wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 09:17 pm GMT

PDB ID	:	4WT1
Title	:	Complex of 70S ribosome with tRNA-Phe and mRNA with A-A mismatch in the second position in the A-site
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2014-10-29
Resolution	:	3.05 Å(reported)

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

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

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

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

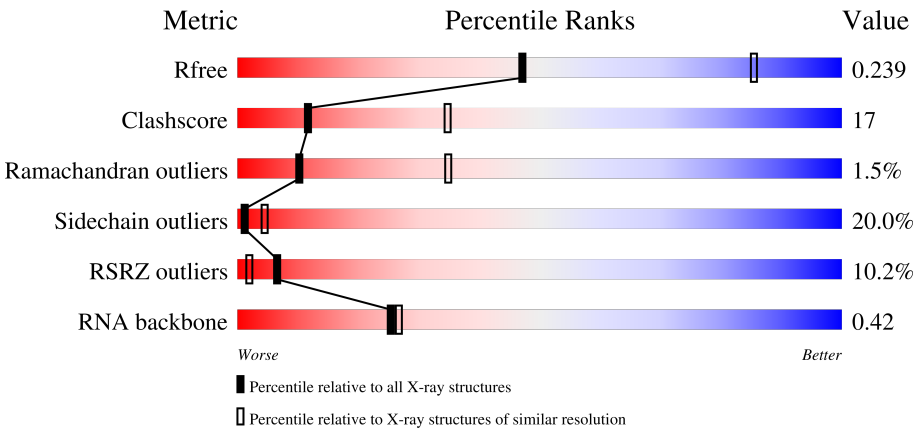
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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	13	1522	3% 33% 43% 19% • •
1	1G	1522	5% 33% 46% 17% • •
2	12	256	7% 45% 38% 10% 7%
2	1E	256	3% 41% 39% 12% 7%

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Mol	Chain	Length	Quality of chain
3	22	239	3% 47% 34% 5% 14%
3	2E	239	56% 24% 5% 14%
4	32	209	9% 51% 39% 10%
4	3E	209	14% 45% 46% 8%
5	42	162	11% 45% 41% 7% 7%
5	4E	162	12% 47% 37% 9% 7%
6	52	101	56% 38% 6%
6	5E	101	66% 28% 6%
7	62	156	17% 55% 38% 6%
7	6E	156	10% 52% 39% 8%
8	72	138	30% 54% 40% 6%
8	7E	138	19% 43% 48% 9%
9	82	128	59% 43% 51% 5%
9	8E	128	35% 43% 45% 12%
10	1A	105	37% 41% 49% 5% 6%
10	1I	105	30% 43% 45% 7% 6%
11	2A	129	9% 50% 36% 10%
11	2I	129	6% 43% 40% 6% 10%
12	3A	132	27% 43% 42% 10% 5%
12	3I	132	8% 57% 33% 5% 5%
13	4A	126	24% 45% 38% 10% 7%
13	4I	126	6% 48% 37% 8% 6%
14	5A	61	75% 41% 48% 7% 5%
14	5I	61	39% 48% 39% 11%
15	6A	89	13% 56% 36% 7%

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Mol	Chain	Length	Quality of chain
15	6I	89	24% 62% 31% 6%
16	7A	88	22% 48% 43% 5% 5%
16	7I	88	63% 25% 56% 15% 5%
17	8A	105	20% 64% 27% 5% 5%
17	8I	105	13% 42% 44% 10% 5%
18	9A	88	2% 33% 41% 8% 18%
18	9I	88	48% 26% 8% 18%
19	AA	93	27% 34% 40% 9% 16%
19	AI	93	5% 40% 35% 10% 13%
20	BA	106	41% 51% 34% 8% 7%
20	BI	106	32% 46% 39% 8% 7%
21	1B	27	85% 33% 56% 7%
21	1F	27	81% 52% 37% 7%
22	1K	76	5% 30% 42% 24%
23	2K	77	39% 35% 22%
23	2L	77	% 34% 42% 23%
24	1L	76	16% 45% 37% 17%
24	3K	76	3% 25% 34% 39%
24	3L	76	12% 28% 46% 25%
25	4K	27	19% 19% 11% 52%
25	4L	27	7% 15% 11% 67%
26	14	2917	2% 31% 43% 22%
26	1H	2917	26% 42% 26% 6%
27	16	122	38% 39% 18% 5%
27	1J	122	% 26% 47% 23%

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Mol	Chain	Length	Quality of chain
28	11	276	3% 48% 41% 9%
28	19	276	14% 59% 32% 7%
29	21	206	13% 44% 39% 16%
29	29	206	33% 38% 48% 12%
30	31	210	% 50% 37% 10%
30	39	210	7% 45% 42% 11%
31	41	182	5% 52% 38% 9%
31	49	182	23% 49% 43% 7%
32	51	180	3% 48% 37% 11%
32	59	180	34% 42% 42% 9% 6%
33	61	148	3% 34% 46% 17%
33	69	148	15% 50% 34% 13%
34	15	140	25% 54% 34% 11%
34	58	140	11% 51% 37% 9%
35	25	122	7% 51% 42% 7%
35	68	122	2% 58% 34% 8%
36	35	150	27% 46% 34% 15% 5%
36	78	150	7% 41% 40% 17%
37	45	141	55% 43% 42% 13%
37	88	141	4% 46% 41% 9%
38	55	118	17% 47% 40% 12%
38	98	118	11% 42% 47% 12%
39	65	112	32% 32% 50% 14%
39	A8	112	4% 36% 46% 14%
40	75	146	7% 39% 41% 14% 6%

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Mol	Chain	Length	Quality of chain
40	B8	146	8% 45% 36% 12% 6%
41	85	118	14% 55% 40%
41	C8	118	16% 46% 45% 8%
42	95	101	14% 44% 42% 14%
42	D8	101	10% 47% 39% 15%
43	A5	113	6% 65% 28% 7%
43	E8	113	3% 52% 36% 12%
44	B5	96	8% 51% 36% 8%
44	F8	96	% 46% 39% 11%
45	C5	110	23% 32% 42% 19% 5%
45	G8	110	40% 41% 13% 5%
46	D5	206	17% 38% 39% 9% 13%
46	H8	206	41% 36% 7% 15%
47	E5	85	41% 46% 35% 8% 11%
47	I8	85	24% 49% 35% 8% 6%
48	F5	98	33% 58% 29% 11%
48	J8	98	14% 63% 28% 7%
49	G5	72	3% 51% 32% 6% 8%
49	K8	72	3% 26% 42% 19% 6% 7%
50	H5	60	22% 52% 40% 7%
50	L8	60	37% 43% 13% 5%
51	I5	71	31% 30% 49% 10% 11%
51	M8	71	8% 32% 46% 13% 7%
52	J5	60	7% 53% 30% 8% 7%
52	N8	60	10% 53% 33% 10%

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Mol	Chain	Length	Quality of chain
53	K5	54	70% 35% 31% 15% • 17%
53	O8	54	59% 22% 39% 22% 17%
54	L5	49	6% 43% 47% • 6%
54	P8	49	45% 43% • 8%
55	M5	65	55% 38% 37% 17% 8%
55	Q8	65	35% 20% 34% 35% 5% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1629	-	-	-	X
56	MG	13	1631	-	-	-	X
56	MG	13	1656	-	-	-	X
56	MG	13	1658	-	-	-	X
56	MG	13	1718	-	-	-	X
56	MG	13	1721	-	-	-	X
56	MG	13	1744	-	-	-	X
56	MG	14	3020	-	-	-	X
56	MG	14	3080	-	-	-	X
56	MG	14	3117	-	-	-	X
56	MG	14	3143	-	-	-	X
56	MG	14	3170	-	-	-	X
56	MG	14	3178	-	-	-	X
56	MG	14	3255	-	-	-	X
56	MG	14	3276	-	-	-	X
56	MG	14	3281	-	-	-	X
56	MG	14	3288	-	-	-	X
56	MG	14	3295	-	-	-	X
56	MG	14	3416	-	-	-	X
56	MG	1G	1632	-	-	-	X
56	MG	1G	1640	-	-	-	X
56	MG	1G	1670	-	-	-	X
56	MG	1H	3013	-	-	-	X
56	MG	1H	3028	-	-	-	X
56	MG	1H	3074	-	-	-	X
56	MG	1H	3119	-	-	-	X
56	MG	1H	3129	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3137	-	-	-	X
56	MG	1H	3142	-	-	-	X
56	MG	1H	3143	-	-	-	X
56	MG	1H	3157	-	-	-	X
56	MG	1H	3158	-	-	-	X
56	MG	1H	3249	-	-	-	X
56	MG	1H	3255	-	-	-	X
56	MG	1H	3266	-	-	-	X
56	MG	1H	3270	-	-	-	X
56	MG	1H	3276	-	-	-	X
56	MG	1H	3280	-	-	-	X
56	MG	1H	3305	-	-	-	X
56	MG	1H	3306	-	-	-	X
56	MG	1H	3309	-	-	-	X
56	MG	1H	3311	-	-	-	X
56	MG	1H	3326	-	-	-	X
56	MG	1H	3328	-	-	-	X
56	MG	1H	3330	-	-	-	X
56	MG	1H	3331	-	-	-	X
56	MG	1H	3332	-	-	-	X
56	MG	1H	3337	-	-	-	X
56	MG	1H	3346	-	-	-	X
56	MG	29	301	-	-	-	X
56	MG	32	301	-	-	-	X
56	MG	39	303	-	-	-	X
56	MG	L8	101	-	-	-	X

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 299951 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	13	1498	32207	14334	5973	10402	1498	0	0	0
1	1G	1497	32182	14324	5968	10394	1496	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	237	1924	1228	344	347	5	0	0	0
2	12	237	1924	1228	344	347	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	1605	1011	313	280	1	0	0	0
3	22	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3E	208	1702	1066	339	290	7	0	0	0
4	32	208	1702	1066	339	290	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	4E	151	1155	729	218	204	4	0	0	0
5	42	151	1155	729	218	204	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	5E	101	842	531	155	153	3	0	0	0
6	52	101	842	531	155	153	3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	6E	155	1256	781	252	217	6	0	0	0
7	62	155	1256	781	252	217	6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	7E	138	1115	705	215	192	3	0	0	0
8	72	138	1115	705	215	192	3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	8E	127	1009	639	197	173	0	0	0
9	82	127	1009	639	197	173	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1I	99	801	504	157	139	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1A	99	801	504	157	139	1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	2I	116	864	537	164	160	3	0	0	0
11	2A	116	864	537	164	160	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	3I	125	975	614	196	164	1	0	0	0
12	3A	125	975	614	196	164	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	118	938	580	193	163	2	0	0	0
13	4A	117	933	577	192	162	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377
4A	119	ALA	GLY	conflict	UNP P80377

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	5I	60	491	312	104	71	4	0	0	0
14	5A	58	475	303	99	69	4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	6I	88	733	459	147	125	2	0	0	0
15	6A	88	733	459	147	125	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	7I	84	705	446	140	118	1	0	0	0
16	7A	84	705	446	140	118	1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	8I	100	834	534	155	143	2	0	0	0
17	8A	100	834	534	155	143	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	9I	72	590	376	117	97	0	0	0
18	9A	72	590	376	117	97	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AI	81	647	413	119	113	2	0	0	0
19	AA	78	624	398	115	109	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	BI	99	762	470	162	128	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	BA	99	762	470	162	128	2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	1F	25	217	134	52	31	0	0	0
21	1B	25	217	134	52	31	0	0	0

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
22	1K	76	1628	731	290	530	75	2	0	0	0

- Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
23	2K	77	1646	735	298	535	77	1	0	0	0
23	2L	77	1646	735	298	535	77	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675818144
2L	18	C	U	conflict	GB 675818144

- Molecule 24 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	3K	76	1619	723	290	531	75	0	0	0
24	1L	76	1619	723	290	531	75	0	0	0
24	3L	76	1619	723	290	531	75	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	4K	13	281	127	57	84	13	0	0	0
25	4L	9	193	87	37	60	9	0	0	0

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	1H	2912	62707	27911	11722	20163	2911	0	0	0
26	14	2909	62647	27884	11716	20139	2908	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	16	122	2617	1166	486	844	121	0	0	0
27	1J	122	2617	1166	486	844	121	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	11	272	2115	1335	420	357	3	0	0	0
28	19	273	2120	1338	421	358	3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	21	205	1568	991	300	271	6	0	0	0
29	29	205	1568	991	300	271	6	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	31	202	1585	1011	297	275	2	0	0	0
30	39	208	1627	1037	304	283	3	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	41	181	1473	942	268	259	4	0	0	0
31	49	181	1473	942	268	259	4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	51	174	1336	848	251	236	1	0	0	0
32	59	169	1299	823	244	231	1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	61	146	1136	726	201	208	1	0	0	0
33	69	146	1136	726	201	208	1	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	58	138	1104	712	206	182	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	15	138	1104	712	206	182	4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	68	122	932	588	171	169	4	0	0	0
			Total	C	N	O	S			
35	25	122	932	588	171	169	4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	78	150	1144	712	232	197	3	0	0	0
			Total	C	N	O	S			
36	35	150	1144	712	232	197	3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	88	138	1086	693	208	179	6	0	0	0
			Total	C	N	O	S			
37	45	141	1121	715	212	187	7	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	98	118	967	604	203	159	1	0	0	0
			Total	C	N	O				
38	55	117	959	599	202	158		0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	A8	111	881	556	176	149	0	0	0
			Total	C	N	O			
39	65	111	881	556	176	149	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	B8	137	1141	710	234	196	1	0	0	0
40	75	137	1141	710	234	196	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	C8	117	963	610	202	150	1	0	0	0
41	85	117	963	610	202	150	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	D8	101	778	501	142	134	1	0	0	0
42	95	101	778	501	142	134	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	E8	113	899	566	177	154	2	0	0	0
43	A5	113	899	566	177	154	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	F8	94	742	482	134	125	1	0	0	0
44	B5	92	725	471	131	123		0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	G8	104	791	510	149	127	5	0	0	0
45	C5	104	794	510	152	127	5	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	H8	175	1397	892	251	251	3	0	0	0
46	D5	179	1428	911	255	259	3	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	I8	80	626	388	132	105	1	0	0	0
47	E5	76	606	376	128	101	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	J8	97	762	481	150	130	1	0	0	0
48	F5	97	762	481	150	130	1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	K8	67	563	349	114	99	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	G5	66	558	346	113	98	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	L8	57	452	288	88	76	0	0	0
50	H5	59	468	298	90	80	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M8	66	533	335	96	97	5	0	0	0
51	I5	63	515	326	93	91	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	N8	58	453	285	89	74	5	0	0	0
52	J5	56	434	272	87	70	5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	O8	45	389	241	79	65	4	0	0	0
53	K5	45	389	241	79	65	4	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	P8	45	391	240	97	52	2	0	0	0
54	L5	46	398	245	98	53	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	Q8	61	485	309	99	75	2	0	0	0
			Total	C	N	O	S			
55	M5	60	477	303	98	74	2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	13	152	152	152	0	0
			Total	Mg		
56	5E	1	1	1	0	0
			Total	Mg		
56	3I	2	2	2	0	0
			Total	Mg		
56	2K	7	7	7	0	0
			Total	Mg		
56	4K	1	1	1	0	0
			Total	Mg		
56	1H	506	506	506	0	0
			Total	Mg		
56	16	15	15	15	0	0
			Total	Mg		
56	11	2	2	2	0	0
			Total	Mg		
56	21	2	2	2	0	0
			Total	Mg		
56	31	1	1	1	0	0
			Total	Mg		
56	41	2	2	2	0	0
			Total	Mg		
56	78	2	2	2	0	0
			Total	Mg		
56	88	2	2	2	0	0
			Total	Mg		
56	G8	1	1	1	0	0
			Total	Mg		
56	I8	2	2	2	0	0
			Total	Mg		
56	J8	1	1	1	0	0
			Total	Mg		
56	L8	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	P8	1	1	1	0	0
56	1G	88	88	88	0	0
56	32	1	1	1	0	0
56	52	1	1	1	0	0
56	6A	1	1	1	0	0
56	2L	3	3	3	0	0
56	14	426	426	426	0	0
56	1J	10	10	10	0	0
56	29	2	2	2	0	0
56	39	3	3	3	0	0
56	49	1	1	1	0	0
56	15	1	1	1	0	0
56	25	2	2	2	0	0
56	35	1	1	1	0	0
56	45	2	2	2	0	0
56	85	1	1	1	0	0
56	C5	1	1	1	0	0
56	E5	1	1	1	0	0
56	M5	1	1	1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	3E	1	Total Zn 1 1	0	0
57	5I	1	Total Zn 1 1	0	0
57	G8	1	Total Zn 1 1	0	0
57	32	1	Total Zn 1 1	0	0
57	5A	1	Total Zn 1 1	0	0
57	C5	1	Total Zn 1 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	164	Total O 164 164	0	0
58	3E	1	Total O 1 1	0	0
58	4E	1	Total O 1 1	0	0
58	1I	1	Total O 1 1	0	0
58	3I	1	Total O 1 1	0	0
58	5I	1	Total O 1 1	0	0
58	6I	1	Total O 1 1	0	0
58	7I	1	Total O 1 1	0	0
58	4K	1	Total O 1 1	0	0
58	1H	920	Total O 920 920	0	0
58	16	6	Total O 6 6	0	0
58	11	9	Total O 9 9	0	0
58	21	5	Total O 5 5	0	0
58	31	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	78	6	Total O 6 6	0	0
58	B8	1	Total O 1 1	0	0
58	C8	2	Total O 2 2	0	0
58	E8	1	Total O 1 1	0	0
58	F8	1	Total O 1 1	0	0
58	G8	3	Total O 3 3	0	0
58	J8	1	Total O 1 1	0	0
58	L8	3	Total O 3 3	0	0
58	P8	1	Total O 1 1	0	0
58	Q8	2	Total O 2 2	0	0
58	1G	64	Total O 64 64	0	0
58	32	1	Total O 1 1	0	0
58	7A	1	Total O 1 1	0	0
58	14	543	Total O 543 543	0	0
58	1J	18	Total O 18 18	0	0
58	19	3	Total O 3 3	0	0
58	29	3	Total O 3 3	0	0
58	39	8	Total O 8 8	0	0
58	15	1	Total O 1 1	0	0
58	35	1	Total O 1 1	0	0
58	85	1	Total O 1 1	0	0

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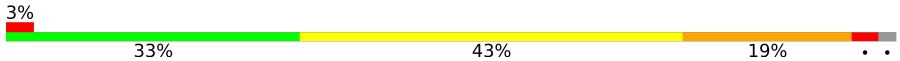
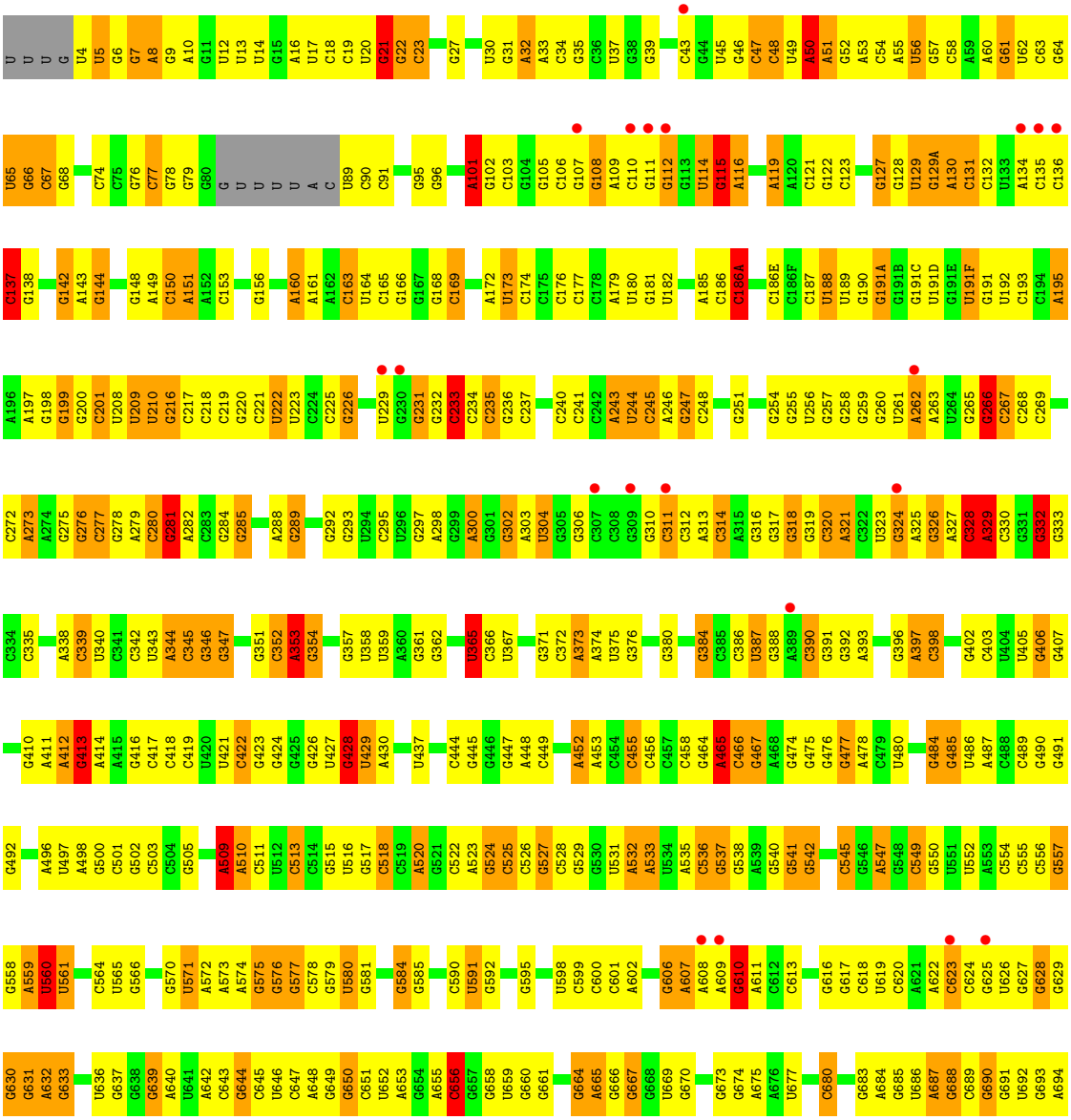
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
58	L5	2	2	2	0	0

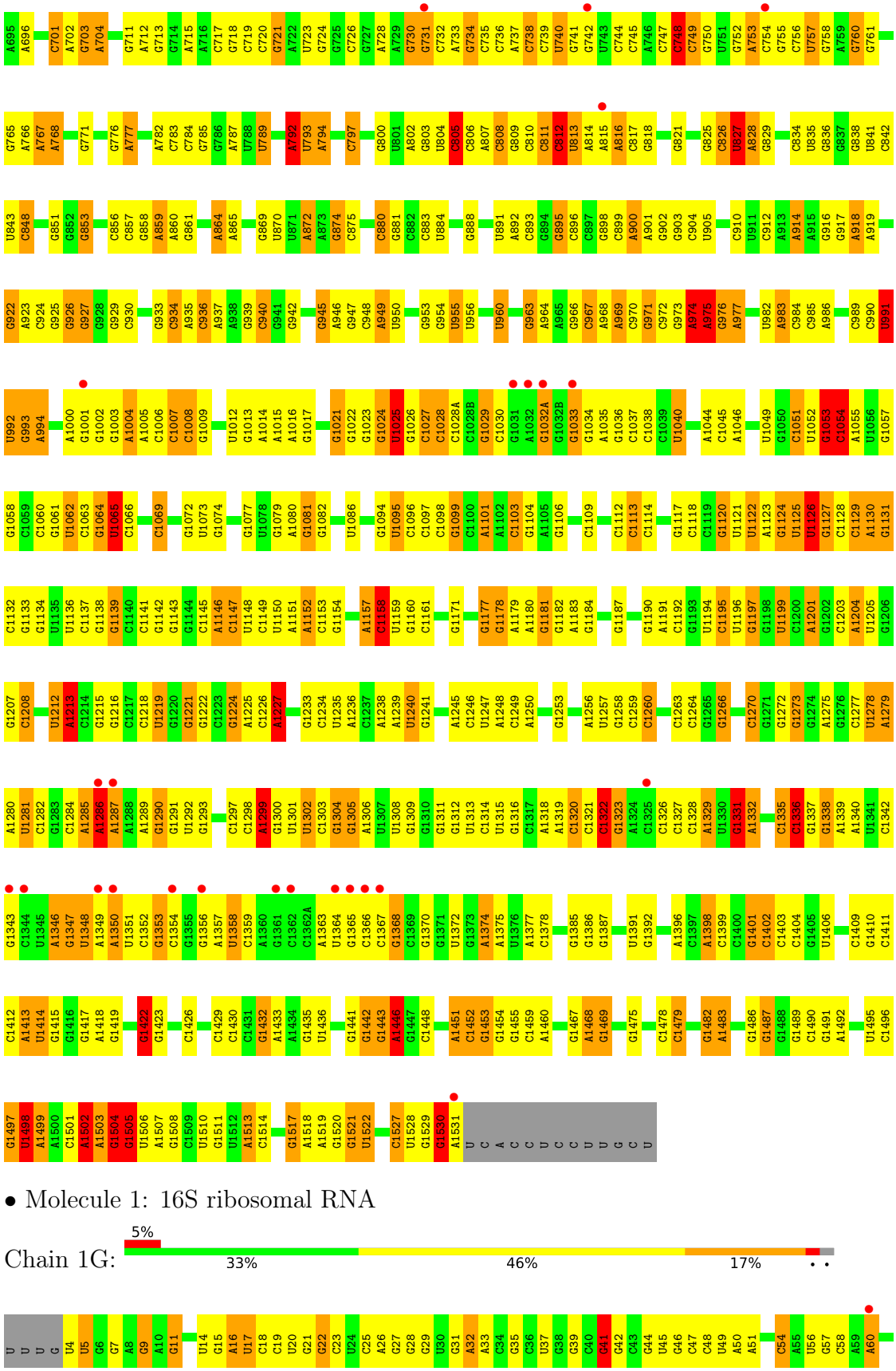
3 Residue-property plots (i)

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: 16S ribosomal RNA

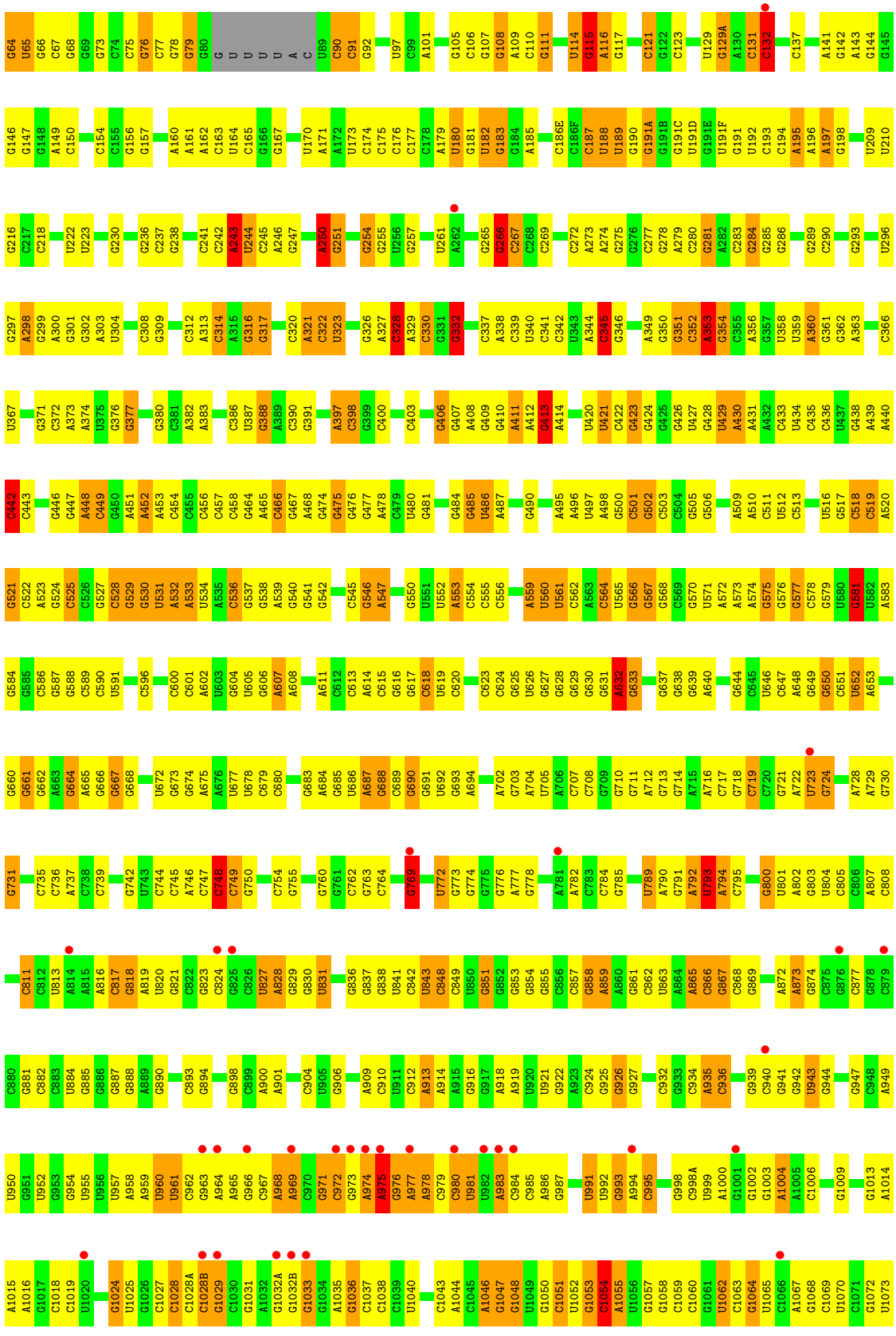
Chain 13: 

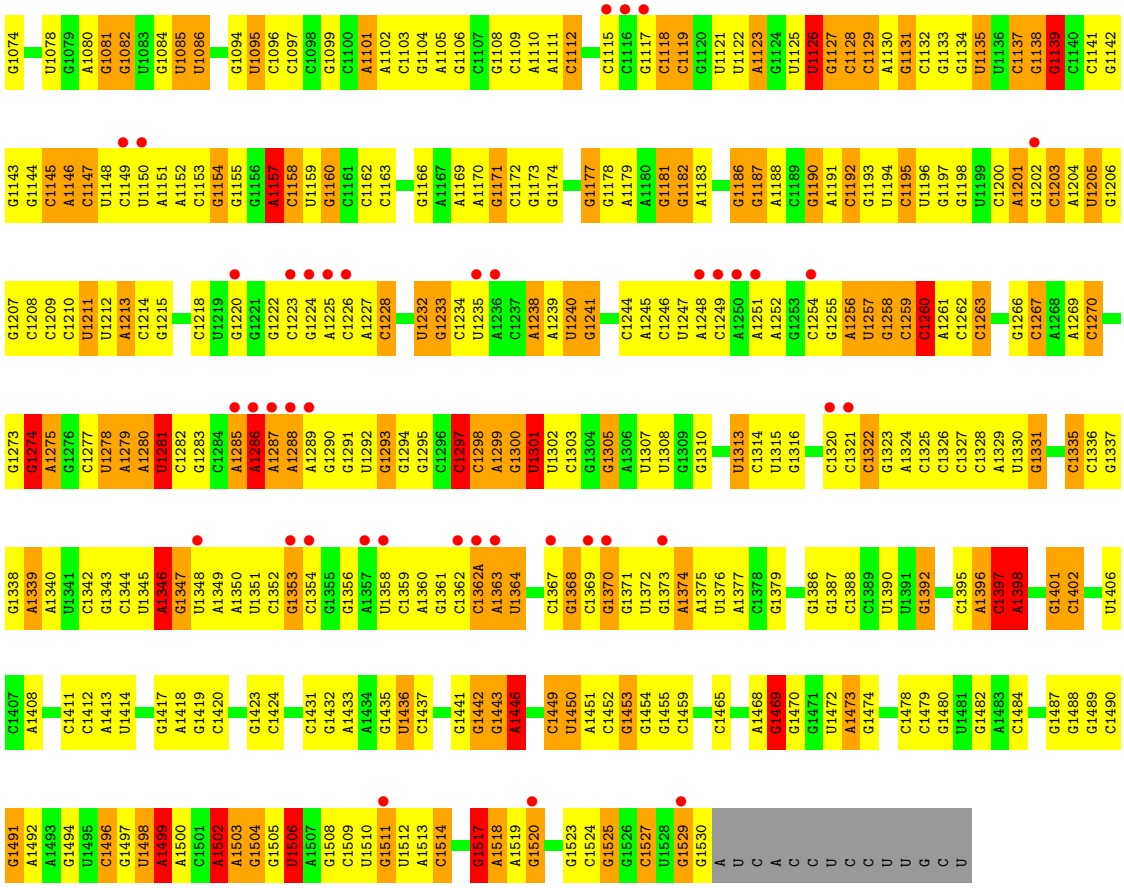




• Molecule 1: 16S ribosomal RNA

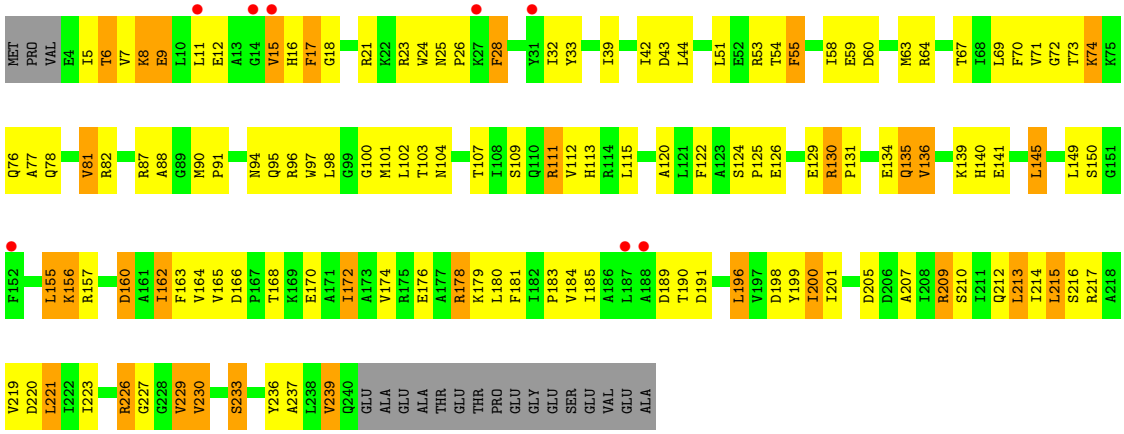
Chain 1G:





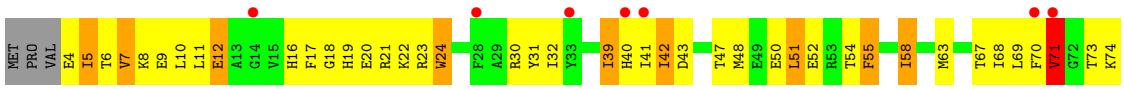
- Molecule 2: 30S ribosomal protein S2

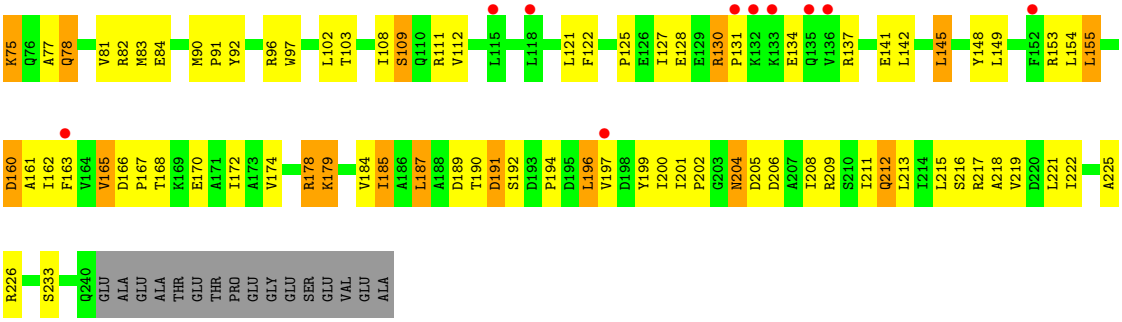
Chain 1E:



- Molecule 2: 30S ribosomal protein S2

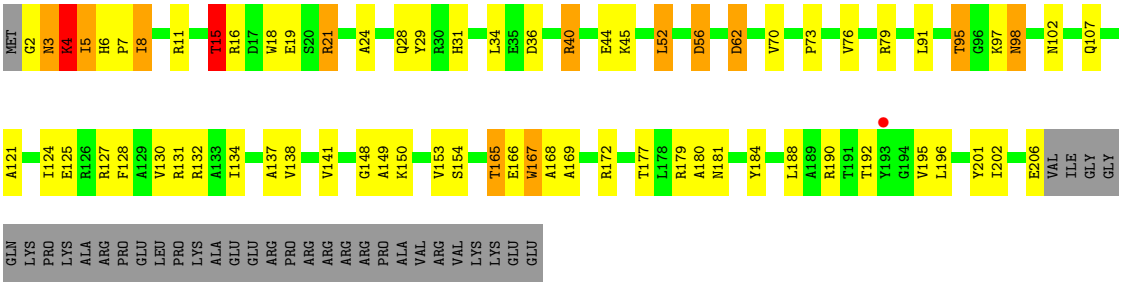
Chain 12:





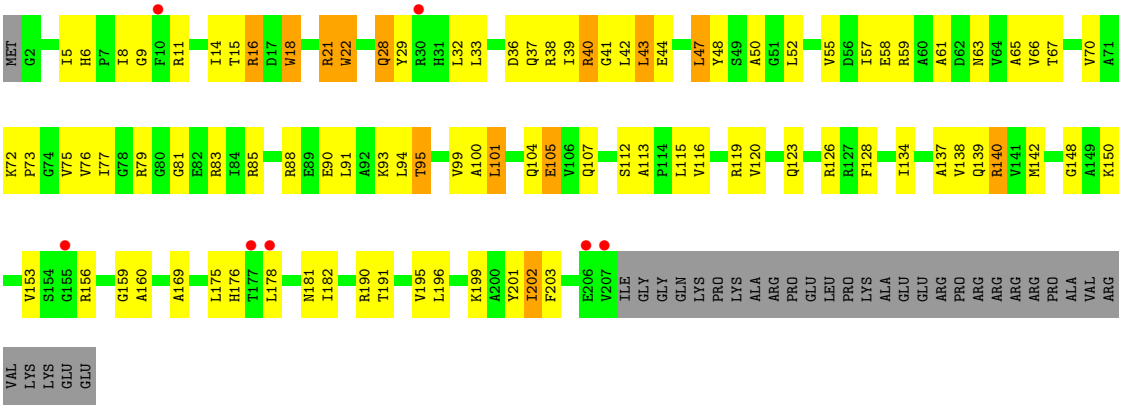
- Molecule 3: 30S ribosomal protein S3

Chain 2E:



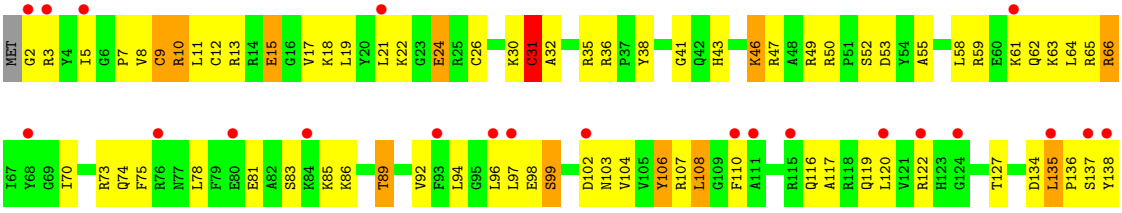
- Molecule 3: 30S ribosomal protein S3

Chain 22:



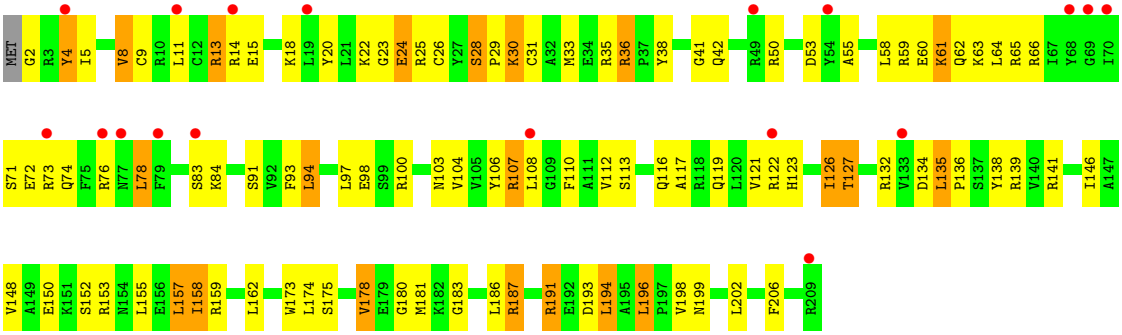
- Molecule 4: 30S ribosomal protein S4

Chain 3E:



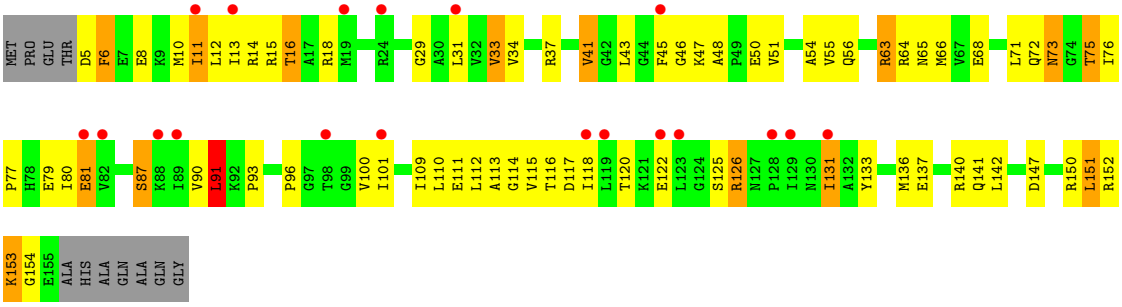
• Molecule 4: 30S ribosomal protein S4

Chain 32:



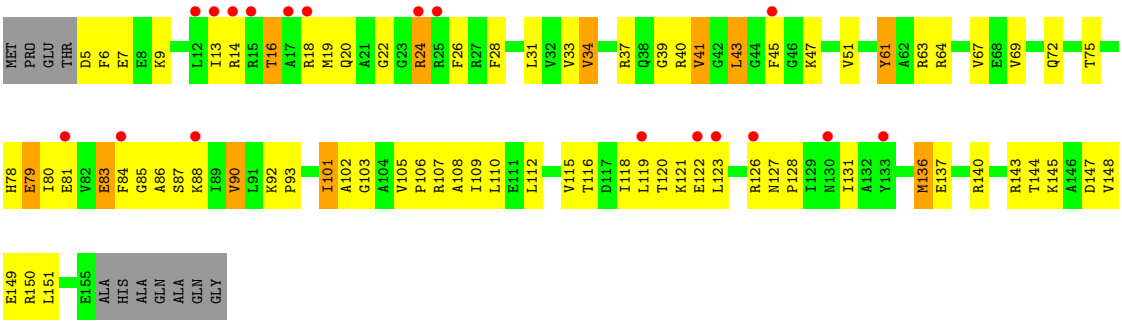
• Molecule 5: 30S ribosomal protein S5

Chain 4E:



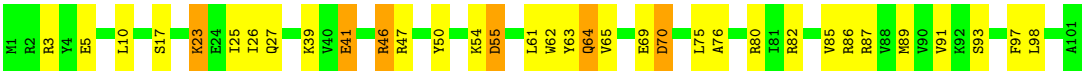
• Molecule 5: 30S ribosomal protein S5

Chain 42:



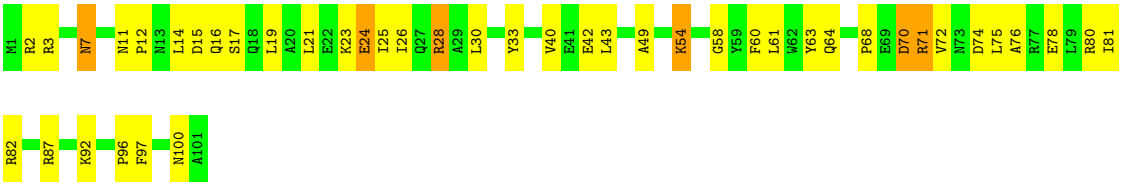
• Molecule 6: 30S ribosomal protein S6

Chain 5E:



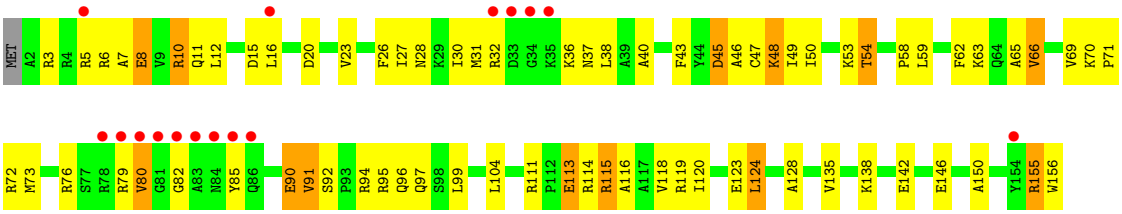
- Molecule 6: 30S ribosomal protein S6

Chain 52:



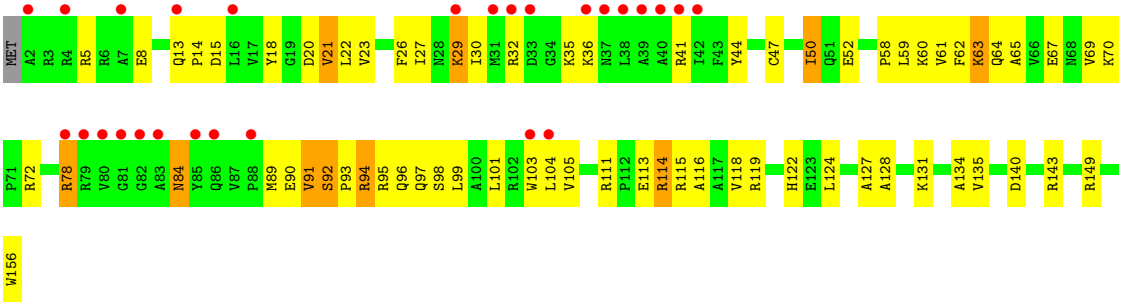
- Molecule 7: 30S ribosomal protein S7

Chain 6E:



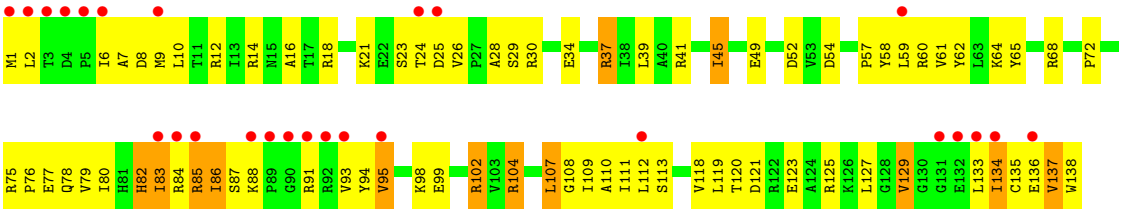
- Molecule 7: 30S ribosomal protein S7

Chain 62:



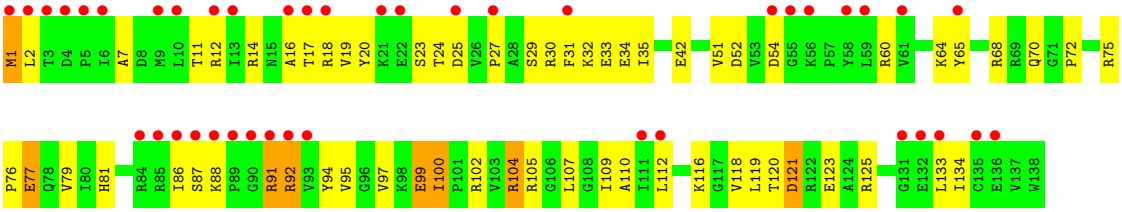
- Molecule 8: 30S ribosomal protein S8

Chain 7E:



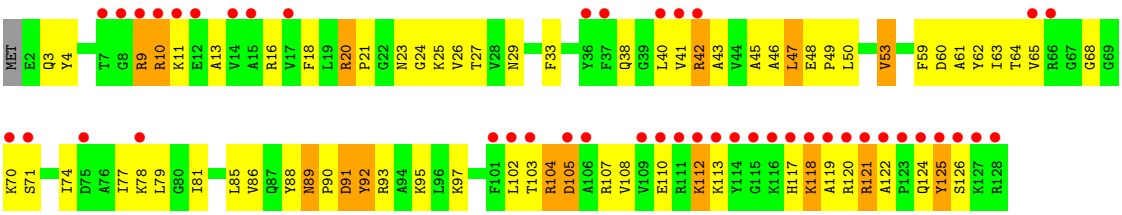
- Molecule 8: 30S ribosomal protein S8

Chain 72:



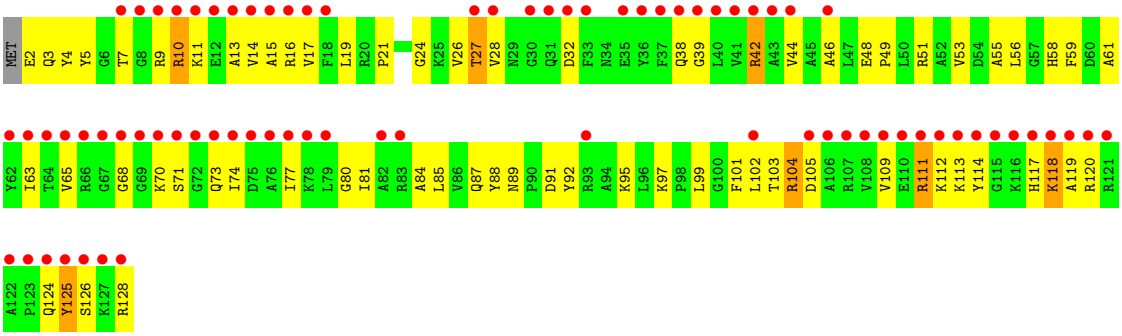
- Molecule 9: 30S ribosomal protein S9

Chain 8E:



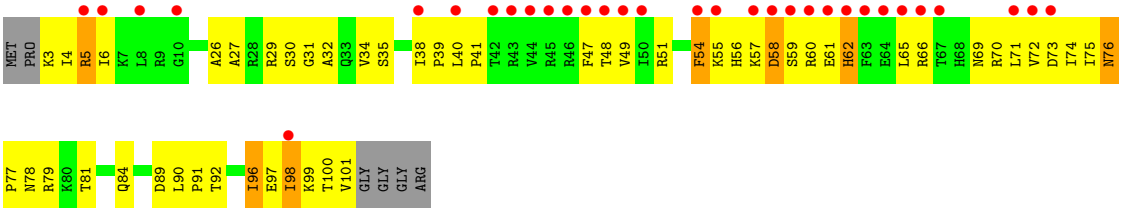
- Molecule 9: 30S ribosomal protein S9

Chain 82:



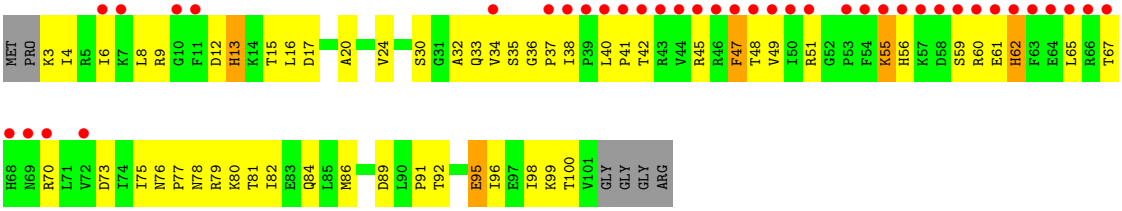
- Molecule 10: 30S ribosomal protein S10

Chain 1I:



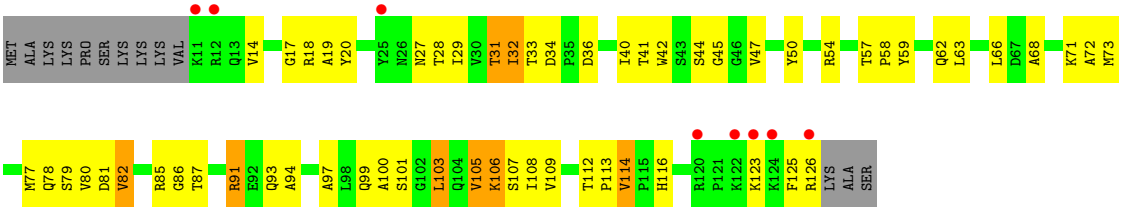
- Molecule 10: 30S ribosomal protein S10

Chain 1A:



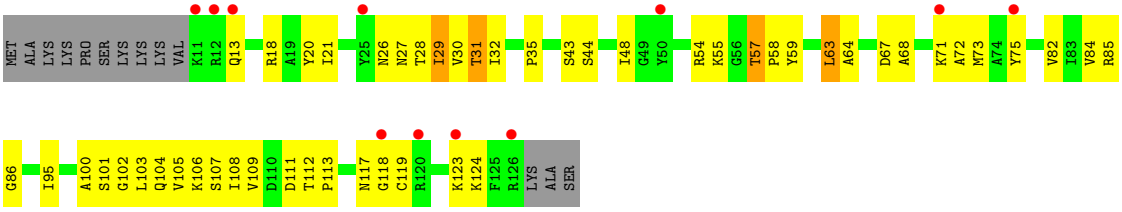
- Molecule 11: 30S ribosomal protein S11

Chain 2I:



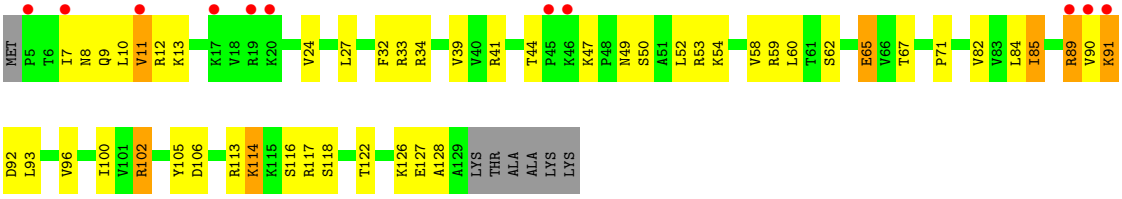
- Molecule 11: 30S ribosomal protein S11

Chain 2A:



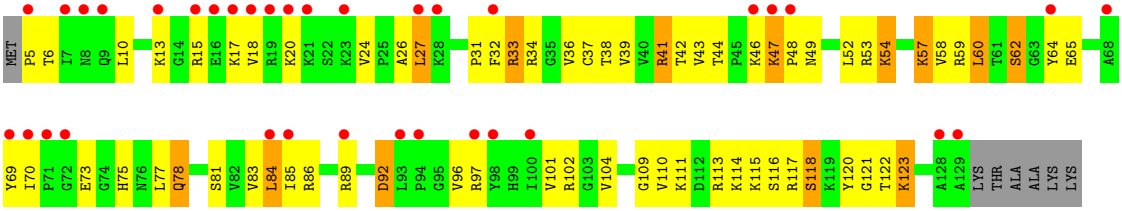
- Molecule 12: 30S ribosomal protein S12

Chain 3I:



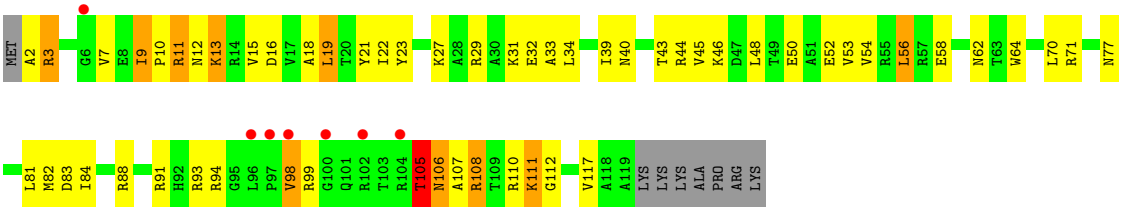
- Molecule 12: 30S ribosomal protein S12

Chain 3A:



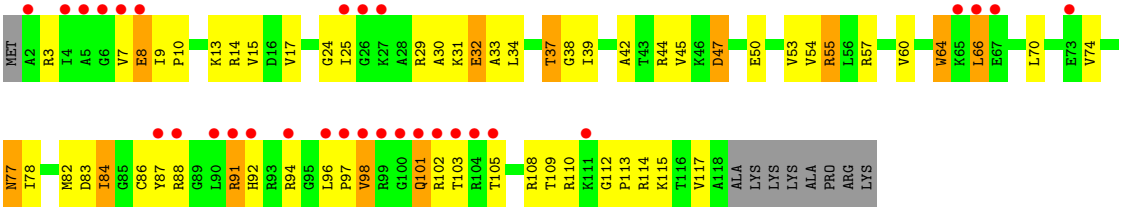
• Molecule 13: 30S ribosomal protein S13

Chain 4I:



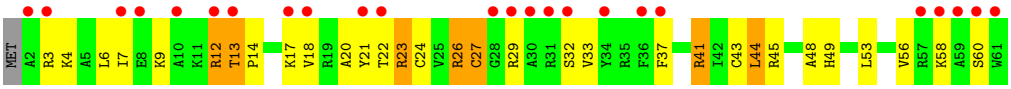
• Molecule 13: 30S ribosomal protein S13

Chain 4A:



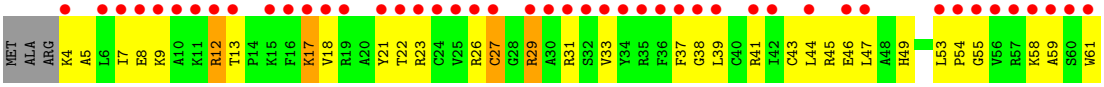
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



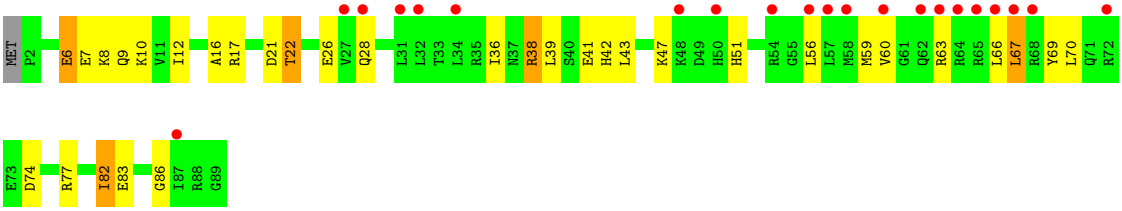
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



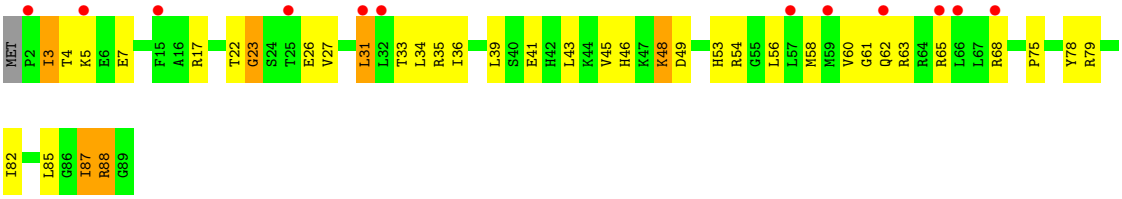
• Molecule 15: 30S ribosomal protein S15

Chain 6I:



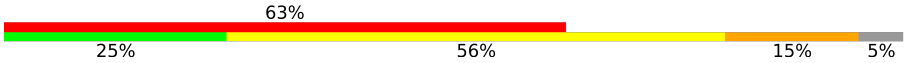
• Molecule 15: 30S ribosomal protein S15

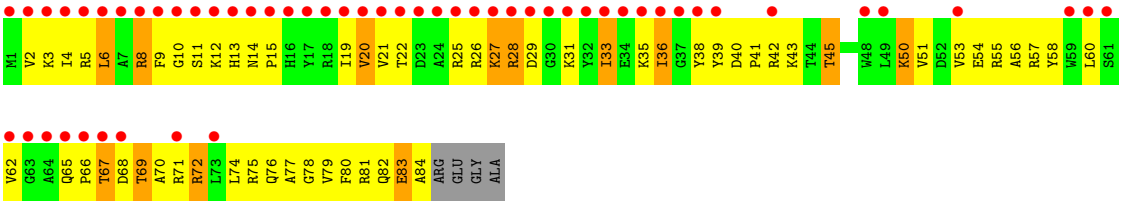
Chain 6A:



- Molecule 16: 30S ribosomal protein S16

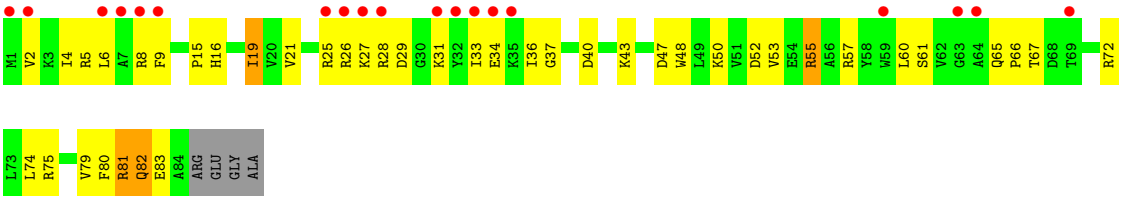
Chain 7I:





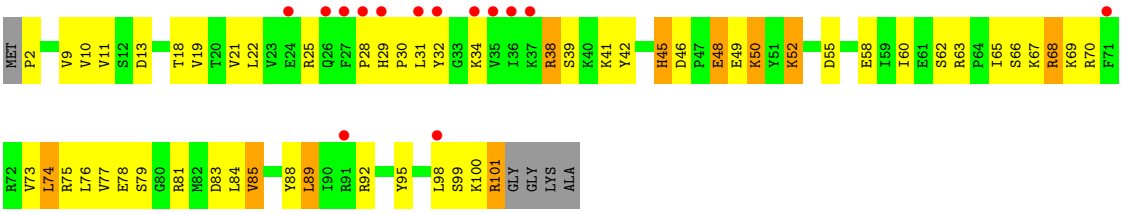
- Molecule 16: 30S ribosomal protein S16

Chain 7A:



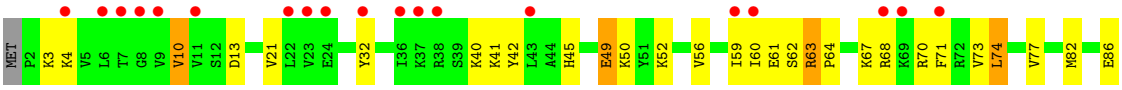
- Molecule 17: 30S ribosomal protein S17

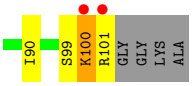
Chain 8I:



- Molecule 17: 30S ribosomal protein S17

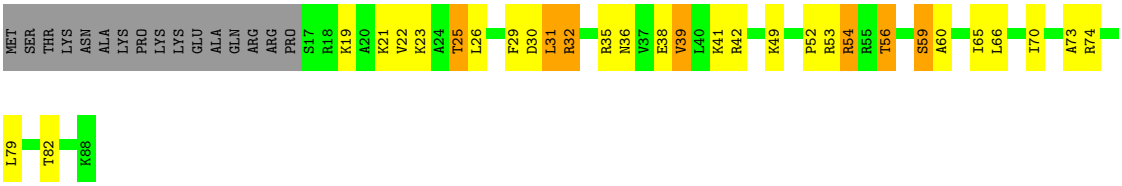
Chain 8A:





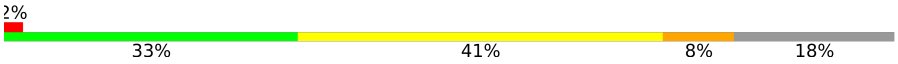
• Molecule 18: 30S ribosomal protein S18

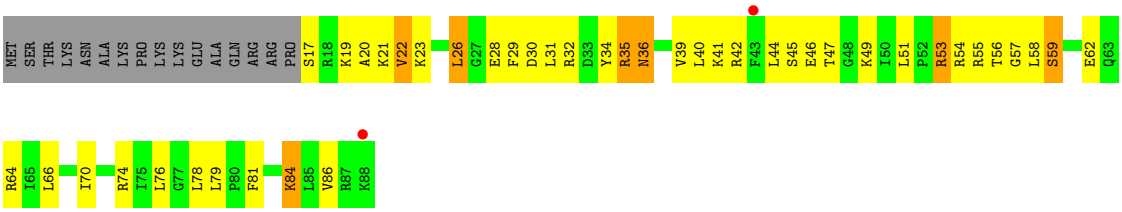
Chain 9I:



• Molecule 18: 30S ribosomal protein S18

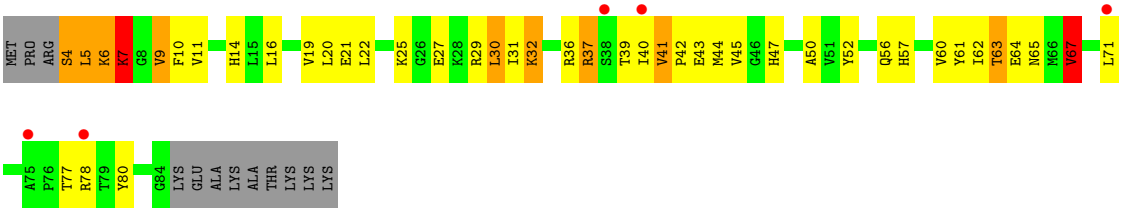
Chain 9A:





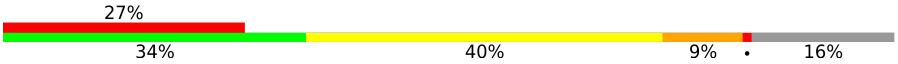
• Molecule 19: 30S ribosomal protein S19

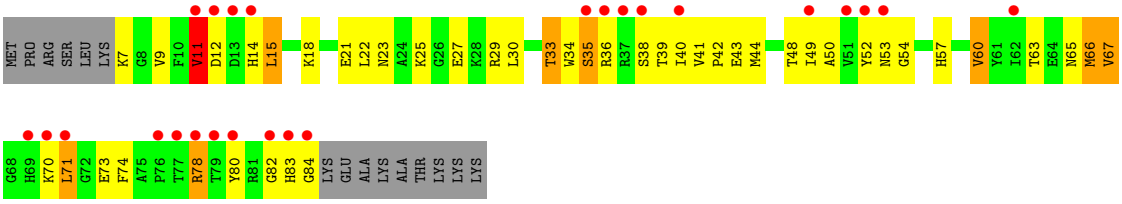
Chain AI:



• Molecule 19: 30S ribosomal protein S19

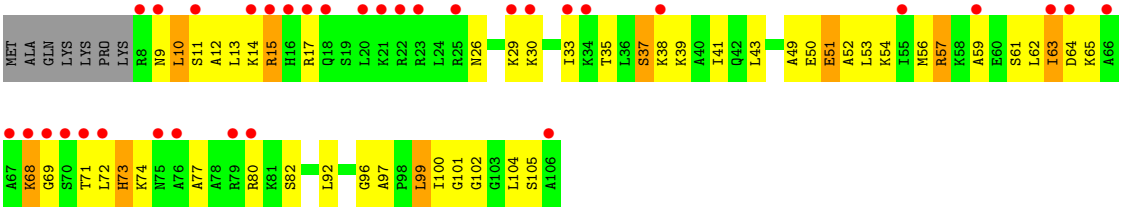
Chain AA:





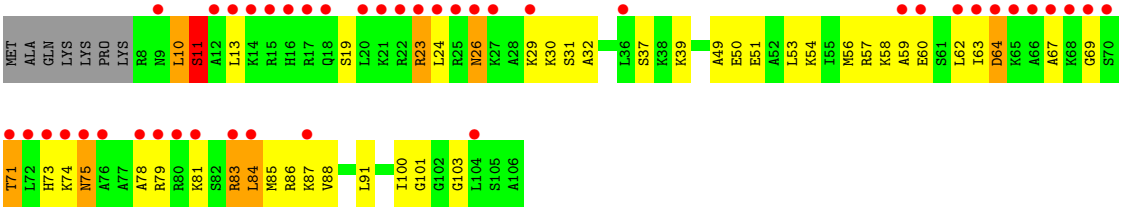
• Molecule 20: 30S ribosomal protein S20

Chain BI:



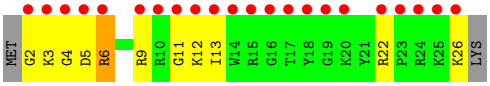
- Molecule 20: 30S ribosomal protein S20

Chain BA:



- Molecule 21: 30S ribosomal protein Thx

Chain 1F:

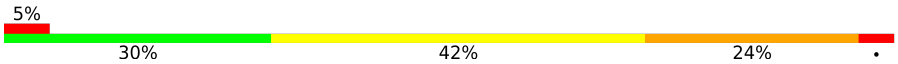


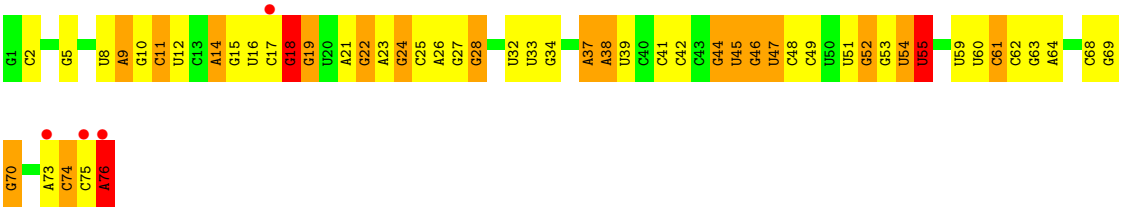
- Molecule 21: 30S ribosomal protein Thx

Chain 1B:

- Molecule 22: tRNA-Phe

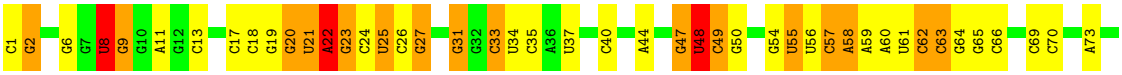
Chain 1K:





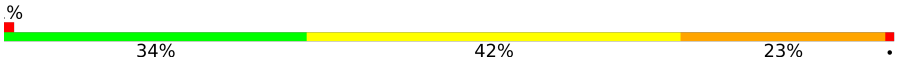
- Molecule 23: tRNA-fMet

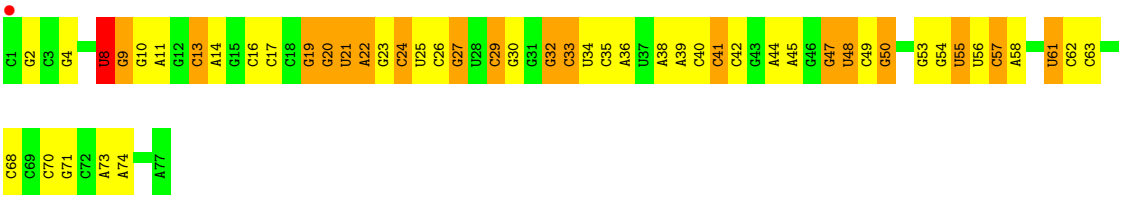
Chain 2K:



• Molecule 23: tRNA-fMet

Chain 2L:



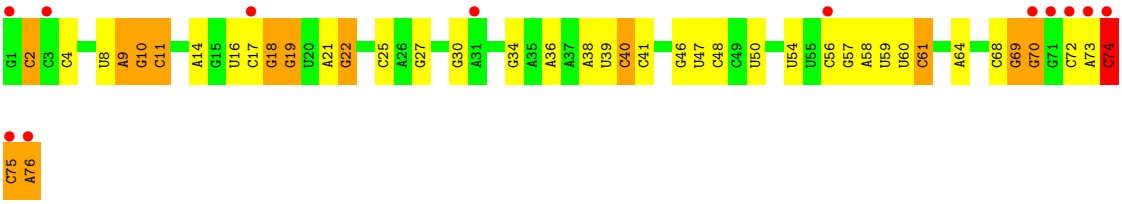


• Molecule 24: tRNA-Phe

Chain 3K:

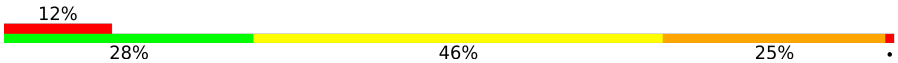
• Molecule 24: tRNA-Phe

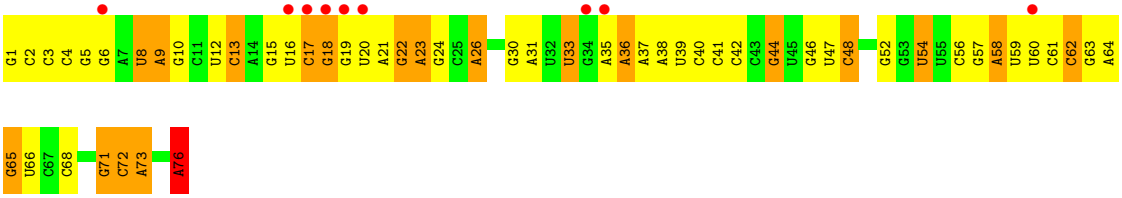
Chain 1L:



• Molecule 24: tRNA-Phe

Chain 3L:





• Molecule 25: mRNA

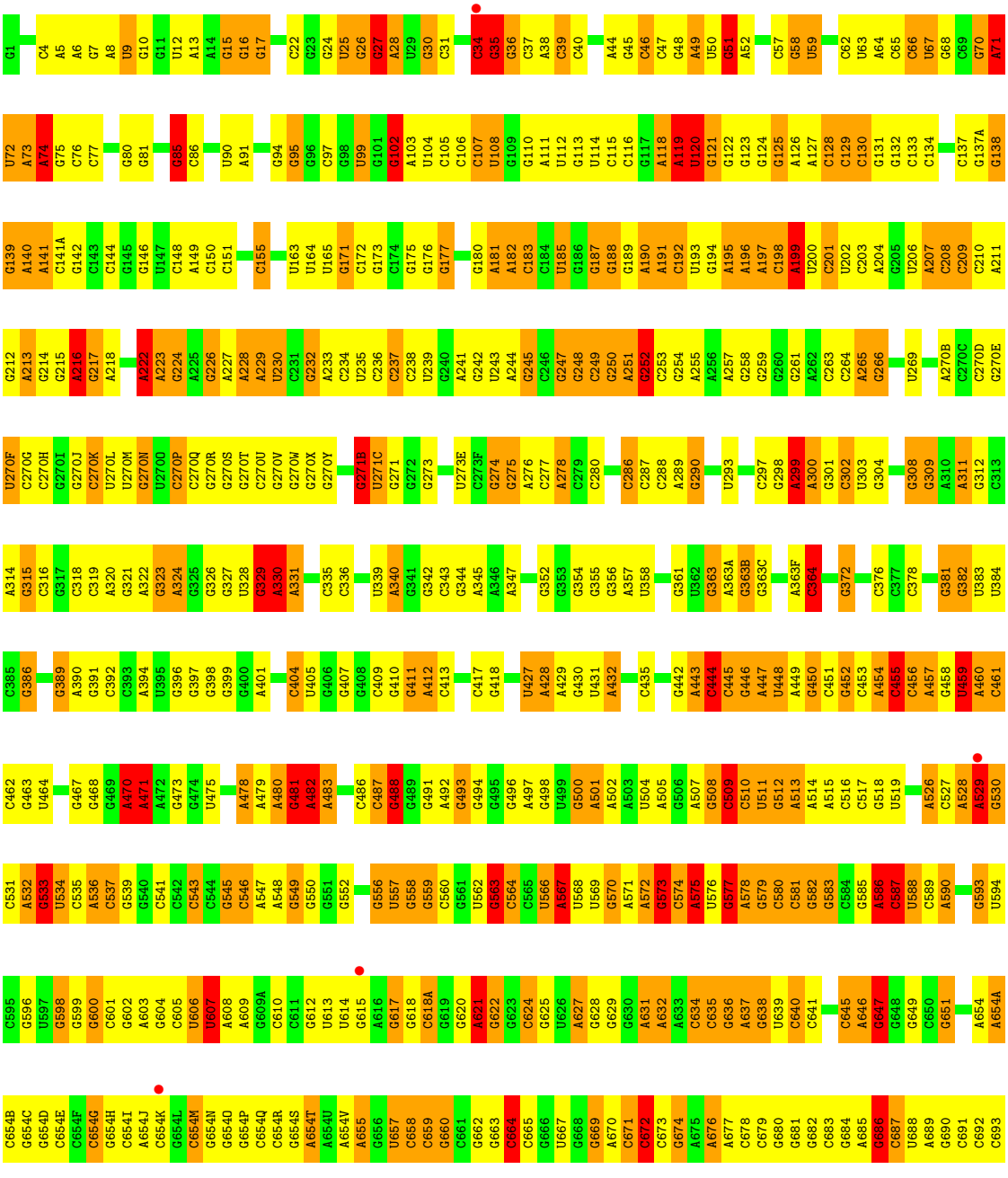
Chain 4K:

- Molecule 25: mRNA

Chain 4L: 7% 15% 11% 67%

- Molecule 26: 23S ribosomal RNA

Chain 1H: 26% 42% 26% 6%



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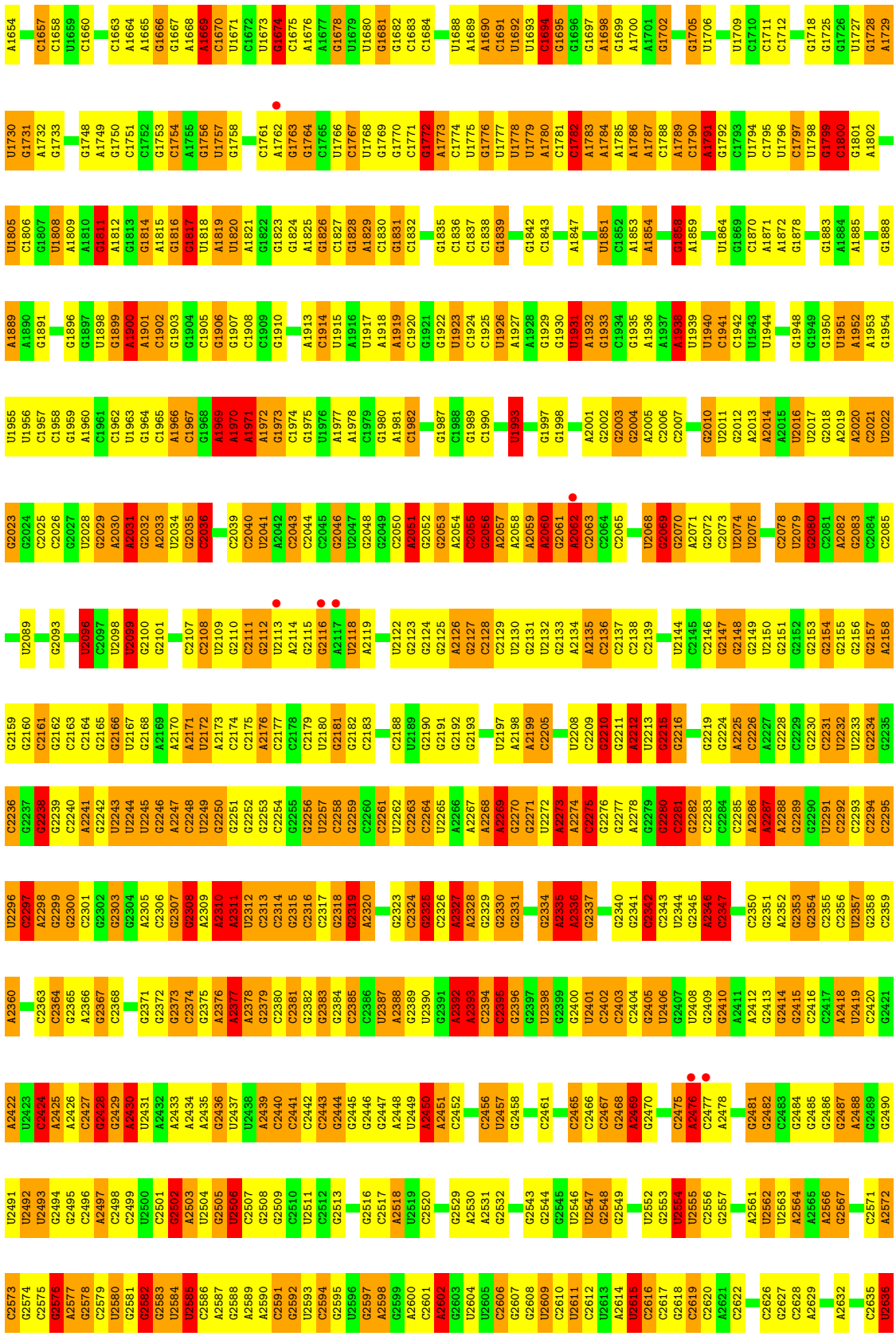
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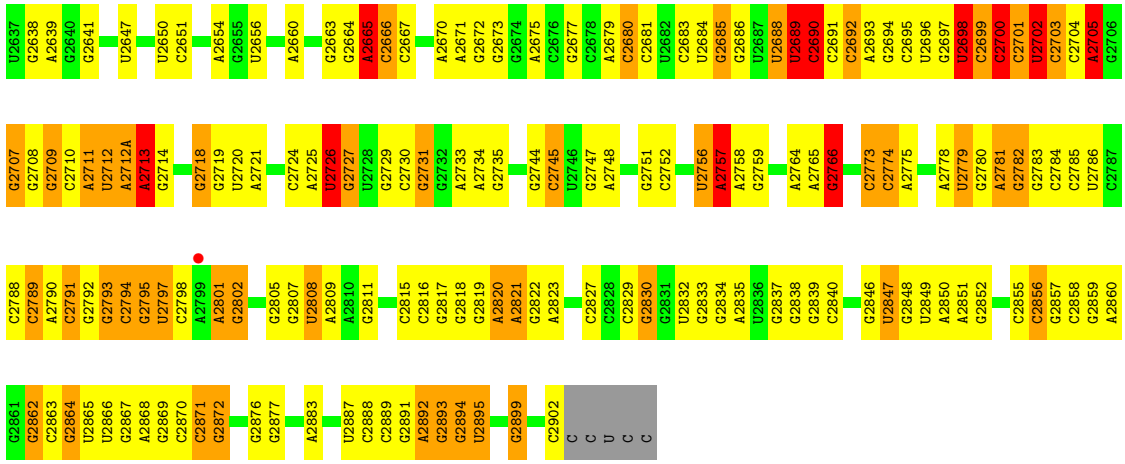

• Molecule 26: 23S ribosomal RNA

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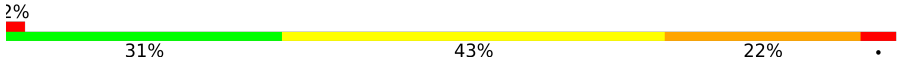

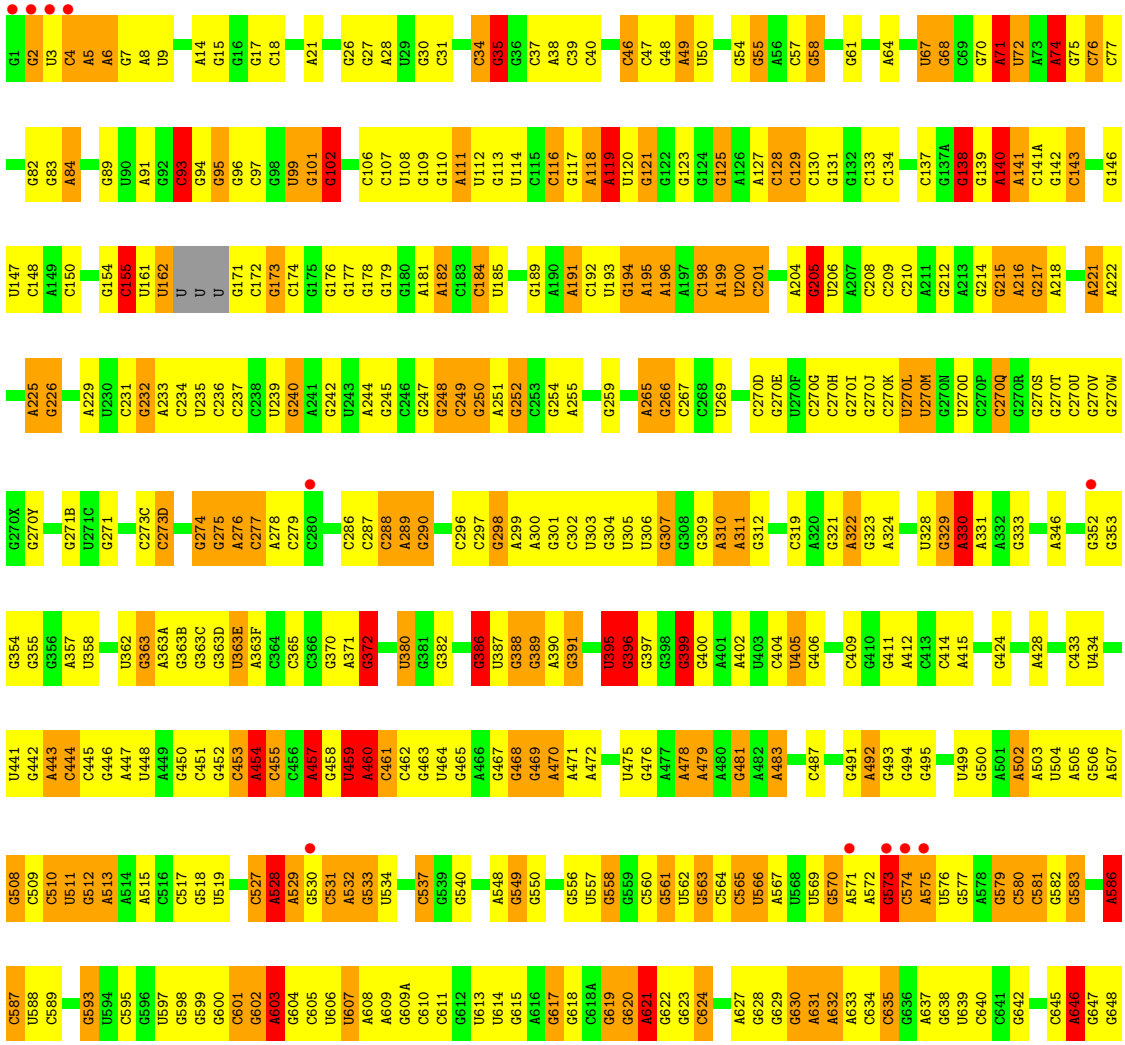

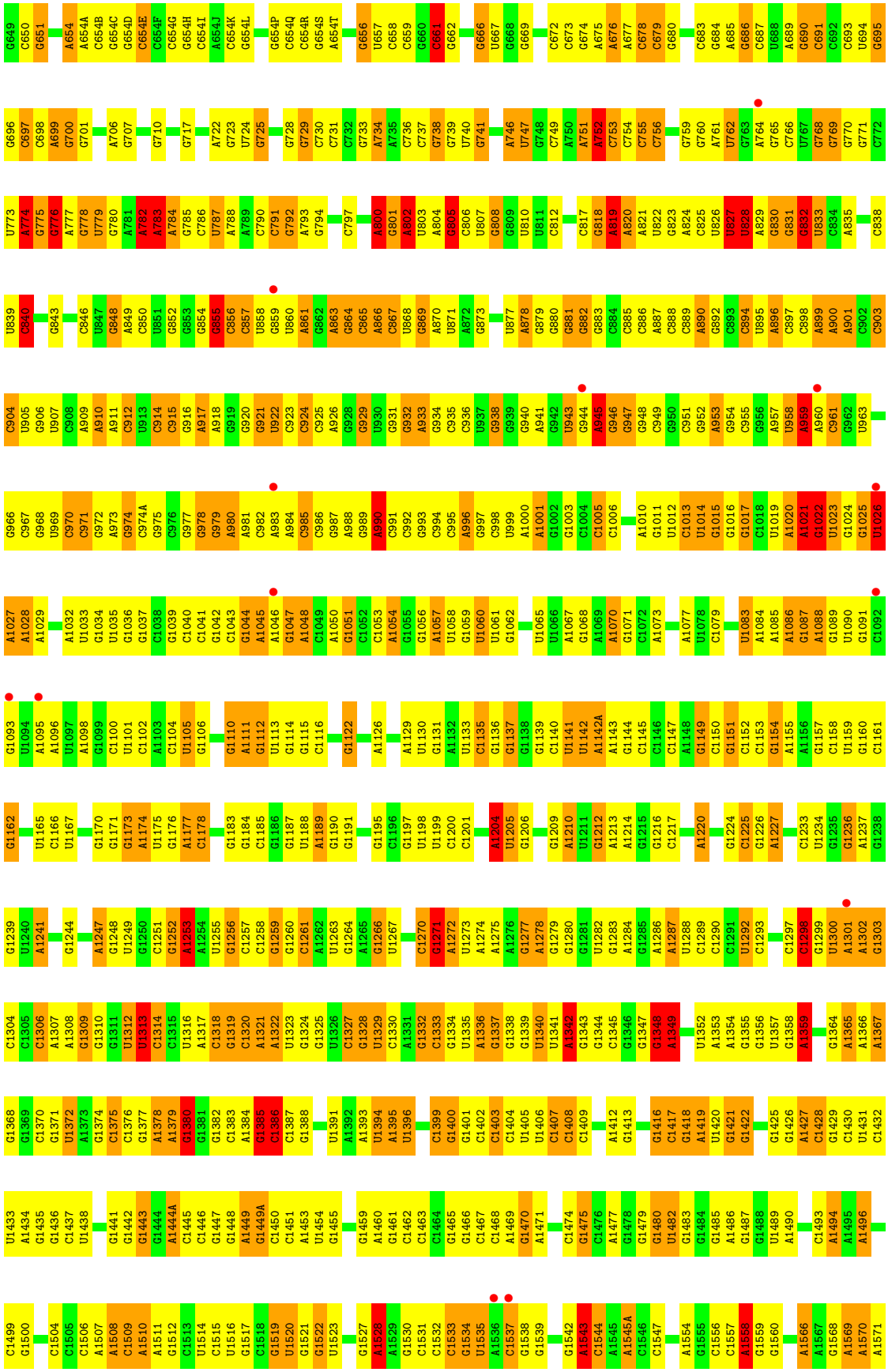
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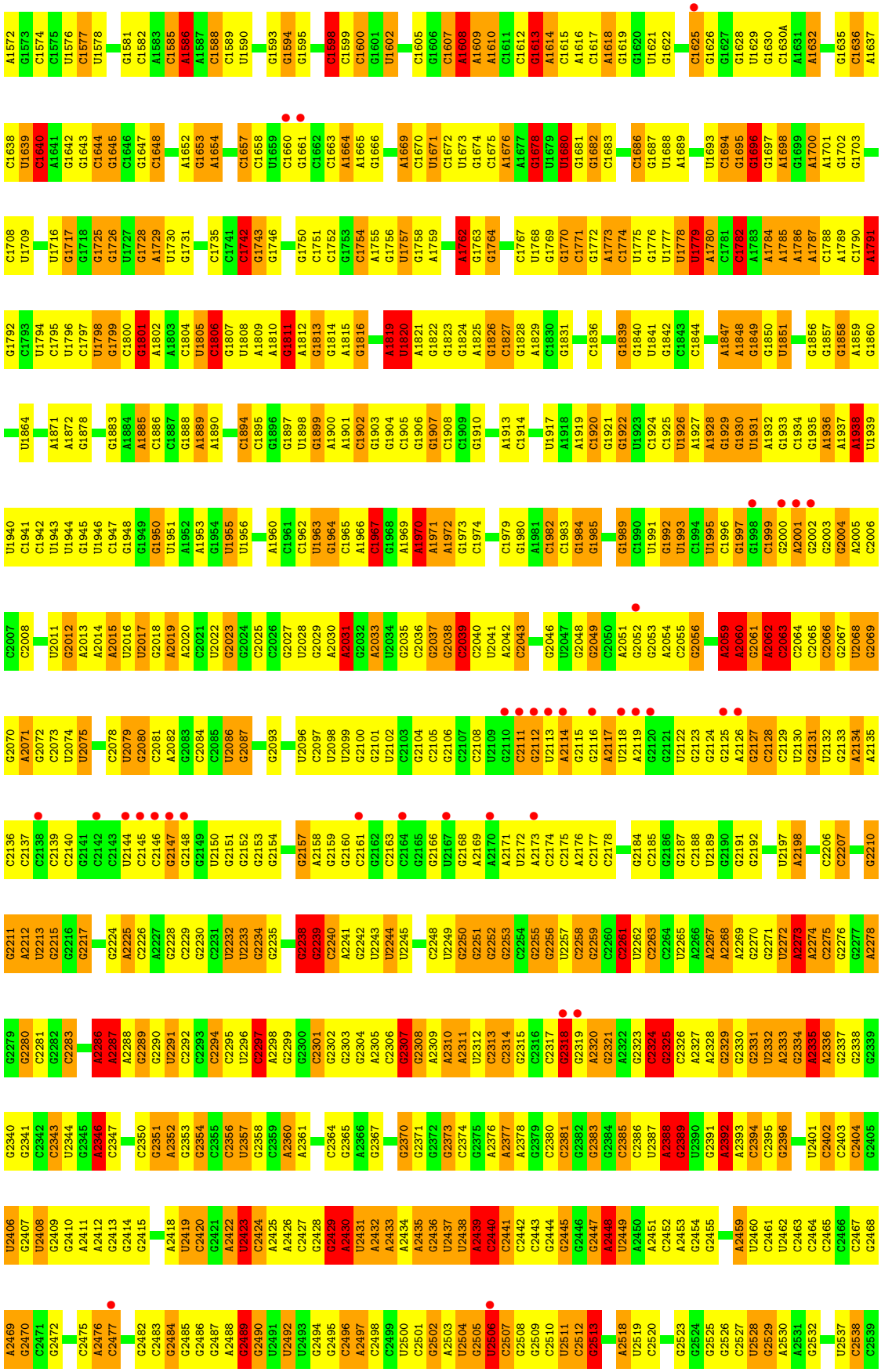
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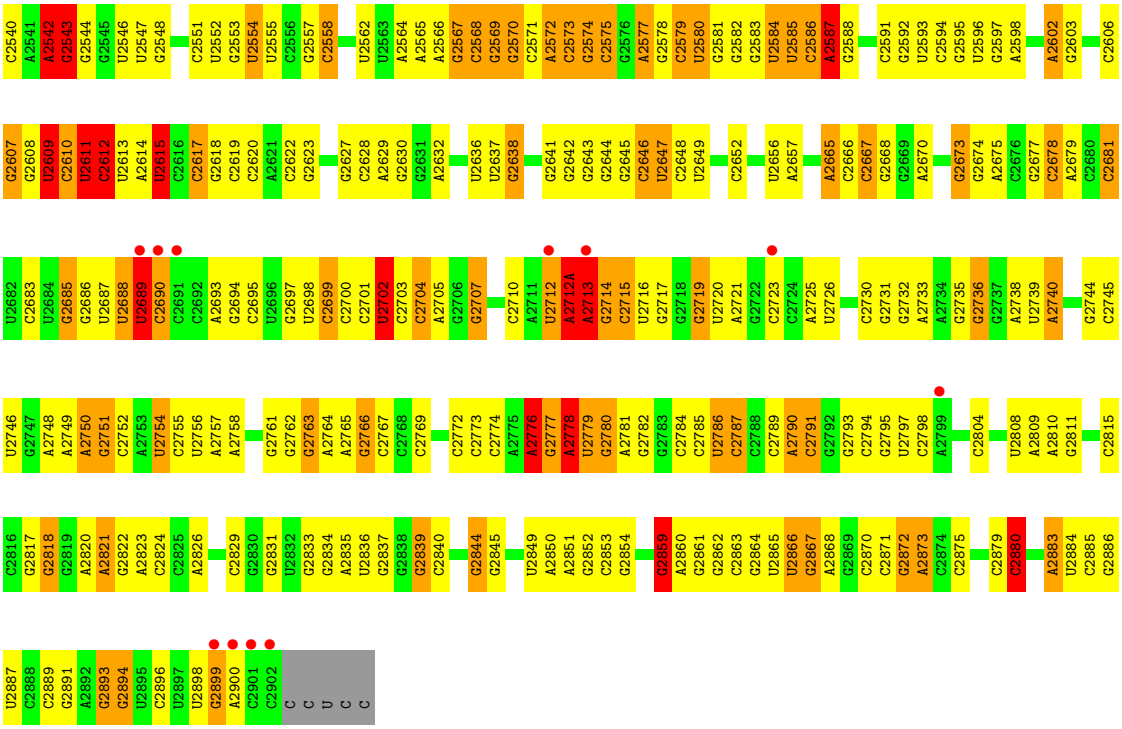

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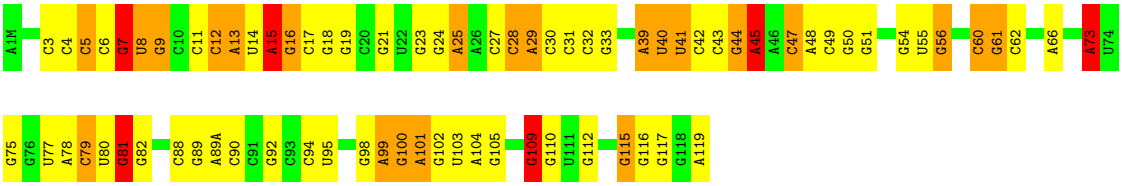

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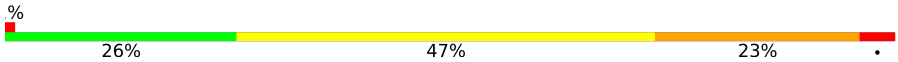
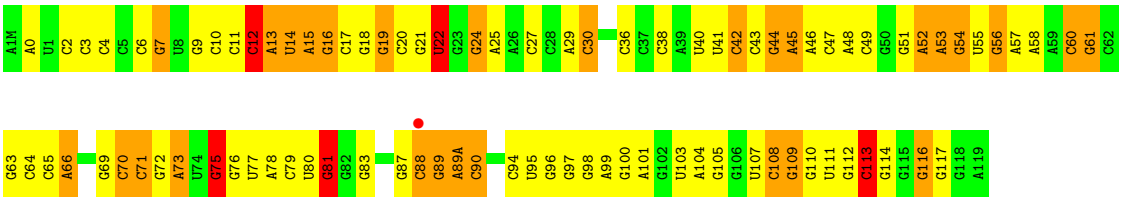
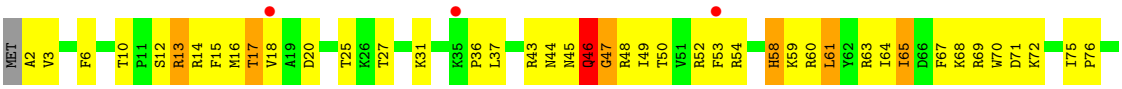
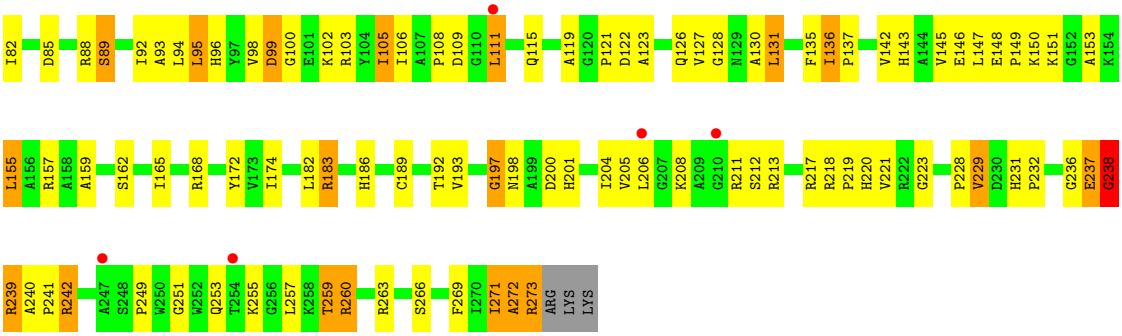




- Molecule 28: 50S ribosomal protein L2

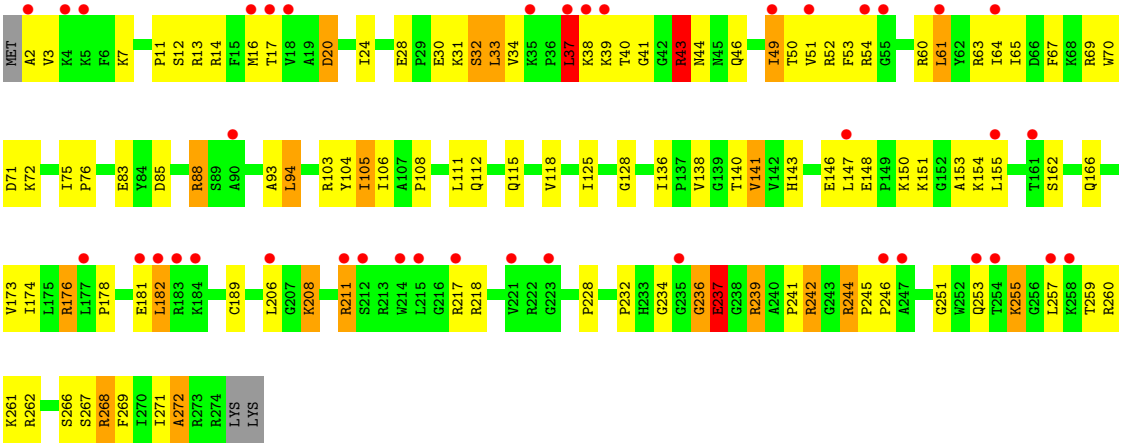
Chain 11:





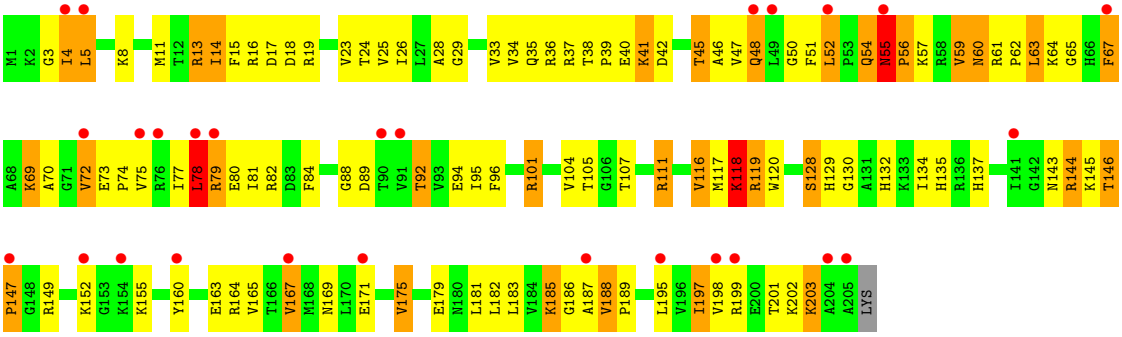
- Molecule 28: 50S ribosomal protein L2

Chain 19:



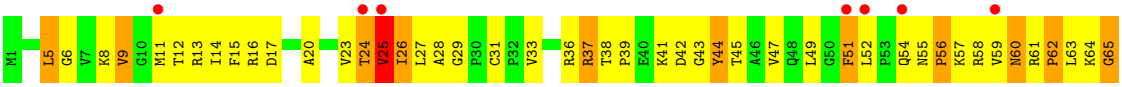
- Molecule 29: 50S ribosomal protein L3

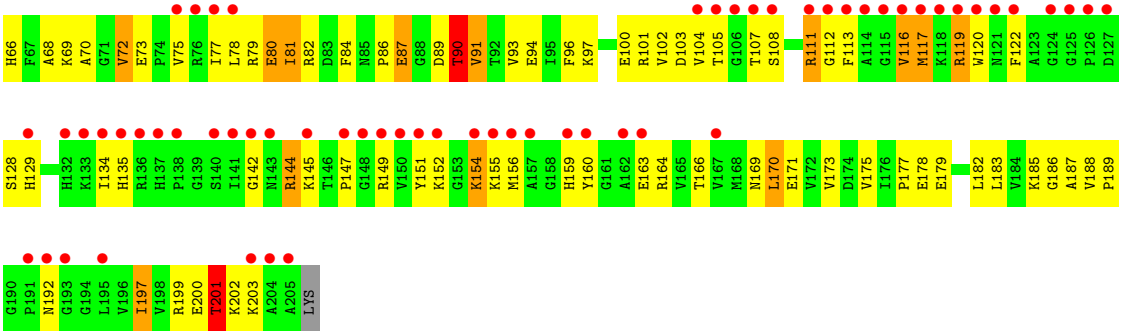
Chain 21:



- Molecule 29: 50S ribosomal protein L3

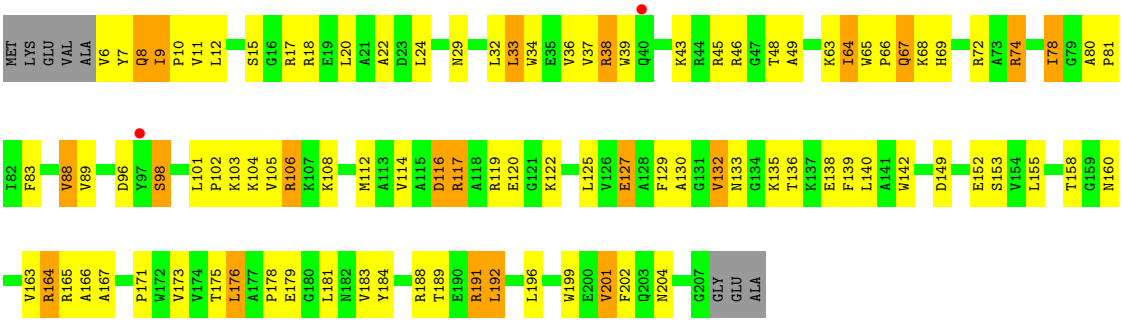
Chain 29:





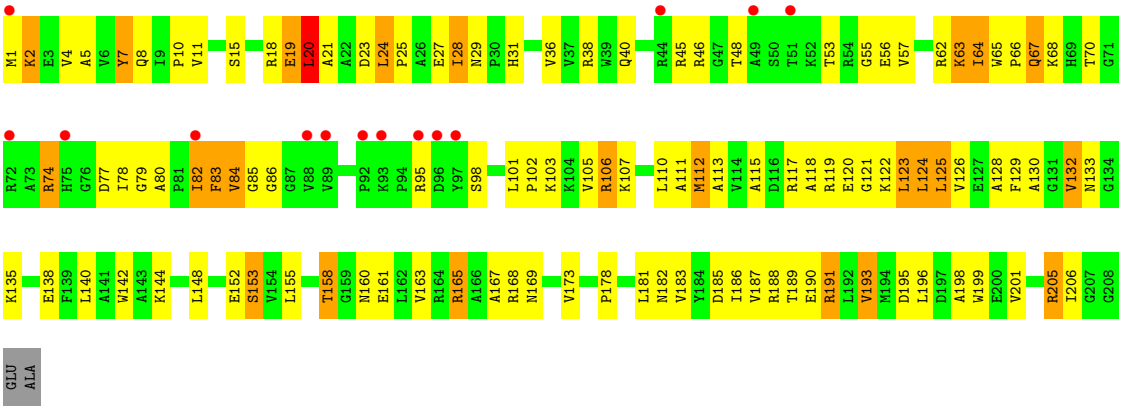
- Molecule 30: 50S ribosomal protein L4

Chain 31:



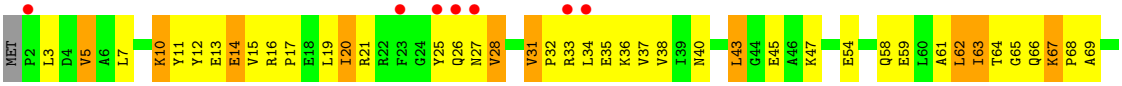
- Molecule 30: 50S ribosomal protein L4

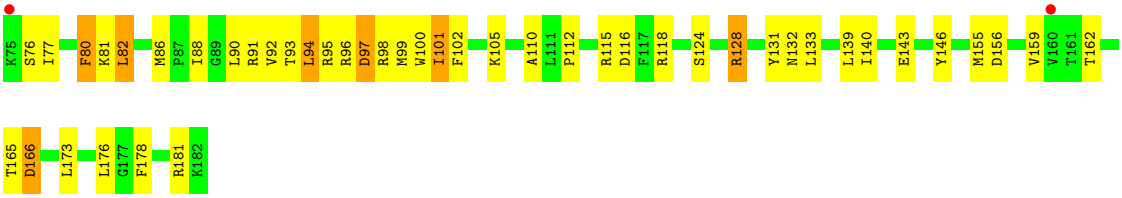
Chain 39:



- Molecule 31: 50S ribosomal protein L5

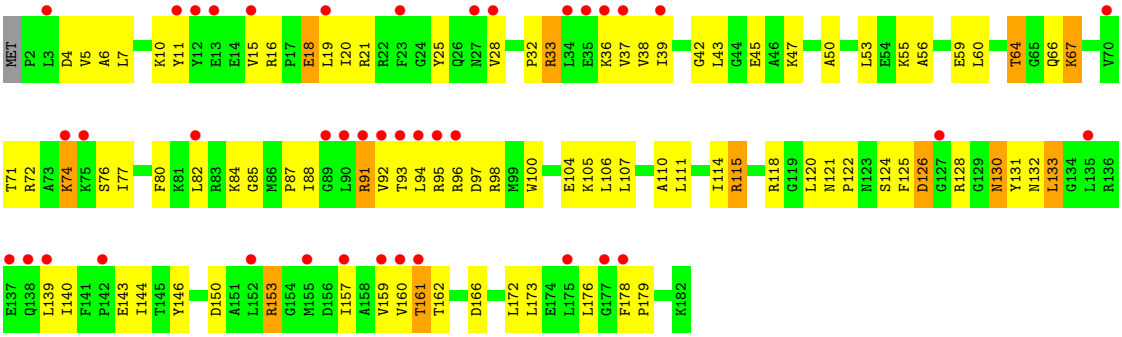
Chain 41:





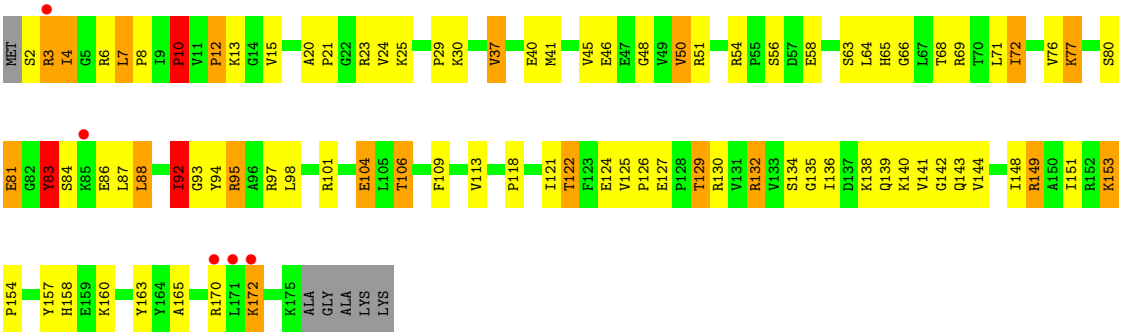
• Molecule 31: 50S ribosomal protein L5

Chain 49:



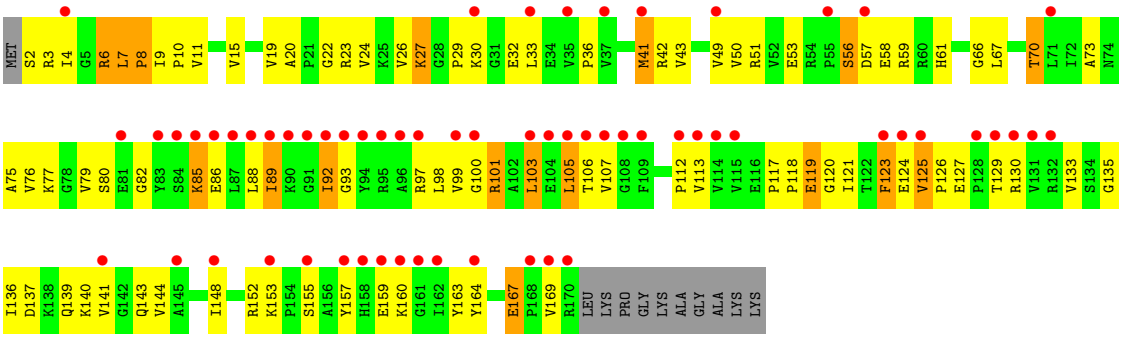
• Molecule 32: 50S ribosomal protein L6

Chain 51:



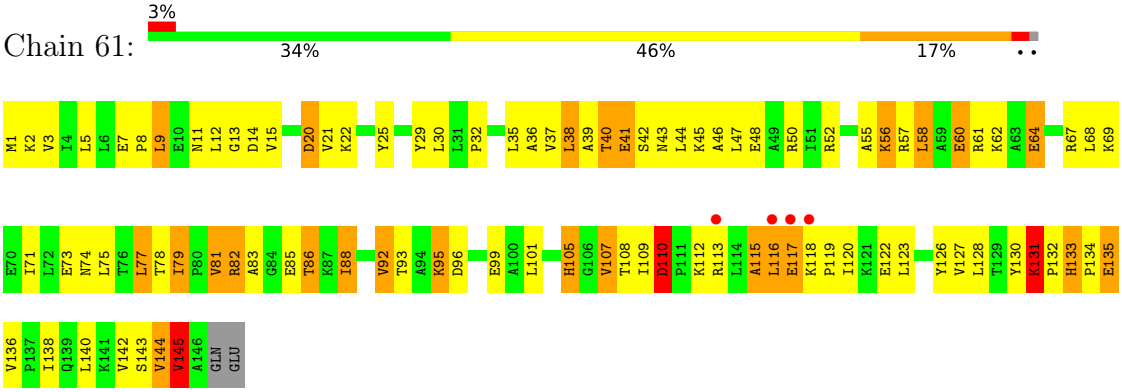
• Molecule 32: 50S ribosomal protein L6

Chain 59:



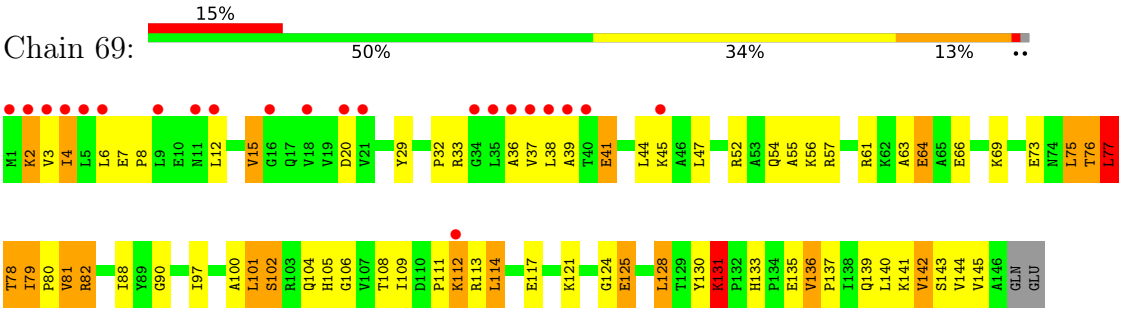
- Molecule 33: 50S ribosomal protein L9

Chain 61:



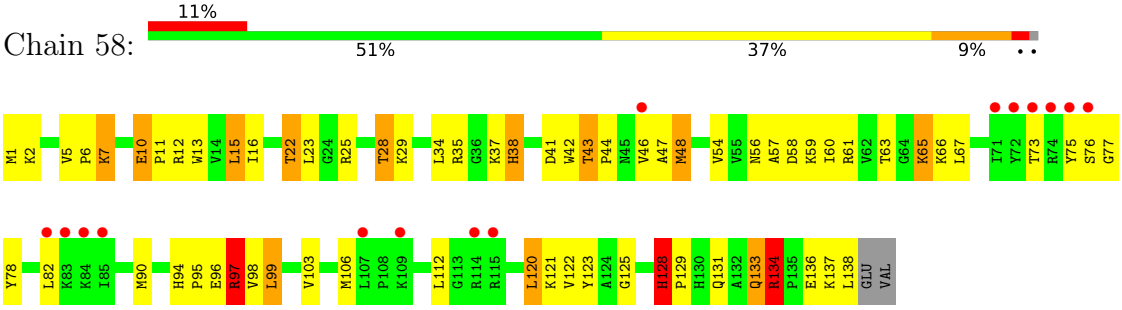
- Molecule 33: 50S ribosomal protein L9

Chain 69:



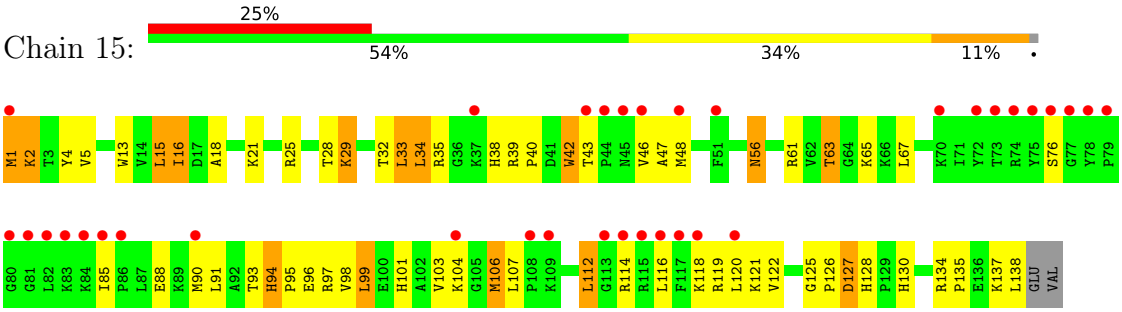
- Molecule 34: 50S ribosomal protein L13

Chain 58:



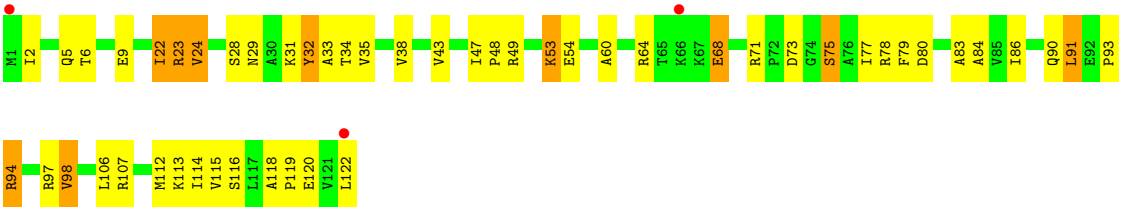
- Molecule 34: 50S ribosomal protein L13

Chain 15:



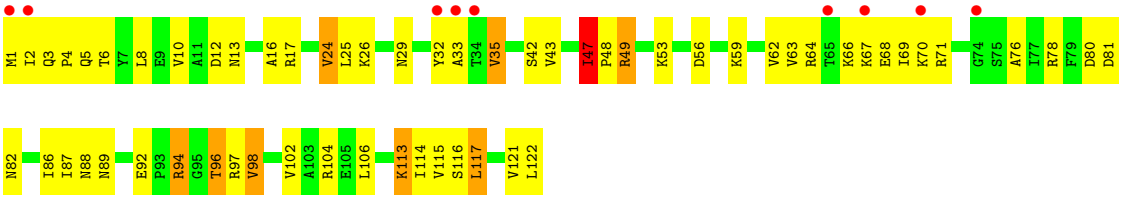
- Molecule 35: 50S ribosomal protein L14

Chain 68:



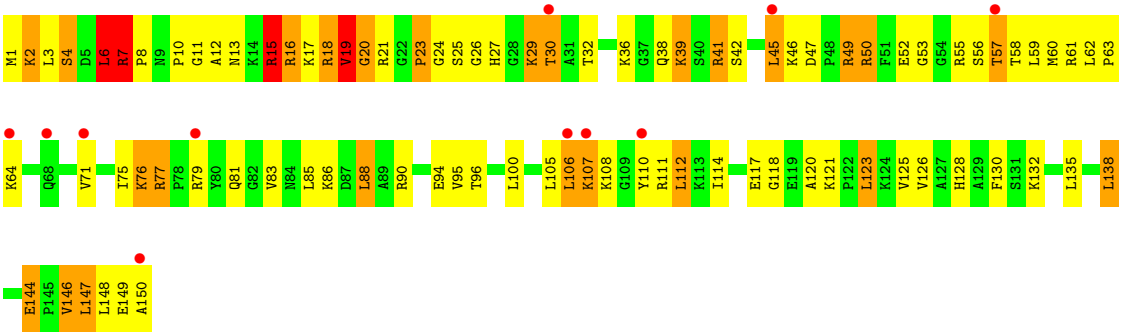
- Molecule 35: 50S ribosomal protein L14

Chain 25:



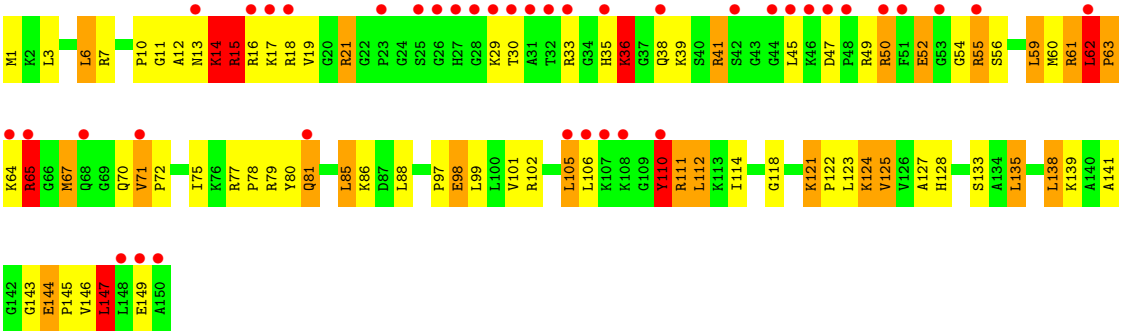
- Molecule 36: 50S ribosomal protein L15

Chain 78:



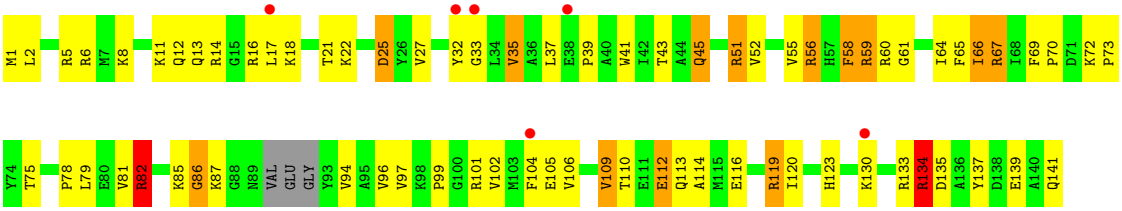
- Molecule 36: 50S ribosomal protein L15

Chain 35:



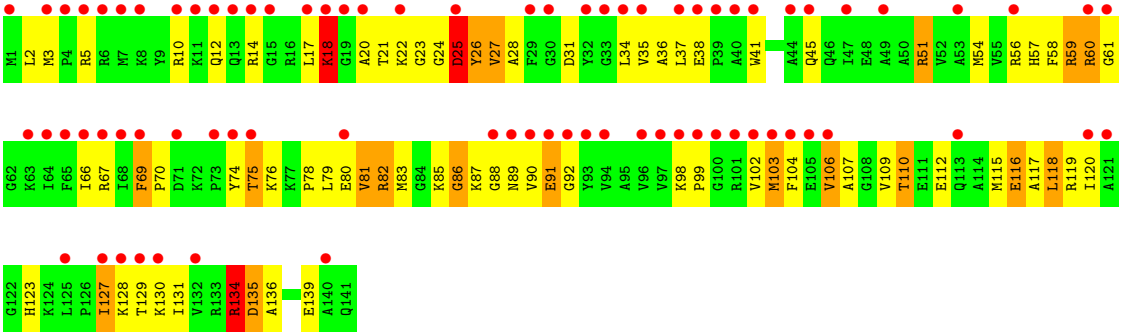
- Molecule 37: 50S ribosomal protein L16

Chain 88:



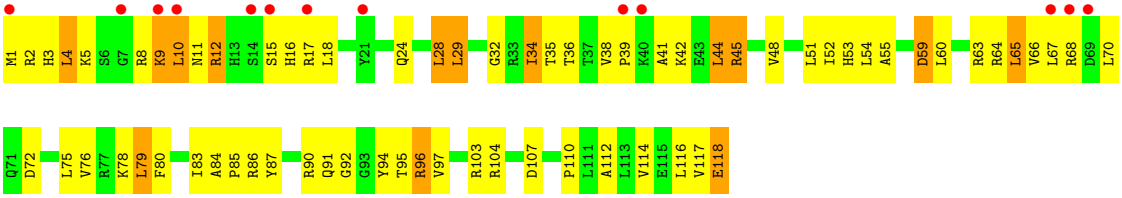
- Molecule 37: 50S ribosomal protein L16

Chain 45:



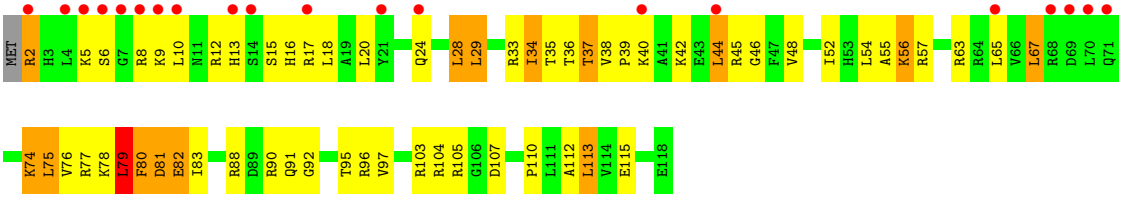
- Molecule 38: 50S ribosomal protein L17

Chain 98:



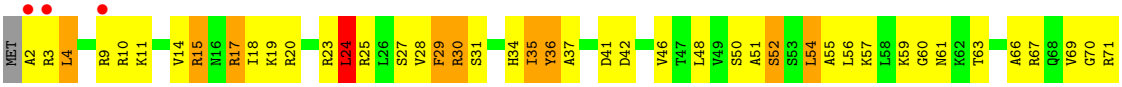
- Molecule 38: 50S ribosomal protein L17

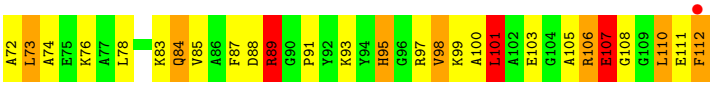
Chain 55:



- Molecule 39: 50S ribosomal protein L18

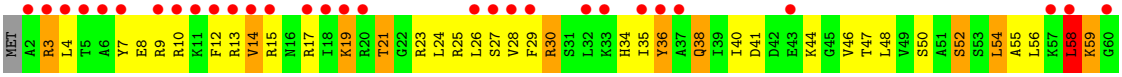
Chain A8:

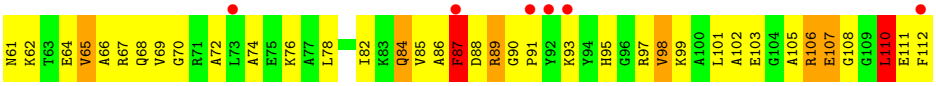




• Molecule 39: 50S ribosomal protein L18

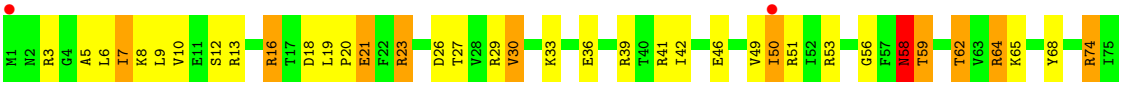
Chain 65:

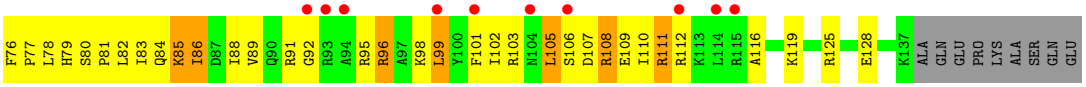




• Molecule 40: 50S ribosomal protein L19

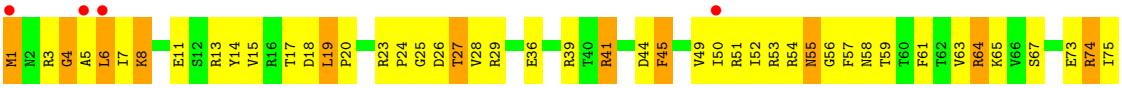
Chain B8:





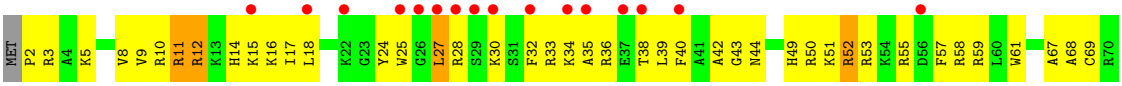
• Molecule 40: 50S ribosomal protein L19

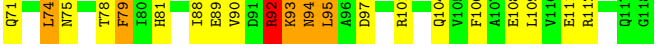
Chain 75:



• Molecule 41: 50S ribosomal protein L20

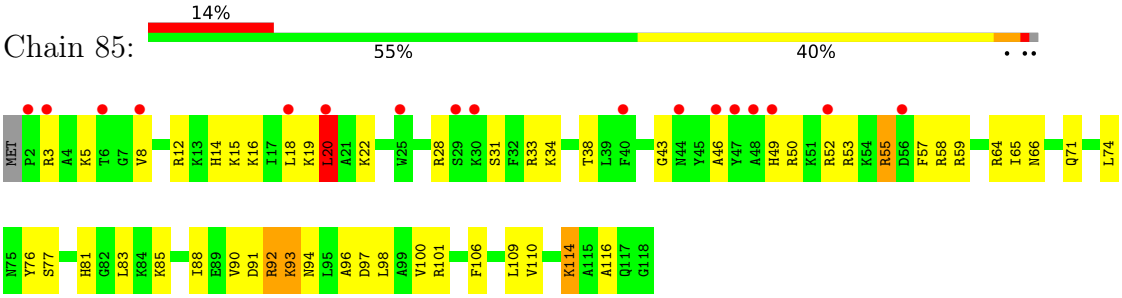
Chain C8:





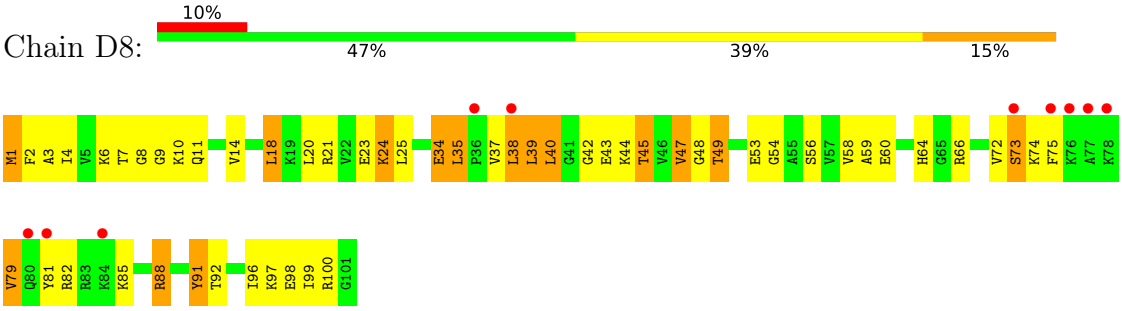
• Molecule 41: 50S ribosomal protein L20

Chain 85:



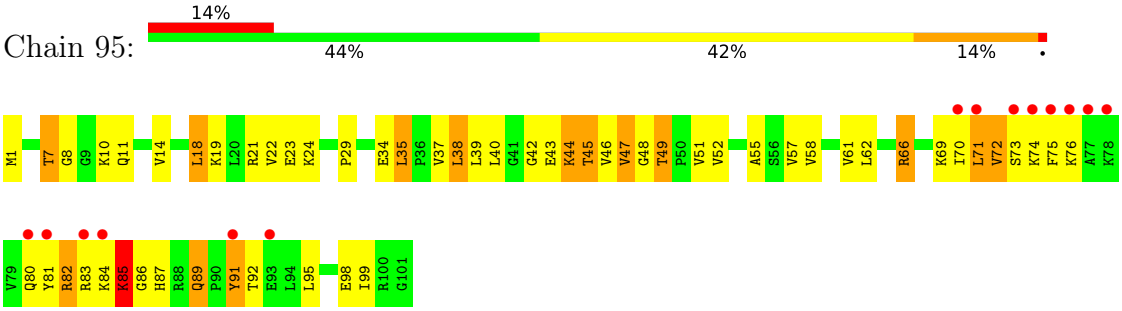
• Molecule 42: 50S ribosomal protein L21

Chain D8:



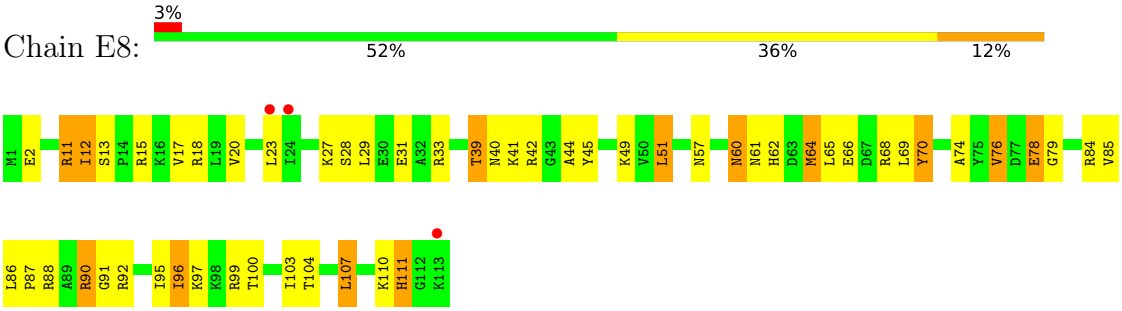
• Molecule 42: 50S ribosomal protein L21

Chain 95:



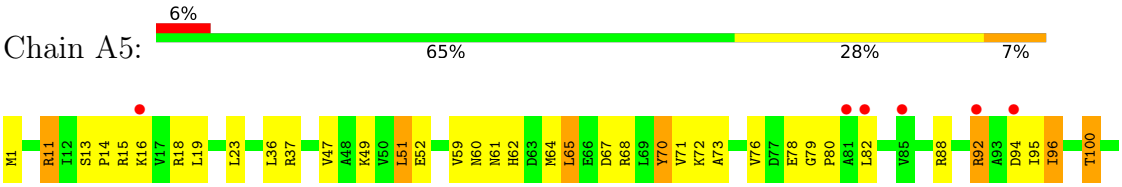
• Molecule 43: 50S ribosomal protein L22

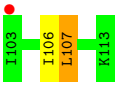
Chain E8:



• Molecule 43: 50S ribosomal protein L22

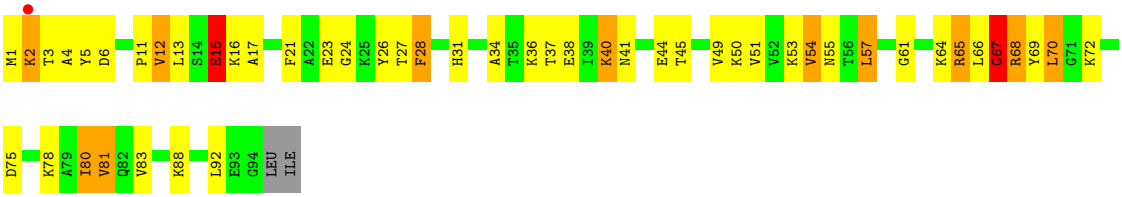
Chain A5:





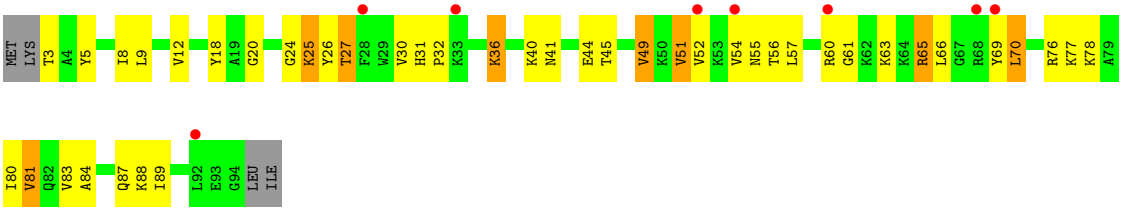
• Molecule 44: 50S ribosomal protein L23

Chain F8:



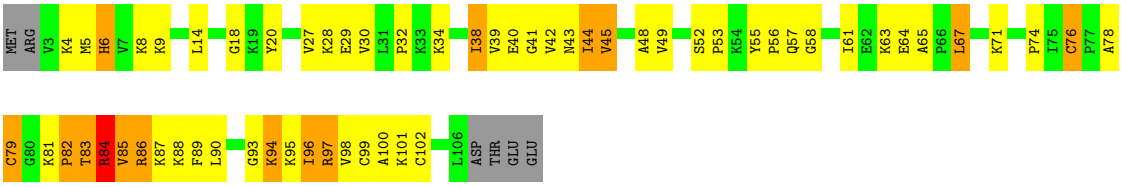
• Molecule 44: 50S ribosomal protein L23

Chain B5:



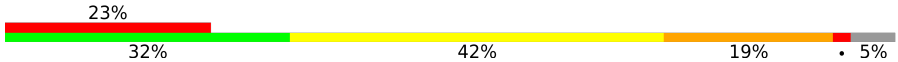
• Molecule 45: 50S ribosomal protein L24

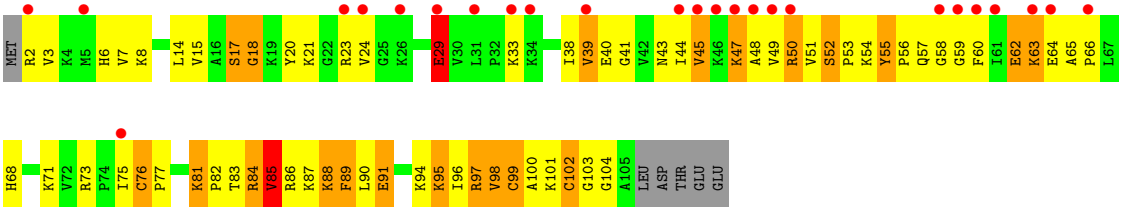
Chain G8:



• Molecule 45: 50S ribosomal protein L24

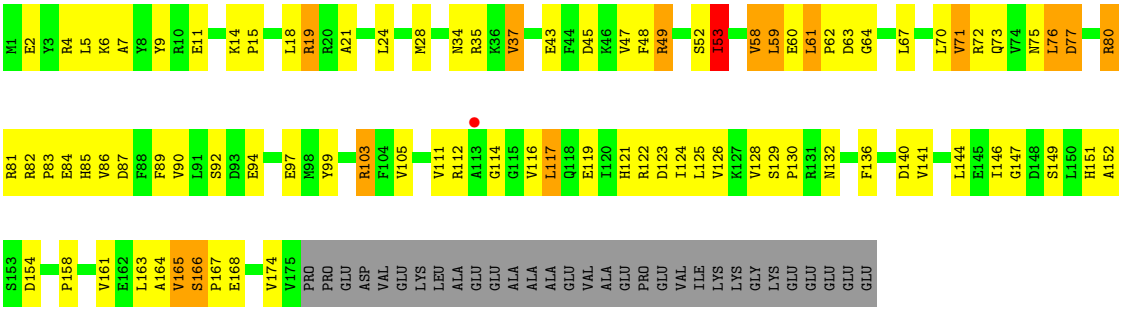
Chain C5:





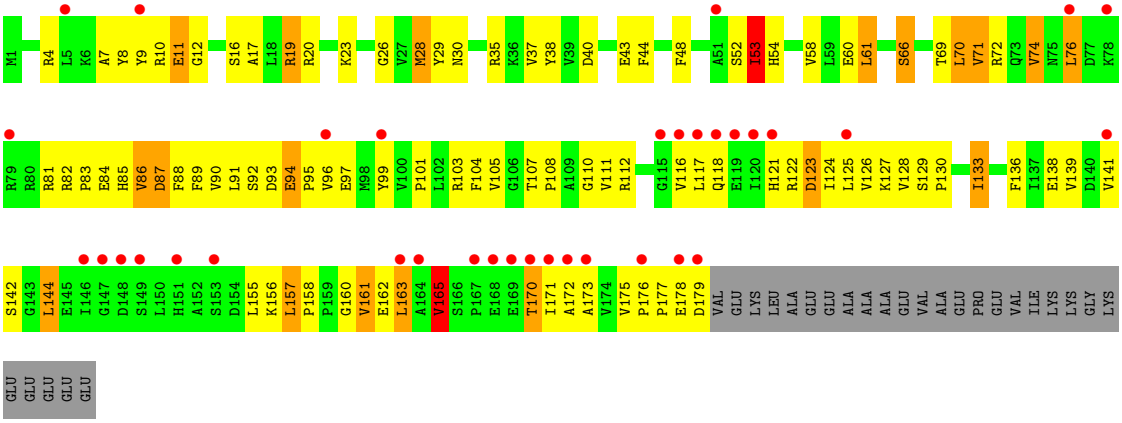
• Molecule 46: 50S ribosomal protein L25

Chain H8:



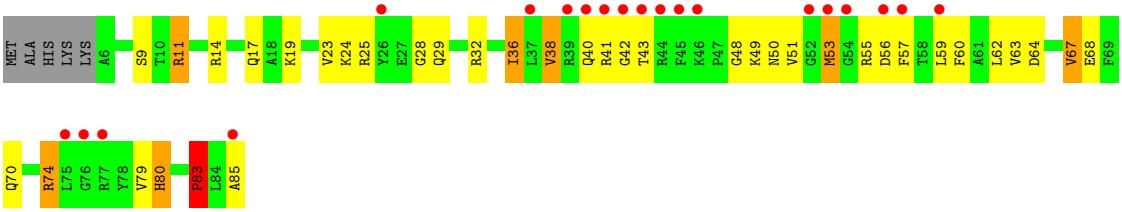
- Molecule 46: 50S ribosomal protein L25

Chain D5:



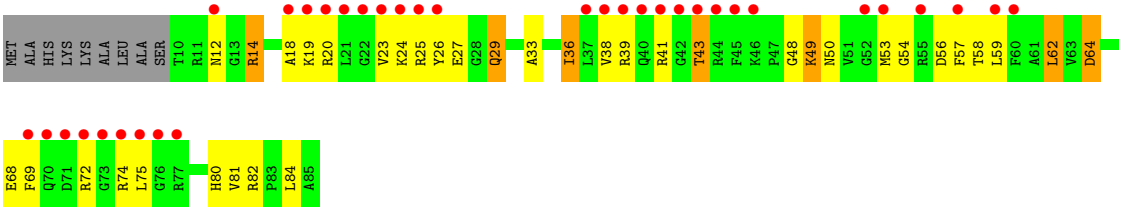
- Molecule 47: 50S ribosomal protein L27

Chain I8:



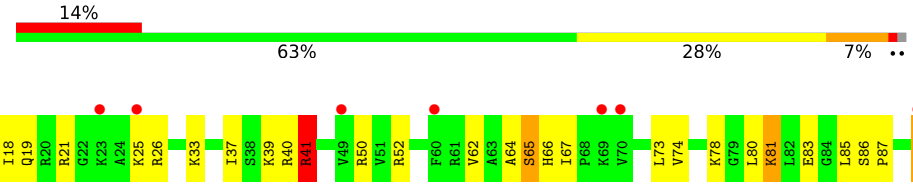
- Molecule 47: 50S ribosomal protein L27

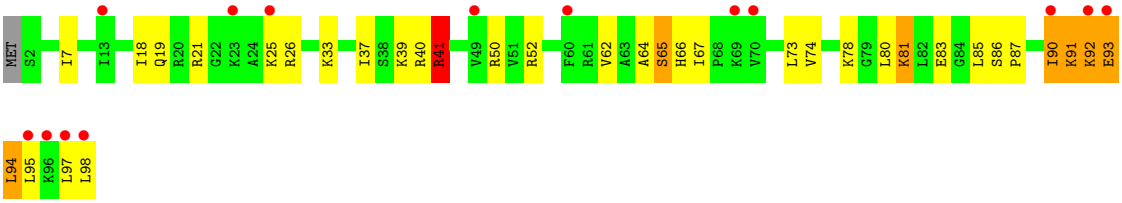
Chain E5:



- Molecule 48: 50S ribosomal protein L28

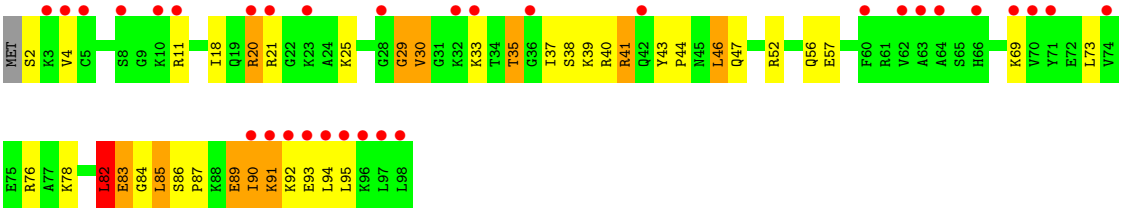
Chain J8:





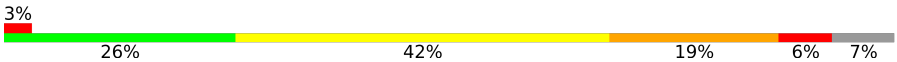
- Molecule 48: 50S ribosomal protein L28

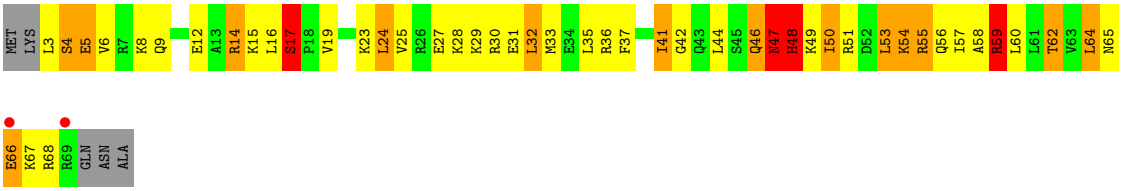
Chain F5:



- Molecule 49: 50S ribosomal protein L29

Chain K8:





- Molecule 49: 50S ribosomal protein L29

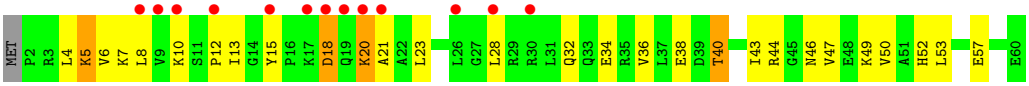
Chain G5:

- Molecule 50: 50S ribosomal protein L30

Chain L8:

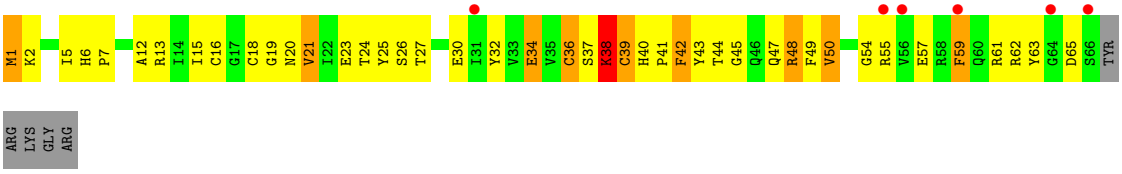
- Molecule 50: 50S ribosomal protein L30

Chain H5:



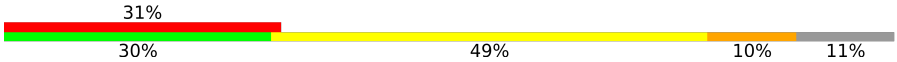
• Molecule 51: 50S ribosomal protein L31

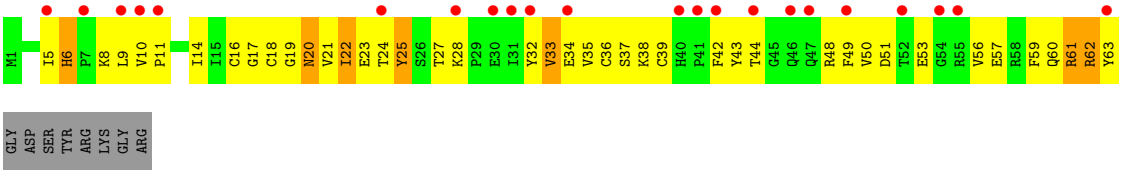
Chain M8:



• Molecule 51: 50S ribosomal protein L31

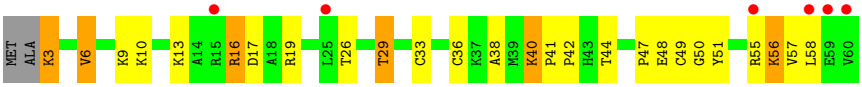
Chain I5:





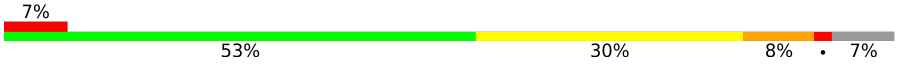
• Molecule 52: 50S ribosomal protein L32

Chain N8:



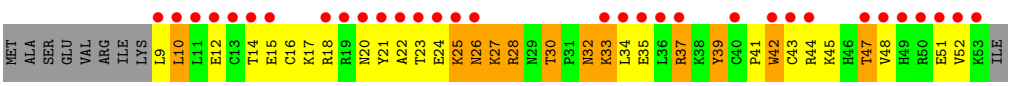
• Molecule 52: 50S ribosomal protein L32

Chain J5:



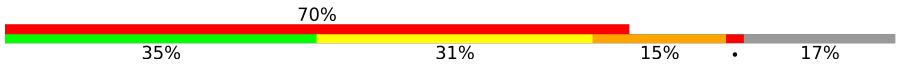
• Molecule 53: 50S ribosomal protein L33

Chain O8:



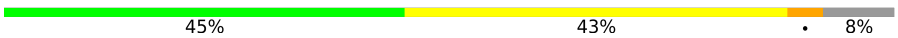
• Molecule 53: 50S ribosomal protein L33

Chain K5:



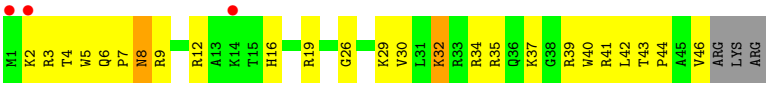
• Molecule 54: 50S ribosomal protein L34

Chain P8:



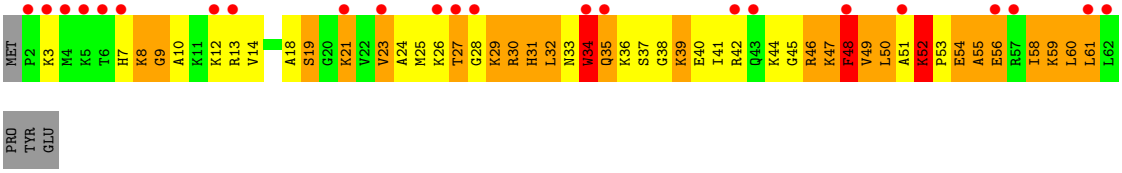
• Molecule 54: 50S ribosomal protein L34

Chain L5:



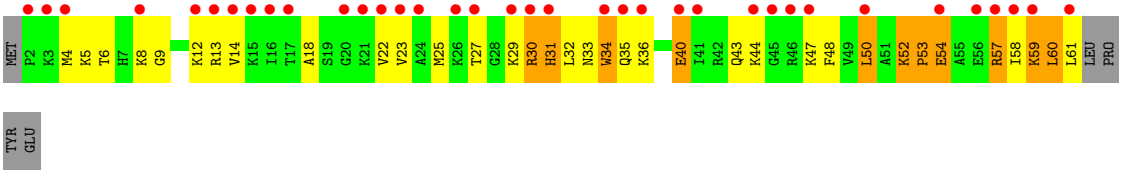
• Molecule 55: 50S ribosomal protein L35

Chain Q8:



• Molecule 55: 50S ribosomal protein L35

Chain M5:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.90Å 447.90Å 621.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.03 – 3.05 223.95 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (188.03-3.05) 91.4 (223.95-3.05)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , (Not available) 0.200 , 0.239	Depositor DCC
R_{free} test set	1998 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 89.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	299951	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: ZN, OMC, 5MU, 4SU, MG, 7MG, PSU, MIA

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	13	0.77	9/36053 (0.0%)	1.46	483/56270 (0.9%)
1	1G	0.65	1/36025 (0.0%)	1.30	249/56227 (0.4%)
2	12	0.37	0/1959	0.58	1/2642 (0.0%)
2	1E	0.42	0/1959	0.65	0/2642
3	22	0.41	0/1636	0.60	0/2205
3	2E	0.52	0/1629	0.67	0/2195
4	32	0.50	0/1732	0.73	1/2318 (0.0%)
4	3E	0.65	2/1732 (0.1%)	0.76	1/2318 (0.0%)
5	42	0.47	0/1171	0.74	0/1576
5	4E	0.55	0/1171	0.76	1/1576 (0.1%)
6	52	0.48	0/855	0.65	0/1154
6	5E	0.58	0/855	0.70	0/1154
7	62	0.42	0/1275	0.60	0/1709
7	6E	0.46	0/1275	0.59	0/1709
8	72	0.39	0/1135	0.60	0/1527
8	7E	0.51	0/1135	0.72	0/1527
9	82	0.39	0/1028	0.59	0/1379
9	8E	0.48	0/1028	0.72	1/1379 (0.1%)
10	1A	0.38	0/814	0.60	0/1095
10	1I	0.46	0/814	0.66	0/1095
11	2A	0.46	0/879	0.65	0/1187
11	2I	0.51	0/879	0.78	0/1187
12	3A	0.54	0/991	0.76	0/1327
12	3I	0.71	0/991	0.92	0/1327
13	4A	0.36	0/943	0.59	0/1265
13	4I	0.51	0/948	0.69	0/1272
14	5A	0.43	0/484	0.65	0/643
14	5I	0.71	1/500 (0.2%)	0.79	0/664
15	6A	0.47	0/744	0.62	1/992 (0.1%)
15	6I	0.54	0/744	0.78	0/992
16	7A	0.47	0/721	0.69	0/970
16	7I	0.48	0/721	0.72	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.52	1/847 (0.1%)	0.64	0/1131
17	8I	0.57	0/847	0.74	0/1131
18	9A	0.51	0/595	0.77	0/790
18	9I	0.56	0/595	0.78	0/790
19	AA	0.40	0/638	0.63	0/860
19	AI	0.58	0/661	0.79	0/890
20	BA	0.48	0/764	0.76	0/1007
20	BI	0.45	0/764	0.70	0/1007
21	1B	0.44	0/221	0.64	0/288
21	1F	0.50	0/221	0.73	0/288
22	1K	0.51	0/1647	1.15	10/2565 (0.4%)
23	2K	1.12	6/1721 (0.3%)	1.64	40/2682 (1.5%)
23	2L	0.99	6/1721 (0.3%)	1.42	20/2682 (0.7%)
24	1L	0.44	0/1809	0.98	4/2819 (0.1%)
24	3K	0.49	1/1809 (0.1%)	1.17	14/2819 (0.5%)
24	3L	0.49	0/1809	1.11	11/2819 (0.4%)
25	4K	0.92	0/316	1.49	5/490 (1.0%)
25	4L	0.80	0/215	1.52	3/330 (0.9%)
26	14	0.91	64/70167 (0.1%)	1.65	1671/109541 (1.5%)
26	1H	1.09	145/70233 (0.2%)	1.89	2868/109643 (2.6%)
27	16	0.92	3/2928 (0.1%)	1.67	74/4568 (1.6%)
27	1J	0.75	0/2928	1.36	17/4568 (0.4%)
28	11	0.84	1/2165 (0.0%)	1.04	7/2919 (0.2%)
28	19	0.71	0/2170	0.96	4/2926 (0.1%)
29	21	0.68	0/1601	0.91	0/2160
29	29	0.69	0/1601	0.97	2/2160 (0.1%)
30	31	0.77	0/1620	0.97	2/2194 (0.1%)
30	39	0.61	0/1662	0.84	1/2249 (0.0%)
31	41	0.58	0/1498	0.83	1/2016 (0.0%)
31	49	0.41	0/1498	0.63	0/2016
32	51	0.66	0/1362	0.87	2/1841 (0.1%)
32	59	0.37	0/1324	0.63	0/1791
33	61	0.56	0/1151	0.79	2/1558 (0.1%)
33	69	0.47	0/1151	0.73	2/1558 (0.1%)
34	15	0.62	1/1131 (0.1%)	0.86	5/1525 (0.3%)
34	58	0.65	0/1131	0.86	3/1525 (0.2%)
35	25	0.64	0/942	0.77	0/1269
35	68	0.71	0/942	0.84	1/1269 (0.1%)
36	35	0.68	0/1161	1.06	4/1544 (0.3%)
36	78	0.75	0/1161	1.08	1/1544 (0.1%)
37	45	0.66	1/1142 (0.1%)	0.88	1/1527 (0.1%)
37	88	0.87	0/1106	1.05	2/1478 (0.1%)
38	55	0.66	0/973	0.88	2/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	98	0.60	0/981	0.87	0/1312
39	65	0.51	0/891	0.91	2/1187 (0.2%)
39	A8	0.71	0/891	0.98	4/1187 (0.3%)
40	75	0.59	0/1155	0.77	0/1542
40	B8	0.66	0/1155	0.84	1/1542 (0.1%)
41	85	0.57	0/981	0.75	1/1306 (0.1%)
41	C8	0.72	0/981	0.93	2/1306 (0.2%)
42	95	0.64	0/789	0.87	1/1057 (0.1%)
42	D8	0.66	0/789	0.84	1/1057 (0.1%)
43	A5	0.69	0/910	0.85	0/1220
43	E8	0.71	0/910	0.95	3/1220 (0.2%)
44	B5	0.77	0/739	0.86	0/993
44	F8	0.90	2/756 (0.3%)	0.98	0/1014
45	C5	0.69	0/807	0.90	1/1076 (0.1%)
45	G8	0.73	0/804	0.96	0/1073
46	D5	0.44	0/1460	0.67	0/1982
46	H8	0.50	0/1427	0.80	2/1935 (0.1%)
47	E5	0.66	0/614	0.88	0/819
47	I8	0.82	0/634	0.98	0/847
48	F5	0.66	0/769	0.93	2/1022 (0.2%)
48	J8	0.74	0/769	0.95	1/1022 (0.1%)
49	G5	0.58	0/560	0.81	1/741 (0.1%)
49	K8	0.94	2/565 (0.4%)	0.94	1/748 (0.1%)
50	H5	0.52	0/473	0.71	0/635
50	L8	0.73	1/457 (0.2%)	0.91	0/613
51	I5	0.46	0/527	0.72	0/709
51	M8	0.53	0/545	0.77	0/733
52	J5	0.71	0/448	0.88	0/606
52	N8	0.68	0/467	0.90	0/632
53	K5	0.74	0/396	0.85	1/529 (0.2%)
53	O8	0.87	1/396 (0.3%)	0.87	1/529 (0.2%)
54	L5	0.79	0/406	0.93	1/536 (0.2%)
54	P8	0.96	0/399	1.13	1/526 (0.2%)
55	M5	0.84	0/483	0.98	0/634
55	Q8	1.25	4/491 (0.8%)	1.62	7/645 (1.1%)
All	All	0.83	252/322599 (0.1%)	1.47	5551/483107 (1.1%)

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
4	3E	0	2
9	8E	0	1
10	1A	0	1
11	2I	0	2
13	4I	0	2
15	6I	0	1
16	7I	0	1
19	AI	0	2
20	BA	0	2
28	11	0	4
28	19	0	5
29	21	0	3
29	29	0	3
30	39	0	2
31	41	0	1
33	61	0	4
33	69	0	1
35	25	0	1
36	35	0	5
37	45	0	4
37	88	0	2
39	65	0	1
39	A8	0	2
40	75	0	2
40	B8	0	1
41	85	0	1
41	C8	0	1
43	E8	0	1
44	B5	0	2
44	F8	0	1
45	C5	0	3
45	G8	0	1
46	D5	0	1
46	H8	0	1
47	I8	0	2
48	F5	0	2
49	G5	0	3
49	K8	0	3
51	M8	0	2
52	J5	0	1
52	N8	0	1
53	O8	0	1
55	M5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	Q8	0	5
All	All	0	88

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	21	U	C5-C6	19.03	1.51	1.34
23	2K	21	U	C5-C6	16.80	1.49	1.34
26	1H	774	A	N9-C4	-13.91	1.29	1.37
26	14	783	A	N9-C4	-12.95	1.30	1.37
23	2K	21	U	C2-N3	12.76	1.46	1.37

The worst 5 of 5551 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1786	A	C2-N3-C4	-22.74	99.23	110.60
26	1H	1899	G	N3-C4-N9	-22.01	112.80	126.00
26	1H	676	A	C2-N3-C4	-20.28	100.46	110.60
26	1H	1899	G	C2-N3-C4	-19.38	102.21	111.90
26	1H	783	A	C2-N3-C4	-18.91	101.14	110.60

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2I	100	ALA	Peptide
11	2I	101	SER	Peptide
4	3E	166	LYS	Peptide
4	3E	30	LYS	Peptide
9	8E	110	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32207	0	16254	745	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1G	32182	0	16245	835	1
2	12	1924	0	1975	96	0
2	1E	1924	0	1975	96	0
3	22	1612	0	1677	71	0
3	2E	1605	0	1668	48	0
4	32	1702	0	1763	86	0
4	3E	1702	0	1762	81	0
5	42	1155	0	1213	60	0
5	4E	1155	0	1213	51	0
6	52	842	0	857	31	0
6	5E	842	0	857	21	0
7	62	1256	0	1296	53	0
7	6E	1256	0	1296	52	0
8	72	1115	0	1177	47	0
8	7E	1115	0	1177	59	0
9	82	1009	0	1037	68	0
9	8E	1009	0	1037	60	0
10	1A	801	0	849	44	0
10	1I	801	0	849	52	0
11	2A	864	0	881	32	0
11	2I	864	0	881	35	0
12	3A	975	0	1062	53	0
12	3I	975	0	1062	37	0
13	4A	933	0	992	64	0
13	4I	938	0	997	51	0
14	5A	475	0	511	30	0
14	5I	491	0	529	24	0
15	6A	733	0	771	29	0
15	6I	733	0	771	29	0
16	7A	705	0	725	25	0
16	7I	705	0	725	58	0
17	8A	834	0	904	22	0
17	8I	834	0	904	47	0
18	9A	590	0	662	32	0
18	9I	590	0	662	22	0
19	AA	624	0	636	40	0
19	AI	647	0	665	33	0
20	BA	762	0	861	34	0
20	BI	762	0	861	48	0
21	1B	217	0	234	15	0
21	1F	217	0	234	10	0
22	1K	1628	0	840	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	845	29	0
23	2L	1646	0	845	32	0
24	1L	1619	0	822	21	0
24	3K	1619	0	822	53	0
24	3L	1619	0	822	40	0
25	4K	281	0	142	6	0
25	4L	193	0	99	8	0
26	14	62647	0	31581	1303	0
26	1H	62707	0	31607	1456	1
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	92	0
28	11	2115	0	2195	101	0
28	19	2120	0	2197	89	0
29	21	1568	0	1634	100	0
29	29	1568	0	1634	119	0
30	31	1585	0	1632	77	0
30	39	1627	0	1680	100	0
31	41	1473	0	1535	75	0
31	49	1473	0	1535	61	0
32	51	1336	0	1418	75	0
32	59	1299	0	1371	68	0
33	61	1136	0	1223	63	0
33	69	1136	0	1223	51	0
34	15	1104	0	1180	56	0
34	58	1104	0	1180	52	0
35	25	932	0	996	37	0
35	68	932	0	996	46	0
36	35	1144	0	1228	81	0
36	78	1144	0	1228	102	0
37	45	1121	0	1179	61	0
37	88	1086	0	1129	65	0
38	55	959	0	1021	47	0
38	98	967	0	1033	58	0
39	65	881	0	943	68	0
39	A8	881	0	943	61	0
40	75	1141	0	1202	69	0
40	B8	1141	0	1202	55	0
41	85	963	0	1022	49	0
41	C8	963	0	1022	62	0
42	95	778	0	852	62	0
42	D8	778	0	852	42	0
43	A5	899	0	964	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	E8	899	0	964	33	0
44	B5	725	0	778	34	0
44	F8	742	0	803	42	0
45	C5	794	0	884	56	0
45	G8	791	0	881	55	0
46	D5	1428	0	1454	69	0
46	H8	1397	0	1430	56	0
47	E5	606	0	628	39	0
47	I8	626	0	642	38	0
48	F5	762	0	848	30	0
48	J8	762	0	848	28	0
49	G5	558	0	610	27	0
49	K8	563	0	612	44	0
50	H5	468	0	518	17	0
50	L8	452	0	503	35	0
51	I5	515	0	514	33	0
51	M8	533	0	526	42	0
52	J5	434	0	454	23	0
52	N8	453	0	475	18	0
53	K5	389	0	404	18	0
53	O8	389	0	404	30	0
54	L5	398	0	441	19	0
54	P8	391	0	432	14	0
55	M5	477	0	540	44	0
55	Q8	485	0	551	72	0
56	11	2	0	0	0	0
56	13	152	0	0	0	0
56	14	426	0	0	0	0
56	15	1	0	0	0	0
56	16	15	0	0	0	0
56	1G	88	0	0	0	0
56	1H	506	0	0	0	0
56	1J	10	0	0	0	0
56	21	2	0	0	0	0
56	25	2	0	0	0	0
56	29	2	0	0	0	0
56	2K	7	0	0	0	0
56	2L	3	0	0	0	0
56	31	1	0	0	0	0
56	32	1	0	0	0	0
56	35	1	0	0	0	0
56	39	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	3I	2	0	0	0	0
56	41	2	0	0	0	0
56	45	2	0	0	0	0
56	49	1	0	0	0	0
56	4K	1	0	0	0	0
56	52	1	0	0	0	0
56	5E	1	0	0	0	0
56	6A	1	0	0	0	0
56	78	2	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	C5	1	0	0	0	0
56	E5	1	0	0	0	0
56	G8	1	0	0	0	0
56	I8	2	0	0	0	0
56	J8	1	0	0	0	0
56	L8	1	0	0	0	0
56	M5	1	0	0	0	0
56	P8	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5A	1	0	0	0	0
57	5I	1	0	0	0	0
57	C5	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	3	0
58	13	164	0	0	12	0
58	14	543	0	0	112	0
58	15	1	0	0	0	0
58	16	6	0	0	2	0
58	19	3	0	0	3	0
58	1G	64	0	0	12	0
58	1H	920	0	0	187	0
58	1I	1	0	0	1	0
58	1J	18	0	0	2	0
58	21	5	0	0	2	0
58	29	3	0	0	0	0
58	31	7	0	0	0	0
58	32	1	0	0	0	0
58	35	1	0	0	0	0
58	39	8	0	0	0	0
58	3E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	3I	1	0	0	0	0
58	4E	1	0	0	0	0
58	4K	1	0	0	0	0
58	5I	1	0	0	0	0
58	6I	1	0	0	0	0
58	78	6	0	0	1	0
58	7A	1	0	0	0	0
58	7I	1	0	0	0	0
58	85	1	0	0	0	0
58	B8	1	0	0	0	0
58	C8	2	0	0	0	0
58	E8	1	0	0	0	0
58	F8	1	0	0	0	0
58	G8	3	0	0	1	0
58	J8	1	0	0	0	0
58	L5	2	0	0	0	0
58	L8	3	0	0	1	0
58	P8	1	0	0	0	0
58	Q8	2	0	0	0	0
All	All	299951	0	200381	8425	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1604:C:OP2	58:1H:3643:HOH:O	1.58	1.18
40:B8:50:ILE:HD11	40:B8:102:ILE:HD11	1.35	1.08
26:1H:2576:G:OP1	58:1H:3756:HOH:O	1.73	1.07
26:1H:1614:A:OP1	58:1H:3859:HOH:O	1.76	1.03
26:14:1774:C:OP1	58:14:3564:HOH:O	1.77	1.03

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.14	0.06

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
2	12	235/256 (92%)	198 (84%)	34 (14%)	3 (1%)	12 38
2	1E	235/256 (92%)	199 (85%)	30 (13%)	6 (3%)	5 22
3	22	204/239 (85%)	178 (87%)	26 (13%)	0	100 100
3	2E	203/239 (85%)	186 (92%)	14 (7%)	3 (2%)	10 35
4	32	206/209 (99%)	179 (87%)	27 (13%)	0	100 100
4	3E	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	10 35
5	42	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22 52
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22 52
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100 100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100 100
7	62	153/156 (98%)	143 (94%)	10 (6%)	0	100 100
7	6E	153/156 (98%)	142 (93%)	11 (7%)	0	100 100
8	72	136/138 (99%)	125 (92%)	11 (8%)	0	100 100
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22 52
9	82	125/128 (98%)	116 (93%)	9 (7%)	0	100 100
9	8E	125/128 (98%)	110 (88%)	15 (12%)	0	100 100
10	1A	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
10	1I	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
11	2A	114/129 (88%)	103 (90%)	10 (9%)	1 (1%)	17 47
11	2I	114/129 (88%)	101 (89%)	12 (10%)	1 (1%)	17 47
12	3A	123/132 (93%)	101 (82%)	18 (15%)	4 (3%)	4 17
12	3I	123/132 (93%)	104 (85%)	19 (15%)	0	100 100
13	4A	115/126 (91%)	95 (83%)	19 (16%)	1 (1%)	17 47
13	4I	116/126 (92%)	95 (82%)	20 (17%)	1 (1%)	17 47
14	5A	56/61 (92%)	47 (84%)	8 (14%)	1 (2%)	8 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	17
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	8A	98/105 (93%)	89 (91%)	9 (9%)	0	100	100
17	8I	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	9A	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	11	36
18	9I	70/88 (80%)	62 (89%)	6 (9%)	2 (3%)	4	20
19	AA	76/93 (82%)	60 (79%)	14 (18%)	2 (3%)	5	22
19	AI	79/93 (85%)	68 (86%)	8 (10%)	3 (4%)	3	15
20	BA	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	15	45
20	BI	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	15	45
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
28	11	270/276 (98%)	247 (92%)	17 (6%)	6 (2%)	6	25
28	19	271/276 (98%)	252 (93%)	16 (6%)	3 (1%)	14	42
29	21	203/206 (98%)	166 (82%)	29 (14%)	8 (4%)	3	15
29	29	203/206 (98%)	160 (79%)	32 (16%)	11 (5%)	2	9
30	31	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	29	60
30	39	206/210 (98%)	174 (84%)	28 (14%)	4 (2%)	8	29
31	41	179/182 (98%)	155 (87%)	20 (11%)	4 (2%)	6	25
31	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	14	42
32	51	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	4	20
32	59	167/180 (93%)	136 (81%)	28 (17%)	3 (2%)	8	30
33	61	144/148 (97%)	118 (82%)	21 (15%)	5 (4%)	3	17
33	69	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	7	26
34	15	136/140 (97%)	122 (90%)	14 (10%)	0	100	100
34	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	6	25
35	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	35	148/150 (99%)	110 (74%)	35 (24%)	3 (2%)	7	27
36	78	148/150 (99%)	115 (78%)	25 (17%)	8 (5%)	2	9
37	45	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	4	20
37	88	134/141 (95%)	112 (84%)	18 (13%)	4 (3%)	4	19
38	55	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	47
39	65	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	5	21
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	47
40	75	135/146 (92%)	113 (84%)	21 (16%)	1 (1%)	22	52
40	B8	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
41	85	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	47
41	C8	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	47
42	95	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	4	19
42	D8	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	45
43	A5	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	E8	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
44	B5	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	14	42
44	F8	92/96 (96%)	83 (90%)	6 (6%)	3 (3%)	4	17
45	C5	102/110 (93%)	73 (72%)	24 (24%)	5 (5%)	2	11
45	G8	102/110 (93%)	84 (82%)	14 (14%)	4 (4%)	3	15
46	D5	177/206 (86%)	136 (77%)	31 (18%)	10 (6%)	2	9
46	H8	173/206 (84%)	142 (82%)	27 (16%)	4 (2%)	6	24
47	E5	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	12	38
48	F5	95/98 (97%)	83 (87%)	11 (12%)	1 (1%)	14	42
48	J8	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
49	G5	64/72 (89%)	57 (89%)	5 (8%)	2 (3%)	4	19
49	K8	65/72 (90%)	56 (86%)	7 (11%)	2 (3%)	4	19
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	49 (89%)	5 (9%)	1 (2%)	8	30
51	I5	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	M8	64/71 (90%)	45 (70%)	16 (25%)	3 (5%)	2 12
52	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100 100
52	N8	56/60 (93%)	52 (93%)	4 (7%)	0	100 100
53	K5	43/54 (80%)	29 (67%)	14 (33%)	0	100 100
53	O8	43/54 (80%)	31 (72%)	12 (28%)	0	100 100
54	L5	44/49 (90%)	43 (98%)	1 (2%)	0	100 100
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100 100
55	M5	58/65 (89%)	46 (79%)	11 (19%)	1 (2%)	9 32
55	Q8	59/65 (91%)	39 (66%)	16 (27%)	4 (7%)	1 6
All	All	11325/12054 (94%)	9841 (87%)	1312 (12%)	172 (2%)	10 35

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	11	239	ARG
31	41	14	GLU
44	F8	68	ARG
49	K8	47	ASN
49	K8	48	HIS

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
2	12	205/220 (93%)	167 (82%)	38 (18%)	1 6
2	1E	205/220 (93%)	167 (82%)	38 (18%)	1 6
3	22	160/188 (85%)	132 (82%)	28 (18%)	2 7
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2 7
4	32	180/181 (99%)	148 (82%)	32 (18%)	2 7
4	3E	180/181 (99%)	147 (82%)	33 (18%)	1 6
5	42	116/123 (94%)	93 (80%)	23 (20%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4E	116/123 (94%)	87 (75%)	29 (25%)	0	1
6	52	90/90 (100%)	76 (84%)	14 (16%)	2	10
6	5E	90/90 (100%)	78 (87%)	12 (13%)	4	14
7	62	126/127 (99%)	105 (83%)	21 (17%)	2	8
7	6E	126/127 (99%)	103 (82%)	23 (18%)	1	6
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	8
8	7E	119/119 (100%)	97 (82%)	22 (18%)	1	6
9	82	98/99 (99%)	81 (83%)	17 (17%)	2	7
9	8E	98/99 (99%)	76 (78%)	22 (22%)	1	3
10	1A	89/92 (97%)	81 (91%)	8 (9%)	9	30
10	1I	89/92 (97%)	78 (88%)	11 (12%)	4	17
11	2A	88/99 (89%)	76 (86%)	12 (14%)	3	14
11	2I	88/99 (89%)	75 (85%)	13 (15%)	3	11
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	3
12	3I	104/109 (95%)	88 (85%)	16 (15%)	2	10
13	4A	94/101 (93%)	79 (84%)	15 (16%)	2	9
13	4I	94/101 (93%)	75 (80%)	19 (20%)	1	4
14	5A	48/50 (96%)	41 (85%)	7 (15%)	3	12
14	5I	49/50 (98%)	37 (76%)	12 (24%)	0	2
15	6A	79/80 (99%)	70 (89%)	9 (11%)	5	20
15	6I	79/80 (99%)	71 (90%)	8 (10%)	7	25
16	7A	72/74 (97%)	58 (81%)	14 (19%)	1	5
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	95/97 (98%)	83 (87%)	12 (13%)	4	16
17	8I	95/97 (98%)	81 (85%)	14 (15%)	3	11
18	9A	63/77 (82%)	49 (78%)	14 (22%)	1	3
18	9I	63/77 (82%)	53 (84%)	10 (16%)	2	9
19	AA	67/80 (84%)	52 (78%)	15 (22%)	1	3
19	AI	70/80 (88%)	49 (70%)	21 (30%)	0	0
20	BA	76/82 (93%)	61 (80%)	15 (20%)	1	5
20	BI	76/82 (93%)	62 (82%)	14 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	25
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	54
28	11	214/218 (98%)	171 (80%)	43 (20%)	1	4
28	19	214/218 (98%)	180 (84%)	34 (16%)	2	9
29	21	165/166 (99%)	122 (74%)	43 (26%)	0	1
29	29	165/166 (99%)	134 (81%)	31 (19%)	1	5
30	31	161/166 (97%)	130 (81%)	31 (19%)	1	5
30	39	165/166 (99%)	132 (80%)	33 (20%)	1	4
31	41	155/156 (99%)	128 (83%)	27 (17%)	2	7
31	49	155/156 (99%)	132 (85%)	23 (15%)	3	11
32	51	145/148 (98%)	114 (79%)	31 (21%)	1	3
32	59	141/148 (95%)	112 (79%)	29 (21%)	1	4
33	61	122/124 (98%)	88 (72%)	34 (28%)	0	1
33	69	122/124 (98%)	93 (76%)	29 (24%)	0	2
34	15	117/119 (98%)	95 (81%)	22 (19%)	1	5
34	58	117/119 (98%)	94 (80%)	23 (20%)	1	5
35	25	100/100 (100%)	77 (77%)	23 (23%)	1	2
35	68	100/100 (100%)	84 (84%)	16 (16%)	2	9
36	35	116/116 (100%)	76 (66%)	40 (34%)	0	0
36	78	116/116 (100%)	80 (69%)	36 (31%)	0	0
37	45	111/111 (100%)	84 (76%)	27 (24%)	0	2
37	88	104/111 (94%)	81 (78%)	23 (22%)	1	3
38	55	100/101 (99%)	78 (78%)	22 (22%)	1	3
38	98	101/101 (100%)	81 (80%)	20 (20%)	1	5
39	65	87/88 (99%)	64 (74%)	23 (26%)	0	1
39	A8	87/88 (99%)	60 (69%)	27 (31%)	0	0
40	75	120/127 (94%)	92 (77%)	28 (23%)	1	2
40	B8	120/127 (94%)	89 (74%)	31 (26%)	0	1
41	85	93/94 (99%)	80 (86%)	13 (14%)	3	13
41	C8	93/94 (99%)	76 (82%)	17 (18%)	1	6
42	95	82/82 (100%)	57 (70%)	25 (30%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	D8	82/82 (100%)	61 (74%)	21 (26%)	0	1
43	A5	92/92 (100%)	78 (85%)	14 (15%)	3	10
43	E8	92/92 (100%)	72 (78%)	20 (22%)	1	3
44	B5	74/78 (95%)	57 (77%)	17 (23%)	1	2
44	F8	76/78 (97%)	59 (78%)	17 (22%)	1	3
45	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
45	G8	85/91 (93%)	67 (79%)	18 (21%)	1	4
46	D5	158/179 (88%)	131 (83%)	27 (17%)	2	7
46	H8	154/179 (86%)	123 (80%)	31 (20%)	1	4
47	E5	61/67 (91%)	52 (85%)	9 (15%)	3	11
47	I8	61/67 (91%)	52 (85%)	9 (15%)	3	11
48	F5	82/83 (99%)	67 (82%)	15 (18%)	1	6
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	4
49	G5	62/67 (92%)	53 (86%)	9 (14%)	3	12
49	K8	62/67 (92%)	41 (66%)	21 (34%)	0	0
50	H5	51/52 (98%)	42 (82%)	9 (18%)	2	7
50	L8	49/52 (94%)	40 (82%)	9 (18%)	1	6
51	I5	57/63 (90%)	47 (82%)	10 (18%)	2	7
51	M8	59/63 (94%)	44 (75%)	15 (25%)	0	1
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	2
52	N8	51/52 (98%)	38 (74%)	13 (26%)	0	1
53	K5	44/52 (85%)	32 (73%)	12 (27%)	0	1
53	O8	44/52 (85%)	26 (59%)	18 (41%)	0	0
54	L5	39/42 (93%)	32 (82%)	7 (18%)	2	6
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	9
55	M5	49/55 (89%)	37 (76%)	12 (24%)	0	2
55	Q8	50/55 (91%)	32 (64%)	18 (36%)	0	0
All	All	9556/9998 (96%)	7642 (80%)	1914 (20%)	1	4

5 of 1914 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	L8	53	LEU

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Mol	Chain	Res	Type
45	C5	38	ILE
7	62	91	VAL
44	B5	27	THR
53	K5	45	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
8	72	15	ASN
51	I5	20	ASN
34	15	56	ASN
49	G5	48	HIS
30	39	203	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	328 (21%)	30 (2%)
1	1G	1495/1522 (98%)	348 (23%)	39 (2%)
22	1K	74/76 (97%)	31 (41%)	2 (2%)
23	2K	76/77 (98%)	15 (19%)	3 (3%)
23	2L	76/77 (98%)	20 (26%)	3 (3%)
24	1L	75/76 (98%)	26 (34%)	2 (2%)
24	3K	75/76 (98%)	38 (50%)	4 (5%)
24	3L	75/76 (98%)	32 (42%)	2 (2%)
25	4K	12/27 (44%)	4 (33%)	0
25	4L	8/27 (29%)	3 (37%)	1 (12%)
26	14	2908/2917 (99%)	736 (25%)	37 (1%)
26	1H	2911/2917 (99%)	688 (23%)	52 (1%)
27	16	121/122 (99%)	19 (15%)	0
27	1J	121/122 (99%)	31 (25%)	3 (2%)
All	All	9523/9634 (98%)	2319 (24%)	178 (1%)

5 of 2319 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A

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Mol	Chain	Res	Type
1	13	9	G

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	992	U
26	14	528	A
1	1G	1126	U
24	1L	10	G
26	14	1085	A

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

17 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	$\#\|Z\| > 2$
23	7MG	2K	47	23	22,26,27	3.19	6 (27%)	29,39,42	2.69	11 (37%)
22	7MG	1K	46	22	22,26,27	3.07	7 (31%)	29,39,42	2.87	9 (31%)
22	5MU	1K	54	22	19,22,23	3.94	5 (26%)	28,32,35	3.10	7 (25%)
23	7MG	2L	47	23	22,26,27	3.11	6 (27%)	29,39,42	2.80	10 (34%)
23	4SU	2L	8	23	18,21,22	1.96	5 (27%)	26,30,33	2.36	7 (26%)
22	PSU	1K	55	22	18,21,22	1.36	1 (5%)	22,30,33	1.49	4 (18%)
23	OMC	2L	33	23	19,22,23	1.84	3 (15%)	26,31,34	1.31	3 (11%)
23	5MU	2L	55	23	19,22,23	3.89	5 (26%)	28,32,35	3.38	8 (28%)
23	5MU	2K	55	23	19,22,23	3.90	5 (26%)	28,32,35	3.38	7 (25%)
22	PSU	1K	32	22	18,21,22	1.26	1 (5%)	22,30,33	1.39	3 (13%)
23	OMC	2K	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.03	1 (3%)
23	PSU	2L	56	23	18,21,22	1.30	2 (11%)	22,30,33	1.68	2 (9%)
22	PSU	1K	39	22	18,21,22	1.06	2 (11%)	22,30,33	1.57	4 (18%)
22	MIA	1K	37	22	24,31,32	2.55	4 (16%)	26,44,47	2.59	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	4SU	1K	8	22	18,21,22	1.88	5 (27%)	26,30,33	2.27	5 (19%)
23	4SU	2K	8	23	18,21,22	1.90	2 (11%)	26,30,33	3.22	10 (38%)
23	PSU	2K	56	23	18,21,22	1.06	2 (11%)	22,30,33	1.74	4 (18%)

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
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
22	7MG	1K	46	22	-	1/7/37/38	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	1/7/37/38	0/3/3/3
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	2/9/27/28	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	32	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
22	MIA	1K	37	22	-	4/11/33/34	0/3/3/3
22	4SU	1K	8	22	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	3/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.68	1.58	1.38
22	1K	54	5MU	C2-N1	12.62	1.58	1.38
23	2K	55	5MU	C2-N1	12.47	1.58	1.38
22	1K	37	MIA	C13-C14	9.50	1.59	1.32
23	2L	47	7MG	C5-N7	8.93	1.45	1.35

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	11.52	125.15	115.31
23	2L	55	5MU	C5-C4-N3	11.10	124.79	115.31
22	1K	54	5MU	C5-C4-N3	10.77	124.50	115.31
23	2K	8	4SU	C4-N3-C2	-10.74	116.91	127.34
22	1K	37	MIA	C12-C13-C14	-7.83	111.90	127.14

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2K	8	4SU	O4'-C4'-C5'-O5'
22	1K	37	MIA	N1-C2-S10-C11
22	1K	37	MIA	N3-C2-S10-C11
22	1K	37	MIA	C12-C13-C14-C15
22	1K	37	MIA	C12-C13-C14-C16

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	47	7MG	2	0
22	1K	46	7MG	3	0
22	1K	54	5MU	1	0
23	2L	47	7MG	1	0
23	2L	8	4SU	1	0
22	1K	55	PSU	1	0
23	2L	33	OMC	5	0
23	2L	55	5MU	3	0
23	2K	55	5MU	3	0
23	2K	33	OMC	1	0
22	1K	37	MIA	3	0
23	2K	8	4SU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1253 ligands modelled in this entry, 1253 are monoatomic - leaving 0 for Mogul analysis.

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	13	1498/1522 (98%)	0.21	45 (3%)	50	25	73, 122, 204, 309	0
1	1G	1497/1522 (98%)	0.24	74 (4%)	29	13	92, 145, 218, 318	0
2	12	237/256 (92%)	0.20	17 (7%)	15	5	168, 199, 220, 228	0
2	1E	237/256 (92%)	0.13	8 (3%)	45	22	132, 167, 193, 205	0
3	22	206/239 (86%)	0.04	7 (3%)	45	22	161, 182, 205, 218	0
3	2E	205/239 (85%)	-0.02	1 (0%)	91	79	103, 128, 161, 170	0
4	32	208/209 (99%)	0.59	18 (8%)	10	3	122, 144, 165, 174	0
4	3E	208/209 (99%)	0.77	30 (14%)	2	1	102, 129, 151, 165	0
5	42	151/162 (93%)	0.52	18 (11%)	4	1	136, 154, 171, 203	0
5	4E	151/162 (93%)	0.57	19 (12%)	3	1	97, 120, 143, 176	0
6	52	101/101 (100%)	-0.27	0	100	100	106, 127, 147, 161	0
6	5E	101/101 (100%)	-0.07	0	100	100	101, 123, 148, 161	0
7	62	155/156 (99%)	0.92	27 (17%)	1	0	136, 154, 182, 207	0
7	6E	155/156 (99%)	0.49	16 (10%)	6	2	124, 139, 168, 193	0
8	72	138/138 (100%)	1.28	42 (30%)	0	0	130, 158, 174, 179	0
8	7E	138/138 (100%)	0.90	26 (18%)	1	0	105, 129, 141, 149	0
9	82	127/128 (99%)	3.27	75 (59%)	0	0	141, 183, 204, 208	0
9	8E	127/128 (99%)	1.66	45 (35%)	0	0	107, 156, 179, 193	0
10	1A	99/105 (94%)	1.96	39 (39%)	0	0	153, 184, 203, 210	0
10	1I	99/105 (94%)	1.40	32 (32%)	0	0	102, 155, 187, 192	0
11	2A	116/129 (89%)	0.50	11 (9%)	8	2	111, 137, 158, 182	0
11	2I	116/129 (89%)	0.27	8 (6%)	16	6	90, 127, 153, 180	0
12	3A	125/132 (94%)	1.24	35 (28%)	0	0	109, 134, 160, 185	0
12	3I	125/132 (94%)	0.44	11 (8%)	10	3	83, 96, 131, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	4A	117/126 (92%)	1.15	30 (25%)	0	0	140, 184, 206, 216	0
13	4I	118/126 (93%)	0.25	7 (5%)	22	9	101, 139, 159, 170	0
14	5A	58/61 (95%)	4.97	46 (79%)	0	0	164, 179, 194, 201	0
14	5I	60/61 (98%)	1.88	24 (40%)	0	0	106, 118, 137, 147	0
15	6A	88/89 (98%)	0.81	12 (13%)	3	1	118, 139, 155, 159	0
15	6I	88/89 (98%)	1.02	21 (23%)	0	0	98, 125, 142, 154	0
16	7A	84/88 (95%)	1.04	19 (22%)	0	0	113, 132, 150, 174	0
16	7I	84/88 (95%)	3.10	55 (65%)	0	0	122, 135, 169, 187	0
17	8A	100/105 (95%)	1.17	21 (21%)	1	0	118, 138, 153, 176	0
17	8I	100/105 (95%)	0.66	14 (14%)	2	1	108, 127, 140, 145	0
18	9A	72/88 (81%)	0.04	2 (2%)	53	28	116, 142, 178, 198	0
18	9I	72/88 (81%)	0.10	0	100	100	109, 127, 162, 187	0
19	AA	78/93 (83%)	1.25	25 (32%)	0	0	172, 203, 216, 222	0
19	AI	81/93 (87%)	0.47	5 (6%)	20	8	109, 135, 160, 166	0
20	BA	99/106 (93%)	1.63	43 (43%)	0	0	108, 130, 158, 173	0
20	BI	99/106 (93%)	1.35	34 (34%)	0	0	129, 144, 177, 183	0
21	1B	25/27 (92%)	6.10	23 (92%)	0	0	147, 163, 179, 196	0
21	1F	25/27 (92%)	4.77	22 (88%)	0	0	114, 126, 139, 164	0
22	1K	69/76 (90%)	0.12	4 (5%)	23	9	101, 222, 265, 271	0
23	2K	72/77 (93%)	0.05	0	100	100	84, 108, 137, 146	0
23	2L	72/77 (93%)	-0.42	1 (1%)	75	53	96, 136, 166, 170	0
24	1L	76/76 (100%)	0.81	12 (15%)	2	0	147, 264, 289, 295	0
24	3K	76/76 (100%)	-0.06	2 (2%)	56	30	92, 255, 286, 289	0
24	3L	76/76 (100%)	0.49	9 (11%)	4	1	104, 264, 294, 299	0
25	4K	13/27 (48%)	0.92	0	100	100	88, 101, 151, 157	0
25	4L	9/27 (33%)	0.59	0	100	100	121, 154, 165, 175	0
26	14	2909/2917 (99%)	0.21	70 (2%)	59	34	67, 105, 270, 378	0
26	1H	2912/2917 (99%)	0.28	12 (0%)	92	82	56, 91, 253, 353	0
27	16	122/122 (100%)	-0.17	0	100	100	83, 111, 133, 217	0
27	1J	122/122 (100%)	-0.13	1 (0%)	86	70	106, 152, 174, 226	0
28	11	272/276 (98%)	0.50	8 (2%)	51	26	57, 82, 100, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	19	273/276 (98%)	0.90	40 (14%)	2	1	67, 94, 110, 125	0
29	21	205/206 (99%)	0.91	27 (13%)	3	1	66, 109, 151, 165	0
29	29	205/206 (99%)	1.30	67 (32%)	0	0	76, 113, 158, 183	0
30	31	202/210 (96%)	0.32	2 (0%)	82	63	60, 94, 130, 150	0
30	39	208/210 (99%)	0.43	14 (6%)	17	7	76, 123, 179, 199	0
31	41	181/182 (99%)	0.31	9 (4%)	28	12	100, 121, 159, 172	0
31	49	181/182 (99%)	1.07	41 (22%)	0	0	148, 169, 198, 209	0
32	51	174/180 (96%)	0.12	5 (2%)	51	26	99, 122, 139, 150	0
32	59	169/180 (93%)	1.64	62 (36%)	0	0	169, 218, 243, 258	0
33	61	146/148 (98%)	-0.02	4 (2%)	54	28	98, 154, 170, 175	0
33	69	146/148 (98%)	0.71	22 (15%)	2	1	102, 146, 170, 175	0
34	15	138/140 (98%)	1.27	35 (25%)	0	0	98, 129, 161, 185	0
34	58	138/140 (98%)	0.79	15 (10%)	5	2	81, 109, 148, 163	0
35	25	122/122 (100%)	0.51	9 (7%)	14	5	85, 107, 125, 135	0
35	68	122/122 (100%)	0.41	3 (2%)	57	32	75, 92, 111, 124	0
36	35	150/150 (100%)	1.13	40 (26%)	0	0	77, 128, 162, 198	0
36	78	150/150 (100%)	0.56	11 (7%)	15	5	64, 98, 124, 176	0
37	45	141/141 (100%)	2.38	78 (55%)	0	0	97, 129, 154, 167	0
37	88	138/141 (97%)	0.52	6 (4%)	35	16	70, 95, 115, 147	0
38	55	117/118 (99%)	0.97	20 (17%)	1	0	77, 97, 113, 133	0
38	98	118/118 (100%)	0.82	13 (11%)	5	2	79, 102, 125, 139	0
39	65	111/112 (99%)	1.38	36 (32%)	0	0	118, 145, 162, 172	0
39	A8	111/112 (99%)	0.36	4 (3%)	42	21	92, 107, 130, 144	0
40	75	137/146 (93%)	0.31	10 (7%)	15	5	96, 115, 173, 208	0
40	B8	137/146 (93%)	0.49	12 (8%)	10	3	86, 111, 170, 202	0
41	85	117/118 (99%)	0.79	17 (14%)	2	1	86, 115, 155, 180	0
41	C8	117/118 (99%)	0.86	19 (16%)	1	0	71, 98, 136, 147	0
42	95	101/101 (100%)	0.51	14 (13%)	2	1	86, 143, 161, 177	0
42	D8	101/101 (100%)	0.31	10 (9%)	7	2	73, 123, 149, 162	0
43	A5	113/113 (100%)	0.42	7 (6%)	20	8	77, 94, 124, 183	0
43	E8	113/113 (100%)	0.38	3 (2%)	54	28	75, 91, 125, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	B5	92/96 (95%)	0.68	8 (8%) 10 3	85, 102, 129, 133	0
44	F8	94/96 (97%)	0.29	1 (1%) 80 60	69, 88, 113, 128	0
45	C5	104/110 (94%)	1.29	25 (24%) 0 0	107, 137, 167, 175	0
45	G8	104/110 (94%)	0.30	0 100 100	87, 113, 147, 166	0
46	D5	179/206 (86%)	0.99	35 (19%) 1 0	139, 176, 263, 269	0
46	H8	175/206 (84%)	-0.05	1 (0%) 89 76	97, 139, 228, 236	0
47	E5	76/85 (89%)	1.90	35 (46%) 0 0	85, 111, 130, 169	0
47	I8	80/85 (94%)	1.09	20 (25%) 0 0	71, 90, 122, 131	0
48	F5	97/98 (98%)	1.73	32 (32%) 0 0	79, 102, 146, 163	0
48	J8	97/98 (98%)	1.14	14 (14%) 2 1	69, 91, 145, 176	0
49	G5	66/72 (91%)	0.19	2 (3%) 50 25	101, 121, 141, 167	0
49	K8	67/72 (93%)	0.39	2 (2%) 50 25	76, 96, 119, 154	0
50	H5	59/60 (98%)	1.04	13 (22%) 0 0	97, 126, 167, 182	0
50	L8	57/60 (95%)	0.18	0 100 100	77, 98, 120, 133	0
51	I5	63/71 (88%)	1.49	22 (34%) 0 0	179, 219, 236, 243	0
51	M8	66/71 (92%)	0.45	6 (9%) 9 3	128, 174, 203, 214	0
52	J5	56/60 (93%)	0.38	4 (7%) 16 6	77, 103, 150, 162	0
52	N8	58/60 (96%)	0.93	6 (10%) 6 2	68, 115, 186, 191	0
53	K5	45/54 (83%)	7.07	38 (84%) 0 0	153, 180, 196, 202	0
53	O8	45/54 (83%)	3.61	32 (71%) 0 0	131, 159, 177, 183	0
54	L5	46/49 (93%)	0.72	3 (6%) 18 7	64, 76, 89, 102	0
54	P8	45/49 (91%)	0.14	0 100 100	59, 64, 78, 92	0
55	M5	60/65 (92%)	2.18	36 (60%) 0 0	89, 101, 125, 147	0
55	Q8	61/65 (93%)	1.77	23 (37%) 0 0	74, 91, 117, 128	0
All	All	21042/21688 (97%)	0.57	2139 (10%) 6 2	56, 122, 214, 378	0

The worst 5 of 2139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	K5	42	TRP	19.7
53	K5	51	GLU	19.1
24	3L	17	C	18.5
7	62	81	GLY	16.8
7	62	82	GLY	16.6

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
22	PSU	1K	55	20/21	0.78	0.12	153,172,191,191	0
22	4SU	1K	8	20/21	0.80	0.14	184,192,200,205	0
22	7MG	1K	46	24/25	0.87	0.12	175,197,203,209	0
23	4SU	2L	8	20/21	0.88	0.14	128,140,143,147	0
22	PSU	1K	32	20/21	0.89	0.32	113,119,123,123	0
23	PSU	2L	56	20/21	0.90	0.09	128,135,142,148	0
22	5MU	1K	54	21/22	0.93	0.10	142,157,168,172	0
22	PSU	1K	39	20/21	0.94	0.17	96,108,116,119	0
23	4SU	2K	8	20/21	0.94	0.21	100,108,123,123	0
22	MIA	1K	37	29/30	0.94	0.30	89,100,118,123	0
23	5MU	2L	55	21/22	0.95	0.11	138,142,147,151	0
23	7MG	2K	47	24/25	0.95	0.17	110,120,128,137	0
23	7MG	2L	47	24/25	0.95	0.12	140,151,156,161	0
23	PSU	2K	56	20/21	0.96	0.14	109,113,120,127	0
23	OMC	2L	33	21/22	0.96	0.20	124,127,132,137	0
23	5MU	2K	55	21/22	0.97	0.15	99,116,125,136	0
23	OMC	2K	33	21/22	0.98	0.32	88,94,101,106	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	1H	3119	1/1	0.35	0.52	101,101,101,101	0
56	MG	1H	3498	1/1	0.39	0.20	119,119,119,119	0
56	MG	1H	3142	1/1	0.41	0.41	88,88,88,88	0
56	MG	13	1720	1/1	0.43	0.24	104,104,104,104	0
56	MG	13	1750	1/1	0.45	0.35	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1710	1/1	0.45	0.30	98,98,98,98	0
56	MG	14	3391	1/1	0.46	0.10	124,124,124,124	0
56	MG	13	1739	1/1	0.47	0.20	120,120,120,120	0
56	MG	13	1697	1/1	0.47	0.26	97,97,97,97	0
56	MG	14	3420	1/1	0.48	0.07	130,130,130,130	0
56	MG	1H	3028	1/1	0.49	0.43	115,115,115,115	0
56	MG	1G	1633	1/1	0.49	0.32	93,93,93,93	0
56	MG	14	3183	1/1	0.51	0.32	110,110,110,110	0
56	MG	13	1631	1/1	0.51	0.70	102,102,102,102	0
56	MG	1H	3322	1/1	0.51	0.22	96,96,96,96	0
56	MG	14	3307	1/1	0.52	0.25	87,87,87,87	0
56	MG	16	205	1/1	0.53	0.20	91,91,91,91	0
56	MG	14	3020	1/1	0.54	0.51	92,92,92,92	0
56	MG	1H	3154	1/1	0.54	0.22	91,91,91,91	0
56	MG	14	3262	1/1	0.54	0.29	81,81,81,81	0
56	MG	1G	1629	1/1	0.55	0.18	124,124,124,124	0
56	MG	13	1692	1/1	0.56	0.22	102,102,102,102	0
56	MG	13	1683	1/1	0.56	0.28	106,106,106,106	0
56	MG	14	3288	1/1	0.56	0.53	107,107,107,107	0
56	MG	29	302	1/1	0.56	0.35	108,108,108,108	0
56	MG	M5	101	1/1	0.56	0.25	94,94,94,94	0
56	MG	1H	3281	1/1	0.57	0.30	85,85,85,85	0
56	MG	14	3284	1/1	0.57	0.30	100,100,100,100	0
56	MG	1H	3313	1/1	0.57	0.24	93,93,93,93	0
56	MG	1H	3200	1/1	0.57	0.35	104,104,104,104	0
56	MG	13	1658	1/1	0.58	0.44	117,117,117,117	0
56	MG	14	3329	1/1	0.58	0.21	120,120,120,120	0
56	MG	1G	1644	1/1	0.59	0.19	115,115,115,115	0
56	MG	1H	3250	1/1	0.59	0.21	104,104,104,104	0
56	MG	13	1606	1/1	0.60	0.33	115,115,115,115	0
56	MG	1H	3243	1/1	0.60	0.36	93,93,93,93	0
56	MG	13	1745	1/1	0.61	0.39	121,121,121,121	0
56	MG	13	1708	1/1	0.61	0.34	119,119,119,119	0
56	MG	14	3181	1/1	0.61	0.21	100,100,100,100	0
56	MG	14	3295	1/1	0.61	0.62	95,95,95,95	0
56	MG	1H	3309	1/1	0.61	0.45	96,96,96,96	0
56	MG	13	1636	1/1	0.62	0.30	100,100,100,100	0
56	MG	1H	3158	1/1	0.62	0.46	104,104,104,104	0
56	MG	13	1629	1/1	0.62	0.45	106,106,106,106	0
56	MG	14	3025	1/1	0.62	0.17	116,116,116,116	0
56	MG	1H	3255	1/1	0.63	0.45	117,117,117,117	0
56	MG	1H	3270	1/1	0.63	0.48	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	14	3201	1/1	0.63	0.30	111,111,111,111	0
56	MG	14	3260	1/1	0.63	0.17	119,119,119,119	0
56	MG	1H	3332	1/1	0.63	0.42	90,90,90,90	0
56	MG	1H	3029	1/1	0.63	0.28	110,110,110,110	0
56	MG	13	1717	1/1	0.63	0.28	114,114,114,114	0
56	MG	1H	3328	1/1	0.64	0.54	87,87,87,87	0
56	MG	1G	1670	1/1	0.64	0.40	138,138,138,138	0
56	MG	1H	3272	1/1	0.65	0.27	96,96,96,96	0
56	MG	1H	3337	1/1	0.65	0.42	106,106,106,106	0
56	MG	1H	3395	1/1	0.65	0.17	118,118,118,118	0
56	MG	1H	3431	1/1	0.65	0.11	163,163,163,163	0
56	MG	1H	3148	1/1	0.65	0.18	79,79,79,79	0
56	MG	13	1664	1/1	0.65	0.28	103,103,103,103	0
56	MG	14	3163	1/1	0.65	0.18	105,105,105,105	0
56	MG	14	3150	1/1	0.66	0.33	80,80,80,80	0
56	MG	14	3019	1/1	0.66	0.22	96,96,96,96	0
56	MG	1H	3276	1/1	0.66	0.44	99,99,99,99	0
56	MG	39	303	1/1	0.66	0.66	87,87,87,87	0
56	MG	E5	101	1/1	0.66	0.23	98,98,98,98	0
56	MG	13	1627	1/1	0.66	0.28	101,101,101,101	0
56	MG	1G	1664	1/1	0.67	0.27	116,116,116,116	0
56	MG	1G	1667	1/1	0.67	0.24	119,119,119,119	0
56	MG	1H	3023	1/1	0.67	0.37	100,100,100,100	0
56	MG	14	3026	1/1	0.68	0.39	92,92,92,92	0
56	MG	14	3133	1/1	0.68	0.13	97,97,97,97	0
56	MG	13	1716	1/1	0.68	0.18	111,111,111,111	0
56	MG	14	3312	1/1	0.68	0.12	93,93,93,93	0
56	MG	1G	1645	1/1	0.68	0.31	113,113,113,113	0
56	MG	13	1744	1/1	0.68	0.41	132,132,132,132	0
56	MG	1H	3464	1/1	0.68	0.14	133,133,133,133	0
56	MG	1H	3306	1/1	0.68	0.60	81,81,81,81	0
56	MG	1H	3273	1/1	0.68	0.25	84,84,84,84	0
56	MG	1H	3311	1/1	0.68	0.48	109,109,109,109	0
56	MG	1H	3343	1/1	0.68	0.36	92,92,92,92	0
56	MG	13	1640	1/1	0.69	0.23	94,94,94,94	0
56	MG	1H	3326	1/1	0.69	0.54	117,117,117,117	0
56	MG	14	3235	1/1	0.69	0.14	83,83,83,83	0
56	MG	14	3029	1/1	0.69	0.22	97,97,97,97	0
56	MG	13	1748	1/1	0.69	0.09	140,140,140,140	0
56	MG	1H	3330	1/1	0.69	0.56	104,104,104,104	0
56	MG	14	3286	1/1	0.69	0.15	92,92,92,92	0
56	MG	1G	1642	1/1	0.69	0.22	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3087	1/1	0.69	0.18	69,69,69,69	0
56	MG	1H	3135	1/1	0.70	0.26	111,111,111,111	0
56	MG	13	1669	1/1	0.70	0.27	110,110,110,110	0
56	MG	14	3143	1/1	0.70	0.43	100,100,100,100	0
56	MG	1H	3143	1/1	0.70	0.44	99,99,99,99	0
56	MG	1H	3331	1/1	0.70	0.82	106,106,106,106	0
56	MG	2L	102	1/1	0.70	0.26	89,89,89,89	0
56	MG	14	3182	1/1	0.70	0.27	98,98,98,98	0
56	MG	13	1749	1/1	0.70	0.23	121,121,121,121	0
56	MG	14	3372	1/1	0.70	0.12	134,134,134,134	0
56	MG	13	1639	1/1	0.70	0.19	109,109,109,109	0
56	MG	14	3403	1/1	0.70	0.09	122,122,122,122	0
56	MG	14	3203	1/1	0.70	0.29	81,81,81,81	0
56	MG	14	3227	1/1	0.70	0.33	97,97,97,97	0
56	MG	13	1714	1/1	0.70	0.22	101,101,101,101	0
56	MG	14	3251	1/1	0.70	0.10	105,105,105,105	0
56	MG	1H	3186	1/1	0.70	0.35	93,93,93,93	0
56	MG	13	1666	1/1	0.71	0.31	105,105,105,105	0
56	MG	14	3319	1/1	0.71	0.29	118,118,118,118	0
56	MG	13	1651	1/1	0.71	0.23	100,100,100,100	0
56	MG	14	3356	1/1	0.71	0.25	118,118,118,118	0
56	MG	14	3272	1/1	0.71	0.32	95,95,95,95	0
56	MG	14	3376	1/1	0.71	0.13	119,119,119,119	0
56	MG	1H	3505	1/1	0.71	0.15	112,112,112,112	0
56	MG	1H	3124	1/1	0.71	0.19	72,72,72,72	0
56	MG	14	3416	1/1	0.71	0.43	126,126,126,126	0
56	MG	13	1675	1/1	0.71	0.19	121,121,121,121	0
56	MG	14	3291	1/1	0.71	0.18	115,115,115,115	0
56	MG	14	3236	1/1	0.71	0.10	99,99,99,99	0
56	MG	14	3297	1/1	0.71	0.24	96,96,96,96	0
56	MG	1H	3157	1/1	0.71	0.51	104,104,104,104	0
56	MG	14	3294	1/1	0.72	0.14	91,91,91,91	0
56	MG	14	3274	1/1	0.72	0.25	122,122,122,122	0
56	MG	1H	3251	1/1	0.72	0.15	93,93,93,93	0
56	MG	13	1688	1/1	0.72	0.33	93,93,93,93	0
56	MG	1H	3266	1/1	0.72	0.58	95,95,95,95	0
56	MG	1H	3179	1/1	0.72	0.40	96,96,96,96	0
56	MG	14	3232	1/1	0.73	0.29	103,103,103,103	0
56	MG	1H	3137	1/1	0.73	0.53	87,87,87,87	0
56	MG	1H	3491	1/1	0.73	0.16	93,93,93,93	0
56	MG	1H	3340	1/1	0.73	0.36	93,93,93,93	0
56	MG	1H	3153	1/1	0.73	0.40	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	1G	1649	1/1	0.73	0.27	105,105,105,105	0
56	MG	14	3265	1/1	0.73	0.29	88,88,88,88	0
56	MG	13	1718	1/1	0.73	0.41	96,96,96,96	0
56	MG	14	3317	1/1	0.73	0.28	98,98,98,98	0
56	MG	1G	1620	1/1	0.73	0.20	107,107,107,107	0
56	MG	1H	3026	1/1	0.73	0.34	94,94,94,94	0
56	MG	13	1656	1/1	0.74	0.42	103,103,103,103	0
56	MG	1H	3062	1/1	0.74	0.23	101,101,101,101	0
56	MG	14	3418	1/1	0.74	0.07	130,130,130,130	0
56	MG	13	1689	1/1	0.74	0.25	98,98,98,98	0
56	MG	29	301	1/1	0.74	0.64	101,101,101,101	0
56	MG	1G	1643	1/1	0.74	0.30	104,104,104,104	0
56	MG	14	3276	1/1	0.74	1.33	103,103,103,103	0
56	MG	14	3252	1/1	0.74	0.15	105,105,105,105	0
56	MG	14	3030	1/1	0.74	0.22	115,115,115,115	0
56	MG	1H	3106	1/1	0.75	0.34	95,95,95,95	0
56	MG	1H	3415	1/1	0.75	0.07	99,99,99,99	0
56	MG	1H	3428	1/1	0.75	0.06	123,123,123,123	0
56	MG	1H	3265	1/1	0.75	0.27	96,96,96,96	0
56	MG	1H	3296	1/1	0.75	0.21	86,86,86,86	0
56	MG	1H	3169	1/1	0.75	0.25	85,85,85,85	0
56	MG	1H	3346	1/1	0.75	0.61	106,106,106,106	0
56	MG	1H	3504	1/1	0.75	0.11	138,138,138,138	0
56	MG	1J	203	1/1	0.75	0.17	114,114,114,114	0
56	MG	14	3313	1/1	0.75	0.19	124,124,124,124	0
56	MG	14	3315	1/1	0.75	0.13	92,92,92,92	0
56	MG	14	3281	1/1	0.75	0.55	105,105,105,105	0
56	MG	14	3170	1/1	0.75	0.60	77,77,77,77	0
56	MG	14	3285	1/1	0.75	0.30	91,91,91,91	0
56	MG	14	3318	1/1	0.76	0.19	99,99,99,99	0
56	MG	1H	3152	1/1	0.76	0.31	93,93,93,93	0
56	MG	1G	1625	1/1	0.76	0.12	131,131,131,131	0
56	MG	14	3311	1/1	0.76	0.17	89,89,89,89	0
56	MG	14	3368	1/1	0.76	0.11	117,117,117,117	0
56	MG	13	1690	1/1	0.76	0.19	108,108,108,108	0
56	MG	13	1641	1/1	0.76	0.35	88,88,88,88	0
56	MG	32	301	1/1	0.76	0.46	120,120,120,120	0
56	MG	14	3264	1/1	0.76	0.30	89,89,89,89	0
56	MG	14	3158	1/1	0.77	0.15	93,93,93,93	0
56	MG	1H	3189	1/1	0.77	0.30	81,81,81,81	0
56	MG	1H	3407	1/1	0.77	0.07	115,115,115,115	0
56	MG	16	214	1/1	0.77	0.22	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	1G	1604	1/1	0.77	0.23	142,142,142,142	0
56	MG	13	1685	1/1	0.77	0.17	112,112,112,112	0
56	MG	14	3196	1/1	0.77	0.34	99,99,99,99	0
56	MG	1H	3307	1/1	0.77	0.28	99,99,99,99	0
56	MG	1H	3206	1/1	0.77	0.14	53,53,53,53	0
56	MG	1G	1632	1/1	0.77	0.41	116,116,116,116	0
56	MG	13	1743	1/1	0.77	0.18	108,108,108,108	0
56	MG	1H	3467	1/1	0.77	0.10	106,106,106,106	0
56	MG	1H	3175	1/1	0.77	0.35	93,93,93,93	0
56	MG	14	3237	1/1	0.77	0.24	95,95,95,95	0
56	MG	14	3064	1/1	0.77	0.27	97,97,97,97	0
56	MG	1H	3147	1/1	0.77	0.32	94,94,94,94	0
56	MG	14	3255	1/1	0.77	0.41	99,99,99,99	0
56	MG	1H	3500	1/1	0.77	0.20	122,122,122,122	0
56	MG	13	1721	1/1	0.77	0.64	101,101,101,101	0
56	MG	14	3178	1/1	0.78	0.44	95,95,95,95	0
56	MG	14	3103	1/1	0.78	0.38	90,90,90,90	0
56	MG	39	302	1/1	0.78	0.30	118,118,118,118	0
56	MG	1H	3027	1/1	0.78	0.32	96,96,96,96	0
56	MG	14	3137	1/1	0.78	0.19	80,80,80,80	0
56	MG	13	1693	1/1	0.78	0.21	103,103,103,103	0
56	MG	14	3147	1/1	0.79	0.19	97,97,97,97	0
56	MG	1H	3476	1/1	0.79	0.12	93,93,93,93	0
56	MG	41	202	1/1	0.79	0.29	96,96,96,96	0
56	MG	L8	101	1/1	0.79	0.43	85,85,85,85	0
56	MG	14	3167	1/1	0.79	0.27	110,110,110,110	0
56	MG	13	1702	1/1	0.79	0.23	109,109,109,109	0
56	MG	14	3176	1/1	0.79	0.39	101,101,101,101	0
56	MG	1H	3267	1/1	0.79	0.34	84,84,84,84	0
56	MG	1G	1657	1/1	0.79	0.25	106,106,106,106	0
56	MG	1H	3072	1/1	0.79	0.29	80,80,80,80	0
56	MG	14	3080	1/1	0.79	0.41	88,88,88,88	0
56	MG	1H	3202	1/1	0.79	0.38	93,93,93,93	0
56	MG	1H	3129	1/1	0.79	0.41	90,90,90,90	0
56	MG	14	3275	1/1	0.79	0.27	105,105,105,105	0
56	MG	1H	3230	1/1	0.79	0.24	91,91,91,91	0
56	MG	1G	1640	1/1	0.79	0.49	106,106,106,106	0
56	MG	14	3320	1/1	0.79	0.22	96,96,96,96	0
56	MG	1H	3280	1/1	0.80	0.70	100,100,100,100	0
56	MG	2K	105	1/1	0.80	0.38	107,107,107,107	0
56	MG	14	3270	1/1	0.80	0.20	107,107,107,107	0
56	MG	1H	3132	1/1	0.80	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3305	1/1	0.80	0.61	104,104,104,104	0
56	MG	1H	3074	1/1	0.80	0.41	80,80,80,80	0
56	MG	1H	3013	1/1	0.80	0.41	104,104,104,104	0
56	MG	14	3422	1/1	0.80	0.09	132,132,132,132	0
56	MG	13	1694	1/1	0.80	0.10	121,121,121,121	0
56	MG	1H	3116	1/1	0.80	0.29	70,70,70,70	0
56	MG	14	3117	1/1	0.80	0.45	98,98,98,98	0
56	MG	14	3254	1/1	0.80	0.17	87,87,87,87	0
56	MG	1H	3034	1/1	0.80	0.34	96,96,96,96	0
56	MG	1H	3249	1/1	0.80	0.42	97,97,97,97	0
56	MG	13	1668	1/1	0.80	0.19	94,94,94,94	0
56	MG	1H	3292	1/1	0.81	0.23	72,72,72,72	0
56	MG	13	1734	1/1	0.81	0.15	133,133,133,133	0
56	MG	16	215	1/1	0.81	0.08	113,113,113,113	0
56	MG	14	3326	1/1	0.81	0.39	117,117,117,117	0
56	MG	1H	3300	1/1	0.81	0.35	87,87,87,87	0
56	MG	14	3280	1/1	0.81	0.31	95,95,95,95	0
56	MG	1G	1659	1/1	0.81	0.29	102,102,102,102	0
56	MG	I8	101	1/1	0.81	0.27	84,84,84,84	0
56	MG	1H	3107	1/1	0.81	0.28	85,85,85,85	0
56	MG	14	3144	1/1	0.81	0.35	93,93,93,93	0
56	MG	1H	3127	1/1	0.81	0.29	92,92,92,92	0
56	MG	14	3405	1/1	0.81	0.22	102,102,102,102	0
56	MG	14	3248	1/1	0.81	0.26	85,85,85,85	0
56	MG	14	3293	1/1	0.81	0.27	95,95,95,95	0
56	MG	1G	1673	1/1	0.81	0.14	108,108,108,108	0
56	MG	13	1684	1/1	0.81	0.33	106,106,106,106	0
56	MG	1H	3479	1/1	0.81	0.16	126,126,126,126	0
56	MG	1J	204	1/1	0.81	0.12	113,113,113,113	0
56	MG	1J	208	1/1	0.81	0.11	121,121,121,121	0
56	MG	1H	3262	1/1	0.81	0.30	89,89,89,89	0
56	MG	1H	3242	1/1	0.81	0.52	105,105,105,105	0
56	MG	1H	3499	1/1	0.81	0.11	110,110,110,110	0
56	MG	1H	3165	1/1	0.81	0.42	95,95,95,95	0
56	MG	1H	3314	1/1	0.81	0.37	76,76,76,76	0
56	MG	1H	3287	1/1	0.81	0.42	92,92,92,92	0
56	MG	14	3162	1/1	0.82	0.19	88,88,88,88	0
56	MG	1G	1628	1/1	0.82	0.21	118,118,118,118	0
56	MG	13	1722	1/1	0.82	0.10	85,85,85,85	0
56	MG	14	3370	1/1	0.82	0.13	110,110,110,110	0
56	MG	14	3169	1/1	0.82	0.29	93,93,93,93	0
56	MG	1H	3372	1/1	0.82	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3173	1/1	0.82	0.28	87,87,87,87	0
56	MG	14	3065	1/1	0.82	0.20	87,87,87,87	0
56	MG	1H	3126	1/1	0.82	0.32	79,79,79,79	0
56	MG	14	3261	1/1	0.82	0.34	83,83,83,83	0
56	MG	14	3301	1/1	0.82	0.29	83,83,83,83	0
56	MG	1H	3485	1/1	0.82	0.08	121,121,121,121	0
56	MG	1G	1680	1/1	0.82	0.11	140,140,140,140	0
56	MG	1G	1686	1/1	0.82	0.07	129,129,129,129	0
56	MG	1H	3490	1/1	0.82	0.13	125,125,125,125	0
56	MG	1J	206	1/1	0.82	0.12	123,123,123,123	0
56	MG	13	1695	1/1	0.82	0.15	112,112,112,112	0
56	MG	1H	3254	1/1	0.82	0.37	80,80,80,80	0
56	MG	14	3211	1/1	0.82	0.40	93,93,93,93	0
56	MG	1H	3232	1/1	0.82	0.32	80,80,80,80	0
56	MG	1H	3140	1/1	0.82	0.52	101,101,101,101	0
56	MG	14	3324	1/1	0.82	0.40	96,96,96,96	0
56	MG	2K	106	1/1	0.82	0.42	115,115,115,115	0
56	MG	14	3193	1/1	0.83	0.09	89,89,89,89	0
56	MG	14	3325	1/1	0.83	0.34	89,89,89,89	0
56	MG	1H	3503	1/1	0.83	0.12	116,116,116,116	0
56	MG	1H	3219	1/1	0.83	0.39	65,65,65,65	0
56	MG	14	3330	1/1	0.83	0.20	105,105,105,105	0
56	MG	1H	3111	1/1	0.83	0.43	91,91,91,91	0
56	MG	14	3204	1/1	0.83	0.13	80,80,80,80	0
56	MG	16	201	1/1	0.83	0.23	79,79,79,79	0
56	MG	1H	3128	1/1	0.83	0.21	88,88,88,88	0
56	MG	14	3374	1/1	0.83	0.08	113,113,113,113	0
56	MG	52	201	1/1	0.83	0.12	107,107,107,107	0
56	MG	14	3151	1/1	0.83	0.24	91,91,91,91	0
56	MG	1H	3477	1/1	0.83	0.10	108,108,108,108	0
56	MG	3I	202	1/1	0.83	0.45	101,101,101,101	0
56	MG	1H	3294	1/1	0.83	0.47	100,100,100,100	0
56	MG	1H	3055	1/1	0.83	0.16	82,82,82,82	0
56	MG	1G	1648	1/1	0.83	0.23	100,100,100,100	0
56	MG	14	3253	1/1	0.83	0.29	82,82,82,82	0
56	MG	1H	3193	1/1	0.83	0.36	95,95,95,95	0
56	MG	13	1682	1/1	0.83	0.28	116,116,116,116	0
56	MG	14	3256	1/1	0.83	0.19	97,97,97,97	0
56	MG	14	3175	1/1	0.83	0.38	99,99,99,99	0
56	MG	1H	3168	1/1	0.83	0.30	83,83,83,83	0
56	MG	1G	1663	1/1	0.83	0.21	92,92,92,92	0
56	MG	1G	1623	1/1	0.83	0.24	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1630	1/1	0.83	0.12	74,74,74,74	0
56	MG	25	201	1/1	0.83	0.43	111,111,111,111	0
56	MG	14	3267	1/1	0.83	0.16	110,110,110,110	0
56	MG	1G	1668	1/1	0.83	0.22	111,111,111,111	0
56	MG	1G	1687	1/1	0.84	0.30	135,135,135,135	0
56	MG	1H	3246	1/1	0.84	0.22	78,78,78,78	0
56	MG	1H	3199	1/1	0.84	0.51	99,99,99,99	0
56	MG	14	3168	1/1	0.84	0.23	67,67,67,67	0
56	MG	6A	101	1/1	0.84	0.21	138,138,138,138	0
56	MG	1G	1638	1/1	0.84	0.43	95,95,95,95	0
56	MG	2L	103	1/1	0.84	0.28	115,115,115,115	0
56	MG	1H	3081	1/1	0.84	0.25	77,77,77,77	0
56	MG	14	3352	1/1	0.84	0.12	74,74,74,74	0
56	MG	1H	3391	1/1	0.84	0.09	96,96,96,96	0
56	MG	1H	3177	1/1	0.84	0.44	98,98,98,98	0
56	MG	1H	3012	1/1	0.84	0.51	93,93,93,93	0
56	MG	1H	3185	1/1	0.84	0.38	88,88,88,88	0
56	MG	1H	3423	1/1	0.84	0.14	102,102,102,102	0
56	MG	14	3279	1/1	0.84	0.25	87,87,87,87	0
56	MG	14	3185	1/1	0.84	0.21	90,90,90,90	0
56	MG	1H	3283	1/1	0.84	0.38	112,112,112,112	0
56	MG	1H	3285	1/1	0.84	0.39	88,88,88,88	0
56	MG	14	3411	1/1	0.84	0.30	104,104,104,104	0
56	MG	1H	3286	1/1	0.84	0.26	85,85,85,85	0
56	MG	14	3202	1/1	0.84	0.26	100,100,100,100	0
56	MG	1H	3258	1/1	0.84	0.31	93,93,93,93	0
56	MG	14	3104	1/1	0.84	0.27	81,81,81,81	0
56	MG	1H	3288	1/1	0.84	0.28	87,87,87,87	0
56	MG	13	1699	1/1	0.84	0.50	102,102,102,102	0
56	MG	14	3136	1/1	0.84	0.10	112,112,112,112	0
56	MG	1H	3122	1/1	0.84	0.30	94,94,94,94	0
56	MG	14	3142	1/1	0.84	0.46	100,100,100,100	0
56	MG	1G	1669	1/1	0.84	0.28	112,112,112,112	0
56	MG	1H	3190	1/1	0.84	0.17	77,77,77,77	0
56	MG	1H	3487	1/1	0.84	0.29	126,126,126,126	0
56	MG	15	201	1/1	0.84	0.54	102,102,102,102	0
56	MG	13	1687	1/1	0.84	0.28	109,109,109,109	0
56	MG	1G	1684	1/1	0.84	0.12	124,124,124,124	0
56	MG	1H	3342	1/1	0.84	0.17	92,92,92,92	0
56	MG	1H	3344	1/1	0.85	0.42	95,95,95,95	0
56	MG	14	3208	1/1	0.85	0.10	84,84,84,84	0
56	MG	14	3209	1/1	0.85	0.33	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3318	1/1	0.85	0.30	87,87,87,87	0
56	MG	1H	3321	1/1	0.85	0.27	99,99,99,99	0
56	MG	1H	3061	1/1	0.85	0.34	85,85,85,85	0
56	MG	1H	3488	1/1	0.85	0.15	114,114,114,114	0
56	MG	P8	101	1/1	0.85	0.41	84,84,84,84	0
56	MG	1G	1602	1/1	0.85	0.39	118,118,118,118	0
56	MG	14	3247	1/1	0.85	0.14	75,75,75,75	0
56	MG	1H	3489	1/1	0.85	0.12	69,69,69,69	0
56	MG	14	3058	1/1	0.85	0.16	128,128,128,128	0
56	MG	14	3412	1/1	0.85	0.08	108,108,108,108	0
56	MG	1H	3298	1/1	0.85	0.33	92,92,92,92	0
56	MG	1H	3146	1/1	0.85	0.32	83,83,83,83	0
56	MG	14	3068	1/1	0.85	0.39	86,86,86,86	0
56	MG	14	3308	1/1	0.85	0.21	106,106,106,106	0
56	MG	1H	3493	1/1	0.85	0.25	130,130,130,130	0
56	MG	14	3093	1/1	0.85	0.51	103,103,103,103	0
56	MG	13	1704	1/1	0.85	0.69	118,118,118,118	0
56	MG	1H	3182	1/1	0.85	0.36	74,74,74,74	0
56	MG	13	1740	1/1	0.85	0.17	106,106,106,106	0
56	MG	1H	3141	1/1	0.85	0.44	89,89,89,89	0
56	MG	1H	3447	1/1	0.85	0.17	105,105,105,105	0
56	MG	1G	1639	1/1	0.85	0.17	89,89,89,89	0
56	MG	14	3200	1/1	0.85	0.18	85,85,85,85	0
56	MG	1H	3092	1/1	0.85	0.30	70,70,70,70	0
56	MG	1H	3174	1/1	0.85	0.31	78,78,78,78	0
56	MG	1H	3256	1/1	0.85	0.26	88,88,88,88	0
56	MG	1H	3030	1/1	0.86	0.19	79,79,79,79	0
56	MG	14	3197	1/1	0.86	0.50	119,119,119,119	0
56	MG	13	1647	1/1	0.86	0.17	93,93,93,93	0
56	MG	1G	1675	1/1	0.86	0.47	99,99,99,99	0
56	MG	1H	3102	1/1	0.86	0.28	67,67,67,67	0
56	MG	14	3278	1/1	0.86	0.26	85,85,85,85	0
56	MG	1H	3434	1/1	0.86	0.19	130,130,130,130	0
56	MG	1H	3439	1/1	0.86	0.15	92,92,92,92	0
56	MG	1H	3260	1/1	0.86	0.28	76,76,76,76	0
56	MG	1G	1635	1/1	0.86	0.39	118,118,118,118	0
56	MG	14	3148	1/1	0.86	0.11	117,117,117,117	0
56	MG	1H	3339	1/1	0.86	0.33	90,90,90,90	0
56	MG	13	1650	1/1	0.86	0.15	87,87,87,87	0
56	MG	14	3152	1/1	0.86	0.23	80,80,80,80	0
56	MG	1H	3263	1/1	0.86	0.22	106,106,106,106	0
56	MG	16	206	1/1	0.86	0.25	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1719	1/1	0.86	0.13	95,95,95,95	0
56	MG	13	1663	1/1	0.86	0.16	87,87,87,87	0
56	MG	31	301	1/1	0.86	0.10	92,92,92,92	0
56	MG	1J	202	1/1	0.86	0.12	157,157,157,157	0
56	MG	1H	3317	1/1	0.86	0.79	85,85,85,85	0
56	MG	1H	3290	1/1	0.86	0.49	92,92,92,92	0
56	MG	1J	205	1/1	0.86	0.23	101,101,101,101	0
56	MG	1G	1650	1/1	0.86	0.36	101,101,101,101	0
56	MG	1G	1653	1/1	0.86	0.11	106,106,106,106	0
56	MG	13	1670	1/1	0.86	0.33	88,88,88,88	0
56	MG	13	1605	1/1	0.86	0.18	93,93,93,93	0
56	MG	1H	3178	1/1	0.86	0.27	76,76,76,76	0
56	MG	1G	1603	1/1	0.86	0.17	118,118,118,118	0
56	MG	1H	3007	1/1	0.86	0.33	97,97,97,97	0
56	MG	1G	1615	1/1	0.86	0.23	115,115,115,115	0
56	MG	45	201	1/1	0.86	0.18	113,113,113,113	0
56	MG	C5	201	1/1	0.86	0.23	123,123,123,123	0
56	MG	14	3266	1/1	0.86	0.38	80,80,80,80	0
56	MG	1H	3492	1/1	0.86	0.23	120,120,120,120	0
56	MG	1H	3284	1/1	0.87	0.27	70,70,70,70	0
56	MG	13	1691	1/1	0.87	0.30	95,95,95,95	0
56	MG	14	3337	1/1	0.87	0.12	76,76,76,76	0
56	MG	1H	3478	1/1	0.87	0.09	118,118,118,118	0
56	MG	1H	3222	1/1	0.87	0.30	79,79,79,79	0
56	MG	1H	3480	1/1	0.87	0.14	109,109,109,109	0
56	MG	1H	3223	1/1	0.87	0.18	82,82,82,82	0
56	MG	88	202	1/1	0.87	0.30	77,77,77,77	0
56	MG	14	3283	1/1	0.87	0.21	98,98,98,98	0
56	MG	1H	3155	1/1	0.87	0.17	78,78,78,78	0
56	MG	14	3381	1/1	0.87	0.22	101,101,101,101	0
56	MG	13	1622	1/1	0.87	0.32	102,102,102,102	0
56	MG	14	3398	1/1	0.87	0.06	127,127,127,127	0
56	MG	1H	3083	1/1	0.87	0.32	92,92,92,92	0
56	MG	1H	3399	1/1	0.87	0.09	59,59,59,59	0
56	MG	1H	3323	1/1	0.87	0.11	110,110,110,110	0
56	MG	1H	3086	1/1	0.87	0.39	72,72,72,72	0
56	MG	14	3413	1/1	0.87	0.31	110,110,110,110	0
56	MG	13	1624	1/1	0.87	0.22	95,95,95,95	0
56	MG	14	3249	1/1	0.87	0.27	97,97,97,97	0
56	MG	1H	3494	1/1	0.87	0.36	121,121,121,121	0
56	MG	1G	1665	1/1	0.87	0.30	110,110,110,110	0
56	MG	14	3305	1/1	0.87	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3174	1/1	0.87	0.18	93,93,93,93	0
56	MG	14	3066	1/1	0.87	0.30	96,96,96,96	0
56	MG	5E	201	1/1	0.87	0.20	104,104,104,104	0
56	MG	1H	3198	1/1	0.87	0.38	90,90,90,90	0
56	MG	1J	207	1/1	0.87	0.27	147,147,147,147	0
56	MG	1H	3015	1/1	0.87	0.24	71,71,71,71	0
56	MG	1H	3335	1/1	0.87	0.42	85,85,85,85	0
56	MG	14	3316	1/1	0.87	0.54	103,103,103,103	0
56	MG	1G	1671	1/1	0.87	0.40	120,120,120,120	0
56	MG	13	1665	1/1	0.87	0.12	91,91,91,91	0
56	MG	14	3123	1/1	0.87	0.16	75,75,75,75	0
56	MG	14	3195	1/1	0.87	0.38	100,100,100,100	0
56	MG	25	202	1/1	0.87	0.33	125,125,125,125	0
56	MG	2K	104	1/1	0.87	0.44	90,90,90,90	0
56	MG	1G	1634	1/1	0.87	0.48	120,120,120,120	0
56	MG	13	1621	1/1	0.87	0.39	115,115,115,115	0
56	MG	14	3328	1/1	0.87	0.12	111,111,111,111	0
57	ZN	G8	202	1/1	0.87	0.31	192,192,192,192	0
56	MG	1H	3282	1/1	0.88	0.15	107,107,107,107	0
56	MG	1G	1679	1/1	0.88	0.09	108,108,108,108	0
56	MG	1H	3144	1/1	0.88	0.23	80,80,80,80	0
56	MG	1G	1682	1/1	0.88	0.09	141,141,141,141	0
56	MG	14	3164	1/1	0.88	0.21	91,91,91,91	0
56	MG	1H	3204	1/1	0.88	0.75	104,104,104,104	0
56	MG	14	3407	1/1	0.88	0.08	116,116,116,116	0
56	MG	13	1680	1/1	0.88	0.19	124,124,124,124	0
56	MG	1G	1652	1/1	0.88	0.26	103,103,103,103	0
56	MG	1H	3381	1/1	0.88	0.09	89,89,89,89	0
56	MG	14	3273	1/1	0.88	0.14	87,87,87,87	0
56	MG	14	3221	1/1	0.88	0.20	87,87,87,87	0
56	MG	1H	3471	1/1	0.88	0.11	128,128,128,128	0
56	MG	13	1652	1/1	0.88	0.23	98,98,98,98	0
56	MG	14	3233	1/1	0.88	0.30	118,118,118,118	0
56	MG	1H	3136	1/1	0.88	0.15	71,71,71,71	0
56	MG	1G	1636	1/1	0.88	0.08	115,115,115,115	0
56	MG	13	1672	1/1	0.88	0.20	100,100,100,100	0
56	MG	14	3282	1/1	0.88	0.31	90,90,90,90	0
56	MG	13	1706	1/1	0.88	0.91	103,103,103,103	0
56	MG	14	3023	1/1	0.88	0.15	86,86,86,86	0
56	MG	13	1654	1/1	0.88	0.28	123,123,123,123	0
56	MG	14	3343	1/1	0.88	0.12	89,89,89,89	0
56	MG	14	3346	1/1	0.88	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	1G	1641	1/1	0.88	0.29	90,90,90,90	0
56	MG	49	201	1/1	0.88	0.10	143,143,143,143	0
56	MG	14	3354	1/1	0.88	0.06	126,126,126,126	0
56	MG	14	3187	1/1	0.88	0.36	100,100,100,100	0
56	MG	14	3363	1/1	0.88	0.06	117,117,117,117	0
56	MG	35	201	1/1	0.88	0.21	91,91,91,91	0
56	MG	14	3192	1/1	0.88	0.14	84,84,84,84	0
56	MG	45	202	1/1	0.88	0.53	82,82,82,82	0
56	MG	14	3369	1/1	0.88	0.18	105,105,105,105	0
56	MG	13	1679	1/1	0.88	0.18	98,98,98,98	0
56	MG	1H	3295	1/1	0.88	0.50	92,92,92,92	0
56	MG	1H	3118	1/1	0.88	0.30	76,76,76,76	0
56	MG	1H	3345	1/1	0.89	0.31	100,100,100,100	0
56	MG	13	1674	1/1	0.89	0.23	118,118,118,118	0
56	MG	1H	3225	1/1	0.89	0.21	69,69,69,69	0
56	MG	14	3166	1/1	0.89	0.14	106,106,106,106	0
56	MG	1H	3457	1/1	0.89	0.05	113,113,113,113	0
56	MG	14	3125	1/1	0.89	0.27	101,101,101,101	0
56	MG	14	3289	1/1	0.89	0.18	86,86,86,86	0
56	MG	14	3130	1/1	0.89	0.10	71,71,71,71	0
56	MG	13	1752	1/1	0.89	0.51	92,92,92,92	0
56	MG	1G	1647	1/1	0.89	0.32	86,86,86,86	0
56	MG	1H	3031	1/1	0.89	0.33	89,89,89,89	0
56	MG	11	302	1/1	0.89	0.25	66,66,66,66	0
56	MG	1H	3237	1/1	0.89	0.17	70,70,70,70	0
56	MG	14	3177	1/1	0.89	0.32	111,111,111,111	0
56	MG	14	3268	1/1	0.89	0.19	100,100,100,100	0
56	MG	14	3371	1/1	0.89	0.21	101,101,101,101	0
56	MG	14	3231	1/1	0.89	0.21	93,93,93,93	0
56	MG	1H	3104	1/1	0.89	0.22	78,78,78,78	0
56	MG	13	1607	1/1	0.89	0.19	78,78,78,78	0
56	MG	1H	3245	1/1	0.89	0.38	96,96,96,96	0
56	MG	14	3149	1/1	0.89	0.21	79,79,79,79	0
56	MG	1H	3210	1/1	0.89	0.17	69,69,69,69	0
56	MG	14	3277	1/1	0.89	0.20	90,90,90,90	0
56	MG	1H	3502	1/1	0.89	0.29	118,118,118,118	0
56	MG	13	1676	1/1	0.89	0.18	111,111,111,111	0
56	MG	13	1727	1/1	0.89	0.24	121,121,121,121	0
56	MG	14	3250	1/1	0.89	0.23	86,86,86,86	0
57	ZN	C5	202	1/1	0.89	0.11	189,189,189,189	0
56	MG	1G	1656	1/1	0.90	0.30	103,103,103,103	0
56	MG	13	1632	1/1	0.90	0.16	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	1H	3238	1/1	0.90	0.32	84,84,84,84	0
56	MG	14	3269	1/1	0.90	0.31	102,102,102,102	0
56	MG	1G	1661	1/1	0.90	0.26	105,105,105,105	0
56	MG	14	3355	1/1	0.90	0.18	102,102,102,102	0
56	MG	13	1644	1/1	0.90	0.12	96,96,96,96	0
56	MG	14	3076	1/1	0.90	0.11	93,93,93,93	0
56	MG	1G	1605	1/1	0.90	0.17	98,98,98,98	0
56	MG	14	3081	1/1	0.90	0.31	90,90,90,90	0
56	MG	1G	1606	1/1	0.90	0.27	129,129,129,129	0
56	MG	1G	1666	1/1	0.90	0.36	89,89,89,89	0
56	MG	13	1646	1/1	0.90	0.24	104,104,104,104	0
56	MG	14	3112	1/1	0.90	0.12	98,98,98,98	0
56	MG	1H	3138	1/1	0.90	0.40	94,94,94,94	0
56	MG	14	3379	1/1	0.90	0.09	77,77,77,77	0
56	MG	1H	3268	1/1	0.90	0.50	125,125,125,125	0
56	MG	14	3383	1/1	0.90	0.16	98,98,98,98	0
56	MG	14	3387	1/1	0.90	0.10	76,76,76,76	0
56	MG	1H	3009	1/1	0.90	0.20	69,69,69,69	0
56	MG	1H	3430	1/1	0.90	0.10	116,116,116,116	0
56	MG	1H	3209	1/1	0.90	0.15	82,82,82,82	0
56	MG	1H	3184	1/1	0.90	0.19	107,107,107,107	0
56	MG	1H	3274	1/1	0.90	0.57	100,100,100,100	0
56	MG	14	3287	1/1	0.90	0.21	95,95,95,95	0
56	MG	1H	3071	1/1	0.90	0.12	94,94,94,94	0
56	MG	14	3217	1/1	0.90	0.80	82,82,82,82	0
56	MG	14	3415	1/1	0.90	0.40	107,107,107,107	0
56	MG	1H	3304	1/1	0.90	0.39	114,114,114,114	0
56	MG	1H	3277	1/1	0.90	0.47	109,109,109,109	0
56	MG	14	3419	1/1	0.90	0.24	112,112,112,112	0
56	MG	1H	3466	1/1	0.90	0.12	94,94,94,94	0
56	MG	1H	3279	1/1	0.90	0.25	80,80,80,80	0
56	MG	14	3296	1/1	0.90	0.20	107,107,107,107	0
56	MG	1H	3469	1/1	0.90	0.07	106,106,106,106	0
56	MG	16	207	1/1	0.90	0.37	84,84,84,84	0
56	MG	14	3303	1/1	0.90	0.11	100,100,100,100	0
56	MG	13	1618	1/1	0.90	0.26	86,86,86,86	0
56	MG	14	3306	1/1	0.90	0.30	93,93,93,93	0
56	MG	1H	3473	1/1	0.90	0.21	127,127,127,127	0
56	MG	1J	209	1/1	0.90	0.07	125,125,125,125	0
56	MG	14	3239	1/1	0.90	0.23	166,166,166,166	0
56	MG	14	3153	1/1	0.90	0.17	70,70,70,70	0
56	MG	1H	3308	1/1	0.90	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3161	1/1	0.90	0.20	104,104,104,104	0
56	MG	14	3013	1/1	0.90	0.17	88,88,88,88	0
56	MG	14	3017	1/1	0.90	0.15	91,91,91,91	0
56	MG	13	1696	1/1	0.90	0.29	108,108,108,108	0
56	MG	1H	3077	1/1	0.90	0.25	67,67,67,67	0
56	MG	14	3022	1/1	0.90	0.48	107,107,107,107	0
56	MG	1H	3108	1/1	0.90	0.22	86,86,86,86	0
56	MG	1H	3366	1/1	0.90	0.12	60,60,60,60	0
56	MG	I8	102	1/1	0.90	0.41	64,64,64,64	0
56	MG	14	3028	1/1	0.90	0.14	98,98,98,98	0
56	MG	13	1707	1/1	0.90	0.25	104,104,104,104	0
56	MG	1H	3316	1/1	0.90	0.57	94,94,94,94	0
56	MG	14	3037	1/1	0.90	0.20	79,79,79,79	0
56	MG	2K	107	1/1	0.91	0.41	106,106,106,106	0
56	MG	14	3388	1/1	0.91	0.12	85,85,85,85	0
56	MG	14	3047	1/1	0.91	0.14	66,66,66,66	0
56	MG	14	3395	1/1	0.91	0.09	96,96,96,96	0
56	MG	14	3396	1/1	0.91	0.16	119,119,119,119	0
56	MG	14	3055	1/1	0.91	0.42	85,85,85,85	0
56	MG	1H	3191	1/1	0.91	0.34	87,87,87,87	0
56	MG	14	3154	1/1	0.91	0.23	86,86,86,86	0
56	MG	1H	3329	1/1	0.91	0.34	99,99,99,99	0
56	MG	14	3207	1/1	0.91	0.14	68,68,68,68	0
56	MG	14	3159	1/1	0.91	0.13	112,112,112,112	0
56	MG	14	3271	1/1	0.91	0.12	87,87,87,87	0
56	MG	13	1637	1/1	0.91	0.26	96,96,96,96	0
56	MG	14	3210	1/1	0.91	0.37	98,98,98,98	0
56	MG	1H	3098	1/1	0.91	0.23	72,72,72,72	0
56	MG	1H	3100	1/1	0.91	0.27	86,86,86,86	0
56	MG	1G	1609	1/1	0.91	0.12	97,97,97,97	0
56	MG	1G	1610	1/1	0.91	0.13	115,115,115,115	0
56	MG	14	3423	1/1	0.91	0.10	133,133,133,133	0
56	MG	14	3424	1/1	0.91	0.43	116,116,116,116	0
56	MG	1G	1688	1/1	0.91	0.13	117,117,117,117	0
56	MG	1H	3334	1/1	0.91	0.50	99,99,99,99	0
56	MG	1H	3312	1/1	0.91	0.37	79,79,79,79	0
56	MG	1G	1655	1/1	0.91	0.21	111,111,111,111	0
56	MG	14	3109	1/1	0.91	0.32	89,89,89,89	0
56	MG	16	204	1/1	0.91	0.40	99,99,99,99	0
56	MG	1H	3181	1/1	0.91	0.35	74,74,74,74	0
56	MG	1H	3426	1/1	0.91	0.13	92,92,92,92	0
56	MG	1H	3133	1/1	0.91	0.14	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	14	3018	1/1	0.91	0.13	70,70,70,70	0
56	MG	13	1677	1/1	0.91	0.39	98,98,98,98	0
56	MG	14	3360	1/1	0.91	0.06	92,92,92,92	0
56	MG	1H	3241	1/1	0.91	0.21	80,80,80,80	0
56	MG	13	1713	1/1	0.91	0.12	119,119,119,119	0
56	MG	13	1724	1/1	0.91	0.06	102,102,102,102	0
56	MG	13	1662	1/1	0.91	0.11	94,94,94,94	0
56	MG	1H	3448	1/1	0.91	0.14	97,97,97,97	0
56	MG	1H	3211	1/1	0.91	0.14	76,76,76,76	0
56	MG	14	3259	1/1	0.91	0.15	100,100,100,100	0
56	MG	14	3375	1/1	0.91	0.06	102,102,102,102	0
56	MG	1H	3358	1/1	0.91	0.15	76,76,76,76	0
56	MG	14	3302	1/1	0.91	0.19	92,92,92,92	0
56	MG	1H	3496	1/1	0.91	0.04	131,131,131,131	0
56	MG	14	3304	1/1	0.91	0.33	121,121,121,121	0
56	MG	1H	3338	1/1	0.92	0.27	110,110,110,110	0
56	MG	1H	3432	1/1	0.92	0.06	113,113,113,113	0
56	MG	1H	3005	1/1	0.92	0.20	70,70,70,70	0
56	MG	14	3218	1/1	0.92	0.13	75,75,75,75	0
56	MG	1H	3495	1/1	0.92	0.32	91,91,91,91	0
56	MG	1H	3437	1/1	0.92	0.06	109,109,109,109	0
56	MG	1H	3438	1/1	0.92	0.05	82,82,82,82	0
56	MG	14	3380	1/1	0.92	0.09	97,97,97,97	0
56	MG	1H	3149	1/1	0.92	0.54	99,99,99,99	0
56	MG	1G	1611	1/1	0.92	0.18	105,105,105,105	0
56	MG	1G	1613	1/1	0.92	0.22	117,117,117,117	0
56	MG	1H	3291	1/1	0.92	0.29	77,77,77,77	0
56	MG	14	3160	1/1	0.92	0.32	85,85,85,85	0
56	MG	14	3394	1/1	0.92	0.07	93,93,93,93	0
56	MG	14	3039	1/1	0.92	0.26	68,68,68,68	0
56	MG	14	3243	1/1	0.92	0.10	91,91,91,91	0
56	MG	14	3246	1/1	0.92	0.21	75,75,75,75	0
56	MG	1G	1617	1/1	0.92	0.27	110,110,110,110	0
56	MG	14	3053	1/1	0.92	0.17	98,98,98,98	0
56	MG	1H	3501	1/1	0.92	0.17	107,107,107,107	0
56	MG	14	3409	1/1	0.92	0.07	114,114,114,114	0
56	MG	14	3056	1/1	0.92	0.11	92,92,92,92	0
56	MG	13	1711	1/1	0.92	0.63	126,126,126,126	0
56	MG	1H	3194	1/1	0.92	0.20	104,104,104,104	0
56	MG	13	1703	1/1	0.92	0.37	96,96,96,96	0
56	MG	14	3309	1/1	0.92	0.48	87,87,87,87	0
56	MG	1H	3320	1/1	0.92	0.73	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3354	1/1	0.92	0.14	64,64,64,64	0
56	MG	1G	1674	1/1	0.92	0.15	111,111,111,111	0
56	MG	14	3258	1/1	0.92	0.13	104,104,104,104	0
56	MG	1H	3278	1/1	0.92	0.29	101,101,101,101	0
56	MG	1H	3297	1/1	0.92	0.10	86,86,86,86	0
56	MG	13	1686	1/1	0.92	0.29	134,134,134,134	0
56	MG	14	3094	1/1	0.92	0.20	83,83,83,83	0
56	MG	14	3098	1/1	0.92	0.28	74,74,74,74	0
56	MG	14	3321	1/1	0.92	0.27	99,99,99,99	0
56	MG	14	3102	1/1	0.92	0.36	93,93,93,93	0
56	MG	1H	3097	1/1	0.92	0.20	89,89,89,89	0
56	MG	1H	3041	1/1	0.92	0.33	67,67,67,67	0
56	MG	14	3107	1/1	0.92	0.21	80,80,80,80	0
56	MG	13	1667	1/1	0.92	0.30	147,147,147,147	0
56	MG	11	301	1/1	0.92	0.32	62,62,62,62	0
56	MG	1H	3162	1/1	0.92	0.24	74,74,74,74	0
56	MG	1H	3163	1/1	0.92	0.20	88,88,88,88	0
56	MG	14	3344	1/1	0.92	0.11	82,82,82,82	0
56	MG	1H	3101	1/1	0.92	0.21	49,49,49,49	0
56	MG	78	201	1/1	0.92	0.15	67,67,67,67	0
56	MG	1H	3420	1/1	0.92	0.10	84,84,84,84	0
56	MG	1H	3333	1/1	0.92	0.34	91,91,91,91	0
56	MG	14	3012	1/1	0.92	0.23	94,94,94,94	0
56	MG	14	3140	1/1	0.92	0.34	93,93,93,93	0
56	MG	1H	3056	1/1	0.92	0.30	72,72,72,72	0
56	MG	14	3365	1/1	0.92	0.10	80,80,80,80	0
56	MG	14	3367	1/1	0.92	0.06	111,111,111,111	0
56	MG	1H	3310	1/1	0.92	0.37	96,96,96,96	0
56	MG	1H	3216	1/1	0.92	0.22	77,77,77,77	0
56	MG	1G	1622	1/1	0.93	0.12	89,89,89,89	0
56	MG	1H	3020	1/1	0.93	0.15	90,90,90,90	0
56	MG	14	3341	1/1	0.93	0.07	78,78,78,78	0
56	MG	1H	3374	1/1	0.93	0.16	71,71,71,71	0
56	MG	1H	3375	1/1	0.93	0.18	76,76,76,76	0
56	MG	1H	3378	1/1	0.93	0.09	94,94,94,94	0
56	MG	1H	3166	1/1	0.93	0.17	73,73,73,73	0
56	MG	1H	3167	1/1	0.93	0.15	92,92,92,92	0
56	MG	1H	3049	1/1	0.93	0.33	60,60,60,60	0
56	MG	14	3156	1/1	0.93	0.18	99,99,99,99	0
56	MG	1H	3247	1/1	0.93	0.28	81,81,81,81	0
56	MG	1H	3248	1/1	0.93	0.23	76,76,76,76	0
56	MG	1G	1637	1/1	0.93	0.16	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3263	1/1	0.93	0.26	88,88,88,88	0
56	MG	1H	3410	1/1	0.93	0.12	73,73,73,73	0
56	MG	14	3024	1/1	0.93	0.28	73,73,73,73	0
56	MG	1H	3319	1/1	0.93	0.27	90,90,90,90	0
56	MG	1H	3417	1/1	0.93	0.12	90,90,90,90	0
56	MG	14	3027	1/1	0.93	0.20	84,84,84,84	0
56	MG	1H	3418	1/1	0.93	0.06	134,134,134,134	0
56	MG	1H	3201	1/1	0.93	0.32	121,121,121,121	0
56	MG	1H	3050	1/1	0.93	0.27	80,80,80,80	0
56	MG	1H	3051	1/1	0.93	0.24	53,53,53,53	0
56	MG	1H	3252	1/1	0.93	0.21	69,69,69,69	0
56	MG	1H	3002	1/1	0.93	0.23	76,76,76,76	0
56	MG	1H	3327	1/1	0.93	0.39	91,91,91,91	0
56	MG	1H	3003	1/1	0.93	0.21	75,75,75,75	0
56	MG	13	1701	1/1	0.93	0.57	103,103,103,103	0
56	MG	1H	3150	1/1	0.93	0.36	86,86,86,86	0
56	MG	14	3063	1/1	0.93	0.18	104,104,104,104	0
56	MG	1H	3293	1/1	0.93	0.17	85,85,85,85	0
56	MG	13	1645	1/1	0.93	0.38	86,86,86,86	0
56	MG	14	3184	1/1	0.93	0.34	94,94,94,94	0
56	MG	1H	3442	1/1	0.93	0.12	57,57,57,57	0
56	MG	14	3186	1/1	0.93	0.21	86,86,86,86	0
56	MG	1H	3217	1/1	0.93	0.12	91,91,91,91	0
56	MG	14	3072	1/1	0.93	0.17	90,90,90,90	0
56	MG	13	1660	1/1	0.93	0.14	94,94,94,94	0
56	MG	14	3078	1/1	0.93	0.11	97,97,97,97	0
56	MG	1G	1660	1/1	0.93	0.43	97,97,97,97	0
56	MG	1H	3264	1/1	0.93	0.29	96,96,96,96	0
56	MG	14	3292	1/1	0.93	0.17	90,90,90,90	0
56	MG	14	3417	1/1	0.93	0.06	148,148,148,148	0
56	MG	14	3083	1/1	0.93	0.26	81,81,81,81	0
56	MG	14	3091	1/1	0.93	0.29	87,87,87,87	0
56	MG	78	202	1/1	0.93	0.20	97,97,97,97	0
56	MG	1H	3458	1/1	0.93	0.13	93,93,93,93	0
56	MG	1H	3461	1/1	0.93	0.08	110,110,110,110	0
56	MG	14	3299	1/1	0.93	0.58	84,84,84,84	0
56	MG	1H	3336	1/1	0.93	0.30	102,102,102,102	0
56	MG	1H	3183	1/1	0.93	0.29	83,83,83,83	0
56	MG	13	1661	1/1	0.93	0.29	91,91,91,91	0
56	MG	1H	3302	1/1	0.93	0.23	90,90,90,90	0
56	MG	1H	3470	1/1	0.93	0.23	99,99,99,99	0
56	MG	14	3213	1/1	0.93	0.17	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3303	1/1	0.93	0.30	76,76,76,76	0
56	MG	14	3113	1/1	0.93	0.35	80,80,80,80	0
56	MG	13	1619	1/1	0.93	0.57	103,103,103,103	0
56	MG	14	3224	1/1	0.93	0.09	80,80,80,80	0
56	MG	39	301	1/1	0.93	0.19	111,111,111,111	0
56	MG	1H	3228	1/1	0.93	0.55	94,94,94,94	0
56	MG	14	3229	1/1	0.93	0.20	83,83,83,83	0
56	MG	1G	1607	1/1	0.93	0.28	98,98,98,98	0
56	MG	1H	3032	1/1	0.93	0.25	78,78,78,78	0
56	MG	14	3132	1/1	0.93	0.22	94,94,94,94	0
56	MG	1H	3231	1/1	0.93	0.49	90,90,90,90	0
56	MG	14	3135	1/1	0.93	0.31	101,101,101,101	0
56	MG	13	1700	1/1	0.93	0.24	109,109,109,109	0
56	MG	1H	3160	1/1	0.93	0.31	84,84,84,84	0
56	MG	1G	1614	1/1	0.93	0.25	140,140,140,140	0
56	MG	1H	3082	1/1	0.93	0.17	77,77,77,77	0
56	MG	1H	3359	1/1	0.93	0.10	83,83,83,83	0
56	MG	1H	3035	1/1	0.93	0.20	55,55,55,55	0
56	MG	14	3146	1/1	0.93	0.19	128,128,128,128	0
56	MG	14	3314	1/1	0.94	0.34	102,102,102,102	0
56	MG	14	3082	1/1	0.94	0.23	71,71,71,71	0
56	MG	13	1626	1/1	0.94	0.20	109,109,109,109	0
56	MG	1G	1654	1/1	0.94	0.38	94,94,94,94	0
56	MG	14	3092	1/1	0.94	0.16	109,109,109,109	0
56	MG	1H	3421	1/1	0.94	0.18	62,62,62,62	0
56	MG	1H	3422	1/1	0.94	0.15	91,91,91,91	0
56	MG	1H	3325	1/1	0.94	0.13	86,86,86,86	0
56	MG	14	3323	1/1	0.94	0.10	101,101,101,101	0
56	MG	16	202	1/1	0.94	0.28	73,73,73,73	0
56	MG	14	3225	1/1	0.94	0.20	65,65,65,65	0
56	MG	1H	3424	1/1	0.94	0.09	119,119,119,119	0
56	MG	1H	3425	1/1	0.94	0.06	95,95,95,95	0
56	MG	14	3106	1/1	0.94	0.20	89,89,89,89	0
56	MG	13	1643	1/1	0.94	0.09	78,78,78,78	0
56	MG	1H	3105	1/1	0.94	0.09	76,76,76,76	0
56	MG	14	3234	1/1	0.94	0.54	98,98,98,98	0
56	MG	16	211	1/1	0.94	0.40	79,79,79,79	0
56	MG	1H	3429	1/1	0.94	0.08	102,102,102,102	0
56	MG	14	3345	1/1	0.94	0.10	84,84,84,84	0
56	MG	1H	3058	1/1	0.94	0.20	107,107,107,107	0
56	MG	14	3350	1/1	0.94	0.08	80,80,80,80	0
56	MG	14	3121	1/1	0.94	0.23	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	14	3240	1/1	0.94	0.10	76,76,76,76	0
56	MG	14	3241	1/1	0.94	0.31	92,92,92,92	0
56	MG	1H	3188	1/1	0.94	0.51	100,100,100,100	0
56	MG	13	1728	1/1	0.94	0.13	131,131,131,131	0
56	MG	14	3362	1/1	0.94	0.17	101,101,101,101	0
56	MG	14	3127	1/1	0.94	0.06	87,87,87,87	0
56	MG	1H	3024	1/1	0.94	0.23	102,102,102,102	0
56	MG	1H	3067	1/1	0.94	0.16	84,84,84,84	0
56	MG	1H	3112	1/1	0.94	0.14	55,55,55,55	0
56	MG	1H	3113	1/1	0.94	0.14	64,64,64,64	0
56	MG	1H	3441	1/1	0.94	0.10	122,122,122,122	0
56	MG	1H	3068	1/1	0.94	0.27	98,98,98,98	0
56	MG	2K	102	1/1	0.94	0.23	97,97,97,97	0
56	MG	14	3141	1/1	0.94	0.19	80,80,80,80	0
56	MG	1G	1681	1/1	0.94	0.18	133,133,133,133	0
56	MG	J8	101	1/1	0.94	0.27	78,78,78,78	0
56	MG	13	1731	1/1	0.94	0.05	91,91,91,91	0
56	MG	1H	3454	1/1	0.94	0.06	85,85,85,85	0
56	MG	1H	3455	1/1	0.94	0.22	99,99,99,99	0
56	MG	1H	3456	1/1	0.94	0.18	79,79,79,79	0
56	MG	1H	3121	1/1	0.94	0.21	80,80,80,80	0
56	MG	1H	3159	1/1	0.94	0.17	77,77,77,77	0
56	MG	1H	3460	1/1	0.94	0.11	110,110,110,110	0
56	MG	1H	3257	1/1	0.94	0.33	80,80,80,80	0
56	MG	1H	3301	1/1	0.94	0.24	79,79,79,79	0
56	MG	14	3003	1/1	0.94	0.14	73,73,73,73	0
56	MG	14	3006	1/1	0.94	0.21	99,99,99,99	0
56	MG	14	3399	1/1	0.94	0.08	78,78,78,78	0
56	MG	14	3400	1/1	0.94	0.22	95,95,95,95	0
56	MG	14	3401	1/1	0.94	0.06	120,120,120,120	0
56	MG	14	3157	1/1	0.94	0.31	76,76,76,76	0
56	MG	1H	3203	1/1	0.94	0.35	73,73,73,73	0
56	MG	14	3406	1/1	0.94	0.07	99,99,99,99	0
56	MG	1H	3073	1/1	0.94	0.24	88,88,88,88	0
56	MG	1H	3161	1/1	0.94	0.36	82,82,82,82	0
56	MG	14	3410	1/1	0.94	0.30	96,96,96,96	0
56	MG	1H	3208	1/1	0.94	0.09	63,63,63,63	0
56	MG	13	1620	1/1	0.94	0.27	119,119,119,119	0
56	MG	13	1715	1/1	0.94	0.31	108,108,108,108	0
56	MG	1G	1618	1/1	0.94	0.12	104,104,104,104	0
56	MG	1H	3474	1/1	0.94	0.20	124,124,124,124	0
56	MG	1H	3475	1/1	0.94	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	1H	3080	1/1	0.94	0.31	86,86,86,86	0
56	MG	13	1615	1/1	0.94	0.24	100,100,100,100	0
56	MG	4K	101	1/1	0.94	0.19	90,90,90,90	0
56	MG	14	3421	1/1	0.94	0.05	130,130,130,130	0
56	MG	13	1741	1/1	0.94	0.08	118,118,118,118	0
56	MG	1H	3220	1/1	0.94	0.29	124,124,124,124	0
56	MG	1H	3482	1/1	0.94	0.10	119,119,119,119	0
56	MG	14	3425	1/1	0.94	0.28	92,92,92,92	0
56	MG	1H	3483	1/1	0.94	0.07	110,110,110,110	0
56	MG	1H	3221	1/1	0.94	0.38	99,99,99,99	0
56	MG	14	3041	1/1	0.94	0.16	80,80,80,80	0
56	MG	14	3179	1/1	0.94	0.30	96,96,96,96	0
56	MG	14	3290	1/1	0.94	0.26	113,113,113,113	0
56	MG	14	3042	1/1	0.94	0.21	87,87,87,87	0
56	MG	13	1678	1/1	0.94	0.09	111,111,111,111	0
56	MG	14	3052	1/1	0.94	0.21	110,110,110,110	0
56	MG	1J	210	1/1	0.94	0.06	109,109,109,109	0
56	MG	1H	3386	1/1	0.94	0.16	82,82,82,82	0
56	MG	1H	3390	1/1	0.94	0.17	83,83,83,83	0
56	MG	1H	3315	1/1	0.94	0.39	105,105,105,105	0
56	MG	13	1603	1/1	0.94	0.21	97,97,97,97	0
56	MG	14	3190	1/1	0.94	0.22	124,124,124,124	0
56	MG	14	3059	1/1	0.94	0.27	74,74,74,74	0
56	MG	1H	3398	1/1	0.94	0.09	92,92,92,92	0
56	MG	13	1671	1/1	0.94	0.24	102,102,102,102	0
56	MG	1H	3400	1/1	0.94	0.10	61,61,61,61	0
56	MG	1H	3404	1/1	0.94	0.09	62,62,62,62	0
56	MG	1H	3094	1/1	0.94	0.39	79,79,79,79	0
56	MG	14	3071	1/1	0.94	0.12	94,94,94,94	0
56	MG	13	1698	1/1	0.94	0.35	95,95,95,95	0
56	MG	13	1709	1/1	0.94	0.28	141,141,141,141	0
56	MG	1H	3416	1/1	0.94	0.07	78,78,78,78	0
56	MG	13	1613	1/1	0.94	0.18	96,96,96,96	0
56	MG	1H	3053	1/1	0.94	0.17	92,92,92,92	0
56	MG	13	1602	1/1	0.95	0.31	87,87,87,87	0
56	MG	14	3336	1/1	0.95	0.14	88,88,88,88	0
56	MG	1H	3010	1/1	0.95	0.34	83,83,83,83	0
56	MG	14	3340	1/1	0.95	0.34	91,91,91,91	0
56	MG	1G	1616	1/1	0.95	0.18	149,149,149,149	0
56	MG	1H	3011	1/1	0.95	0.51	91,91,91,91	0
56	MG	1H	3419	1/1	0.95	0.16	94,94,94,94	0
56	MG	14	3001	1/1	0.95	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3138	1/1	0.95	0.20	73,73,73,73	0
56	MG	14	3139	1/1	0.95	0.19	67,67,67,67	0
56	MG	13	1642	1/1	0.95	0.11	98,98,98,98	0
56	MG	14	3005	1/1	0.95	0.18	66,66,66,66	0
56	MG	1H	3170	1/1	0.95	0.33	100,100,100,100	0
56	MG	14	3007	1/1	0.95	0.23	94,94,94,94	0
56	MG	14	3359	1/1	0.95	0.13	114,114,114,114	0
56	MG	1H	3173	1/1	0.95	0.36	98,98,98,98	0
56	MG	1H	3109	1/1	0.95	0.20	84,84,84,84	0
56	MG	2K	103	1/1	0.95	0.10	98,98,98,98	0
56	MG	14	3364	1/1	0.95	0.07	87,87,87,87	0
56	MG	1H	3176	1/1	0.95	0.30	91,91,91,91	0
56	MG	1G	1630	1/1	0.95	0.47	116,116,116,116	0
56	MG	1G	1631	1/1	0.95	0.23	113,113,113,113	0
56	MG	14	3021	1/1	0.95	0.40	79,79,79,79	0
56	MG	1H	3212	1/1	0.95	0.14	61,61,61,61	0
56	MG	1H	3213	1/1	0.95	0.27	113,113,113,113	0
56	MG	1H	3215	1/1	0.95	0.14	81,81,81,81	0
56	MG	1H	3261	1/1	0.95	0.48	99,99,99,99	0
56	MG	1H	3341	1/1	0.95	0.27	100,100,100,100	0
56	MG	1H	3047	1/1	0.95	0.30	65,65,65,65	0
56	MG	1H	3433	1/1	0.95	0.09	76,76,76,76	0
56	MG	13	1657	1/1	0.95	0.24	104,104,104,104	0
56	MG	1H	3218	1/1	0.95	0.17	78,78,78,78	0
56	MG	13	1726	1/1	0.95	0.12	90,90,90,90	0
56	MG	14	3384	1/1	0.95	0.14	60,60,60,60	0
56	MG	1H	3021	1/1	0.95	0.32	79,79,79,79	0
56	MG	1H	3347	1/1	0.95	0.13	57,57,57,57	0
56	MG	14	3390	1/1	0.95	0.18	94,94,94,94	0
56	MG	1H	3052	1/1	0.95	0.30	80,80,80,80	0
56	MG	14	3393	1/1	0.95	0.14	80,80,80,80	0
56	MG	14	3044	1/1	0.95	0.14	78,78,78,78	0
56	MG	1H	3444	1/1	0.95	0.28	102,102,102,102	0
56	MG	14	3049	1/1	0.95	0.25	87,87,87,87	0
56	MG	13	1673	1/1	0.95	0.28	91,91,91,91	0
56	MG	14	3171	1/1	0.95	0.19	73,73,73,73	0
56	MG	16	208	1/1	0.95	0.55	94,94,94,94	0
56	MG	16	210	1/1	0.95	0.45	107,107,107,107	0
56	MG	1H	3090	1/1	0.95	0.47	91,91,91,91	0
56	MG	16	213	1/1	0.95	0.43	85,85,85,85	0
56	MG	13	1616	1/1	0.95	0.10	82,82,82,82	0
56	MG	14	3060	1/1	0.95	0.27	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3367	1/1	0.95	0.13	82,82,82,82	0
56	MG	14	3180	1/1	0.95	0.32	83,83,83,83	0
56	MG	1H	3025	1/1	0.95	0.48	78,78,78,78	0
56	MG	1H	3229	1/1	0.95	0.23	83,83,83,83	0
56	MG	1H	3275	1/1	0.95	0.30	97,97,97,97	0
56	MG	1G	1658	1/1	0.95	0.21	110,110,110,110	0
56	MG	14	3069	1/1	0.95	0.08	63,63,63,63	0
56	MG	41	201	1/1	0.95	0.16	89,89,89,89	0
56	MG	1H	3376	1/1	0.95	0.04	96,96,96,96	0
56	MG	14	3074	1/1	0.95	0.13	79,79,79,79	0
56	MG	1H	3095	1/1	0.95	0.43	74,74,74,74	0
56	MG	1G	1662	1/1	0.95	0.16	155,155,155,155	0
56	MG	1H	3463	1/1	0.95	0.04	113,113,113,113	0
56	MG	88	201	1/1	0.95	0.22	95,95,95,95	0
56	MG	14	3298	1/1	0.95	0.42	115,115,115,115	0
56	MG	13	1730	1/1	0.95	0.03	113,113,113,113	0
56	MG	1J	201	1/1	0.95	0.15	123,123,123,123	0
56	MG	G8	201	1/1	0.95	0.11	83,83,83,83	0
56	MG	1H	3384	1/1	0.95	0.07	59,59,59,59	0
56	MG	1H	3385	1/1	0.95	0.14	75,75,75,75	0
56	MG	13	1625	1/1	0.95	0.30	77,77,77,77	0
56	MG	1H	3235	1/1	0.95	0.25	75,75,75,75	0
56	MG	1H	3236	1/1	0.95	0.26	77,77,77,77	0
56	MG	14	3099	1/1	0.95	0.14	106,106,106,106	0
56	MG	14	3100	1/1	0.95	0.12	87,87,87,87	0
56	MG	1G	1672	1/1	0.95	0.26	126,126,126,126	0
56	MG	1H	3099	1/1	0.95	0.33	69,69,69,69	0
56	MG	13	1635	1/1	0.95	0.14	88,88,88,88	0
56	MG	14	3216	1/1	0.95	0.43	111,111,111,111	0
56	MG	1H	3066	1/1	0.95	0.27	71,71,71,71	0
56	MG	1G	1676	1/1	0.95	0.35	121,121,121,121	0
56	MG	14	3219	1/1	0.95	0.20	102,102,102,102	0
56	MG	1H	3196	1/1	0.95	0.70	110,110,110,110	0
56	MG	14	3222	1/1	0.95	0.24	99,99,99,99	0
56	MG	1H	3324	1/1	0.95	0.15	107,107,107,107	0
56	MG	1H	3405	1/1	0.95	0.13	86,86,86,86	0
56	MG	14	3114	1/1	0.95	0.39	97,97,97,97	0
56	MG	13	1653	1/1	0.95	0.21	78,78,78,78	0
56	MG	85	201	1/1	0.95	0.28	93,93,93,93	0
56	MG	1H	3408	1/1	0.95	0.09	87,87,87,87	0
56	MG	1H	3164	1/1	0.95	0.43	102,102,102,102	0
56	MG	1G	1612	1/1	0.95	0.15	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3126	1/1	0.95	0.29	103,103,103,103	0
57	ZN	5A	101	1/1	0.95	0.13	172,172,172,172	0
56	MG	3I	201	1/1	0.95	0.18	81,81,81,81	0
56	MG	1G	1646	1/1	0.96	0.15	102,102,102,102	0
56	MG	1H	3117	1/1	0.96	0.29	87,87,87,87	0
56	MG	1H	3462	1/1	0.96	0.11	75,75,75,75	0
56	MG	13	1655	1/1	0.96	0.14	89,89,89,89	0
56	MG	21	302	1/1	0.96	0.16	82,82,82,82	0
56	MG	14	3242	1/1	0.96	0.16	94,94,94,94	0
56	MG	14	3349	1/1	0.96	0.14	71,71,71,71	0
56	MG	1H	3396	1/1	0.96	0.17	87,87,87,87	0
56	MG	14	3245	1/1	0.96	0.18	71,71,71,71	0
56	MG	1H	3038	1/1	0.96	0.26	58,58,58,58	0
56	MG	14	3031	1/1	0.96	0.29	76,76,76,76	0
56	MG	1H	3214	1/1	0.96	0.13	103,103,103,103	0
56	MG	1H	3180	1/1	0.96	0.17	84,84,84,84	0
56	MG	14	3040	1/1	0.96	0.20	79,79,79,79	0
56	MG	1H	3402	1/1	0.96	0.12	81,81,81,81	0
56	MG	1H	3151	1/1	0.96	0.17	110,110,110,110	0
56	MG	1H	3093	1/1	0.96	0.16	81,81,81,81	0
56	MG	14	3045	1/1	0.96	0.17	70,70,70,70	0
56	MG	1H	3064	1/1	0.96	0.27	76,76,76,76	0
56	MG	1H	3065	1/1	0.96	0.27	71,71,71,71	0
56	MG	14	3050	1/1	0.96	0.13	60,60,60,60	0
56	MG	13	1648	1/1	0.96	0.26	76,76,76,76	0
56	MG	1H	3156	1/1	0.96	0.36	110,110,110,110	0
56	MG	14	3054	1/1	0.96	0.12	93,93,93,93	0
56	MG	14	3373	1/1	0.96	0.08	81,81,81,81	0
56	MG	1H	3187	1/1	0.96	0.24	89,89,89,89	0
56	MG	1H	3042	1/1	0.96	0.19	53,53,53,53	0
56	MG	14	3057	1/1	0.96	0.15	91,91,91,91	0
56	MG	14	3378	1/1	0.96	0.16	101,101,101,101	0
56	MG	1H	3046	1/1	0.96	0.30	72,72,72,72	0
56	MG	1H	3069	1/1	0.96	0.37	89,89,89,89	0
56	MG	13	1612	1/1	0.96	0.27	89,89,89,89	0
56	MG	14	3165	1/1	0.96	0.33	70,70,70,70	0
56	MG	1H	3269	1/1	0.96	0.52	90,90,90,90	0
56	MG	1H	3486	1/1	0.96	0.07	98,98,98,98	0
56	MG	1H	3192	1/1	0.96	0.11	78,78,78,78	0
56	MG	14	3389	1/1	0.96	0.17	72,72,72,72	0
56	MG	13	1609	1/1	0.96	0.19	83,83,83,83	0
56	MG	14	3067	1/1	0.96	0.18	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	1H	3134	1/1	0.96	0.13	57,57,57,57	0
56	MG	14	3172	1/1	0.96	0.21	107,107,107,107	0
56	MG	13	1751	1/1	0.96	0.16	94,94,94,94	0
56	MG	14	3070	1/1	0.96	0.19	66,66,66,66	0
56	MG	1H	3349	1/1	0.96	0.16	69,69,69,69	0
56	MG	1H	3350	1/1	0.96	0.14	64,64,64,64	0
56	MG	14	3073	1/1	0.96	0.26	74,74,74,74	0
56	MG	1H	3197	1/1	0.96	0.41	89,89,89,89	0
56	MG	14	3402	1/1	0.96	0.11	99,99,99,99	0
56	MG	1G	1678	1/1	0.96	0.13	108,108,108,108	0
56	MG	14	3404	1/1	0.96	0.08	97,97,97,97	0
56	MG	13	1681	1/1	0.96	0.25	107,107,107,107	0
56	MG	1H	3075	1/1	0.96	0.08	59,59,59,59	0
56	MG	1H	3360	1/1	0.96	0.14	58,58,58,58	0
56	MG	1H	3497	1/1	0.96	0.10	119,119,119,119	0
56	MG	1G	1683	1/1	0.96	0.14	129,129,129,129	0
56	MG	14	3084	1/1	0.96	0.22	78,78,78,78	0
56	MG	14	3086	1/1	0.96	0.28	84,84,84,84	0
56	MG	14	3087	1/1	0.96	0.16	82,82,82,82	0
56	MG	14	3088	1/1	0.96	0.23	66,66,66,66	0
56	MG	14	3090	1/1	0.96	0.20	89,89,89,89	0
56	MG	1G	1619	1/1	0.96	0.21	72,72,72,72	0
56	MG	1H	3363	1/1	0.96	0.21	71,71,71,71	0
56	MG	1H	3364	1/1	0.96	0.12	80,80,80,80	0
56	MG	1H	3436	1/1	0.96	0.10	79,79,79,79	0
56	MG	14	3199	1/1	0.96	0.35	126,126,126,126	0
56	MG	1H	3240	1/1	0.96	0.25	94,94,94,94	0
56	MG	13	1623	1/1	0.96	0.15	84,84,84,84	0
56	MG	1H	3139	1/1	0.96	0.40	79,79,79,79	0
56	MG	13	1628	1/1	0.96	0.35	102,102,102,102	0
56	MG	1H	3244	1/1	0.96	0.20	90,90,90,90	0
56	MG	14	3206	1/1	0.96	0.08	83,83,83,83	0
56	MG	1H	3506	1/1	0.96	0.33	57,57,57,57	0
56	MG	1H	3054	1/1	0.96	0.19	71,71,71,71	0
56	MG	14	3004	1/1	0.96	0.25	64,64,64,64	0
56	MG	14	3108	1/1	0.96	0.15	92,92,92,92	0
56	MG	1H	3377	1/1	0.96	0.17	97,97,97,97	0
56	MG	13	1617	1/1	0.96	0.08	106,106,106,106	0
56	MG	14	3214	1/1	0.96	0.14	70,70,70,70	0
56	MG	1H	3450	1/1	0.96	0.13	66,66,66,66	0
56	MG	14	3009	1/1	0.96	0.24	65,65,65,65	0
56	MG	14	3115	1/1	0.96	0.18	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	14	3011	1/1	0.96	0.20	61,61,61,61	0
56	MG	14	3220	1/1	0.96	0.32	94,94,94,94	0
56	MG	1H	3451	1/1	0.96	0.11	87,87,87,87	0
56	MG	1H	3033	1/1	0.96	0.59	100,100,100,100	0
56	MG	1H	3057	1/1	0.96	0.19	72,72,72,72	0
56	MG	16	209	1/1	0.96	0.21	88,88,88,88	0
56	MG	14	3226	1/1	0.96	0.21	123,123,123,123	0
56	MG	1H	3114	1/1	0.96	0.42	82,82,82,82	0
56	MG	14	3228	1/1	0.96	0.20	86,86,86,86	0
56	MG	14	3129	1/1	0.96	0.20	78,78,78,78	0
56	MG	2K	101	1/1	0.96	0.22	76,76,76,76	0
56	MG	14	3131	1/1	0.96	0.20	56,56,56,56	0
56	MG	16	212	1/1	0.96	0.43	99,99,99,99	0
56	MG	14	3334	1/1	0.96	0.11	91,91,91,91	0
56	MG	1H	3387	1/1	0.96	0.17	70,70,70,70	0
56	MG	1H	3289	1/1	0.96	0.22	93,93,93,93	0
56	MG	14	3338	1/1	0.96	0.09	68,68,68,68	0
56	MG	14	3353	1/1	0.97	0.15	91,91,91,91	0
56	MG	1H	3115	1/1	0.97	0.34	95,95,95,95	0
56	MG	14	3085	1/1	0.97	0.18	81,81,81,81	0
56	MG	1H	3401	1/1	0.97	0.16	87,87,87,87	0
56	MG	1H	3239	1/1	0.97	0.17	88,88,88,88	0
56	MG	1H	3403	1/1	0.97	0.16	73,73,73,73	0
56	MG	14	3361	1/1	0.97	0.17	86,86,86,86	0
56	MG	14	3089	1/1	0.97	0.21	85,85,85,85	0
56	MG	1H	3008	1/1	0.97	0.41	79,79,79,79	0
56	MG	13	1746	1/1	0.97	0.07	110,110,110,110	0
56	MG	1H	3468	1/1	0.97	0.07	95,95,95,95	0
56	MG	13	1747	1/1	0.97	0.28	103,103,103,103	0
56	MG	14	3015	1/1	0.97	0.08	81,81,81,81	0
56	MG	14	3095	1/1	0.97	0.20	78,78,78,78	0
56	MG	14	3097	1/1	0.97	0.12	69,69,69,69	0
56	MG	13	1608	1/1	0.97	0.20	91,91,91,91	0
56	MG	1H	3120	1/1	0.97	0.13	80,80,80,80	0
56	MG	1H	3413	1/1	0.97	0.15	77,77,77,77	0
56	MG	1H	3348	1/1	0.97	0.14	84,84,84,84	0
56	MG	1H	3096	1/1	0.97	0.17	57,57,57,57	0
56	MG	13	1610	1/1	0.97	0.20	79,79,79,79	0
56	MG	14	3105	1/1	0.97	0.14	74,74,74,74	0
56	MG	1G	1651	1/1	0.97	0.20	138,138,138,138	0
56	MG	13	1659	1/1	0.97	0.31	109,109,109,109	0
56	MG	14	3191	1/1	0.97	0.21	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	14	3382	1/1	0.97	0.29	86,86,86,86	0
56	MG	1H	3356	1/1	0.97	0.10	58,58,58,58	0
56	MG	13	1649	1/1	0.97	0.27	85,85,85,85	0
56	MG	14	3194	1/1	0.97	0.23	97,97,97,97	0
56	MG	14	3111	1/1	0.97	0.17	72,72,72,72	0
56	MG	1H	3018	1/1	0.97	0.41	79,79,79,79	0
56	MG	1H	3481	1/1	0.97	0.11	70,70,70,70	0
56	MG	14	3198	1/1	0.97	0.11	88,88,88,88	0
56	MG	1H	3019	1/1	0.97	0.28	54,54,54,54	0
56	MG	1H	3078	1/1	0.97	0.23	70,70,70,70	0
56	MG	14	3116	1/1	0.97	0.21	73,73,73,73	0
56	MG	1H	3131	1/1	0.97	0.17	56,56,56,56	0
56	MG	14	3397	1/1	0.97	0.13	101,101,101,101	0
56	MG	14	3036	1/1	0.97	0.15	67,67,67,67	0
56	MG	1H	3253	1/1	0.97	0.20	91,91,91,91	0
56	MG	14	3205	1/1	0.97	0.45	72,72,72,72	0
56	MG	14	3124	1/1	0.97	0.26	85,85,85,85	0
56	MG	1H	3103	1/1	0.97	0.15	60,60,60,60	0
56	MG	1H	3369	1/1	0.97	0.15	92,92,92,92	0
56	MG	1H	3371	1/1	0.97	0.08	91,91,91,91	0
56	MG	14	3128	1/1	0.97	0.21	97,97,97,97	0
56	MG	13	1725	1/1	0.97	0.11	102,102,102,102	0
56	MG	1H	3037	1/1	0.97	0.37	76,76,76,76	0
56	MG	14	3300	1/1	0.97	0.15	98,98,98,98	0
56	MG	13	1614	1/1	0.97	0.16	98,98,98,98	0
56	MG	14	3046	1/1	0.97	0.24	88,88,88,88	0
56	MG	1H	3039	1/1	0.97	0.39	55,55,55,55	0
56	MG	14	3134	1/1	0.97	0.10	103,103,103,103	0
56	MG	13	1638	1/1	0.97	0.09	115,115,115,115	0
56	MG	13	1712	1/1	0.97	0.19	99,99,99,99	0
56	MG	1H	3226	1/1	0.97	0.26	88,88,88,88	0
56	MG	1H	3383	1/1	0.97	0.10	67,67,67,67	0
56	MG	14	3223	1/1	0.97	0.82	81,81,81,81	0
56	MG	14	3310	1/1	0.97	0.20	96,96,96,96	0
56	MG	1H	3227	1/1	0.97	0.26	123,123,123,123	0
56	MG	1H	3110	1/1	0.97	0.31	67,67,67,67	0
56	MG	1H	3299	1/1	0.97	0.17	71,71,71,71	0
56	MG	1H	3195	1/1	0.97	0.11	94,94,94,94	0
56	MG	1H	3445	1/1	0.97	0.12	83,83,83,83	0
56	MG	14	3426	1/1	0.97	0.24	67,67,67,67	0
56	MG	1G	1677	1/1	0.97	0.08	91,91,91,91	0
56	MG	14	3230	1/1	0.97	0.27	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	14	3145	1/1	0.97	0.25	105,105,105,105	0
56	MG	1H	3388	1/1	0.97	0.14	65,65,65,65	0
56	MG	14	3062	1/1	0.97	0.29	85,85,85,85	0
56	MG	1G	1621	1/1	0.97	0.11	88,88,88,88	0
56	MG	14	3322	1/1	0.97	0.14	90,90,90,90	0
56	MG	1H	3088	1/1	0.97	0.33	52,52,52,52	0
56	MG	1H	3449	1/1	0.97	0.15	78,78,78,78	0
56	MG	1G	1624	1/1	0.97	0.17	93,93,93,93	0
56	MG	14	3238	1/1	0.97	0.16	110,110,110,110	0
56	MG	1H	3089	1/1	0.97	0.28	58,58,58,58	0
56	MG	1G	1626	1/1	0.97	0.27	102,102,102,102	0
56	MG	1G	1627	1/1	0.97	0.23	116,116,116,116	0
56	MG	14	3155	1/1	0.97	0.17	76,76,76,76	0
56	MG	1H	3392	1/1	0.97	0.13	65,65,65,65	0
56	MG	14	3244	1/1	0.97	0.23	99,99,99,99	0
56	MG	1H	3394	1/1	0.97	0.09	62,62,62,62	0
56	MG	16	203	1/1	0.97	0.17	107,107,107,107	0
56	MG	13	1729	1/1	0.97	0.12	109,109,109,109	0
56	MG	1H	3091	1/1	0.97	0.36	70,70,70,70	0
56	MG	2L	101	1/1	0.97	0.18	98,98,98,98	0
56	MG	1H	3397	1/1	0.97	0.15	77,77,77,77	0
56	MG	1H	3171	1/1	0.97	0.51	75,75,75,75	0
56	MG	14	3347	1/1	0.97	0.07	85,85,85,85	0
56	MG	14	3348	1/1	0.97	0.10	71,71,71,71	0
57	ZN	5I	101	1/1	0.97	0.20	114,114,114,114	0
56	MG	1H	3459	1/1	0.97	0.14	81,81,81,81	0
56	MG	14	3002	1/1	0.97	0.24	70,70,70,70	0
56	MG	1H	3172	1/1	0.97	0.26	98,98,98,98	0
56	MG	14	3212	1/1	0.98	0.16	104,104,104,104	0
56	MG	1H	3414	1/1	0.98	0.15	65,65,65,65	0
56	MG	1H	3361	1/1	0.98	0.16	56,56,56,56	0
56	MG	1H	3043	1/1	0.98	0.27	72,72,72,72	0
56	MG	14	3377	1/1	0.98	0.08	82,82,82,82	0
56	MG	1H	3045	1/1	0.98	0.20	63,63,63,63	0
56	MG	21	301	1/1	0.98	0.23	75,75,75,75	0
56	MG	1H	3365	1/1	0.98	0.13	69,69,69,69	0
56	MG	1H	3259	1/1	0.98	0.52	105,105,105,105	0
56	MG	13	1735	1/1	0.98	0.07	96,96,96,96	0
56	MG	1H	3145	1/1	0.98	0.20	57,57,57,57	0
56	MG	13	1737	1/1	0.98	0.14	72,72,72,72	0
56	MG	14	3386	1/1	0.98	0.25	105,105,105,105	0
56	MG	14	3075	1/1	0.98	0.23	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	1H	3048	1/1	0.98	0.21	65,65,65,65	0
56	MG	14	3008	1/1	0.98	0.25	78,78,78,78	0
56	MG	1H	3373	1/1	0.98	0.12	63,63,63,63	0
56	MG	14	3010	1/1	0.98	0.19	65,65,65,65	0
56	MG	1H	3070	1/1	0.98	0.54	125,125,125,125	0
56	MG	1H	3233	1/1	0.98	0.19	65,65,65,65	0
56	MG	1H	3427	1/1	0.98	0.09	75,75,75,75	0
56	MG	1H	3234	1/1	0.98	0.29	91,91,91,91	0
56	MG	1H	3484	1/1	0.98	0.09	79,79,79,79	0
56	MG	13	1738	1/1	0.98	0.13	77,77,77,77	0
56	MG	13	1634	1/1	0.98	0.30	85,85,85,85	0
56	MG	1G	1601	1/1	0.98	0.19	109,109,109,109	0
56	MG	1H	3379	1/1	0.98	0.12	74,74,74,74	0
56	MG	13	1604	1/1	0.98	0.27	108,108,108,108	0
56	MG	1H	3207	1/1	0.98	0.18	60,60,60,60	0
56	MG	1H	3271	1/1	0.98	0.46	93,93,93,93	0
56	MG	1H	3125	1/1	0.98	0.16	68,68,68,68	0
56	MG	1H	3014	1/1	0.98	0.42	57,57,57,57	0
56	MG	1G	1608	1/1	0.98	0.14	98,98,98,98	0
56	MG	14	3408	1/1	0.98	0.08	79,79,79,79	0
56	MG	13	1601	1/1	0.98	0.27	74,74,74,74	0
56	MG	1H	3016	1/1	0.98	0.31	66,66,66,66	0
56	MG	1H	3389	1/1	0.98	0.16	69,69,69,69	0
56	MG	14	3101	1/1	0.98	0.15	80,80,80,80	0
56	MG	1H	3001	1/1	0.98	0.29	64,64,64,64	0
56	MG	14	3414	1/1	0.98	0.06	93,93,93,93	0
56	MG	14	3032	1/1	0.98	0.20	52,52,52,52	0
56	MG	14	3033	1/1	0.98	0.18	66,66,66,66	0
56	MG	14	3034	1/1	0.98	0.23	69,69,69,69	0
56	MG	14	3327	1/1	0.98	0.43	117,117,117,117	0
56	MG	1H	3130	1/1	0.98	0.24	78,78,78,78	0
56	MG	13	1742	1/1	0.98	0.10	82,82,82,82	0
56	MG	1H	3446	1/1	0.98	0.12	74,74,74,74	0
56	MG	14	3333	1/1	0.98	0.12	73,73,73,73	0
56	MG	1H	3393	1/1	0.98	0.17	60,60,60,60	0
56	MG	14	3110	1/1	0.98	0.23	61,61,61,61	0
56	MG	13	1705	1/1	0.98	0.14	98,98,98,98	0
56	MG	13	1732	1/1	0.98	0.09	81,81,81,81	0
56	MG	14	3043	1/1	0.98	0.21	101,101,101,101	0
56	MG	1H	3059	1/1	0.98	0.49	92,92,92,92	0
56	MG	1H	3084	1/1	0.98	0.31	61,61,61,61	0
56	MG	1H	3453	1/1	0.98	0.15	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	14	3188	1/1	0.98	0.31	91,91,91,91	0
56	MG	14	3189	1/1	0.98	0.12	83,83,83,83	0
56	MG	1H	3085	1/1	0.98	0.22	62,62,62,62	0
56	MG	14	3118	1/1	0.98	0.24	71,71,71,71	0
56	MG	14	3119	1/1	0.98	0.32	66,66,66,66	0
56	MG	14	3120	1/1	0.98	0.17	80,80,80,80	0
56	MG	14	3351	1/1	0.98	0.12	60,60,60,60	0
56	MG	14	3048	1/1	0.98	0.20	73,73,73,73	0
56	MG	14	3122	1/1	0.98	0.19	68,68,68,68	0
56	MG	1H	3060	1/1	0.98	0.24	74,74,74,74	0
56	MG	1H	3351	1/1	0.98	0.18	65,65,65,65	0
56	MG	14	3051	1/1	0.98	0.20	100,100,100,100	0
56	MG	14	3358	1/1	0.98	0.09	85,85,85,85	0
56	MG	1H	3352	1/1	0.98	0.14	61,61,61,61	0
56	MG	1H	3353	1/1	0.98	0.11	77,77,77,77	0
56	MG	1H	3006	1/1	0.98	0.17	91,91,91,91	0
56	MG	1H	3355	1/1	0.98	0.18	64,64,64,64	0
56	MG	13	1733	1/1	0.98	0.10	102,102,102,102	0
56	MG	1H	3406	1/1	0.98	0.17	77,77,77,77	0
56	MG	1G	1685	1/1	0.98	0.08	112,112,112,112	0
56	MG	1H	3357	1/1	0.98	0.07	57,57,57,57	0
56	MG	1H	3063	1/1	0.98	0.28	83,83,83,83	0
57	ZN	3E	301	1/1	0.98	0.41	115,115,115,115	0
56	MG	14	3061	1/1	0.98	0.15	79,79,79,79	0
56	MG	1H	3465	1/1	0.98	0.10	83,83,83,83	0
56	MG	1H	3224	1/1	0.98	0.28	82,82,82,82	0
56	MG	13	1633	1/1	0.98	0.15	75,75,75,75	0
56	MG	1H	3017	1/1	0.99	0.23	79,79,79,79	0
56	MG	1H	3370	1/1	0.99	0.16	84,84,84,84	0
56	MG	1H	3452	1/1	0.99	0.14	65,65,65,65	0
56	MG	14	3331	1/1	0.99	0.29	112,112,112,112	0
56	MG	14	3332	1/1	0.99	0.12	72,72,72,72	0
56	MG	1H	3044	1/1	0.99	0.20	68,68,68,68	0
56	MG	1H	3036	1/1	0.99	0.46	61,61,61,61	0
56	MG	14	3335	1/1	0.99	0.12	73,73,73,73	0
56	MG	1H	3409	1/1	0.99	0.18	76,76,76,76	0
56	MG	14	3096	1/1	0.99	0.15	77,77,77,77	0
56	MG	13	1611	1/1	0.99	0.18	95,95,95,95	0
56	MG	14	3339	1/1	0.99	0.12	74,74,74,74	0
56	MG	14	3035	1/1	0.99	0.27	79,79,79,79	0
56	MG	1H	3411	1/1	0.99	0.12	80,80,80,80	0
56	MG	14	3342	1/1	0.99	0.12	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	14	3385	1/1	0.99	0.12	73,73,73,73	0
56	MG	1H	3412	1/1	0.99	0.12	64,64,64,64	0
56	MG	14	3038	1/1	0.99	0.16	72,72,72,72	0
56	MG	13	1723	1/1	0.99	0.14	105,105,105,105	0
56	MG	1H	3435	1/1	0.99	0.16	72,72,72,72	0
56	MG	13	1736	1/1	0.99	0.17	102,102,102,102	0
56	MG	1H	3076	1/1	0.99	0.26	73,73,73,73	0
56	MG	14	3392	1/1	0.99	0.08	70,70,70,70	0
56	MG	1H	3205	1/1	0.99	0.23	64,64,64,64	0
56	MG	14	3014	1/1	0.99	0.27	73,73,73,73	0
56	MG	1H	3362	1/1	0.99	0.14	61,61,61,61	0
56	MG	14	3016	1/1	0.99	0.24	71,71,71,71	0
56	MG	14	3077	1/1	0.99	0.28	80,80,80,80	0
56	MG	1H	3440	1/1	0.99	0.10	83,83,83,83	0
56	MG	14	3079	1/1	0.99	0.23	84,84,84,84	0
56	MG	1H	3040	1/1	0.99	0.21	78,78,78,78	0
56	MG	14	3357	1/1	0.99	0.13	80,80,80,80	0
56	MG	1H	3380	1/1	0.99	0.16	61,61,61,61	0
56	MG	1H	3443	1/1	0.99	0.17	76,76,76,76	0
56	MG	14	3215	1/1	0.99	0.15	104,104,104,104	0
56	MG	1H	3004	1/1	0.99	0.30	68,68,68,68	0
56	MG	1H	3382	1/1	0.99	0.10	58,58,58,58	0
56	MG	1H	3123	1/1	0.99	0.24	68,68,68,68	0
56	MG	1H	3472	1/1	0.99	0.08	98,98,98,98	0
56	MG	1H	3079	1/1	0.99	0.33	83,83,83,83	0
56	MG	14	3366	1/1	0.99	0.15	88,88,88,88	0
56	MG	1H	3022	1/1	0.99	0.38	64,64,64,64	0
57	ZN	32	302	1/1	0.99	0.39	131,131,131,131	0
56	MG	1H	3368	1/1	0.99	0.17	79,79,79,79	0
56	MG	14	3257	1/1	0.99	0.20	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.