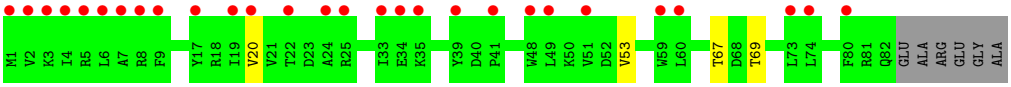
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



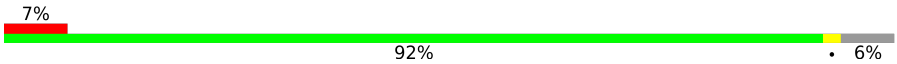
• Molecule 47: 30S ribosomal protein S16

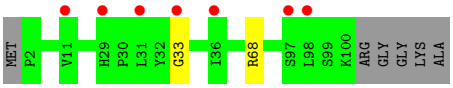
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

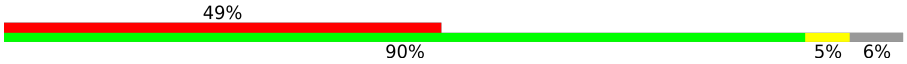
Chain 1q:

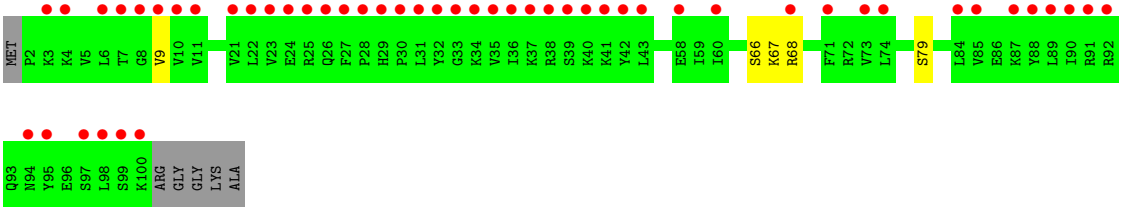




• Molecule 48: 30S ribosomal protein S17

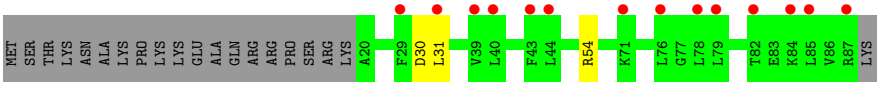
Chain 2q:





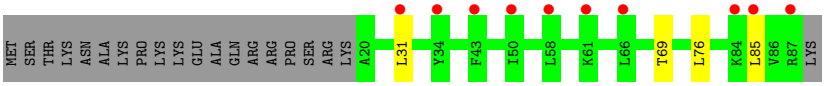
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



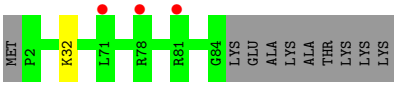
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



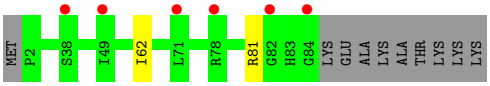
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



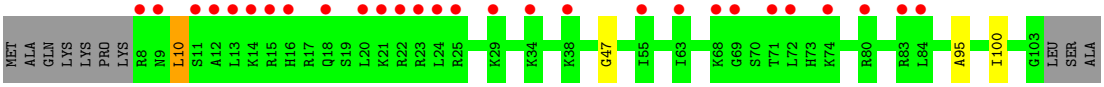
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



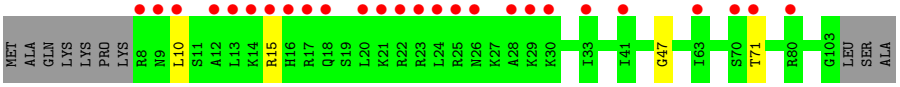
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



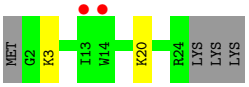
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



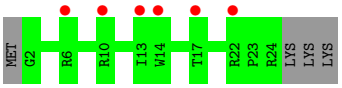
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



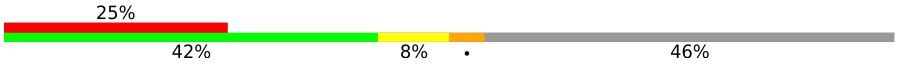
• Molecule 52: 30S ribosomal protein Thx

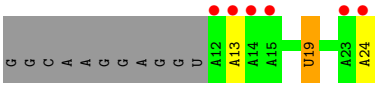
Chain 2u:



• Molecule 53: mRNA

Chain 1v:



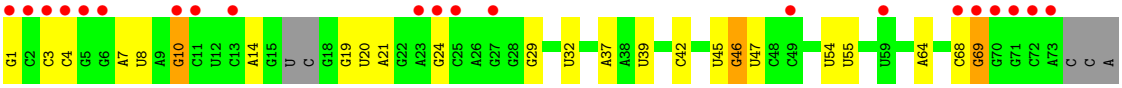


• Molecule 53: mRNA

Chain 2v:

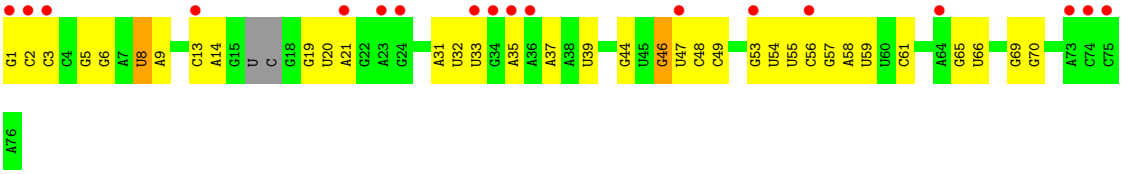
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



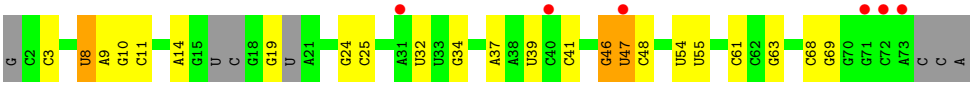
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



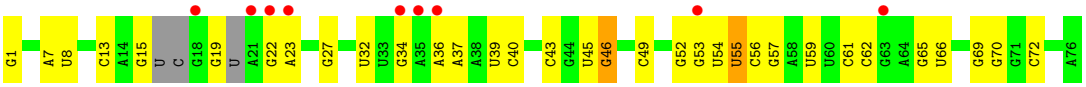
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



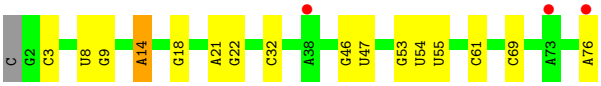
• Molecule 54: A-site and E-site tRNAs

Chain 2y:



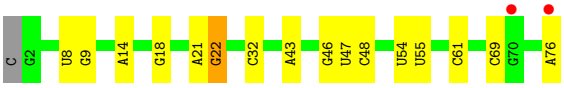
• Molecule 55: P-site tRNA

Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:



4 Data and refinement statistics (i)

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

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

[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 (i)

5.1 Standard geometry (i)

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

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

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

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

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

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1
41	2j	0	1
All	All	0	2

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

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

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

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide
41	2j	32	ALA	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	34	69
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	64
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	48
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	64
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	48
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	60
6	2G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	25	60
7	1H	172/180 (96%)	159 (92%)	13 (8%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	43
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22	56
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	22	56
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	53
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11	39
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	51
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	53
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	2V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	48
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22	56
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	46
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	7
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	7
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	6	28
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	23 (10%)	4 (2%)	9	34
33	2b	229/256 (90%)	205 (90%)	20 (9%)	4 (2%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	64
34	2c	204/239 (85%)	192 (94%)	10 (5%)	2 (1%)	15	48
35	1d	206/209 (99%)	200 (97%)	4 (2%)	2 (1%)	15	48
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	64
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	39
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	39
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	7	30
38	2g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22	56
39	1h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	56
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	116 (93%)	7 (6%)	2 (2%)	9	36
40	2i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	9	36
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	6
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	12
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	33
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	33
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	34
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	43
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
47	2p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	41
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	48
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	48
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	43
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	12
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	29
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10654 (94%)	629 (6%)	87 (1%)	19	53

5 of 87 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	207 (96%)	8 (4%)	34	66
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26	59
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	58
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	53
5	1F	160/166 (96%)	155 (97%)	5 (3%)	40	71
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	44
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	63
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	53
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	37
8	2I	105/124 (85%)	97 (92%)	8 (8%)	13	39
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	50
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16	45
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	50
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	64
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	62
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	62
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	61
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	37
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	78
14	2S	85/88 (97%)	82 (96%)	3 (4%)	36	68
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	68
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	62
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	54
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	48
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	48
18	1W	90/92 (98%)	88 (98%)	2 (2%)	52	79
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	62
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	65
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	16
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	50
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	50
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	79
22	1O	65/67 (97%)	65 (100%)	0	100	100
22	2O	65/67 (97%)	63 (97%)	2 (3%)	40	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	66
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	76
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	71
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	65
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	80
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	34
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	81
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	26
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	50
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	15
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	26
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	27
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	41
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	53
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	81
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	73
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	50
33	1b	192/220 (87%)	181 (94%)	11 (6%)	20	52
33	2b	187/220 (85%)	172 (92%)	15 (8%)	12	37
34	1c	142/188 (76%)	135 (95%)	7 (5%)	25	58
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	62
35	1d	169/181 (93%)	158 (94%)	11 (6%)	17	46
35	2d	173/181 (96%)	161 (93%)	12 (7%)	15	44
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	62
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	55
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	59
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	69
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38	70
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22	55
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21	53
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	22
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	72
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	62
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	77
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	59
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	63
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	48
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	89
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	19
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	64
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	66
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	39
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	42
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	62
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	89
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	62
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	56
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	86
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	85
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42	73
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	22
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8839 (95%)	464 (5%)	24	57

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

Mol	Chain	Res	Type
3	2D	61	LEU

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Mol	Chain	Res	Type
45	2n	33	VAL
9	2N	58	ASP
43	2l	73	GLU
36	2e	51	VAL

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

Mol	Chain	Res	Type
21	2Z	32	HIS
35	2d	125	HIS
21	2Z	73	GLN
33	2b	94	ASN
38	2g	37	ASN

5.3.3 RNA (i)

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

5 of 1736 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	1A	45	C

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	528	A
1	2A	1530	C
1	2A	752	A
1	2A	1210	A
1	2A	1913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.48	3 (11%)
55	4SU	2x	8	55,56	18,21,22	1.92	6 (33%)	26,30,33	1.71	6 (23%)
54	5MU	2w	54	54	19,22,23	1.42	6 (31%)	28,32,35	1.87	6 (21%)
54	PSU	2w	39	54	18,21,22	1.27	2 (11%)	22,30,33	2.08	4 (18%)
32	5MC	2a	1400	32	18,22,23	1.01	1 (5%)	26,32,35	1.43	5 (19%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	28,32,35	2.19	6 (21%)
1	5MC	2A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.18	2 (7%)
54	5MU	1w	54	54	19,22,23	1.44	6 (31%)	28,32,35	1.81	8 (28%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	PSU	2y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.68	4 (22%)
1	OMG	1A	2251	55,56,1	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
54	7MG	1y	46	54	22,26,27	1.36	3 (13%)	29,39,42	2.63	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	4SU	2y	8	54,56	18,21,22	1.67	4 (22%)	26,30,33	2.31	6 (23%)
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
54	7MG	2w	46	54	22,26,27	1.34	4 (18%)	29,39,42	2.49	7 (24%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.98	4 (18%)
43	0TD	1l	92	43	7,9,10	4.69	1 (14%)	6,11,13	7.22	2 (33%)
1	PSU	1A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	4 (18%)
1	2MU	1A	2552	56,1	19,22,24	1.26	3 (15%)	26,31,36	1.85	6 (23%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
1	2MA	2A	2503	1	17,25,26	0.99	1 (5%)	17,37,40	0.97	2 (11%)
32	5MC	1a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.11	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	22,30,33	1.94	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
54	PSU	1y	39	54	18,21,22	1.30	2 (11%)	22,30,33	1.99	3 (13%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.60	5 (27%)
32	7MG	2a	527	32	22,26,27	1.34	3 (13%)	29,39,42	2.50	6 (20%)
54	7MG	2y	46	54	22,26,27	1.41	3 (13%)	29,39,42	2.61	6 (20%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.92	1 (3%)
53	PSU	1v	19	53,54	18,21,22	1.44	3 (16%)	22,30,33	1.48	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.97	1 (5%)	26,32,35	1.17	3 (11%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.72	6 (33%)
53	PSU	2v	19	53,54,56	18,21,22	1.38	2 (11%)	22,30,33	1.82	3 (13%)
54	4SU	1w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.11	5 (19%)
32	7MG	1a	527	32,56	22,26,27	1.34	3 (13%)	29,39,42	2.51	6 (20%)
1	5MC	1A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
54	MIA	2w	37	54	20,27,32	1.84	2 (10%)	22,39,47	1.87	7 (31%)
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	0.93	2 (9%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.80	4 (18%)
1	2MA	1A	2503	56,1	17,25,26	1.00	1 (5%)	17,37,40	0.98	2 (11%)
32	5MC	2a	1407	32,56	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.03	7 (25%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.54	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MU	2A	2552	56,1	19,22,24	1.24	3 (15%)	26,31,36	1.79	6 (23%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	28,32,35	2.03	7 (25%)
54	PSU	2y	39	54	18,21,22	1.36	2 (11%)	22,30,33	1.71	3 (13%)
54	4SU	1y	8	54	18,21,22	1.63	4 (22%)	26,30,33	2.11	4 (15%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.48	1 (3%)
1	5MU	1A	1939	1	19,22,23	1.44	5 (26%)	28,32,35	2.19	6 (21%)
32	5MC	1a	967	32	18,22,23	0.92	2 (11%)	26,32,35	1.11	2 (7%)
43	0TD	2l	92	43	7,9,10	4.71	1 (14%)	6,11,13	8.18	2 (33%)
54	4SU	2w	8	54	18,21,22	1.69	5 (27%)	26,30,33	2.06	4 (15%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.88	1 (3%)
1	4OC	1A	1920	1	19,22,24	0.81	0	26,31,35	0.90	0
1	OMG	2A	2251	55,1	18,26,27	0.93	1 (5%)	19,38,41	1.10	3 (15%)
54	MIA	1y	37	54	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
54	5MU	2y	54	54	19,22,23	1.44	5 (26%)	28,32,35	2.02	5 (17%)
54	5MU	1y	54	54	19,22,23	1.37	4 (21%)	28,32,35	2.15	6 (21%)
54	PSU	1y	32	54	18,21,22	1.31	2 (11%)	22,30,33	1.87	4 (18%)
32	2MG	2a	1207	32,56	18,26,27	0.88	1 (5%)	16,38,41	1.04	2 (12%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
54	PSU	1w	39	54	18,21,22	1.24	1 (5%)	22,30,33	2.11	4 (18%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.65	4 (22%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.21	2 (7%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	28,32,35	2.10	6 (21%)
32	4OC	2a	1402	32,56	20,23,24	0.77	0	26,32,35	0.96	0
55	5MC	2x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.21	3 (11%)
32	M2G	1a	966	32	20,27,28	1.42	3 (15%)	22,40,43	0.96	2 (9%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
55	5MU	1x	54	55	19,22,23	1.37	5 (26%)	28,32,35	1.98	7 (25%)
55	4SU	1x	8	55,56	18,21,22	1.99	4 (22%)	26,30,33	1.63	5 (19%)
54	MIA	2y	37	54,32	18,24,32	1.13	2 (11%)	18,35,47	1.22	2 (11%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.07	2 (12%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	22,30,33	1.76	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	1a	1407	32	18,22,23	0.95	2 (11%)	26,32,35	1.09	2 (7%)
54	7MG	1w	46	54	22,26,27	1.32	3 (13%)	29,39,42	2.54	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	2/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	5/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	2/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	4SU	2y	8	54,56	-	1/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
53	PSU	1v	19	53,54	-	3/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	3/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
53	PSU	2v	19	53,54,56	-	2/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55,56	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54,32	-	2/3/25/34	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3

The worst 5 of 207 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.15	1.69	1.82
43	1l	92	0TD	CB-SB	-12.07	1.69	1.82
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
54	1w	37	MIA	C2-S10	-7.02	1.69	1.75
54	2w	37	MIA	C2-S10	-6.89	1.69	1.75

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-19.84	66.54	102.44
43	1l	92	0TD	CSB-SB-CB	-17.44	70.90	102.44
54	2y	46	7MG	N9-C4-N3	9.74	140.03	125.47
54	1y	46	7MG	N9-C4-N3	9.71	139.99	125.47
54	1w	46	7MG	N9-C4-N3	8.86	138.72	125.47

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1466 ligands modelled in this entry, 1464 are monoatomic - leaving 2 for Mogul analysis.

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

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

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

The worst 5 of 3414 RSRZ outliers are listed below:

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

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

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

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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	4SU	2x	8	20/21	0.91	0.11	97,110,116,120	0
54	PSU	2w	32	20/21	0.91	0.29	108,114,123,126	0
54	PSU	1w	39	20/21	0.91	0.29	97,105,119,120	0
32	5MC	2a	967	21/22	0.91	0.16	99,102,110,118	0
32	5MC	2a	1404	21/22	0.91	0.17	84,99,105,110	0
1	5MU	1A	1915	21/22	0.93	0.17	82,100,104,110	0
32	4OC	2a	1402	22/23	0.93	0.17	97,104,109,114	0
1	PSU	1A	2605	20/21	0.93	0.28	66,79,85,86	0
53	PSU	1v	19	20/21	0.93	0.14	79,95,102,102	0
43	0TD	1l	92	10/11	0.93	0.22	88,91,97,113	0
32	7MG	2a	527	24/25	0.93	0.18	89,95,101,112	0
55	5MC	2x	32	21/22	0.93	0.22	99,105,110,112	0
55	4SU	1x	8	20/21	0.93	0.15	93,100,106,110	0
1	PSU	2A	1911	20/21	0.94	0.14	86,98,105,106	0
55	5MU	2x	54	21/22	0.94	0.13	103,111,114,124	0
1	5MU	2A	1915	21/22	0.94	0.13	101,107,111,116	0
1	PSU	2A	1917	20/21	0.94	0.13	86,103,108,111	0
32	4OC	1a	1402	22/23	0.94	0.26	82,92,98,100	0
1	4OC	2A	1920	21/23	0.94	0.15	89,98,103,108	0
54	5MU	1w	54	21/22	0.94	0.25	104,108,117,119	0
1	5MC	2A	1962	21/22	0.94	0.17	77,89,95,99	0
32	5MC	1a	1407	21/22	0.94	0.23	76,88,93,97	0
32	UR3	2a	1498	21/22	0.94	0.24	88,98,102,106	0
32	MA6	2a	1519	24/25	0.94	0.30	86,99,103,105	0
43	0TD	2l	92	10/11	0.94	0.15	95,101,103,110	0
32	PSU	1a	516	20/21	0.94	0.17	84,92,98,104	0
1	PSU	1A	1911	20/21	0.94	0.18	70,90,95,100	0
1	OMG	2A	2251	24/25	0.95	0.33	74,88,94,96	0
1	2MA	2A	2503	23/24	0.95	0.27	70,81,88,92	0
1	PSU	1A	1917	20/21	0.95	0.18	83,90,95,96	0
32	5MC	1a	1404	21/22	0.95	0.28	74,83,96,97	0
1	PSU	2A	2605	20/21	0.95	0.25	79,88,93,96	0
55	5MC	1x	32	21/22	0.95	0.23	84,95,100,102	0
32	5MC	2a	1407	21/22	0.95	0.16	93,98,101,106	0
55	5MU	1x	54	21/22	0.95	0.14	86,97,101,105	0
1	5MC	2A	1942	21/22	0.95	0.17	88,94,99,106	0
32	M2G	2a	966	25/26	0.95	0.19	93,99,106,113	0
1	5MC	1A	1962	21/22	0.95	0.22	72,83,91,94	0
32	2MG	1a	1207	24/25	0.95	0.17	77,95,102,105	0
55	PSU	1x	55	20/21	0.95	0.12	94,100,107,116	0
32	7MG	1a	527	24/25	0.96	0.20	78,89,96,98	0
1	2MU	1A	2552	21/23	0.96	0.31	58,78,84,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	M2G	1a	966	25/26	0.96	0.26	81,87,96,98	0
1	5MU	1A	1939	21/22	0.96	0.26	66,78,86,90	0
32	5MC	1a	967	21/22	0.96	0.23	77,88,95,101	0
1	5MU	2A	1939	21/22	0.96	0.23	75,86,91,95	0
1	5MC	1A	1942	21/22	0.96	0.20	65,81,86,88	0
1	4OC	1A	1920	21/23	0.96	0.21	76,89,95,96	0
32	MA6	2a	1518	24/25	0.96	0.22	90,97,101,102	0
32	5MC	1a	1400	21/22	0.96	0.26	81,91,96,104	0
32	UR3	1a	1498	21/22	0.97	0.28	78,85,89,93	0
1	2MU	2A	2552	21/23	0.97	0.17	74,84,89,91	0
32	MA6	1a	1518	24/25	0.97	0.24	58,85,89,93	0
1	OMG	1A	2251	24/25	0.97	0.25	66,80,85,86	0
32	MA6	1a	1519	24/25	0.97	0.34	82,87,92,99	0
1	2MA	1A	2503	23/24	0.97	0.32	58,74,81,83	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	3317	1/1	0.32	0.65	92,92,92,92	0
56	MG	2A	3201	1/1	0.34	0.22	102,102,102,102	0
56	MG	1A	3190	1/1	0.34	0.48	118,118,118,118	0
56	MG	1A	3242	1/1	0.37	0.33	78,78,78,78	0
56	MG	2a	3060	1/1	0.37	0.43	101,101,101,101	0
56	MG	2a	3082	1/1	0.37	0.31	109,109,109,109	0
56	MG	2a	3154	1/1	0.38	0.16	101,101,101,101	0
56	MG	1A	3557	1/1	0.40	0.36	89,89,89,89	0
56	MG	2A	3315	1/1	0.40	0.84	103,103,103,103	0
56	MG	1a	3094	1/1	0.44	1.77	96,96,96,96	0
56	MG	1a	3214	1/1	0.45	0.26	103,103,103,103	0
56	MG	2A	3031	1/1	0.45	0.20	100,100,100,100	0
56	MG	1A	3104	1/1	0.46	0.98	90,90,90,90	0
56	MG	1A	3497	1/1	0.46	0.22	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3017	1/1	0.48	0.30	98,98,98,98	0
56	MG	1A	3377	1/1	0.48	0.45	102,102,102,102	0
56	MG	1A	3429	1/1	0.50	0.25	87,87,87,87	0
56	MG	1a	3111	1/1	0.51	0.42	103,103,103,103	0
56	MG	1A	3194	1/1	0.53	0.26	72,72,72,72	0
56	MG	1A	3240	1/1	0.53	0.37	101,101,101,101	0
56	MG	1A	3157	1/1	0.54	0.13	92,92,92,92	0
56	MG	1A	3036	1/1	0.54	0.80	99,99,99,99	0
56	MG	1A	3099	1/1	0.55	0.40	77,77,77,77	0
56	MG	1A	3133	1/1	0.55	0.36	76,76,76,76	0
56	MG	1A	3359	1/1	0.56	0.77	89,89,89,89	0
56	MG	1A	3433	1/1	0.56	1.77	97,97,97,97	0
56	MG	2a	3080	1/1	0.56	0.28	85,85,85,85	0
56	MG	1A	3041	1/1	0.56	0.23	105,105,105,105	0
56	MG	1A	3534	1/1	0.56	0.30	86,86,86,86	0
56	MG	2A	3205	1/1	0.57	0.32	111,111,111,111	0
56	MG	2a	3059	1/1	0.57	0.46	79,79,79,79	0
56	MG	1A	3441	1/1	0.57	0.38	103,103,103,103	0
56	MG	1a	3077	1/1	0.58	0.22	84,84,84,84	0
56	MG	1A	3367	1/1	0.58	0.25	104,104,104,104	0
56	MG	1A	3148	1/1	0.58	0.42	79,79,79,79	0
56	MG	2a	3034	1/1	0.59	0.23	79,79,79,79	0
56	MG	1a	3005	1/1	0.60	0.21	80,80,80,80	0
56	MG	2A	3146	1/1	0.60	0.23	79,79,79,79	0
56	MG	2a	3107	1/1	0.60	0.10	106,106,106,106	0
56	MG	1A	3615	1/1	0.60	0.22	95,95,95,95	0
56	MG	2A	3074	1/1	0.61	0.30	102,102,102,102	0
56	MG	2A	3111	1/1	0.61	0.67	81,81,81,81	0
56	MG	1A	3527	1/1	0.61	0.24	74,74,74,74	0
56	MG	1A	3651	1/1	0.61	0.19	90,90,90,90	0
56	MG	1a	3211	1/1	0.61	0.30	77,77,77,77	0
56	MG	2a	3102	1/1	0.61	0.23	90,90,90,90	0
56	MG	2A	3034	1/1	0.61	0.17	71,71,71,71	0
56	MG	2A	3057	1/1	0.61	0.71	89,89,89,89	0
56	MG	2A	3316	1/1	0.62	0.48	93,93,93,93	0
56	MG	2A	3302	1/1	0.63	0.14	82,82,82,82	0
56	MG	1A	3142	1/1	0.64	0.53	73,73,73,73	0
56	MG	2a	3087	1/1	0.64	0.46	94,94,94,94	0
56	MG	1A	3105	1/1	0.64	0.25	74,74,74,74	0
56	MG	1a	3043	1/1	0.64	0.41	95,95,95,95	0
56	MG	2a	3007	1/1	0.64	0.54	99,99,99,99	0
56	MG	1a	3167	1/1	0.65	0.48	109,109,109,109	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	0.65	0.15	98,98,98,98	0
56	MG	2A	3158	1/1	0.65	0.67	78,78,78,78	0
56	MG	2a	3058	1/1	0.65	0.61	93,93,93,93	0
56	MG	1A	3569	1/1	0.65	0.11	95,95,95,95	0
56	MG	1a	3122	1/1	0.65	1.05	93,93,93,93	0
56	MG	2a	3017	1/1	0.66	2.14	89,89,89,89	0
56	MG	1A	3364	1/1	0.66	0.30	96,96,96,96	0
56	MG	2a	3051	1/1	0.66	0.31	79,79,79,79	0
56	MG	2A	3323	1/1	0.66	0.15	104,104,104,104	0
56	MG	1A	3145	1/1	0.67	0.27	93,93,93,93	0
56	MG	1A	3191	1/1	0.67	0.26	90,90,90,90	0
56	MG	1A	3098	1/1	0.67	1.35	80,80,80,80	0
56	MG	1A	3123	1/1	0.67	0.47	93,93,93,93	0
56	MG	2A	3160	1/1	0.67	0.13	88,88,88,88	0
56	MG	2A	3184	1/1	0.67	0.28	82,82,82,82	0
56	MG	1a	3116	1/1	0.67	0.47	90,90,90,90	0
56	MG	2a	3106	1/1	0.67	0.22	124,124,124,124	0
56	MG	1a	3008	1/1	0.67	0.15	66,66,66,66	0
56	MG	1a	3149	1/1	0.67	0.21	110,110,110,110	0
57	ZN	14	501	1/1	0.67	0.04	162,162,162,162	0
56	MG	2A	3287	1/1	0.68	0.16	83,83,83,83	0
56	MG	1a	3085	1/1	0.68	0.34	89,89,89,89	0
56	MG	2a	3049	1/1	0.68	0.18	79,79,79,79	0
56	MG	2a	3138	1/1	0.68	0.28	95,95,95,95	0
56	MG	1A	3408	1/1	0.68	0.20	96,96,96,96	0
56	MG	1A	3524	1/1	0.68	0.36	84,84,84,84	0
56	MG	2A	3162	1/1	0.69	0.23	77,77,77,77	0
56	MG	1A	3565	1/1	0.69	0.28	83,83,83,83	0
56	MG	1A	3034	1/1	0.69	0.10	79,79,79,79	0
56	MG	2a	3158	1/1	0.69	0.22	116,116,116,116	0
56	MG	1A	3573	1/1	0.69	0.21	88,88,88,88	0
56	MG	1A	3128	1/1	0.70	0.22	75,75,75,75	0
56	MG	2A	3094	1/1	0.71	0.22	85,85,85,85	0
56	MG	1a	3173	1/1	0.71	0.25	75,75,75,75	0
56	MG	1A	3585	1/1	0.71	0.19	76,76,76,76	0
56	MG	2a	3070	1/1	0.71	0.21	87,87,87,87	0
56	MG	1A	3303	1/1	0.71	0.27	78,78,78,78	0
56	MG	1A	3160	1/1	0.71	0.26	76,76,76,76	0
56	MG	1A	3506	1/1	0.71	0.52	118,118,118,118	0
56	MG	2a	3100	1/1	0.71	0.26	94,94,94,94	0
56	MG	2A	3166	1/1	0.71	0.27	79,79,79,79	0
56	MG	1A	3151	1/1	0.71	0.27	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	2A	3196	1/1	0.71	0.33	81,81,81,81	0
56	MG	1A	3572	1/1	0.71	0.18	85,85,85,85	0
56	MG	1A	3277	1/1	0.71	0.21	73,73,73,73	0
56	MG	2A	3278	1/1	0.71	0.16	89,89,89,89	0
56	MG	2a	3053	1/1	0.71	0.82	90,90,90,90	0
56	MG	1a	3082	1/1	0.72	0.80	75,75,75,75	0
56	MG	1a	3028	1/1	0.72	0.20	76,76,76,76	0
56	MG	2A	3290	1/1	0.72	0.14	94,94,94,94	0
56	MG	1A	3533	1/1	0.72	0.37	114,114,114,114	0
56	MG	1a	3162	1/1	0.72	0.31	93,93,93,93	0
56	MG	2A	3099	1/1	0.72	0.62	89,89,89,89	0
56	MG	2A	3022	1/1	0.72	0.16	96,96,96,96	0
56	MG	2A	3119	1/1	0.72	0.15	90,90,90,90	0
56	MG	2a	3006	1/1	0.72	0.31	104,104,104,104	0
56	MG	1A	3239	1/1	0.72	0.25	93,93,93,93	0
56	MG	2a	3077	1/1	0.72	0.17	95,95,95,95	0
56	MG	1A	3612	1/1	0.73	0.24	95,95,95,95	0
56	MG	2a	3054	1/1	0.73	0.18	90,90,90,90	0
56	MG	1A	3505	1/1	0.73	0.15	70,70,70,70	0
56	MG	2A	3019	1/1	0.73	0.21	101,101,101,101	0
56	MG	2A	3092	1/1	0.73	0.48	99,99,99,99	0
56	MG	2a	3130	1/1	0.73	0.09	74,74,74,74	0
56	MG	1A	3636	1/1	0.73	0.34	73,73,73,73	0
56	MG	2a	3037	1/1	0.73	0.21	106,106,106,106	0
56	MG	2A	3245	1/1	0.73	0.41	94,94,94,94	0
56	MG	2a	3179	1/1	0.73	0.12	106,106,106,106	0
56	MG	1A	3513	1/1	0.73	0.63	88,88,88,88	0
56	MG	2a	3031	1/1	0.74	0.88	109,109,109,109	0
56	MG	2A	3244	1/1	0.74	0.11	90,90,90,90	0
56	MG	2A	3070	1/1	0.74	0.35	74,74,74,74	0
56	MG	2A	3192	1/1	0.74	0.12	77,77,77,77	0
56	MG	2A	3193	1/1	0.74	0.35	86,86,86,86	0
56	MG	1A	3583	1/1	0.74	0.15	88,88,88,88	0
56	MG	1A	3390	1/1	0.74	0.27	87,87,87,87	0
56	MG	2a	3088	1/1	0.74	0.32	97,97,97,97	0
56	MG	1a	3105	1/1	0.74	0.25	86,86,86,86	0
56	MG	2A	3197	1/1	0.75	0.20	78,78,78,78	0
56	MG	1a	3163	1/1	0.75	0.41	66,66,66,66	0
56	MG	1a	3092	1/1	0.75	0.71	85,85,85,85	0
56	MG	1A	3368	1/1	0.75	0.78	99,99,99,99	0
56	MG	2A	3087	1/1	0.75	0.28	88,88,88,88	0
56	MG	2a	3097	1/1	0.75	0.31	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3352	1/1	0.75	0.26	95,95,95,95	0
56	MG	1A	3268	1/1	0.75	0.21	68,68,68,68	0
56	MG	1A	3423	1/1	0.76	0.38	78,78,78,78	0
56	MG	1A	3257	1/1	0.76	0.27	80,80,80,80	0
56	MG	1a	3182	1/1	0.76	0.21	102,102,102,102	0
56	MG	1A	3149	1/1	0.76	0.53	76,76,76,76	0
56	MG	2A	3058	1/1	0.76	0.32	78,78,78,78	0
56	MG	2A	3123	1/1	0.76	0.18	81,81,81,81	0
56	MG	1a	3016	1/1	0.76	0.92	87,87,87,87	0
56	MG	2A	3156	1/1	0.76	0.17	69,69,69,69	0
56	MG	2a	3166	1/1	0.76	0.14	115,115,115,115	0
56	MG	1A	3014	1/1	0.76	0.39	93,93,93,93	0
56	MG	1A	3555	1/1	0.76	0.23	80,80,80,80	0
56	MG	1a	3027	1/1	0.77	0.18	76,76,76,76	0
56	MG	1A	3304	1/1	0.77	0.21	76,76,76,76	0
56	MG	2A	3198	1/1	0.77	0.17	83,83,83,83	0
56	MG	1A	3415	1/1	0.77	0.21	78,78,78,78	0
56	MG	2A	3138	1/1	0.77	0.20	102,102,102,102	0
56	MG	2A	3243	1/1	0.77	0.13	88,88,88,88	0
56	MG	1a	3067	1/1	0.77	0.18	80,80,80,80	0
56	MG	2A	3148	1/1	0.77	0.16	96,96,96,96	0
56	MG	1A	3045	1/1	0.77	0.23	94,94,94,94	0
56	MG	1A	3629	1/1	0.77	0.28	106,106,106,106	0
56	MG	1A	3280	1/1	0.77	0.20	77,77,77,77	0
56	MG	1A	3518	1/1	0.77	0.27	97,97,97,97	0
56	MG	1A	3244	1/1	0.77	0.23	81,81,81,81	0
56	MG	1A	3394	1/1	0.77	0.46	91,91,91,91	0
56	MG	2A	3003	1/1	0.77	0.23	84,84,84,84	0
56	MG	1A	3442	1/1	0.77	0.15	77,77,77,77	0
56	MG	1A	3549	1/1	0.78	0.26	83,83,83,83	0
56	MG	1A	3121	1/1	0.78	0.42	76,76,76,76	0
56	MG	1A	3176	1/1	0.78	0.23	95,95,95,95	0
56	MG	2A	3318	1/1	0.78	0.21	87,87,87,87	0
56	MG	2A	3142	1/1	0.78	0.61	81,81,81,81	0
56	MG	2A	3331	1/1	0.78	0.28	67,67,67,67	0
56	MG	1A	3198	1/1	0.78	0.11	83,83,83,83	0
56	MG	2a	3090	1/1	0.78	0.22	91,91,91,91	0
56	MG	1A	3252	1/1	0.78	0.20	73,73,73,73	0
56	MG	2A	3206	1/1	0.78	0.35	73,73,73,73	0
56	MG	1A	3428	1/1	0.78	0.26	79,79,79,79	0
56	MG	1A	3125	1/1	0.78	0.30	77,77,77,77	0
56	MG	1A	3376	1/1	0.78	0.19	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3249	1/1	0.78	0.11	81,81,81,81	0
56	MG	1A	3318	1/1	0.78	0.46	99,99,99,99	0
56	MG	1A	3320	1/1	0.78	0.23	65,65,65,65	0
56	MG	2A	3110	1/1	0.78	0.15	79,79,79,79	0
56	MG	2A	3294	1/1	0.78	0.38	104,104,104,104	0
56	MG	2A	3297	1/1	0.78	0.19	93,93,93,93	0
56	MG	1a	3051	1/1	0.78	0.33	99,99,99,99	0
56	MG	1A	3199	1/1	0.79	0.23	70,70,70,70	0
56	MG	1a	3152	1/1	0.79	0.18	102,102,102,102	0
56	MG	1A	3479	1/1	0.79	0.14	86,86,86,86	0
56	MG	1A	3571	1/1	0.79	0.05	98,98,98,98	0
56	MG	1a	3037	1/1	0.79	0.42	82,82,82,82	0
56	MG	2A	3143	1/1	0.79	0.24	93,93,93,93	0
56	MG	1A	3486	1/1	0.79	0.23	68,68,68,68	0
56	MG	2a	3092	1/1	0.79	0.19	88,88,88,88	0
56	MG	1a	3106	1/1	0.79	0.07	98,98,98,98	0
56	MG	2a	3028	1/1	0.79	0.14	85,85,85,85	0
56	MG	2A	3071	1/1	0.79	0.20	75,75,75,75	0
56	MG	1a	3189	1/1	0.79	0.23	85,85,85,85	0
56	MG	2A	3078	1/1	0.79	0.23	75,75,75,75	0
56	MG	1A	3554	1/1	0.79	0.14	109,109,109,109	0
56	MG	1A	3161	1/1	0.79	0.17	90,90,90,90	0
56	MG	2a	3141	1/1	0.79	0.10	82,82,82,82	0
56	MG	1a	3238	1/1	0.79	0.15	99,99,99,99	0
56	MG	1A	3114	1/1	0.79	0.42	93,93,93,93	0
56	MG	2A	3310	1/1	0.79	0.06	91,91,91,91	0
56	MG	2a	3169	1/1	0.79	0.25	78,78,78,78	0
56	MG	2A	3101	1/1	0.79	0.46	83,83,83,83	0
56	MG	1a	3134	1/1	0.79	0.39	77,77,77,77	0
56	MG	1A	3420	1/1	0.80	0.36	76,76,76,76	0
56	MG	1a	3053	1/1	0.80	1.62	79,79,79,79	0
56	MG	1a	3222	1/1	0.80	0.11	91,91,91,91	0
56	MG	2a	3063	1/1	0.80	0.25	83,83,83,83	0
56	MG	1a	3230	1/1	0.80	0.23	84,84,84,84	0
56	MG	1a	3117	1/1	0.80	0.14	83,83,83,83	0
56	MG	1A	3661	1/1	0.80	0.35	87,87,87,87	0
56	MG	1a	3068	1/1	0.80	0.15	95,95,95,95	0
56	MG	1a	3072	1/1	0.80	0.20	94,94,94,94	0
56	MG	2A	3112	1/1	0.80	0.31	89,89,89,89	0
56	MG	2A	3114	1/1	0.80	0.37	79,79,79,79	0
56	MG	1A	3579	1/1	0.80	0.51	118,118,118,118	0
56	MG	1A	3159	1/1	0.80	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3227	1/1	0.80	0.11	81,81,81,81	0
56	MG	2A	3234	1/1	0.80	0.72	84,84,84,84	0
56	MG	2A	3237	1/1	0.80	0.18	92,92,92,92	0
56	MG	1A	3258	1/1	0.80	0.29	95,95,95,95	0
56	MG	2A	3051	1/1	0.80	0.29	80,80,80,80	0
56	MG	2a	3036	1/1	0.80	0.10	95,95,95,95	0
56	MG	1A	3181	1/1	0.80	1.48	78,78,78,78	0
56	MG	2a	3144	1/1	0.80	0.24	101,101,101,101	0
56	MG	2a	3048	1/1	0.80	0.33	94,94,94,94	0
56	MG	1A	3056	1/1	0.80	0.27	80,80,80,80	0
56	MG	2a	3050	1/1	0.80	0.29	105,105,105,105	0
56	MG	1a	3179	1/1	0.80	0.13	90,90,90,90	0
56	MG	1A	3058	1/1	0.80	0.15	80,80,80,80	0
56	MG	1A	3511	1/1	0.80	0.17	62,62,62,62	0
56	MG	1A	3400	1/1	0.81	0.25	90,90,90,90	0
56	MG	2A	3055	1/1	0.81	0.13	92,92,92,92	0
56	MG	1A	3447	1/1	0.81	0.30	91,91,91,91	0
56	MG	1a	3069	1/1	0.81	0.18	81,81,81,81	0
56	MG	1a	3004	1/1	0.81	0.19	101,101,101,101	0
56	MG	1A	3168	1/1	0.81	0.19	78,78,78,78	0
56	MG	1A	3291	1/1	0.81	0.18	79,79,79,79	0
56	MG	1A	3580	1/1	0.81	0.15	74,74,74,74	0
56	MG	1a	3019	1/1	0.81	0.53	96,96,96,96	0
56	MG	1a	3201	1/1	0.81	0.50	93,93,93,93	0
56	MG	1a	3203	1/1	0.81	0.34	105,105,105,105	0
56	MG	1A	3295	1/1	0.81	0.34	66,66,66,66	0
56	MG	1A	3174	1/1	0.81	0.39	77,77,77,77	0
56	MG	2A	3332	1/1	0.81	0.48	116,116,116,116	0
56	MG	2A	3336	1/1	0.81	0.21	77,77,77,77	0
56	MG	2A	3337	1/1	0.81	0.14	78,78,78,78	0
56	MG	2a	3099	1/1	0.81	0.20	93,93,93,93	0
56	MG	2A	3351	1/1	0.81	0.15	84,84,84,84	0
56	MG	2a	3004	1/1	0.81	0.29	98,98,98,98	0
56	MG	1a	3030	1/1	0.81	0.47	105,105,105,105	0
56	MG	1a	3110	1/1	0.81	0.10	90,90,90,90	0
56	MG	2a	3116	1/1	0.81	0.20	82,82,82,82	0
56	MG	1a	3033	1/1	0.81	0.28	87,87,87,87	0
56	MG	2A	3216	1/1	0.81	0.75	87,87,87,87	0
56	MG	1A	3016	1/1	0.81	0.28	66,66,66,66	0
56	MG	1a	3039	1/1	0.81	0.21	80,80,80,80	0
56	MG	1A	3002	1/1	0.81	0.17	72,72,72,72	0
56	MG	2A	3134	1/1	0.81	0.42	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3053	1/1	0.81	0.38	95,95,95,95	0
56	MG	2a	3167	1/1	0.81	0.30	101,101,101,101	0
56	MG	1a	3136	1/1	0.81	0.23	84,84,84,84	0
56	MG	1A	3015	1/1	0.81	0.13	86,86,86,86	0
56	MG	2A	3258	1/1	0.81	0.34	103,103,103,103	0
56	MG	1A	3192	1/1	0.82	0.14	74,74,74,74	0
56	MG	2a	3085	1/1	0.82	0.16	83,83,83,83	0
56	MG	1A	3647	1/1	0.82	0.15	93,93,93,93	0
56	MG	1a	3220	1/1	0.82	0.35	80,80,80,80	0
56	MG	1A	3385	1/1	0.82	0.30	74,74,74,74	0
56	MG	1A	3657	1/1	0.82	0.43	79,79,79,79	0
56	MG	1a	3233	1/1	0.82	0.19	76,76,76,76	0
56	MG	1A	3567	1/1	0.82	0.13	87,87,87,87	0
56	MG	2A	3298	1/1	0.82	0.56	76,76,76,76	0
56	MG	1A	3180	1/1	0.82	0.77	93,93,93,93	0
56	MG	1A	3196	1/1	0.82	0.23	81,81,81,81	0
56	MG	2A	3090	1/1	0.82	0.22	98,98,98,98	0
56	MG	1A	3293	1/1	0.82	0.13	78,78,78,78	0
56	MG	2A	3217	1/1	0.82	0.52	82,82,82,82	0
56	MG	2A	3222	1/1	0.82	0.23	89,89,89,89	0
56	MG	1a	3133	1/1	0.82	0.15	90,90,90,90	0
56	MG	2A	3097	1/1	0.82	0.41	91,91,91,91	0
56	MG	2A	3098	1/1	0.82	0.57	79,79,79,79	0
56	MG	1a	3090	1/1	0.82	0.53	87,87,87,87	0
56	MG	2a	3061	1/1	0.82	0.07	92,92,92,92	0
56	MG	1A	3249	1/1	0.82	0.34	77,77,77,77	0
56	MG	2A	3344	1/1	0.82	0.10	106,106,106,106	0
56	MG	2a	3177	1/1	0.82	0.16	86,86,86,86	0
56	MG	2A	3165	1/1	0.82	0.14	77,77,77,77	0
56	MG	2A	3247	1/1	0.82	0.16	101,101,101,101	0
56	MG	2a	3047	1/1	0.83	0.14	83,83,83,83	0
56	MG	1a	3126	1/1	0.83	0.15	100,100,100,100	0
56	MG	2A	3011	1/1	0.83	0.21	87,87,87,87	0
56	MG	2A	3131	1/1	0.83	0.41	95,95,95,95	0
56	MG	1a	3063	1/1	0.83	0.27	89,89,89,89	0
56	MG	1A	3203	1/1	0.83	0.29	74,74,74,74	0
56	MG	2A	3277	1/1	0.83	0.40	93,93,93,93	0
56	MG	1A	3208	1/1	0.83	0.22	74,74,74,74	0
56	MG	2A	3283	1/1	0.83	0.20	84,84,84,84	0
56	MG	1a	3143	1/1	0.83	0.27	91,91,91,91	0
56	MG	2A	3033	1/1	0.83	0.33	81,81,81,81	0
56	MG	1A	3234	1/1	0.83	0.36	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3151	1/1	0.83	0.13	78,78,78,78	0
56	MG	2A	3153	1/1	0.83	0.35	81,81,81,81	0
56	MG	1A	3265	1/1	0.83	0.26	65,65,65,65	0
56	MG	1A	3319	1/1	0.83	0.54	100,100,100,100	0
56	MG	2A	3313	1/1	0.83	0.15	96,96,96,96	0
56	MG	1A	3391	1/1	0.83	0.27	80,80,80,80	0
56	MG	1a	3165	1/1	0.83	0.49	87,87,87,87	0
56	MG	2a	3089	1/1	0.83	0.14	86,86,86,86	0
56	MG	2A	3060	1/1	0.83	0.17	79,79,79,79	0
56	MG	1a	3083	1/1	0.83	0.30	93,93,93,93	0
56	MG	1a	3169	1/1	0.83	0.16	80,80,80,80	0
56	MG	2A	3186	1/1	0.83	0.20	79,79,79,79	0
56	MG	1A	3444	1/1	0.83	0.23	83,83,83,83	0
56	MG	1a	3089	1/1	0.83	0.16	78,78,78,78	0
56	MG	1A	3147	1/1	0.83	0.15	86,86,86,86	0
56	MG	1a	3187	1/1	0.83	0.27	78,78,78,78	0
56	MG	1A	3459	1/1	0.83	0.11	62,62,62,62	0
56	MG	1A	3620	1/1	0.83	0.51	91,91,91,91	0
56	MG	1a	3097	1/1	0.83	0.88	95,95,95,95	0
56	MG	1A	3087	1/1	0.83	0.14	79,79,79,79	0
56	MG	2a	3009	1/1	0.83	0.32	84,84,84,84	0
56	MG	2a	3010	1/1	0.83	0.08	86,86,86,86	0
56	MG	1A	3197	1/1	0.83	0.25	72,72,72,72	0
56	MG	2a	3161	1/1	0.83	0.14	104,104,104,104	0
56	MG	1A	3144	1/1	0.83	0.18	85,85,85,85	0
56	MG	2A	3104	1/1	0.83	0.16	98,98,98,98	0
56	MG	1a	3049	1/1	0.83	0.21	87,87,87,87	0
56	MG	1A	3419	1/1	0.83	0.16	87,87,87,87	0
56	MG	1A	3113	1/1	0.83	0.14	75,75,75,75	0
56	MG	1a	3062	1/1	0.83	0.27	71,71,71,71	0
57	ZN	24	501	1/1	0.83	0.06	168,168,168,168	0
56	MG	2A	3266	1/1	0.84	0.10	88,88,88,88	0
56	MG	2A	3026	1/1	0.84	0.19	92,92,92,92	0
56	MG	1A	3030	1/1	0.84	0.50	69,69,69,69	0
56	MG	1A	3299	1/1	0.84	0.20	90,90,90,90	0
56	MG	1a	3007	1/1	0.84	0.19	67,67,67,67	0
56	MG	1A	3453	1/1	0.84	0.19	84,84,84,84	0
56	MG	1A	3457	1/1	0.84	0.18	77,77,77,77	0
56	MG	1A	3548	1/1	0.84	0.62	91,91,91,91	0
56	MG	1A	3601	1/1	0.84	0.91	102,102,102,102	0
56	MG	1a	3174	1/1	0.84	0.15	87,87,87,87	0
56	MG	2A	3061	1/1	0.84	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3078	1/1	0.84	0.15	85,85,85,85	0
56	MG	1A	3012	1/1	0.84	0.13	78,78,78,78	0
56	MG	1A	3001	1/1	0.84	0.10	70,70,70,70	0
56	MG	1A	3617	1/1	0.84	0.14	69,69,69,69	0
56	MG	1A	3371	1/1	0.84	0.29	52,52,52,52	0
56	MG	1a	3191	1/1	0.84	0.12	93,93,93,93	0
56	MG	1A	3622	1/1	0.84	0.19	91,91,91,91	0
56	MG	2A	3328	1/1	0.84	0.12	90,90,90,90	0
56	MG	2A	3194	1/1	0.84	0.16	85,85,85,85	0
56	MG	1a	3107	1/1	0.84	0.17	84,84,84,84	0
56	MG	1a	3205	1/1	0.84	0.11	102,102,102,102	0
56	MG	1A	3253	1/1	0.84	0.28	71,71,71,71	0
56	MG	1A	3633	1/1	0.84	0.22	75,75,75,75	0
56	MG	2A	3204	1/1	0.84	0.53	90,90,90,90	0
56	MG	1a	3115	1/1	0.84	0.12	89,89,89,89	0
56	MG	2A	3100	1/1	0.84	0.21	86,86,86,86	0
56	MG	2a	3121	1/1	0.84	0.26	114,114,114,114	0
56	MG	2A	3215	1/1	0.84	0.18	86,86,86,86	0
56	MG	1A	3287	1/1	0.84	0.13	80,80,80,80	0
56	MG	1a	3052	1/1	0.84	0.15	84,84,84,84	0
56	MG	2a	3012	1/1	0.84	0.14	79,79,79,79	0
56	MG	1A	3026	1/1	0.84	0.27	77,77,77,77	0
56	MG	1A	3339	1/1	0.84	1.46	112,112,112,112	0
56	MG	2a	3159	1/1	0.84	0.33	92,92,92,92	0
56	MG	2a	3160	1/1	0.84	0.11	104,104,104,104	0
56	MG	1A	3343	1/1	0.84	0.20	72,72,72,72	0
56	MG	1A	3658	1/1	0.84	0.23	98,98,98,98	0
56	MG	2A	3013	1/1	0.84	0.36	79,79,79,79	0
56	MG	1A	3137	1/1	0.84	0.20	82,82,82,82	0
56	MG	2A	3127	1/1	0.84	0.10	78,78,78,78	0
56	MG	2A	3018	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3674	1/1	0.84	0.33	81,81,81,81	0
56	MG	1a	3070	1/1	0.84	0.20	85,85,85,85	0
56	MG	1A	3019	1/1	0.85	0.19	81,81,81,81	0
56	MG	1a	3060	1/1	0.85	0.17	83,83,83,83	0
56	MG	2a	3062	1/1	0.85	0.32	94,94,94,94	0
56	MG	1A	3608	1/1	0.85	0.12	87,87,87,87	0
56	MG	2A	3195	1/1	0.85	0.31	84,84,84,84	0
56	MG	2a	3076	1/1	0.85	0.17	99,99,99,99	0
56	MG	1a	3108	1/1	0.85	0.24	93,93,93,93	0
56	MG	2A	3024	1/1	0.85	0.22	95,95,95,95	0
56	MG	1A	3552	1/1	0.85	0.14	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3028	1/1	0.85	0.40	68,68,68,68	0
56	MG	2A	3203	1/1	0.85	0.43	87,87,87,87	0
56	MG	1a	3180	1/1	0.85	0.19	90,90,90,90	0
56	MG	1A	3205	1/1	0.85	0.15	78,78,78,78	0
56	MG	1A	3007	1/1	0.85	0.12	91,91,91,91	0
56	MG	2A	3207	1/1	0.85	0.46	68,68,68,68	0
56	MG	2A	3209	1/1	0.85	0.38	83,83,83,83	0
56	MG	2A	3041	1/1	0.85	0.23	69,69,69,69	0
56	MG	1A	3372	1/1	0.85	0.17	63,63,63,63	0
56	MG	1A	3417	1/1	0.85	0.19	79,79,79,79	0
56	MG	1A	3246	1/1	0.85	0.14	78,78,78,78	0
56	MG	1A	3519	1/1	0.85	0.17	88,88,88,88	0
56	MG	1a	3127	1/1	0.85	0.21	82,82,82,82	0
56	MG	1A	3521	1/1	0.85	0.15	64,64,64,64	0
56	MG	2a	3118	1/1	0.85	0.04	115,115,115,115	0
56	MG	2a	3120	1/1	0.85	0.67	103,103,103,103	0
56	MG	1a	3036	1/1	0.85	0.14	90,90,90,90	0
56	MG	1A	3455	1/1	0.85	0.15	63,63,63,63	0
56	MG	2A	3152	1/1	0.85	0.68	85,85,85,85	0
56	MG	1A	3219	1/1	0.85	0.13	84,84,84,84	0
56	MG	1a	3224	1/1	0.85	0.21	77,77,77,77	0
56	MG	2A	3253	1/1	0.85	0.17	74,74,74,74	0
56	MG	2A	3080	1/1	0.85	0.08	80,80,80,80	0
56	MG	2A	3263	1/1	0.85	0.52	86,86,86,86	0
56	MG	1A	3354	1/1	0.85	0.21	83,83,83,83	0
56	MG	1A	3153	1/1	0.85	0.37	72,72,72,72	0
56	MG	2a	3162	1/1	0.85	0.15	126,126,126,126	0
56	MG	1A	3543	1/1	0.85	0.28	86,86,86,86	0
56	MG	1A	3063	1/1	0.85	0.16	80,80,80,80	0
56	MG	2A	3181	1/1	0.85	0.69	90,90,90,90	0
56	MG	1a	3099	1/1	0.85	0.10	90,90,90,90	0
56	MG	1a	3166	1/1	0.85	0.15	100,100,100,100	0
56	MG	2A	3295	1/1	0.85	0.31	91,91,91,91	0
56	MG	2A	3190	1/1	0.85	0.11	98,98,98,98	0
56	MG	1A	3065	1/1	0.86	0.43	71,71,71,71	0
56	MG	1A	3431	1/1	0.86	0.14	76,76,76,76	0
56	MG	2a	3066	1/1	0.86	0.22	106,106,106,106	0
56	MG	1a	3140	1/1	0.86	0.33	84,84,84,84	0
56	MG	1A	3330	1/1	0.86	0.26	96,96,96,96	0
56	MG	1A	3103	1/1	0.86	0.86	68,68,68,68	0
56	MG	1A	3150	1/1	0.86	0.20	91,91,91,91	0
56	MG	1A	3443	1/1	0.86	0.09	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3139	1/1	0.86	0.21	79,79,79,79	0
56	MG	1A	3525	1/1	0.86	0.21	101,101,101,101	0
56	MG	1a	3018	1/1	0.86	0.37	74,74,74,74	0
56	MG	2A	3025	1/1	0.86	0.21	88,88,88,88	0
56	MG	2A	3333	1/1	0.86	0.12	101,101,101,101	0
56	MG	1A	3177	1/1	0.86	0.66	89,89,89,89	0
56	MG	1A	3589	1/1	0.86	0.11	86,86,86,86	0
56	MG	1A	3529	1/1	0.86	0.16	71,71,71,71	0
56	MG	1A	3452	1/1	0.86	0.16	97,97,97,97	0
56	MG	1A	3609	1/1	0.86	0.67	74,74,74,74	0
56	MG	1a	3103	1/1	0.86	0.19	79,79,79,79	0
56	MG	2A	3048	1/1	0.86	0.23	83,83,83,83	0
56	MG	1A	3122	1/1	0.86	0.24	77,77,77,77	0
56	MG	2A	3144	1/1	0.86	0.42	75,75,75,75	0
56	MG	2A	3053	1/1	0.86	0.10	77,77,77,77	0
56	MG	1A	3251	1/1	0.86	0.43	69,69,69,69	0
56	MG	1A	3154	1/1	0.86	0.18	59,59,59,59	0
56	MG	1A	3075	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3621	1/1	0.86	0.13	69,69,69,69	0
56	MG	2A	3154	1/1	0.86	0.70	74,74,74,74	0
56	MG	2a	3142	1/1	0.86	0.24	103,103,103,103	0
56	MG	1A	3011	1/1	0.86	0.38	65,65,65,65	0
56	MG	1A	3022	1/1	0.86	0.38	83,83,83,83	0
56	MG	2a	3043	1/1	0.86	0.66	70,70,70,70	0
56	MG	1A	3493	1/1	0.86	0.16	69,69,69,69	0
56	MG	2A	3072	1/1	0.86	0.18	74,74,74,74	0
56	MG	1a	3213	1/1	0.86	1.10	117,117,117,117	0
56	MG	1a	3058	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3286	1/1	0.86	0.15	93,93,93,93	0
56	MG	1A	3556	1/1	0.86	0.18	81,81,81,81	0
56	MG	2a	3168	1/1	0.86	0.15	112,112,112,112	0
56	MG	2A	3084	1/1	0.86	0.26	90,90,90,90	0
56	MG	1A	3425	1/1	0.86	0.31	62,62,62,62	0
56	MG	2A	3188	1/1	0.86	0.12	92,92,92,92	0
56	MG	1A	3237	1/1	0.86	0.33	74,74,74,74	0
56	MG	1A	3566	1/1	0.86	0.10	93,93,93,93	0
56	MG	1A	3437	1/1	0.87	0.31	79,79,79,79	0
56	MG	1A	3183	1/1	0.87	0.42	74,74,74,74	0
56	MG	1a	3020	1/1	0.87	0.15	74,74,74,74	0
56	MG	1a	3184	1/1	0.87	0.27	71,71,71,71	0
56	MG	1A	3541	1/1	0.87	0.15	72,72,72,72	0
56	MG	1a	3120	1/1	0.87	0.57	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3254	1/1	0.87	0.15	78,78,78,78	0
56	MG	1a	3071	1/1	0.87	0.84	75,75,75,75	0
56	MG	2A	3106	1/1	0.87	0.25	73,73,73,73	0
56	MG	2A	3038	1/1	0.87	0.39	65,65,65,65	0
56	MG	1A	3186	1/1	0.87	0.15	95,95,95,95	0
56	MG	1A	3545	1/1	0.87	0.17	67,67,67,67	0
56	MG	2a	3024	1/1	0.87	0.10	90,90,90,90	0
56	MG	1A	3167	1/1	0.87	0.20	90,90,90,90	0
56	MG	2A	3115	1/1	0.87	1.18	80,80,80,80	0
56	MG	1a	3035	1/1	0.87	0.23	81,81,81,81	0
56	MG	1A	3637	1/1	0.87	0.13	100,100,100,100	0
56	MG	2a	3117	1/1	0.87	0.11	92,92,92,92	0
56	MG	1a	3139	1/1	0.87	0.41	81,81,81,81	0
56	MG	2a	3042	1/1	0.87	0.19	82,82,82,82	0
56	MG	1A	3032	1/1	0.87	0.14	75,75,75,75	0
56	MG	2a	3129	1/1	0.87	0.14	92,92,92,92	0
56	MG	1A	3048	1/1	0.87	0.51	74,74,74,74	0
56	MG	1a	3042	1/1	0.87	0.11	74,74,74,74	0
56	MG	2A	3140	1/1	0.87	0.45	81,81,81,81	0
56	MG	1A	3322	1/1	0.87	0.15	92,92,92,92	0
56	MG	1A	3600	1/1	0.87	0.10	77,77,77,77	0
56	MG	1A	3288	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3138	1/1	0.87	0.48	82,82,82,82	0
56	MG	2a	3055	1/1	0.87	0.23	95,95,95,95	0
56	MG	1A	3100	1/1	0.87	0.60	61,61,61,61	0
56	MG	1A	3023	1/1	0.87	1.07	88,88,88,88	0
56	MG	1A	3613	1/1	0.87	0.15	64,64,64,64	0
56	MG	2A	3327	1/1	0.87	0.52	96,96,96,96	0
56	MG	1a	3170	1/1	0.87	0.13	76,76,76,76	0
56	MG	1A	3118	1/1	0.87	0.11	60,60,60,60	0
56	MG	2a	3064	1/1	0.87	0.14	99,99,99,99	0
56	MG	2a	3176	1/1	0.87	0.14	83,83,83,83	0
56	MG	1A	3358	1/1	0.87	0.19	83,83,83,83	0
56	MG	2a	3069	1/1	0.87	0.19	103,103,103,103	0
56	MG	2a	3183	1/1	0.87	0.07	98,98,98,98	0
56	MG	2A	3157	1/1	0.87	0.84	70,70,70,70	0
56	MG	2A	3334	1/1	0.87	0.46	105,105,105,105	0
56	MG	1A	3175	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	3066	1/1	0.88	0.37	78,78,78,78	0
56	MG	1A	3261	1/1	0.88	0.22	72,72,72,72	0
56	MG	1A	3263	1/1	0.88	0.20	78,78,78,78	0
56	MG	2a	3074	1/1	0.88	0.14	98,98,98,98	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	0.88	0.16	72,72,72,72	0
56	MG	1a	3146	1/1	0.88	0.20	79,79,79,79	0
56	MG	1a	3147	1/1	0.88	0.27	71,71,71,71	0
56	MG	1a	3073	1/1	0.88	0.16	78,78,78,78	0
56	MG	1A	3267	1/1	0.88	0.22	76,76,76,76	0
56	MG	1a	3153	1/1	0.88	0.15	84,84,84,84	0
56	MG	1A	3396	1/1	0.88	0.28	99,99,99,99	0
56	MG	1A	3004	1/1	0.88	0.17	56,56,56,56	0
56	MG	1a	3024	1/1	0.88	0.41	83,83,83,83	0
56	MG	2A	3121	1/1	0.88	0.34	79,79,79,79	0
56	MG	1A	3544	1/1	0.88	0.18	71,71,71,71	0
56	MG	2a	3096	1/1	0.88	0.27	84,84,84,84	0
56	MG	2A	3343	1/1	0.88	0.23	99,99,99,99	0
56	MG	1A	3021	1/1	0.88	1.00	55,55,55,55	0
56	MG	1A	3614	1/1	0.88	0.15	89,89,89,89	0
56	MG	2a	3101	1/1	0.88	0.80	101,101,101,101	0
56	MG	1a	3032	1/1	0.88	0.07	76,76,76,76	0
56	MG	2a	3105	1/1	0.88	0.26	95,95,95,95	0
56	MG	2A	3136	1/1	0.88	0.23	71,71,71,71	0
56	MG	2A	3223	1/1	0.88	0.21	72,72,72,72	0
56	MG	2A	3035	1/1	0.88	0.16	92,92,92,92	0
56	MG	1A	3279	1/1	0.88	0.15	82,82,82,82	0
56	MG	1A	3465	1/1	0.88	0.18	80,80,80,80	0
56	MG	1a	3175	1/1	0.88	0.07	87,87,87,87	0
56	MG	1A	3347	1/1	0.88	0.23	70,70,70,70	0
56	MG	2a	3124	1/1	0.88	0.18	83,83,83,83	0
56	MG	1A	3481	1/1	0.88	0.22	83,83,83,83	0
56	MG	2A	3147	1/1	0.88	0.13	84,84,84,84	0
56	MG	1A	3052	1/1	0.88	0.21	77,77,77,77	0
56	MG	2A	3150	1/1	0.88	0.43	88,88,88,88	0
56	MG	1A	3286	1/1	0.88	0.12	96,96,96,96	0
56	MG	2a	3143	1/1	0.88	0.10	107,107,107,107	0
56	MG	1A	3494	1/1	0.88	0.11	75,75,75,75	0
56	MG	1A	3184	1/1	0.88	1.24	73,73,73,73	0
56	MG	2A	3265	1/1	0.88	0.34	93,93,93,93	0
56	MG	1a	3190	1/1	0.88	1.15	95,95,95,95	0
56	MG	1A	3185	1/1	0.88	1.14	80,80,80,80	0
56	MG	1a	3113	1/1	0.88	0.13	86,86,86,86	0
56	MG	1A	3645	1/1	0.88	0.24	82,82,82,82	0
56	MG	2a	3164	1/1	0.88	0.10	114,114,114,114	0
56	MG	1A	3173	1/1	0.88	0.16	74,74,74,74	0
56	MG	1A	3042	1/1	0.88	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	3210	1/1	0.88	0.15	71,71,71,71	0
56	MG	1A	3214	1/1	0.88	0.27	96,96,96,96	0
56	MG	1a	3217	1/1	0.88	0.10	85,85,85,85	0
56	MG	2A	3296	1/1	0.88	0.21	102,102,102,102	0
56	MG	2a	3178	1/1	0.88	0.26	96,96,96,96	0
56	MG	1A	3436	1/1	0.88	0.18	68,68,68,68	0
56	MG	2a	3180	1/1	0.88	0.26	102,102,102,102	0
56	MG	1a	3064	1/1	0.88	0.32	87,87,87,87	0
56	MG	2A	3301	1/1	0.88	0.22	83,83,83,83	0
56	MG	1A	3301	1/1	0.88	0.24	85,85,85,85	0
56	MG	1A	3676	1/1	0.89	0.15	84,84,84,84	0
56	MG	2A	3126	1/1	0.89	0.21	80,80,80,80	0
56	MG	1A	3092	1/1	0.89	0.09	70,70,70,70	0
56	MG	2A	3039	1/1	0.89	0.32	88,88,88,88	0
56	MG	1A	3407	1/1	0.89	0.14	91,91,91,91	0
56	MG	2A	3042	1/1	0.89	0.12	89,89,89,89	0
56	MG	2A	3047	1/1	0.89	0.26	89,89,89,89	0
56	MG	1A	3363	1/1	0.89	0.18	79,79,79,79	0
56	MG	2a	3003	1/1	0.89	0.48	69,69,69,69	0
56	MG	2A	3141	1/1	0.89	0.72	81,81,81,81	0
56	MG	2a	3005	1/1	0.89	0.43	96,96,96,96	0
56	MG	1a	3121	1/1	0.89	0.41	88,88,88,88	0
56	MG	1A	3112	1/1	0.89	0.29	66,66,66,66	0
56	MG	1a	3192	1/1	0.89	0.19	85,85,85,85	0
56	MG	1a	3124	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3515	1/1	0.89	0.30	63,63,63,63	0
56	MG	1A	3416	1/1	0.89	0.34	82,82,82,82	0
56	MG	2a	3115	1/1	0.89	0.24	103,103,103,103	0
56	MG	1A	3560	1/1	0.89	0.27	88,88,88,88	0
56	MG	1A	3164	1/1	0.89	0.14	72,72,72,72	0
56	MG	1A	3323	1/1	0.89	0.20	81,81,81,81	0
56	MG	1A	3165	1/1	0.89	0.41	86,86,86,86	0
56	MG	1A	3078	1/1	0.89	0.91	79,79,79,79	0
56	MG	1A	3062	1/1	0.89	0.84	92,92,92,92	0
56	MG	2A	3079	1/1	0.89	0.25	89,89,89,89	0
56	MG	1A	3346	1/1	0.89	0.41	92,92,92,92	0
56	MG	2A	3282	1/1	0.89	0.12	87,87,87,87	0
56	MG	1A	3169	1/1	0.89	0.25	84,84,84,84	0
56	MG	1A	3575	1/1	0.89	0.25	83,83,83,83	0
56	MG	1a	3236	1/1	0.89	0.15	85,85,85,85	0
56	MG	1A	3639	1/1	0.89	0.20	67,67,67,67	0
56	MG	2A	3293	1/1	0.89	0.13	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3306	1/1	0.89	0.28	82,82,82,82	0
56	MG	2A	3008	1/1	0.89	0.11	79,79,79,79	0
56	MG	1a	3158	1/1	0.89	0.15	81,81,81,81	0
56	MG	1A	3353	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3648	1/1	0.89	0.32	127,127,127,127	0
56	MG	2a	3163	1/1	0.89	0.19	103,103,103,103	0
56	MG	1A	3434	1/1	0.89	0.10	81,81,81,81	0
56	MG	1a	3101	1/1	0.89	0.39	88,88,88,88	0
56	MG	2A	3105	1/1	0.89	0.18	71,71,71,71	0
56	MG	1a	3045	1/1	0.89	0.12	85,85,85,85	0
56	MG	1a	3048	1/1	0.89	0.20	73,73,73,73	0
56	MG	2a	3170	1/1	0.89	0.13	80,80,80,80	0
56	MG	2a	3175	1/1	0.89	0.20	76,76,76,76	0
56	MG	1A	3308	1/1	0.89	0.13	80,80,80,80	0
56	MG	1a	3050	1/1	0.89	0.11	80,80,80,80	0
56	MG	1A	3588	1/1	0.89	0.23	82,82,82,82	0
56	MG	1A	3136	1/1	0.89	0.69	78,78,78,78	0
56	MG	2A	3118	1/1	0.89	0.62	72,72,72,72	0
56	MG	1A	3662	1/1	0.89	0.16	90,90,90,90	0
56	MG	1A	3503	1/1	0.89	0.27	90,90,90,90	0
56	MG	2a	3079	1/1	0.89	0.37	90,90,90,90	0
56	MG	2a	3072	1/1	0.90	0.12	107,107,107,107	0
56	MG	2A	3004	1/1	0.90	0.16	91,91,91,91	0
56	MG	1A	3439	1/1	0.90	0.30	84,84,84,84	0
56	MG	1A	3405	1/1	0.90	0.18	78,78,78,78	0
56	MG	1A	3044	1/1	0.90	0.16	89,89,89,89	0
56	MG	1A	3231	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3067	1/1	0.90	0.08	65,65,65,65	0
56	MG	1A	3094	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3324	1/1	0.90	0.36	67,67,67,67	0
56	MG	2A	3330	1/1	0.90	0.16	101,101,101,101	0
56	MG	1A	3327	1/1	0.90	0.18	78,78,78,78	0
56	MG	1a	3093	1/1	0.90	0.39	88,88,88,88	0
56	MG	1A	3520	1/1	0.90	0.10	88,88,88,88	0
56	MG	1A	3568	1/1	0.90	0.09	79,79,79,79	0
56	MG	1A	3096	1/1	0.90	0.09	90,90,90,90	0
56	MG	1A	3374	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3188	1/1	0.90	0.27	91,91,91,91	0
56	MG	2A	3213	1/1	0.90	0.14	90,90,90,90	0
56	MG	1A	3070	1/1	0.90	0.23	52,52,52,52	0
56	MG	1A	3468	1/1	0.90	0.73	83,83,83,83	0
56	MG	1A	3577	1/1	0.90	0.12	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3130	1/1	0.90	0.24	90,90,90,90	0
56	MG	2A	3040	1/1	0.90	0.14	82,82,82,82	0
56	MG	1a	3046	1/1	0.90	0.24	73,73,73,73	0
56	MG	1a	3109	1/1	0.90	0.61	103,103,103,103	0
56	MG	1A	3531	1/1	0.90	0.20	92,92,92,92	0
56	MG	2a	3011	1/1	0.90	0.10	101,101,101,101	0
56	MG	2A	3139	1/1	0.90	0.25	101,101,101,101	0
56	MG	2a	3014	1/1	0.90	0.30	89,89,89,89	0
56	MG	1A	3472	1/1	0.90	0.14	72,72,72,72	0
56	MG	1A	3049	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3584	1/1	0.90	0.16	92,92,92,92	0
56	MG	1A	3009	1/1	0.90	0.28	75,75,75,75	0
56	MG	2a	3139	1/1	0.90	0.15	81,81,81,81	0
56	MG	2a	3029	1/1	0.90	0.20	87,87,87,87	0
56	MG	1A	3665	1/1	0.90	0.21	74,74,74,74	0
56	MG	1a	3118	1/1	0.90	0.75	101,101,101,101	0
56	MG	2A	3256	1/1	0.90	0.08	98,98,98,98	0
56	MG	2a	3151	1/1	0.90	0.20	111,111,111,111	0
56	MG	1A	3270	1/1	0.90	0.41	75,75,75,75	0
56	MG	2a	3155	1/1	0.90	0.11	84,84,84,84	0
56	MG	2a	3157	1/1	0.90	0.29	114,114,114,114	0
56	MG	2a	3040	1/1	0.90	0.14	78,78,78,78	0
56	MG	1a	3209	1/1	0.90	0.33	90,90,90,90	0
56	MG	1A	3489	1/1	0.90	0.34	78,78,78,78	0
56	MG	1A	3679	1/1	0.90	0.59	83,83,83,83	0
56	MG	2A	3273	1/1	0.90	0.20	86,86,86,86	0
56	MG	1A	3156	1/1	0.90	0.14	66,66,66,66	0
56	MG	1a	3215	1/1	0.90	0.15	84,84,84,84	0
56	MG	2A	3076	1/1	0.90	0.47	77,77,77,77	0
56	MG	2A	3077	1/1	0.90	0.42	77,77,77,77	0
56	MG	1A	3547	1/1	0.90	0.18	71,71,71,71	0
56	MG	1a	3065	1/1	0.90	0.19	87,87,87,87	0
56	MG	2A	3159	1/1	0.90	0.14	91,91,91,91	0
56	MG	1a	3066	1/1	0.90	0.11	101,101,101,101	0
56	MG	1A	3607	1/1	0.90	0.12	58,58,58,58	0
56	MG	1A	3250	1/1	0.90	0.30	94,94,94,94	0
56	MG	2A	3089	1/1	0.90	0.15	82,82,82,82	0
56	MG	2A	3173	1/1	0.90	0.11	70,70,70,70	0
56	MG	1a	3009	1/1	0.90	0.36	91,91,91,91	0
56	MG	1a	3012	1/1	0.90	0.49	93,93,93,93	0
56	MG	1a	3014	1/1	0.90	0.10	78,78,78,78	0
57	ZN	2Y	501	1/1	0.90	0.13	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3218	1/1	0.90	0.21	96,96,96,96	0
56	MG	1A	3140	1/1	0.91	0.20	89,89,89,89	0
56	MG	1a	3015	1/1	0.91	0.39	90,90,90,90	0
56	MG	1A	3380	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3036	1/1	0.91	0.94	87,87,87,87	0
56	MG	2A	3268	1/1	0.91	0.06	82,82,82,82	0
56	MG	1A	3141	1/1	0.91	0.21	70,70,70,70	0
56	MG	1A	3388	1/1	0.91	0.34	69,69,69,69	0
56	MG	1A	3328	1/1	0.91	0.34	94,94,94,94	0
56	MG	1a	3021	1/1	0.91	0.24	102,102,102,102	0
56	MG	1A	3033	1/1	0.91	0.31	86,86,86,86	0
56	MG	2A	3284	1/1	0.91	0.09	79,79,79,79	0
56	MG	1a	3025	1/1	0.91	0.09	85,85,85,85	0
56	MG	2a	3071	1/1	0.91	0.41	88,88,88,88	0
56	MG	2A	3149	1/1	0.91	0.27	84,84,84,84	0
56	MG	1a	3095	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3454	1/1	0.91	0.20	66,66,66,66	0
56	MG	1a	3098	1/1	0.91	0.35	87,87,87,87	0
56	MG	2A	3054	1/1	0.91	0.17	89,89,89,89	0
56	MG	1A	3333	1/1	0.91	0.30	73,73,73,73	0
56	MG	1a	3185	1/1	0.91	0.11	90,90,90,90	0
56	MG	1a	3186	1/1	0.91	0.19	85,85,85,85	0
56	MG	1A	3335	1/1	0.91	0.14	66,66,66,66	0
56	MG	1a	3031	1/1	0.91	0.49	103,103,103,103	0
56	MG	2A	3303	1/1	0.91	0.65	98,98,98,98	0
56	MG	1A	3010	1/1	0.91	0.64	65,65,65,65	0
56	MG	1A	3616	1/1	0.91	0.27	84,84,84,84	0
56	MG	2a	3091	1/1	0.91	0.24	92,92,92,92	0
56	MG	2A	3314	1/1	0.91	0.13	94,94,94,94	0
56	MG	2a	3095	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3460	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3256	1/1	0.91	0.42	84,84,84,84	0
56	MG	2A	3168	1/1	0.91	0.30	98,98,98,98	0
56	MG	2A	3169	1/1	0.91	0.26	79,79,79,79	0
56	MG	2A	3320	1/1	0.91	0.10	79,79,79,79	0
56	MG	2A	3321	1/1	0.91	0.10	101,101,101,101	0
56	MG	2A	3170	1/1	0.91	0.20	95,95,95,95	0
56	MG	1a	3202	1/1	0.91	0.22	89,89,89,89	0
56	MG	1A	3294	1/1	0.91	0.38	87,87,87,87	0
56	MG	1A	3470	1/1	0.91	0.31	100,100,100,100	0
56	MG	1A	3553	1/1	0.91	0.22	89,89,89,89	0
56	MG	1a	3112	1/1	0.91	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3095	1/1	0.91	0.17	81,81,81,81	0
56	MG	2A	3086	1/1	0.91	0.92	78,78,78,78	0
56	MG	1A	3478	1/1	0.91	0.30	83,83,83,83	0
56	MG	1A	3350	1/1	0.91	0.13	76,76,76,76	0
56	MG	2a	3126	1/1	0.91	0.31	86,86,86,86	0
56	MG	2a	3127	1/1	0.91	0.10	100,100,100,100	0
56	MG	1a	3216	1/1	0.91	0.14	81,81,81,81	0
56	MG	2A	3091	1/1	0.91	0.28	74,74,74,74	0
56	MG	2A	3348	1/1	0.91	0.25	79,79,79,79	0
56	MG	1A	3232	1/1	0.91	0.24	52,52,52,52	0
56	MG	2a	3001	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3559	1/1	0.91	0.10	115,115,115,115	0
56	MG	1A	3300	1/1	0.91	0.19	77,77,77,77	0
56	MG	1A	3178	1/1	0.91	0.43	82,82,82,82	0
56	MG	2a	3145	1/1	0.91	0.20	90,90,90,90	0
56	MG	1a	3226	1/1	0.91	0.27	89,89,89,89	0
56	MG	1A	3357	1/1	0.91	0.32	76,76,76,76	0
56	MG	1a	3232	1/1	0.91	0.19	76,76,76,76	0
56	MG	1A	3652	1/1	0.91	0.13	86,86,86,86	0
56	MG	1A	3035	1/1	0.91	0.15	70,70,70,70	0
56	MG	2A	3210	1/1	0.91	0.12	75,75,75,75	0
56	MG	1A	3006	1/1	0.91	0.45	69,69,69,69	0
56	MG	1a	3061	1/1	0.91	0.35	79,79,79,79	0
56	MG	1A	3426	1/1	0.91	0.25	72,72,72,72	0
56	MG	2a	3023	1/1	0.91	0.47	80,80,80,80	0
56	MG	1A	3504	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3009	1/1	0.91	0.90	89,89,89,89	0
56	MG	1A	3427	1/1	0.91	0.20	78,78,78,78	0
56	MG	1A	3361	1/1	0.91	0.27	71,71,71,71	0
56	MG	1A	3060	1/1	0.91	0.17	75,75,75,75	0
56	MG	1A	3201	1/1	0.91	0.29	68,68,68,68	0
56	MG	1A	3310	1/1	0.91	0.14	76,76,76,76	0
56	MG	2A	3124	1/1	0.91	0.20	86,86,86,86	0
56	MG	1A	3243	1/1	0.91	0.12	81,81,81,81	0
56	MG	2A	3246	1/1	0.91	0.88	105,105,105,105	0
56	MG	1A	3119	1/1	0.91	0.23	107,107,107,107	0
56	MG	1A	3024	1/1	0.91	0.82	83,83,83,83	0
56	MG	1a	3154	1/1	0.91	0.32	78,78,78,78	0
56	MG	1A	3050	1/1	0.91	0.16	76,76,76,76	0
56	MG	1A	3285	1/1	0.91	0.26	56,56,56,56	0
56	MG	2A	3257	1/1	0.91	0.26	76,76,76,76	0
56	MG	1a	3079	1/1	0.92	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3252	1/1	0.92	0.13	73,73,73,73	0
56	MG	1A	3124	1/1	0.92	0.79	86,86,86,86	0
56	MG	1A	3207	1/1	0.92	0.11	74,74,74,74	0
56	MG	2A	3135	1/1	0.92	0.25	78,78,78,78	0
56	MG	1a	3084	1/1	0.92	0.20	94,94,94,94	0
56	MG	1A	3340	1/1	0.92	0.32	78,78,78,78	0
56	MG	1A	3283	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3115	1/1	0.92	0.23	87,87,87,87	0
56	MG	1a	3091	1/1	0.92	0.57	83,83,83,83	0
56	MG	1a	3178	1/1	0.92	0.32	81,81,81,81	0
56	MG	1A	3384	1/1	0.92	0.46	75,75,75,75	0
56	MG	1a	3022	1/1	0.92	0.21	89,89,89,89	0
56	MG	2A	3145	1/1	0.92	0.11	77,77,77,77	0
56	MG	2A	3043	1/1	0.92	0.21	82,82,82,82	0
56	MG	2A	3044	1/1	0.92	0.22	78,78,78,78	0
56	MG	2A	3046	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3488	1/1	0.92	0.16	80,80,80,80	0
56	MG	2a	3073	1/1	0.92	0.19	113,113,113,113	0
56	MG	1A	3550	1/1	0.92	0.31	101,101,101,101	0
56	MG	2a	3075	1/1	0.92	0.30	98,98,98,98	0
56	MG	2A	3050	1/1	0.92	0.36	81,81,81,81	0
56	MG	1a	3026	1/1	0.92	0.22	80,80,80,80	0
56	MG	1A	3551	1/1	0.92	0.24	97,97,97,97	0
56	MG	1A	3126	1/1	0.92	0.64	76,76,76,76	0
56	MG	1A	3491	1/1	0.92	0.23	84,84,84,84	0
56	MG	1A	3618	1/1	0.92	0.19	98,98,98,98	0
56	MG	1A	3313	1/1	0.92	0.29	72,72,72,72	0
56	MG	2a	3086	1/1	0.92	0.14	87,87,87,87	0
56	MG	1A	3389	1/1	0.92	0.49	75,75,75,75	0
56	MG	1a	3197	1/1	0.92	0.12	102,102,102,102	0
56	MG	2A	3066	1/1	0.92	0.13	92,92,92,92	0
56	MG	2A	3305	1/1	0.92	0.11	85,85,85,85	0
56	MG	2A	3164	1/1	0.92	0.16	82,82,82,82	0
56	MG	2A	3312	1/1	0.92	0.10	74,74,74,74	0
56	MG	2A	3068	1/1	0.92	0.18	106,106,106,106	0
56	MG	1a	3034	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3495	1/1	0.92	0.23	66,66,66,66	0
56	MG	1A	3211	1/1	0.92	0.30	88,88,88,88	0
56	MG	1A	3500	1/1	0.92	0.17	86,86,86,86	0
56	MG	1a	3207	1/1	0.92	0.20	96,96,96,96	0
56	MG	2A	3180	1/1	0.92	0.15	74,74,74,74	0
56	MG	1A	3143	1/1	0.92	0.32	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3182	1/1	0.92	0.23	81,81,81,81	0
56	MG	2A	3326	1/1	0.92	0.16	91,91,91,91	0
56	MG	2a	3113	1/1	0.92	0.08	111,111,111,111	0
56	MG	1A	3563	1/1	0.92	0.17	97,97,97,97	0
56	MG	1A	3638	1/1	0.92	0.13	80,80,80,80	0
56	MG	2A	3187	1/1	0.92	0.14	81,81,81,81	0
56	MG	1A	3290	1/1	0.92	0.35	90,90,90,90	0
56	MG	2a	3119	1/1	0.92	0.12	107,107,107,107	0
56	MG	2A	3081	1/1	0.92	0.10	79,79,79,79	0
56	MG	1A	3642	1/1	0.92	0.29	74,74,74,74	0
56	MG	2a	3123	1/1	0.92	0.16	79,79,79,79	0
56	MG	1A	3356	1/1	0.92	0.67	61,61,61,61	0
56	MG	2A	3335	1/1	0.92	0.09	100,100,100,100	0
56	MG	1A	3187	1/1	0.92	0.14	75,75,75,75	0
56	MG	1A	3110	1/1	0.92	0.67	82,82,82,82	0
56	MG	1A	3171	1/1	0.92	0.14	77,77,77,77	0
56	MG	1A	3449	1/1	0.92	0.27	76,76,76,76	0
56	MG	1a	3123	1/1	0.92	0.16	72,72,72,72	0
56	MG	1a	3229	1/1	0.92	0.24	85,85,85,85	0
56	MG	1A	3325	1/1	0.92	0.19	69,69,69,69	0
56	MG	1A	3409	1/1	0.92	0.33	70,70,70,70	0
56	MG	1a	3059	1/1	0.92	0.68	82,82,82,82	0
56	MG	1A	3411	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3055	1/1	0.92	0.22	79,79,79,79	0
56	MG	2a	3152	1/1	0.92	0.19	111,111,111,111	0
56	MG	1A	3274	1/1	0.92	0.24	78,78,78,78	0
56	MG	1A	3672	1/1	0.92	0.28	68,68,68,68	0
56	MG	2a	3156	1/1	0.92	0.08	104,104,104,104	0
56	MG	2A	3211	1/1	0.92	0.29	81,81,81,81	0
56	MG	2A	3007	1/1	0.92	0.14	80,80,80,80	0
56	MG	1A	3365	1/1	0.92	0.31	75,75,75,75	0
56	MG	1A	3581	1/1	0.92	0.13	84,84,84,84	0
56	MG	1A	3582	1/1	0.92	0.20	73,73,73,73	0
56	MG	1A	3329	1/1	0.92	0.20	77,77,77,77	0
56	MG	1A	3461	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3116	1/1	0.92	0.35	91,91,91,91	0
56	MG	2a	3026	1/1	0.92	0.15	90,90,90,90	0
56	MG	2A	3229	1/1	0.92	0.18	90,90,90,90	0
56	MG	2A	3231	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3275	1/1	0.92	0.19	61,61,61,61	0
56	MG	2a	3033	1/1	0.92	0.13	86,86,86,86	0
56	MG	1A	3466	1/1	0.92	0.16	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3238	1/1	0.92	0.17	93,93,93,93	0
56	MG	2A	3242	1/1	0.92	0.18	70,70,70,70	0
56	MG	2a	3039	1/1	0.92	0.13	89,89,89,89	0
56	MG	2A	3020	1/1	0.92	0.29	69,69,69,69	0
56	MG	1A	3204	1/1	0.92	0.19	60,60,60,60	0
56	MG	1a	3010	1/1	0.92	0.26	85,85,85,85	0
56	MG	2a	3046	1/1	0.92	0.10	85,85,85,85	0
56	MG	1A	3596	1/1	0.92	0.16	81,81,81,81	0
56	MG	1A	3599	1/1	0.92	0.30	100,100,100,100	0
56	MG	1A	3221	1/1	0.93	0.31	79,79,79,79	0
56	MG	2A	3308	1/1	0.93	0.13	103,103,103,103	0
56	MG	2A	3309	1/1	0.93	0.12	85,85,85,85	0
56	MG	1A	3223	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3311	1/1	0.93	0.22	106,106,106,106	0
56	MG	2A	3107	1/1	0.93	0.27	92,92,92,92	0
56	MG	1A	3523	1/1	0.93	0.11	96,96,96,96	0
56	MG	1a	3041	1/1	0.93	0.14	81,81,81,81	0
56	MG	1a	3102	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	3229	1/1	0.93	0.21	74,74,74,74	0
56	MG	1A	3255	1/1	0.93	0.26	59,59,59,59	0
56	MG	2A	3202	1/1	0.93	0.32	88,88,88,88	0
56	MG	1A	3289	1/1	0.93	0.71	92,92,92,92	0
56	MG	2a	3084	1/1	0.93	0.14	78,78,78,78	0
56	MG	1A	3038	1/1	0.93	0.16	74,74,74,74	0
56	MG	2A	3322	1/1	0.93	0.15	86,86,86,86	0
56	MG	1A	3530	1/1	0.93	0.79	79,79,79,79	0
56	MG	1A	3469	1/1	0.93	0.37	84,84,84,84	0
56	MG	2A	3037	1/1	0.93	0.26	75,75,75,75	0
56	MG	2A	3208	1/1	0.93	0.12	71,71,71,71	0
56	MG	1A	3202	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3670	1/1	0.93	0.13	76,76,76,76	0
56	MG	1A	3233	1/1	0.93	0.09	58,58,58,58	0
56	MG	2A	3129	1/1	0.93	0.32	73,73,73,73	0
56	MG	1A	3537	1/1	0.93	1.62	113,113,113,113	0
56	MG	1A	3476	1/1	0.93	0.11	89,89,89,89	0
56	MG	2A	3133	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3219	1/1	0.93	0.13	80,80,80,80	0
56	MG	2A	3341	1/1	0.93	0.15	94,94,94,94	0
56	MG	2a	3104	1/1	0.93	0.11	100,100,100,100	0
56	MG	1A	3592	1/1	0.93	0.25	84,84,84,84	0
56	MG	1a	3196	1/1	0.93	0.15	85,85,85,85	0
56	MG	1a	3003	1/1	0.93	0.11	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3137	1/1	0.93	0.28	91,91,91,91	0
56	MG	2a	3114	1/1	0.93	0.34	92,92,92,92	0
56	MG	2A	3230	1/1	0.93	0.35	82,82,82,82	0
56	MG	1a	3198	1/1	0.93	0.28	89,89,89,89	0
56	MG	1A	3542	1/1	0.93	0.42	77,77,77,77	0
56	MG	1A	3331	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	3132	1/1	0.93	0.22	82,82,82,82	0
56	MG	1a	3204	1/1	0.93	0.17	80,80,80,80	0
56	MG	2a	3008	1/1	0.93	0.10	85,85,85,85	0
56	MG	1A	3334	1/1	0.93	0.18	64,64,64,64	0
56	MG	1a	3206	1/1	0.93	0.10	89,89,89,89	0
56	MG	1A	3235	1/1	0.93	0.13	73,73,73,73	0
56	MG	1A	3189	1/1	0.93	0.49	78,78,78,78	0
56	MG	1a	3125	1/1	0.93	0.21	106,106,106,106	0
56	MG	1A	3025	1/1	0.93	0.29	87,87,87,87	0
56	MG	1A	3166	1/1	0.93	0.33	77,77,77,77	0
56	MG	2a	3020	1/1	0.93	0.08	98,98,98,98	0
56	MG	1a	3132	1/1	0.93	0.12	101,101,101,101	0
56	MG	1A	3241	1/1	0.93	0.32	68,68,68,68	0
56	MG	2a	3025	1/1	0.93	0.08	86,86,86,86	0
56	MG	1A	3438	1/1	0.93	0.10	71,71,71,71	0
56	MG	2a	3027	1/1	0.93	0.12	83,83,83,83	0
56	MG	2a	3148	1/1	0.93	0.13	92,92,92,92	0
56	MG	1A	3273	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3496	1/1	0.93	0.24	72,72,72,72	0
56	MG	2A	3260	1/1	0.93	0.24	87,87,87,87	0
56	MG	2A	3075	1/1	0.93	0.34	83,83,83,83	0
56	MG	1A	3074	1/1	0.93	0.14	81,81,81,81	0
56	MG	1a	3141	1/1	0.93	0.20	59,59,59,59	0
56	MG	1A	3047	1/1	0.93	0.99	68,68,68,68	0
56	MG	2A	3271	1/1	0.93	0.18	83,83,83,83	0
56	MG	1A	3029	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3312	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3355	1/1	0.93	0.23	68,68,68,68	0
56	MG	2A	3280	1/1	0.93	0.83	94,94,94,94	0
56	MG	1a	3235	1/1	0.93	0.32	93,93,93,93	0
56	MG	1a	3151	1/1	0.93	0.21	80,80,80,80	0
56	MG	1A	3624	1/1	0.93	0.29	64,64,64,64	0
56	MG	2A	3285	1/1	0.93	0.11	82,82,82,82	0
56	MG	2A	3001	1/1	0.93	0.14	75,75,75,75	0
56	MG	1A	3278	1/1	0.93	0.28	59,59,59,59	0
56	MG	2a	3173	1/1	0.93	0.35	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3158	1/1	0.93	0.19	67,67,67,67	0
56	MG	2A	3177	1/1	0.93	0.22	74,74,74,74	0
56	MG	1A	3512	1/1	0.93	0.29	82,82,82,82	0
56	MG	1a	3159	1/1	0.93	0.28	72,72,72,72	0
56	MG	1a	3160	1/1	0.93	0.23	76,76,76,76	0
56	MG	1A	3081	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3120	1/1	0.93	0.23	111,111,111,111	0
56	MG	1A	3413	1/1	0.93	0.24	71,71,71,71	0
56	MG	1A	3640	1/1	0.93	0.26	81,81,81,81	0
56	MG	1A	3414	1/1	0.93	0.36	82,82,82,82	0
56	MG	1A	3017	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3039	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3326	1/1	0.94	0.20	83,83,83,83	0
56	MG	1A	3677	1/1	0.94	0.23	55,55,55,55	0
56	MG	1a	3078	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	3586	1/1	0.94	0.32	71,71,71,71	0
56	MG	2A	3261	1/1	0.94	0.40	98,98,98,98	0
56	MG	1A	3418	1/1	0.94	0.35	75,75,75,75	0
56	MG	1A	3473	1/1	0.94	0.12	86,86,86,86	0
56	MG	2a	3056	1/1	0.94	0.11	97,97,97,97	0
56	MG	1A	3264	1/1	0.94	0.43	67,67,67,67	0
56	MG	1a	3006	1/1	0.94	0.21	90,90,90,90	0
56	MG	1A	3593	1/1	0.94	0.17	65,65,65,65	0
56	MG	1A	3595	1/1	0.94	0.32	69,69,69,69	0
56	MG	2A	3045	1/1	0.94	0.21	76,76,76,76	0
56	MG	1A	3366	1/1	0.94	0.14	72,72,72,72	0
56	MG	1A	3422	1/1	0.94	0.32	67,67,67,67	0
56	MG	1A	3134	1/1	0.94	0.30	63,63,63,63	0
56	MG	2a	3067	1/1	0.94	0.09	112,112,112,112	0
56	MG	1A	3266	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3603	1/1	0.94	0.21	67,67,67,67	0
56	MG	1A	3605	1/1	0.94	0.20	93,93,93,93	0
56	MG	1a	3017	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3370	1/1	0.94	0.17	82,82,82,82	0
56	MG	2A	3289	1/1	0.94	0.07	102,102,102,102	0
56	MG	2A	3056	1/1	0.94	0.67	73,73,73,73	0
56	MG	1a	3193	1/1	0.94	0.24	88,88,88,88	0
56	MG	1A	3088	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3220	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3610	1/1	0.94	0.21	79,79,79,79	0
56	MG	1a	3199	1/1	0.94	0.31	93,93,93,93	0
56	MG	2a	3081	1/1	0.94	0.10	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	1A	3332	1/1	0.94	0.24	77,77,77,77	0
56	MG	2a	3083	1/1	0.94	0.52	76,76,76,76	0
56	MG	1A	3077	1/1	0.94	0.30	93,93,93,93	0
56	MG	1A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3245	1/1	0.94	0.31	56,56,56,56	0
56	MG	2A	3304	1/1	0.94	0.46	92,92,92,92	0
56	MG	1A	3381	1/1	0.94	0.27	68,68,68,68	0
56	MG	2A	3171	1/1	0.94	0.19	86,86,86,86	0
56	MG	1A	3383	1/1	0.94	0.24	69,69,69,69	0
56	MG	2A	3174	1/1	0.94	0.13	79,79,79,79	0
56	MG	1A	3337	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3558	1/1	0.94	0.14	97,97,97,97	0
56	MG	1A	3116	1/1	0.94	0.41	113,113,113,113	0
56	MG	1A	3387	1/1	0.94	0.17	80,80,80,80	0
56	MG	1A	3623	1/1	0.94	0.15	87,87,87,87	0
56	MG	2A	3185	1/1	0.94	0.32	76,76,76,76	0
56	MG	1A	3561	1/1	0.94	0.17	64,64,64,64	0
56	MG	2A	3082	1/1	0.94	0.05	85,85,85,85	0
56	MG	1A	3305	1/1	0.94	0.20	65,65,65,65	0
56	MG	1A	3564	1/1	0.94	0.10	97,97,97,97	0
56	MG	1a	3218	1/1	0.94	0.21	80,80,80,80	0
56	MG	2A	3088	1/1	0.94	0.17	77,77,77,77	0
56	MG	2a	3109	1/1	0.94	0.11	82,82,82,82	0
56	MG	2a	3110	1/1	0.94	0.13	80,80,80,80	0
56	MG	2a	3111	1/1	0.94	0.13	86,86,86,86	0
56	MG	2a	3112	1/1	0.94	0.14	87,87,87,87	0
56	MG	1A	3224	1/1	0.94	0.22	65,65,65,65	0
56	MG	1A	3227	1/1	0.94	0.18	72,72,72,72	0
56	MG	1A	3051	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3079	1/1	0.94	0.12	96,96,96,96	0
56	MG	1A	3351	1/1	0.94	0.24	58,58,58,58	0
56	MG	2A	3095	1/1	0.94	0.43	89,89,89,89	0
56	MG	1A	3206	1/1	0.94	0.07	76,76,76,76	0
56	MG	1A	3644	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3316	1/1	0.94	0.29	83,83,83,83	0
56	MG	1a	3234	1/1	0.94	0.18	85,85,85,85	0
56	MG	1A	3254	1/1	0.94	0.14	78,78,78,78	0
56	MG	2A	3103	1/1	0.94	0.24	83,83,83,83	0
56	MG	2A	3342	1/1	0.94	0.26	78,78,78,78	0
56	MG	2a	3128	1/1	0.94	0.17	74,74,74,74	0
56	MG	1A	3574	1/1	0.94	0.23	77,77,77,77	0
56	MG	1A	3649	1/1	0.94	0.05	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3131	1/1	0.94	0.13	84,84,84,84	0
56	MG	2a	3132	1/1	0.94	0.20	83,83,83,83	0
56	MG	2a	3136	1/1	0.94	0.27	85,85,85,85	0
56	MG	2a	3137	1/1	0.94	0.09	81,81,81,81	0
56	MG	2A	3346	1/1	0.94	0.27	78,78,78,78	0
56	MG	1a	3137	1/1	0.94	0.10	79,79,79,79	0
56	MG	1A	3650	1/1	0.94	1.24	90,90,90,90	0
56	MG	2A	3212	1/1	0.94	0.52	83,83,83,83	0
56	MG	2A	3108	1/1	0.94	0.25	72,72,72,72	0
56	MG	2A	3214	1/1	0.94	0.49	92,92,92,92	0
56	MG	2A	3109	1/1	0.94	0.14	93,93,93,93	0
56	MG	1a	3055	1/1	0.94	0.18	83,83,83,83	0
56	MG	1a	3056	1/1	0.94	0.11	83,83,83,83	0
56	MG	2A	3218	1/1	0.94	0.23	83,83,83,83	0
56	MG	2a	3153	1/1	0.94	0.13	106,106,106,106	0
56	MG	1A	3152	1/1	0.94	0.67	84,84,84,84	0
56	MG	2A	3220	1/1	0.94	0.33	74,74,74,74	0
56	MG	2A	3113	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3576	1/1	0.94	0.14	76,76,76,76	0
56	MG	2a	3013	1/1	0.94	0.28	85,85,85,85	0
56	MG	2A	3226	1/1	0.94	0.11	73,73,73,73	0
56	MG	1A	3656	1/1	0.94	0.20	70,70,70,70	0
56	MG	2A	3228	1/1	0.94	0.10	68,68,68,68	0
56	MG	2a	3018	1/1	0.94	0.13	71,71,71,71	0
56	MG	2A	3012	1/1	0.94	0.30	92,92,92,92	0
56	MG	1A	3080	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3578	1/1	0.94	0.12	86,86,86,86	0
56	MG	2A	3233	1/1	0.94	0.25	71,71,71,71	0
56	MG	1A	3659	1/1	0.94	0.18	80,80,80,80	0
56	MG	2A	3235	1/1	0.94	0.19	69,69,69,69	0
56	MG	1A	3321	1/1	0.94	0.21	62,62,62,62	0
56	MG	1A	3412	1/1	0.94	0.45	79,79,79,79	0
56	MG	2a	3174	1/1	0.94	0.12	101,101,101,101	0
56	MG	1a	3155	1/1	0.94	0.08	74,74,74,74	0
56	MG	2a	3032	1/1	0.94	0.17	79,79,79,79	0
56	MG	1A	3663	1/1	0.94	0.23	89,89,89,89	0
56	MG	2A	3128	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3209	1/1	0.94	0.19	56,56,56,56	0
56	MG	1A	3666	1/1	0.94	0.17	92,92,92,92	0
56	MG	2a	3182	1/1	0.94	0.17	106,106,106,106	0
56	MG	1A	3668	1/1	0.94	0.11	82,82,82,82	0
56	MG	1A	3130	1/1	0.94	0.36	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3251	1/1	0.94	0.13	73,73,73,73	0
56	MG	2A	3032	1/1	0.94	0.25	78,78,78,78	0
56	MG	2A	3200	1/1	0.95	0.26	86,86,86,86	0
56	MG	1A	3546	1/1	0.95	0.21	69,69,69,69	0
56	MG	2A	3010	1/1	0.95	0.14	85,85,85,85	0
56	MG	1a	3157	1/1	0.95	0.45	89,89,89,89	0
56	MG	1A	3373	1/1	0.95	0.35	54,54,54,54	0
56	MG	1A	3341	1/1	0.95	0.21	70,70,70,70	0
56	MG	2A	3015	1/1	0.95	0.53	84,84,84,84	0
56	MG	2A	3016	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3342	1/1	0.95	0.20	64,64,64,64	0
56	MG	1a	3081	1/1	0.95	0.16	81,81,81,81	0
56	MG	1A	3131	1/1	0.95	0.18	84,84,84,84	0
56	MG	1a	3164	1/1	0.95	0.73	81,81,81,81	0
56	MG	2A	3324	1/1	0.95	0.27	83,83,83,83	0
56	MG	1A	3484	1/1	0.95	0.25	80,80,80,80	0
56	MG	1A	3260	1/1	0.95	0.26	62,62,62,62	0
56	MG	1A	3487	1/1	0.95	0.11	81,81,81,81	0
56	MG	1A	3238	1/1	0.95	0.13	60,60,60,60	0
56	MG	2A	3027	1/1	0.95	0.16	87,87,87,87	0
56	MG	1A	3382	1/1	0.95	0.23	60,60,60,60	0
56	MG	1a	3172	1/1	0.95	0.14	90,90,90,90	0
56	MG	2A	3125	1/1	0.95	0.28	88,88,88,88	0
56	MG	1A	3349	1/1	0.95	0.25	72,72,72,72	0
56	MG	1A	3083	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3162	1/1	0.95	0.09	83,83,83,83	0
56	MG	2A	3338	1/1	0.95	0.64	97,97,97,97	0
56	MG	1A	3432	1/1	0.95	0.32	57,57,57,57	0
56	MG	1A	3386	1/1	0.95	0.49	68,68,68,68	0
56	MG	1A	3054	1/1	0.95	0.24	86,86,86,86	0
56	MG	1a	3181	1/1	0.95	0.28	66,66,66,66	0
56	MG	1A	3182	1/1	0.95	0.69	72,72,72,72	0
56	MG	2A	3347	1/1	0.95	0.16	86,86,86,86	0
56	MG	1A	3626	1/1	0.95	0.16	86,86,86,86	0
56	MG	2A	3349	1/1	0.95	0.26	81,81,81,81	0
56	MG	1A	3501	1/1	0.95	0.28	71,71,71,71	0
56	MG	1A	3631	1/1	0.95	0.08	82,82,82,82	0
56	MG	2a	3002	1/1	0.95	0.13	98,98,98,98	0
56	MG	1A	3076	1/1	0.95	0.60	54,54,54,54	0
56	MG	1a	3104	1/1	0.95	0.15	74,74,74,74	0
56	MG	1A	3091	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3108	1/1	0.95	0.43	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3393	1/1	0.95	0.18	82,82,82,82	0
56	MG	1A	3225	1/1	0.95	0.38	65,65,65,65	0
56	MG	2A	3049	1/1	0.95	0.15	81,81,81,81	0
56	MG	1a	3195	1/1	0.95	0.22	80,80,80,80	0
56	MG	1A	3570	1/1	0.95	0.32	99,99,99,99	0
56	MG	2a	3122	1/1	0.95	0.09	114,114,114,114	0
56	MG	2A	3248	1/1	0.95	0.11	85,85,85,85	0
56	MG	2A	3052	1/1	0.95	0.15	72,72,72,72	0
56	MG	1A	3395	1/1	0.95	0.14	72,72,72,72	0
56	MG	1A	3109	1/1	0.95	0.16	78,78,78,78	0
56	MG	1A	3446	1/1	0.95	0.16	65,65,65,65	0
56	MG	1a	3040	1/1	0.95	0.08	89,89,89,89	0
56	MG	2a	3019	1/1	0.95	0.13	95,95,95,95	0
56	MG	2A	3255	1/1	0.95	0.60	91,91,91,91	0
56	MG	2a	3021	1/1	0.95	0.09	101,101,101,101	0
56	MG	2a	3134	1/1	0.95	0.19	100,100,100,100	0
56	MG	2a	3135	1/1	0.95	0.14	108,108,108,108	0
56	MG	1a	3114	1/1	0.95	0.09	86,86,86,86	0
56	MG	1A	3397	1/1	0.95	0.09	83,83,83,83	0
56	MG	1A	3302	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3402	1/1	0.95	0.21	51,51,51,51	0
56	MG	2A	3062	1/1	0.95	0.12	84,84,84,84	0
56	MG	2A	3262	1/1	0.95	0.66	84,84,84,84	0
56	MG	1A	3403	1/1	0.95	0.36	59,59,59,59	0
56	MG	2a	3030	1/1	0.95	0.12	77,77,77,77	0
56	MG	1A	3522	1/1	0.95	0.10	69,69,69,69	0
56	MG	2a	3147	1/1	0.95	0.36	89,89,89,89	0
56	MG	1A	3404	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3360	1/1	0.95	0.14	68,68,68,68	0
56	MG	1a	3212	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3020	1/1	0.95	0.36	89,89,89,89	0
56	MG	2A	3274	1/1	0.95	0.23	92,92,92,92	0
56	MG	1A	3458	1/1	0.95	0.14	82,82,82,82	0
56	MG	1A	3528	1/1	0.95	0.28	78,78,78,78	0
56	MG	1A	3230	1/1	0.95	0.20	72,72,72,72	0
56	MG	2A	3281	1/1	0.95	0.10	88,88,88,88	0
56	MG	1A	3031	1/1	0.95	0.10	62,62,62,62	0
56	MG	1a	3128	1/1	0.95	0.22	98,98,98,98	0
56	MG	1A	3008	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3664	1/1	0.95	0.21	82,82,82,82	0
56	MG	1A	3587	1/1	0.95	0.18	80,80,80,80	0
56	MG	1A	3462	1/1	0.95	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	3228	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3018	1/1	0.95	0.56	84,84,84,84	0
56	MG	2A	3183	1/1	0.95	0.15	80,80,80,80	0
56	MG	1A	3669	1/1	0.95	0.19	79,79,79,79	0
56	MG	2a	3057	1/1	0.95	0.13	74,74,74,74	0
56	MG	2a	3172	1/1	0.95	0.38	89,89,89,89	0
56	MG	1A	3536	1/1	0.95	0.22	74,74,74,74	0
56	MG	1A	3309	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3540	1/1	0.95	0.10	94,94,94,94	0
56	MG	1a	3145	1/1	0.95	0.48	97,97,97,97	0
56	MG	1A	3675	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3336	1/1	0.95	0.41	81,81,81,81	0
56	MG	1A	3369	1/1	0.95	0.31	86,86,86,86	0
56	MG	1A	3003	1/1	0.95	0.39	60,60,60,60	0
56	MG	1A	3082	1/1	0.95	0.15	69,69,69,69	0
56	MG	2a	3068	1/1	0.95	0.16	83,83,83,83	0
56	MG	2A	3005	1/1	0.95	0.09	84,84,84,84	0
56	MG	1A	3602	1/1	0.95	0.22	67,67,67,67	0
56	MG	1A	3236	1/1	0.95	0.29	60,60,60,60	0
56	MG	1A	3222	1/1	0.96	0.22	64,64,64,64	0
56	MG	1A	3163	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3170	1/1	0.96	0.30	99,99,99,99	0
56	MG	1A	3421	1/1	0.96	0.22	68,68,68,68	0
56	MG	1A	3467	1/1	0.96	0.11	73,73,73,73	0
56	MG	1A	3641	1/1	0.96	0.17	68,68,68,68	0
56	MG	1a	3208	1/1	0.96	0.14	80,80,80,80	0
56	MG	1A	3027	1/1	0.96	1.18	68,68,68,68	0
56	MG	2A	3176	1/1	0.96	0.22	89,89,89,89	0
56	MG	1a	3210	1/1	0.96	0.23	91,91,91,91	0
56	MG	1A	3226	1/1	0.96	0.22	62,62,62,62	0
56	MG	1A	3172	1/1	0.96	0.26	94,94,94,94	0
56	MG	2A	3299	1/1	0.96	0.48	66,66,66,66	0
56	MG	1A	3471	1/1	0.96	0.19	88,88,88,88	0
56	MG	1A	3281	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3282	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3535	1/1	0.96	0.34	90,90,90,90	0
56	MG	1a	3044	1/1	0.96	0.29	90,90,90,90	0
56	MG	2A	3307	1/1	0.96	0.17	79,79,79,79	0
56	MG	1A	3392	1/1	0.96	0.36	80,80,80,80	0
56	MG	2A	3083	1/1	0.96	0.10	80,80,80,80	0
56	MG	2A	3189	1/1	0.96	0.23	89,89,89,89	0
56	MG	1A	3362	1/1	0.96	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3653	1/1	0.96	0.17	95,95,95,95	0
56	MG	1a	3223	1/1	0.96	0.24	84,84,84,84	0
56	MG	1A	3654	1/1	0.96	0.16	89,89,89,89	0
56	MG	1a	3225	1/1	0.96	0.57	85,85,85,85	0
56	MG	1a	3130	1/1	0.96	0.27	99,99,99,99	0
56	MG	1A	3538	1/1	0.96	0.09	87,87,87,87	0
56	MG	1A	3539	1/1	0.96	0.33	85,85,85,85	0
56	MG	2A	3199	1/1	0.96	0.37	74,74,74,74	0
56	MG	1A	3430	1/1	0.96	0.24	61,61,61,61	0
56	MG	1A	3480	1/1	0.96	0.27	104,104,104,104	0
56	MG	2a	3093	1/1	0.96	0.23	87,87,87,87	0
56	MG	2a	3094	1/1	0.96	0.29	89,89,89,89	0
56	MG	2A	3096	1/1	0.96	0.17	90,90,90,90	0
56	MG	1A	3590	1/1	0.96	0.21	68,68,68,68	0
56	MG	2A	3325	1/1	0.96	0.20	91,91,91,91	0
56	MG	1A	3591	1/1	0.96	0.34	83,83,83,83	0
56	MG	1a	3057	1/1	0.96	0.24	92,92,92,92	0
56	MG	1A	3228	1/1	0.96	0.17	59,59,59,59	0
56	MG	2A	3329	1/1	0.96	0.29	100,100,100,100	0
56	MG	1a	3237	1/1	0.96	0.06	106,106,106,106	0
56	MG	1a	3142	1/1	0.96	0.16	85,85,85,85	0
56	MG	1A	3284	1/1	0.96	0.16	86,86,86,86	0
56	MG	1A	3059	1/1	0.96	0.13	81,81,81,81	0
56	MG	2a	3108	1/1	0.96	0.05	98,98,98,98	0
56	MG	1A	3213	1/1	0.96	0.16	66,66,66,66	0
56	MG	1A	3597	1/1	0.96	0.16	87,87,87,87	0
56	MG	2A	3006	1/1	0.96	0.24	71,71,71,71	0
56	MG	1A	3598	1/1	0.96	0.27	74,74,74,74	0
56	MG	1a	3150	1/1	0.96	0.15	83,83,83,83	0
56	MG	2A	3340	1/1	0.96	0.19	67,67,67,67	0
56	MG	1A	3398	1/1	0.96	0.14	67,67,67,67	0
56	MG	1A	3671	1/1	0.96	0.16	79,79,79,79	0
56	MG	1A	3399	1/1	0.96	0.28	68,68,68,68	0
56	MG	1A	3673	1/1	0.96	0.30	77,77,77,77	0
56	MG	1A	3037	1/1	0.96	0.18	83,83,83,83	0
56	MG	2A	3221	1/1	0.96	0.14	107,107,107,107	0
56	MG	2A	3014	1/1	0.96	0.38	72,72,72,72	0
56	MG	1A	3315	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3440	1/1	0.96	0.14	77,77,77,77	0
56	MG	1A	3248	1/1	0.96	0.20	76,76,76,76	0
56	MG	1A	3678	1/1	0.96	0.23	75,75,75,75	0
56	MG	1a	3161	1/1	0.96	0.10	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3317	1/1	0.96	0.30	56,56,56,56	0
56	MG	1a	3074	1/1	0.96	0.12	88,88,88,88	0
56	MG	1a	3001	1/1	0.96	0.25	90,90,90,90	0
56	MG	1A	3216	1/1	0.96	0.32	50,50,50,50	0
56	MG	1A	3406	1/1	0.96	0.22	59,59,59,59	0
56	MG	2a	3133	1/1	0.96	0.23	92,92,92,92	0
56	MG	2A	3236	1/1	0.96	0.18	69,69,69,69	0
56	MG	1A	3445	1/1	0.96	0.20	80,80,80,80	0
56	MG	1a	3168	1/1	0.96	0.14	111,111,111,111	0
56	MG	2A	3240	1/1	0.96	0.12	84,84,84,84	0
56	MG	2A	3132	1/1	0.96	0.19	97,97,97,97	0
56	MG	2A	3029	1/1	0.96	0.21	94,94,94,94	0
56	MG	1A	3344	1/1	0.96	0.19	79,79,79,79	0
56	MG	2a	3016	1/1	0.96	0.29	91,91,91,91	0
56	MG	1A	3117	1/1	0.96	0.10	98,98,98,98	0
56	MG	1a	3171	1/1	0.96	0.23	86,86,86,86	0
56	MG	1A	3269	1/1	0.96	0.15	69,69,69,69	0
56	MG	2a	3146	1/1	0.96	0.17	100,100,100,100	0
56	MG	1A	3450	1/1	0.96	0.38	76,76,76,76	0
56	MG	1a	3087	1/1	0.96	0.13	100,100,100,100	0
56	MG	1A	3508	1/1	0.96	0.12	86,86,86,86	0
56	MG	1a	3176	1/1	0.96	0.10	84,84,84,84	0
56	MG	1a	3011	1/1	0.96	0.20	94,94,94,94	0
56	MG	1A	3410	1/1	0.96	0.17	77,77,77,77	0
56	MG	1a	3013	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3562	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3348	1/1	0.96	0.34	74,74,74,74	0
56	MG	1A	3193	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3259	1/1	0.96	0.21	76,76,76,76	0
56	MG	1a	3096	1/1	0.96	0.10	95,95,95,95	0
56	MG	1A	3514	1/1	0.96	0.12	94,94,94,94	0
56	MG	1A	3378	1/1	0.96	0.43	73,73,73,73	0
56	MG	2a	3035	1/1	0.96	0.15	94,94,94,94	0
56	MG	1A	3516	1/1	0.96	0.07	81,81,81,81	0
56	MG	2A	3264	1/1	0.96	0.10	91,91,91,91	0
56	MG	2a	3038	1/1	0.96	0.20	101,101,101,101	0
56	MG	1a	3100	1/1	0.96	0.13	78,78,78,78	0
56	MG	1A	3625	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3090	1/1	0.96	0.50	84,84,84,84	0
56	MG	2a	3171	1/1	0.96	0.07	115,115,115,115	0
56	MG	2A	3269	1/1	0.96	0.75	74,74,74,74	0
56	MG	2A	3270	1/1	0.96	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3155	1/1	0.96	0.07	66,66,66,66	0
56	MG	2A	3272	1/1	0.96	0.15	89,89,89,89	0
56	MG	1A	3627	1/1	0.96	0.20	60,60,60,60	0
56	MG	1a	3023	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3195	1/1	0.96	0.33	78,78,78,78	0
56	MG	2a	3052	1/1	0.96	0.09	95,95,95,95	0
56	MG	1A	3630	1/1	0.96	0.17	77,77,77,77	0
56	MG	2a	3181	1/1	0.96	0.17	90,90,90,90	0
56	MG	2A	3279	1/1	0.96	0.25	70,70,70,70	0
56	MG	1A	3297	1/1	0.96	0.13	77,77,77,77	0
56	MG	2A	3161	1/1	0.96	0.11	69,69,69,69	0
57	ZN	16	501	1/1	0.96	0.23	87,87,87,87	0
56	MG	1A	3298	1/1	0.96	0.42	83,83,83,83	0
56	MG	1A	3634	1/1	0.96	0.19	83,83,83,83	0
57	ZN	29	501	1/1	0.96	0.19	105,105,105,105	0
56	MG	2A	3275	1/1	0.97	0.34	81,81,81,81	0
56	MG	2a	3098	1/1	0.97	0.37	101,101,101,101	0
56	MG	2A	3276	1/1	0.97	0.12	82,82,82,82	0
56	MG	1A	3635	1/1	0.97	0.20	78,78,78,78	0
56	MG	1A	3271	1/1	0.97	0.17	49,49,49,49	0
56	MG	1A	3594	1/1	0.97	0.17	77,77,77,77	0
56	MG	2a	3103	1/1	0.97	0.27	73,73,73,73	0
56	MG	1a	3054	1/1	0.97	0.21	85,85,85,85	0
56	MG	1A	3483	1/1	0.97	0.07	77,77,77,77	0
56	MG	1A	3424	1/1	0.97	1.40	81,81,81,81	0
56	MG	1A	3401	1/1	0.97	0.27	90,90,90,90	0
56	MG	1A	3526	1/1	0.97	0.12	76,76,76,76	0
56	MG	1a	3231	1/1	0.97	0.16	82,82,82,82	0
56	MG	1A	3040	1/1	0.97	0.24	115,115,115,115	0
56	MG	2a	3022	1/1	0.97	0.15	83,83,83,83	0
56	MG	1A	3643	1/1	0.97	0.13	86,86,86,86	0
56	MG	1A	3311	1/1	0.97	0.34	61,61,61,61	0
56	MG	1A	3071	1/1	0.97	0.21	74,74,74,74	0
56	MG	2A	3291	1/1	0.97	0.10	87,87,87,87	0
56	MG	2A	3292	1/1	0.97	0.08	91,91,91,91	0
56	MG	1A	3490	1/1	0.97	0.19	79,79,79,79	0
56	MG	1A	3292	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3063	1/1	0.97	0.07	67,67,67,67	0
56	MG	2A	3065	1/1	0.97	0.36	88,88,88,88	0
56	MG	1A	3492	1/1	0.97	0.12	77,77,77,77	0
56	MG	1a	3119	1/1	0.97	0.58	88,88,88,88	0
56	MG	2A	3002	1/1	0.97	0.22	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3606	1/1	0.97	0.47	71,71,71,71	0
56	MG	1A	3043	1/1	0.97	0.13	74,74,74,74	0
56	MG	2A	3073	1/1	0.97	0.16	85,85,85,85	0
56	MG	1A	3061	1/1	0.97	0.21	77,77,77,77	0
56	MG	1A	3338	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3005	1/1	0.97	0.13	74,74,74,74	0
56	MG	2a	3041	1/1	0.97	0.20	69,69,69,69	0
56	MG	1A	3611	1/1	0.97	0.30	75,75,75,75	0
56	MG	1a	3183	1/1	0.97	0.34	78,78,78,78	0
56	MG	2a	3044	1/1	0.97	0.29	86,86,86,86	0
56	MG	1A	3296	1/1	0.97	0.12	76,76,76,76	0
56	MG	1A	3499	1/1	0.97	0.09	72,72,72,72	0
56	MG	1A	3463	1/1	0.97	0.29	75,75,75,75	0
56	MG	1A	3660	1/1	0.97	0.25	65,65,65,65	0
56	MG	1a	3131	1/1	0.97	0.25	107,107,107,107	0
56	MG	1A	3464	1/1	0.97	0.15	73,73,73,73	0
56	MG	2A	3232	1/1	0.97	0.24	53,53,53,53	0
56	MG	2A	3085	1/1	0.97	0.66	101,101,101,101	0
56	MG	1A	3155	1/1	0.97	0.15	65,65,65,65	0
56	MG	2A	3319	1/1	0.97	0.14	78,78,78,78	0
56	MG	1a	3029	1/1	0.97	0.12	64,64,64,64	0
56	MG	1a	3135	1/1	0.97	0.10	82,82,82,82	0
56	MG	1a	3194	1/1	0.97	0.22	102,102,102,102	0
56	MG	2a	3149	1/1	0.97	0.09	74,74,74,74	0
56	MG	2a	3150	1/1	0.97	0.21	87,87,87,87	0
56	MG	1A	3106	1/1	0.97	0.26	63,63,63,63	0
56	MG	2A	3239	1/1	0.97	0.08	77,77,77,77	0
56	MG	2A	3021	1/1	0.97	0.43	98,98,98,98	0
56	MG	2A	3241	1/1	0.97	0.12	89,89,89,89	0
56	MG	1A	3093	1/1	0.97	0.15	73,73,73,73	0
56	MG	2A	3093	1/1	0.97	0.16	71,71,71,71	0
56	MG	2A	3023	1/1	0.97	0.07	71,71,71,71	0
56	MG	1a	3138	1/1	0.97	0.20	91,91,91,91	0
56	MG	1A	3619	1/1	0.97	0.15	86,86,86,86	0
56	MG	1A	3212	1/1	0.97	0.21	54,54,54,54	0
56	MG	1A	3068	1/1	0.97	0.08	74,74,74,74	0
56	MG	1A	3510	1/1	0.97	0.17	64,64,64,64	0
56	MG	2A	3172	1/1	0.97	0.23	80,80,80,80	0
56	MG	1A	3146	1/1	0.97	0.17	62,62,62,62	0
56	MG	1a	3144	1/1	0.97	0.18	71,71,71,71	0
56	MG	2A	3175	1/1	0.97	0.16	65,65,65,65	0
56	MG	2A	3102	1/1	0.97	0.55	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3215	1/1	0.97	0.15	49,49,49,49	0
56	MG	2A	3179	1/1	0.97	0.14	74,74,74,74	0
56	MG	1a	3038	1/1	0.97	0.12	88,88,88,88	0
56	MG	1A	3084	1/1	0.97	0.28	71,71,71,71	0
56	MG	2A	3345	1/1	0.97	0.60	77,77,77,77	0
56	MG	1a	3148	1/1	0.97	0.21	112,112,112,112	0
56	MG	1A	3217	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3474	1/1	0.97	0.24	74,74,74,74	0
56	MG	1A	3628	1/1	0.97	0.16	56,56,56,56	0
56	MG	2A	3350	1/1	0.97	0.33	70,70,70,70	0
56	MG	1A	3475	1/1	0.97	0.30	88,88,88,88	0
56	MG	1A	3085	1/1	0.97	0.37	92,92,92,92	0
56	MG	1A	3307	1/1	0.97	0.28	60,60,60,60	0
56	MG	1A	3086	1/1	0.97	0.17	70,70,70,70	0
56	MG	1a	3156	1/1	0.97	0.19	73,73,73,73	0
56	MG	2A	3191	1/1	0.97	0.36	74,74,74,74	0
56	MG	1A	3680	1/1	0.97	0.19	85,85,85,85	0
57	ZN	1n	501	1/1	0.97	0.20	105,105,105,105	0
56	MG	1A	3448	1/1	0.97	0.15	78,78,78,78	0
56	MG	2A	3117	1/1	0.97	0.17	83,83,83,83	0
56	MG	1a	3002	1/1	0.97	0.12	83,83,83,83	0
57	ZN	2n	501	1/1	0.97	0.10	117,117,117,117	0
56	MG	1A	3604	1/1	0.98	0.14	67,67,67,67	0
56	MG	1A	3482	1/1	0.98	0.22	75,75,75,75	0
56	MG	2A	3064	1/1	0.98	0.34	82,82,82,82	0
56	MG	1a	3219	1/1	0.98	0.20	74,74,74,74	0
56	MG	1A	3632	1/1	0.98	0.16	63,63,63,63	0
56	MG	2A	3067	1/1	0.98	0.14	82,82,82,82	0
56	MG	1a	3221	1/1	0.98	0.20	79,79,79,79	0
56	MG	2A	3069	1/1	0.98	0.15	82,82,82,82	0
56	MG	1A	3069	1/1	0.98	0.90	67,67,67,67	0
56	MG	2a	3140	1/1	0.98	0.14	88,88,88,88	0
56	MG	2A	3163	1/1	0.98	0.22	79,79,79,79	0
56	MG	2A	3267	1/1	0.98	0.21	93,93,93,93	0
56	MG	1A	3507	1/1	0.98	0.25	92,92,92,92	0
56	MG	1a	3075	1/1	0.98	0.24	72,72,72,72	0
56	MG	1a	3076	1/1	0.98	0.21	58,58,58,58	0
56	MG	2A	3167	1/1	0.98	0.12	87,87,87,87	0
56	MG	1A	3532	1/1	0.98	0.09	88,88,88,88	0
56	MG	2A	3120	1/1	0.98	0.13	94,94,94,94	0
56	MG	2A	3030	1/1	0.98	0.11	81,81,81,81	0
56	MG	2A	3122	1/1	0.98	0.21	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3259	1/1	0.98	0.20	54,54,54,54	0
56	MG	1a	3188	1/1	0.98	0.12	81,81,81,81	0
56	MG	2A	3224	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3509	1/1	0.98	0.28	75,75,75,75	0
56	MG	1a	3080	1/1	0.98	0.17	88,88,88,88	0
56	MG	1a	3047	1/1	0.98	0.20	82,82,82,82	0
56	MG	1A	3667	1/1	0.98	0.45	68,68,68,68	0
56	MG	2A	3178	1/1	0.98	0.17	63,63,63,63	0
56	MG	2A	3339	1/1	0.98	0.14	92,92,92,92	0
56	MG	1A	3101	1/1	0.98	0.23	86,86,86,86	0
56	MG	2a	3045	1/1	0.98	0.08	102,102,102,102	0
56	MG	1A	3179	1/1	0.98	0.34	90,90,90,90	0
56	MG	1A	3262	1/1	0.98	0.22	64,64,64,64	0
56	MG	1A	3314	1/1	0.98	0.29	54,54,54,54	0
56	MG	2a	3165	1/1	0.98	0.08	116,116,116,116	0
56	MG	1a	3088	1/1	0.98	0.18	96,96,96,96	0
56	MG	1A	3451	1/1	0.98	0.11	85,85,85,85	0
56	MG	1A	3435	1/1	0.98	0.17	59,59,59,59	0
56	MG	1a	3200	1/1	0.98	0.17	83,83,83,83	0
56	MG	1A	3129	1/1	0.98	0.16	93,93,93,93	0
56	MG	1A	3517	1/1	0.98	0.20	77,77,77,77	0
56	MG	1A	3646	1/1	0.98	0.31	92,92,92,92	0
56	MG	1a	3129	1/1	0.98	0.11	88,88,88,88	0
56	MG	1A	3276	1/1	0.98	0.24	64,64,64,64	0
56	MG	1A	3345	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3456	1/1	0.98	0.25	96,96,96,96	0
56	MG	2A	3300	1/1	0.98	0.35	79,79,79,79	0
56	MG	1A	3072	1/1	0.98	0.47	67,67,67,67	0
56	MG	1A	3097	1/1	0.98	0.11	94,94,94,94	0
56	MG	1A	3477	1/1	0.98	0.15	56,56,56,56	0
56	MG	1A	3089	1/1	0.98	0.66	59,59,59,59	0
56	MG	2a	3065	1/1	0.98	0.17	83,83,83,83	0
56	MG	1A	3200	1/1	0.98	0.22	63,63,63,63	0
57	ZN	1Y	501	1/1	0.98	0.18	100,100,100,100	0
56	MG	2A	3306	1/1	0.98	0.19	74,74,74,74	0
56	MG	2a	3125	1/1	0.98	0.14	75,75,75,75	0
56	MG	1A	3655	1/1	0.98	0.35	67,67,67,67	0
56	MG	1A	3502	1/1	0.98	0.27	61,61,61,61	0
56	MG	2A	3059	1/1	0.98	0.12	93,93,93,93	0
56	MG	1A	3046	1/1	0.98	0.09	54,54,54,54	0
56	MG	1A	3247	1/1	0.98	0.10	55,55,55,55	0
56	MG	1a	3177	1/1	0.99	0.14	73,73,73,73	0

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

6.5 Other polymers (i)

There are no such residues in this entry.