



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:07 PM UTC

PDB ID : 4WRA / pdb_00004wra
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in the first position in the A-site and with antibiotic paromomycin.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-23
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

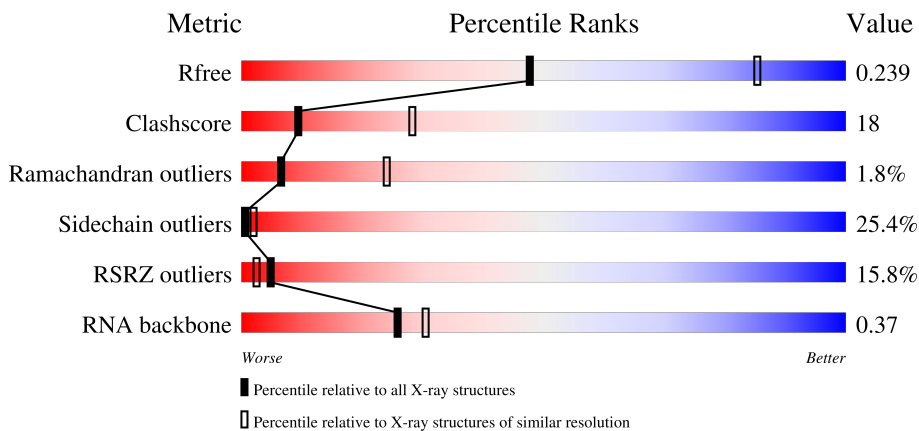
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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Mol	Chain	Length	Quality of chain
15	6I	89	11% 47% 44% 8%
16	7A	88	16% 40% 42% 14% 5%
16	7I	88	11% 33% 47% 15% 5%
17	8A	105	15% 47% 42% 5% 5%
17	8I	105	21% 37% 47% 10% 5%
18	9A	88	9% 41% 31% 9% 19%
18	9I	88	15% 36% 35% 9% 18%
19	AA	93	22% 38% 34% 10% 16%
19	AI	93	16% 40% 40% 6% 11%
20	BA	106	28% 44% 38% 8% 7%
20	BI	106	39% 39% 40% 15% 7%
21	1B	27	19% 37% 48% 7% 7%
21	1F	27	30% 30% 63% 7%
22	1K	85	35% 20% 45% 34%
23	2K	77	16% 34% 51% 14%
23	2L	77	25% 49% 35% 13%
24	1L	85	46% 36% 36% 27%
24	3K	85	20% 32% 47% 21%
25	4K	30	10% 20% 7% 13% 60%
25	4L	30	7% 13% 10% 13% 60%
26	14	2918	10% 41% 43% 15%
26	1H	2918	10% 41% 44% 14%
27	16	122	4% 43% 47% 11%
27	1J	122	8% 30% 48% 22%
28	11	276	3% 49% 39% 10%

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Mol	Chain	Length	Quality of chain
28	19	276	4% 51% 35% 11% ..
29	21	206	11% 32% 43% 21% .
29	29	206	19% 37% 37% 20% .
30	31	210	10% 47% 34% 13% ..
30	39	210	20% 33% 42% 20% ..
31	41	182	28% 45% 45% 9% ..
31	49	182	18% 48% 40% 12% .
32	51	180	22% 36% 41% 17% ..
32	59	180	48% 39% 38% 16% . 6%
33	61	148	27% 27% 51% 20% ..
33	69	148	32% 34% 48% 12% 5% .
34	15	140	31% 51% 31% 15% ..
34	58	140	12% 39% 40% 16% ..
35	25	122	11% 52% 38% 10% .
35	68	122	9% 52% 38% 10% .
36	35	150	15% 37% 37% 18% 7%
36	78	150	14% 39% 36% 19% 5%
37	45	141	15% 35% 43% 15% 5% .
37	88	141	12% 43% 41% 11% .
38	55	118	20% 42% 42% 13% ..
38	98	118	18% 33% 52% 14% .
39	65	112	10% 36% 45% 17% ..
39	A8	112	8% 39% 44% 15% .
40	75	146	23% 38% 41% 13% . 6%
40	B8	146	26% 39% 35% 18% . 6%


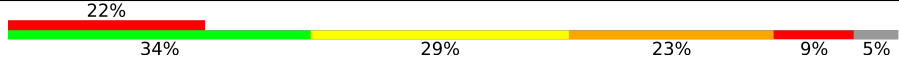
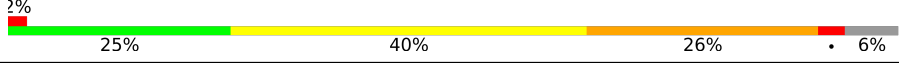
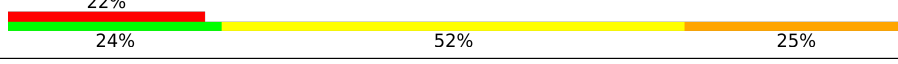
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Mol	Chain	Length	Quality of chain
41	85	118	23% 56% 29% 14% ..
41	C8	118	14% 43% 40% 14% ..
42	95	101	40% 35% 37% 25% .
42	D8	101	30% 43% 43% 12% .
43	A5	113	9% 49% 42% 9%
43	E8	113	4% 57% 31% 12% .
44	B5	96	6% 44% 42% 9% ..
44	F8	96	4% 43% 44% 9% ..
45	C5	110	33% 33% 37% 25% 5%
45	G8	110	13% 33% 43% 14% 5% 5%
46	D5	206	13% 31% 24% 10% . 33%
46	H8	206	17% 33% 37% 13% . 15%
47	E5	85	8% 42% 35% 11% . 9%
47	I8	85	9% 44% 34% 11% . 11%
48	F5	98	21% 47% 38% 13% ..
48	J8	98	9% 52% 31% 15% ..
49	G5	72	14% 28% 46% 14% . 8%
49	K8	72	18% 22% 44% 22% . 8%
50	H5	60	18% 52% 38% 8% .
50	L8	60	5% 47% 42% 10% .
51	I5	71	17% 21% 46% 18% . 11%
51	M8	71	27% 32% 39% 17% . 7%
52	J5	60	35% 53% 37% 8% .
52	N8	60	23% 48% 28% 22% .
53	L5	49	6% 53% 37% . 8%

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Mol	Chain	Length	Quality of chain
53	P8	49	
54	M5	65	
54	Q8	65	
55	3L	85	

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	1615	-	-	-	X
56	MG	13	1616	-	-	-	X
56	MG	13	1647	-	-	-	X
56	MG	13	1685	-	-	-	X
56	MG	13	1707	-	-	-	X
56	MG	13	1714	-	-	-	X
56	MG	14	3122	-	-	-	X
56	MG	14	3140	-	-	-	X
56	MG	14	3148	-	-	-	X
56	MG	14	3192	-	-	-	X
56	MG	14	3228	-	-	-	X
56	MG	14	3293	-	-	-	X
56	MG	14	3298	-	-	-	X
56	MG	14	3301	-	-	-	X
56	MG	1G	1610	-	-	-	X
56	MG	1G	1648	-	-	-	X
56	MG	1H	3075	-	-	-	X
56	MG	1H	3117	-	-	-	X
56	MG	1H	3163	-	-	-	X
56	MG	1H	3172	-	-	-	X
56	MG	1H	3207	-	-	-	X
56	MG	1H	3290	-	-	-	X
56	MG	1H	3293	-	-	-	X
56	MG	1H	3306	-	-	-	X
56	MG	1H	3311	-	-	-	X
56	MG	1H	3328	-	-	-	X
56	MG	1H	3342	-	-	-	X
56	MG	1H	3349	-	-	-	X
56	MG	1J	203	-	-	-	X
56	MG	25	201	-	-	-	X

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 299607 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	1505	Total 32352	C 14399	N 5994	O 10454	P 1505	0	0	0
1	1G	1504	Total 32327	C 14389	N 5989	O 10446	P 1503	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	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	12	237	Total 1924	C 1228	N 344	O 347	S 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	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	22	206	Total 1612	C 1016	N 314	O 281	S 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	Total 1702	C 1066	N 339	O 290	S 7	0	0	0
4	32	208	Total 1702	C 1066	N 339	O 290	S 7	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	152	Total	C	N	O	S	0	0	0
			1243	774	249	214	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			
9	82	122	Total	C	N	O	0	0	0
			971	616	189	166			

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

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

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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	117	873	543	166	161	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	122	956	603	193	159	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	116	928	574	191	161	2	0	0	0
13	4A	117	933	577	192	162	2	0	0	0

- 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	59	480	306	100	70	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
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			
18	9A	71	Total	C	N	O	0	0	0
			581	370	115	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	85	Total	C	N	O	P	S	0	0	0
			1824	821	323	594	85	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 723229079
2L	18	C	U	conflict	GB 723229079

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			
24	1L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	12	Total	C	N	O	P	0	1	0
			283	128	60	82	13			
25	4L	12	Total	C	N	O	P	0	0	0
			261	118	55	76	12			

- 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	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
26	14	2909	Total 62647	C 27884	N 11716	O 20139	P 2908	0	0	0

There are 18 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	654A	A	G	conflict	GB 48268
1H	654E	C	G	conflict	GB 48268
1H	654P	G	C	conflict	GB 48268
1H	654T	A	C	conflict	GB 48268
1H	1058	U	G	conflict	GB 48268
1H	1080	A	C	conflict	GB 48268
1H	1228	G	-	insertion	GB 48268
14	158	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	654A	A	G	conflict	GB 48268
14	654E	C	G	conflict	GB 48268
14	654P	G	C	conflict	GB 48268
14	654T	A	C	conflict	GB 48268
14	1058	U	G	conflict	GB 48268
14	1080	A	C	conflict	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	Total 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 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	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0
28	19	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	173	Total	C	N	O	S	0	0	0
			1321	837	248	235	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
37	45	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	110	Total	C	N	O	0	0	0
			876	553	175	148			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			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
44	F8	93	730	474	132	124	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
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
45	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
46	D5	138	Total	C	N	O	S	0	0	0
			1139	732	205	199	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
47	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
49	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			
52	J5	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	46	Total	C	N	O	S	0	0	0
			396	243	98	53	2			
53	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	M5	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			

- Molecule 55 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
55	3L	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

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

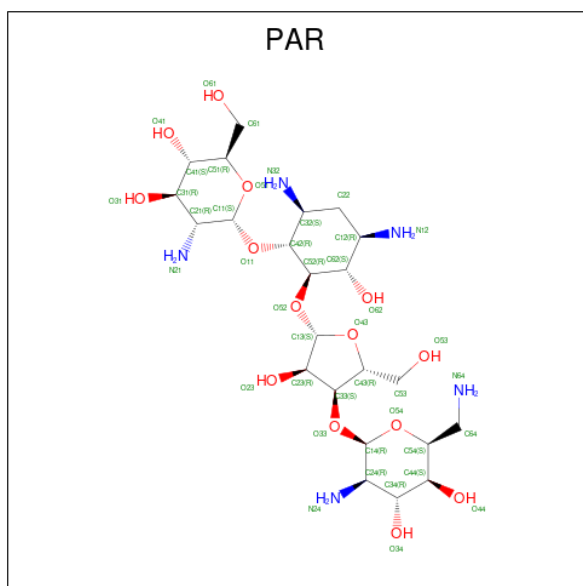
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	13	146	Total Mg 146 146	0	0
56	3E	1	Total Mg 1 1	0	0
56	5E	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	7	Total Mg 7 7	0	0
56	1H	481	Total Mg 481 481	0	0
56	16	12	Total Mg 12 12	0	0
56	11	2	Total Mg 2 2	0	0
56	21	2	Total Mg 2 2	0	0
56	31	1	Total Mg 1 1	0	0
56	41	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	88	1	Total Mg 1 1	0	0
56	I8	1	Total Mg 1 1	0	0
56	L8	1	Total Mg 1 1	0	0
56	P8	1	Total Mg 1 1	0	0
56	1G	86	Total Mg 86 86	0	0
56	2L	4	Total Mg 4 4	0	0
56	14	391	Total Mg 391 391	0	0
56	1J	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	29	3	Total Mg 3 3	0	0
56	39	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	35	1	Total Mg 1 1	0	0
56	45	1	Total Mg 1 1	0	0
56	85	1	Total Mg 1 1	0	0
56	C5	1	Total Mg 1 1	0	0
56	L5	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	3E	1	Total Zn 1 1	0	0
58	5I	1	Total Zn 1 1	0	0
58	G8	1	Total Zn 1 1	0	0
58	32	1	Total Zn 1 1	0	0
58	5A	1	Total Zn 1 1	0	0
58	C5	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	141	Total O 141 141	0	0
59	3E	1	Total O 1 1	0	0
59	1I	1	Total O 1 1	0	0
59	3I	2	Total O 2 2	0	0
59	5I	1	Total O 1 1	0	0
59	1K	1	Total O 1 1	0	0
59	2K	6	Total O 6 6	0	0
59	4K	3	Total O 3 3	0	0
59	1H	633	Total O 633 633	0	0
59	16	11	Total O 11 11	0	0
59	11	10	Total O 10 10	0	0
59	21	5	Total O 5 5	0	0
59	31	5	Total O 5 5	0	0
59	78	4	Total O 4 4	0	0

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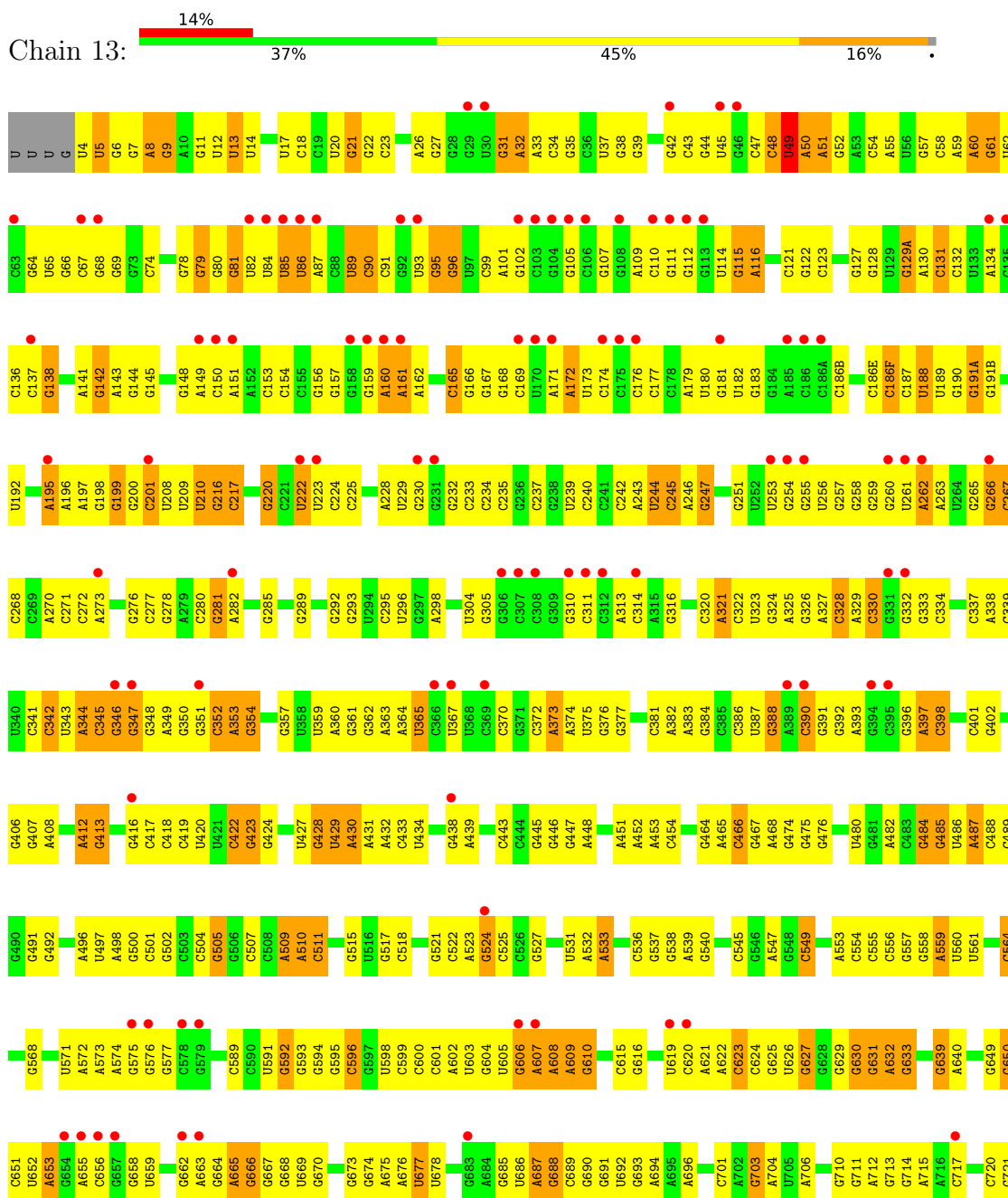
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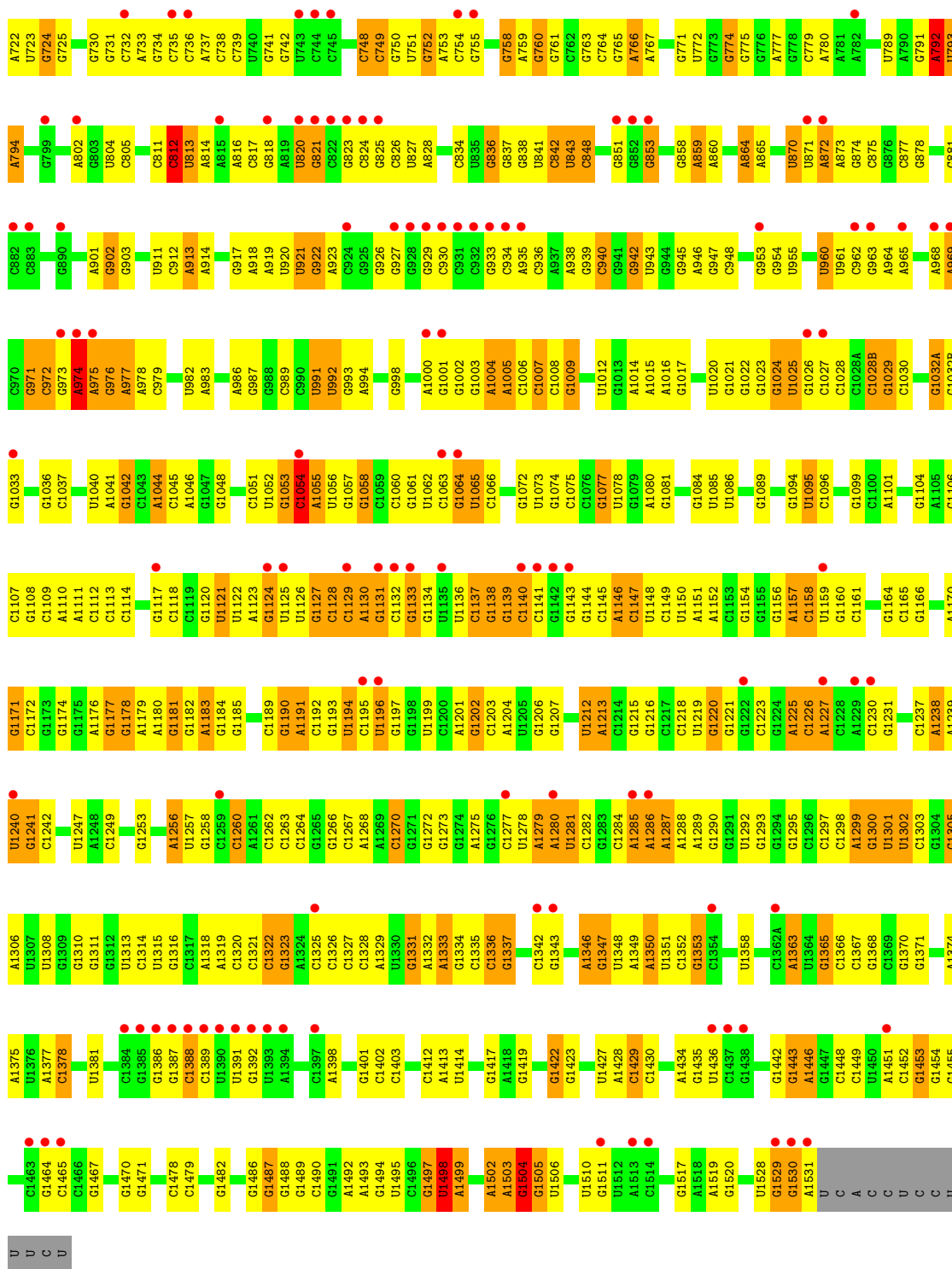
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59	G8	2	Total O 2 2	0	0
59	J8	1	Total O 1 1	0	0
59	L8	2	Total O 2 2	0	0
59	1G	87	Total O 87 87	0	0
59	5A	1	Total O 1 1	0	0
59	6A	1	Total O 1 1	0	0
59	BA	1	Total O 1 1	0	0
59	14	474	Total O 474 474	0	0
59	1J	6	Total O 6 6	0	0
59	19	9	Total O 9 9	0	0
59	29	3	Total O 3 3	0	0
59	39	5	Total O 5 5	0	0
59	55	1	Total O 1 1	0	0
59	75	1	Total O 1 1	0	0
59	85	1	Total O 1 1	0	0
59	A5	1	Total O 1 1	0	0
59	M5	2	Total O 2 2	0	0

3 Residue-property plots i

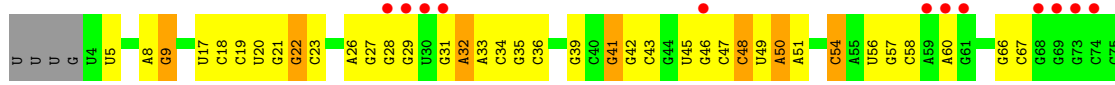
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

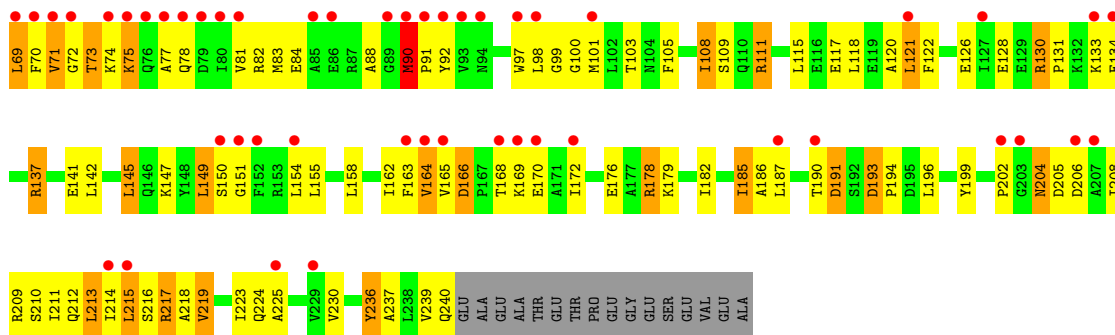
• Molecule 1: 16S ribosomal RNA



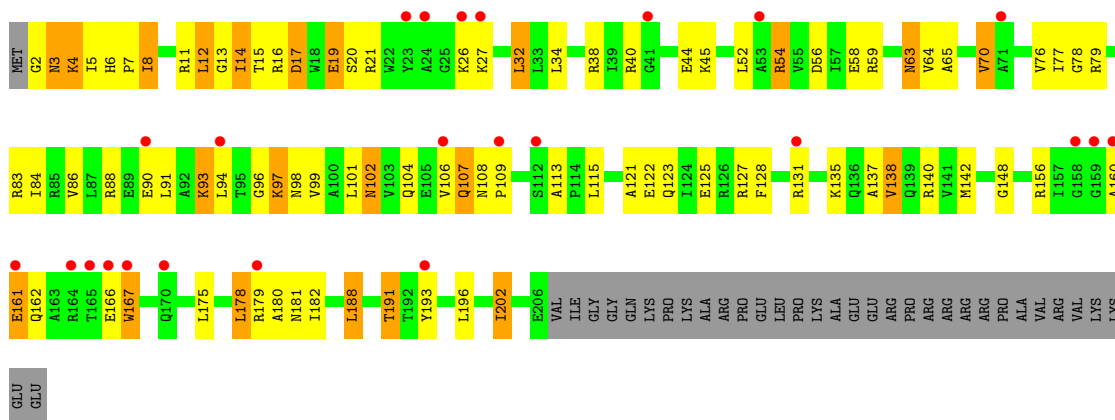


● Molecule 1: 16S ribosomal RNA

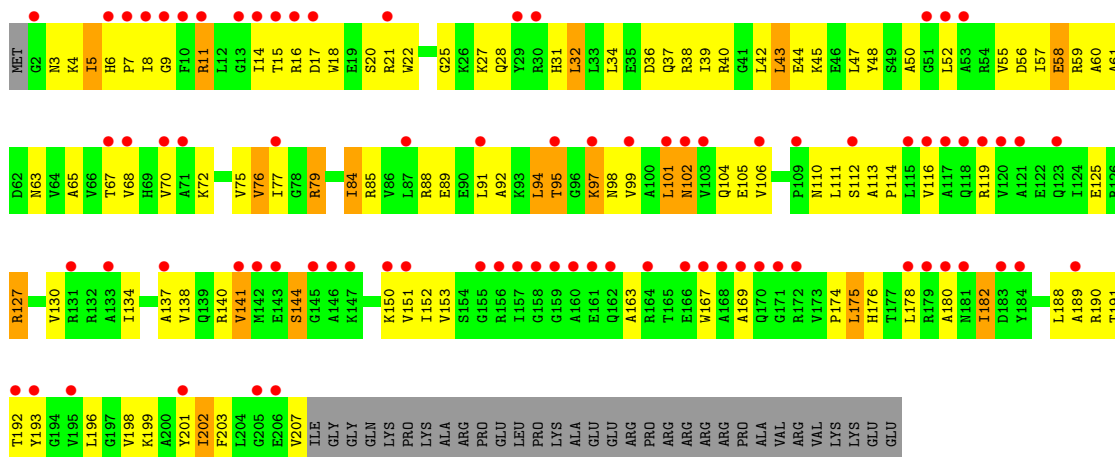




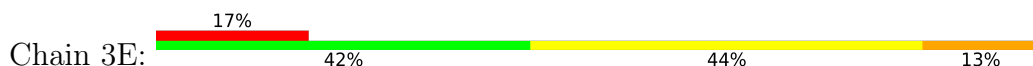
• Molecule 3: 30S ribosomal protein S3

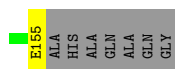


• Molecule 3: 30S ribosomal protein S3

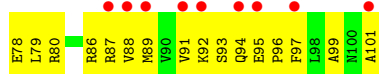


• Molecule 4: 30S ribosomal protein S4

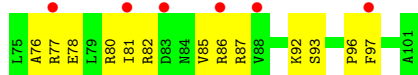




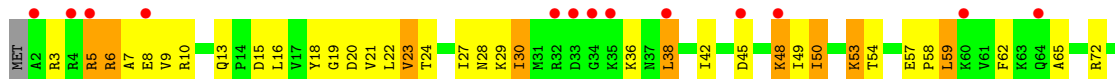
- Molecule 6: 30S ribosomal protein S6



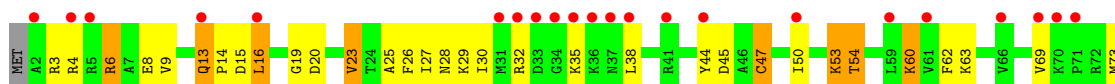
- Molecule 6: 30S ribosomal protein S6

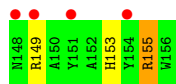


- Molecule 7: 30S ribosomal protein S7

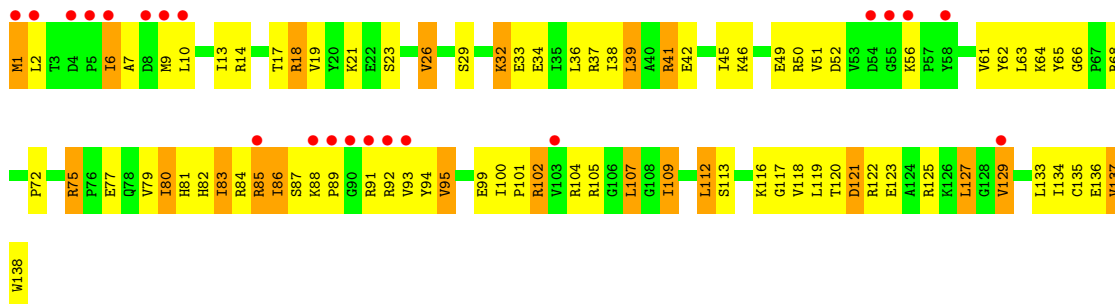


- Molecule 7: 30S ribosomal protein S7

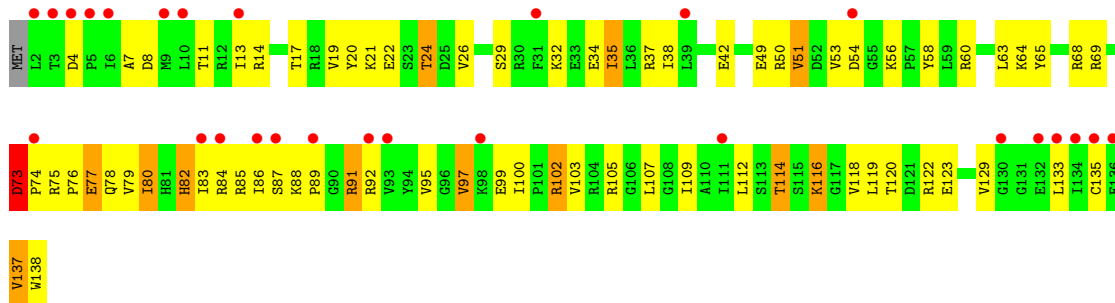




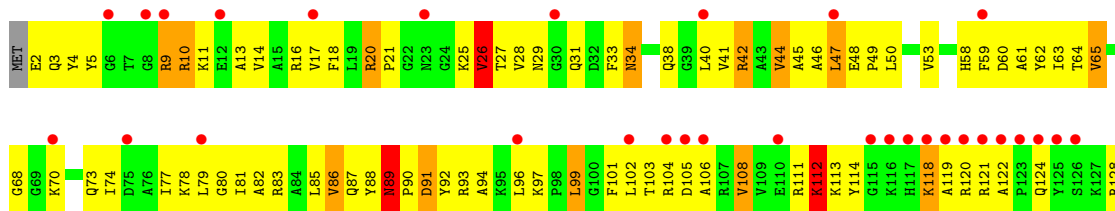
• Molecule 8: 30S ribosomal protein S8



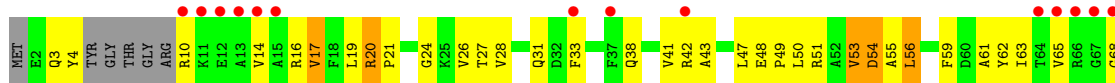
• Molecule 8: 30S ribosomal protein S8

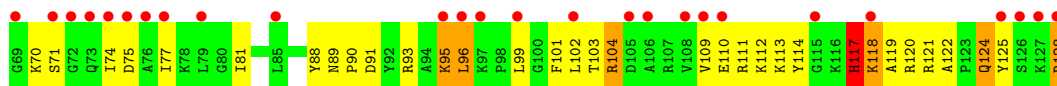


• Molecule 9: 30S ribosomal protein S9

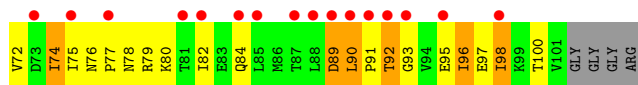
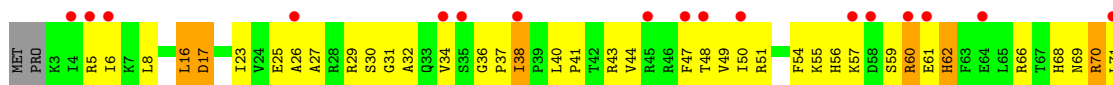


• Molecule 9: 30S ribosomal protein S9

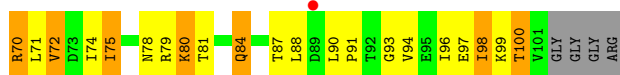
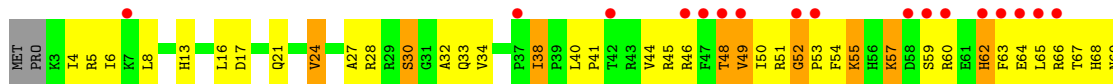




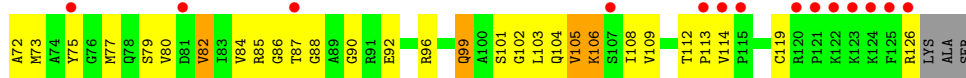
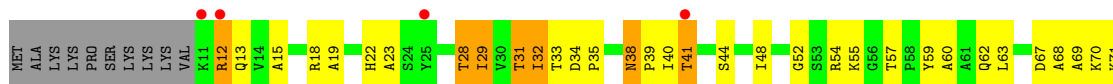
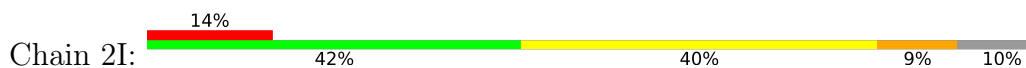
- Molecule 10: 30S ribosomal protein S10



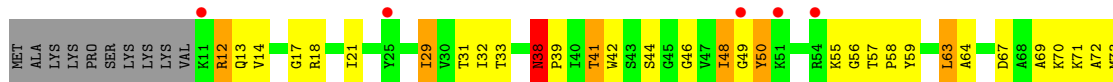
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

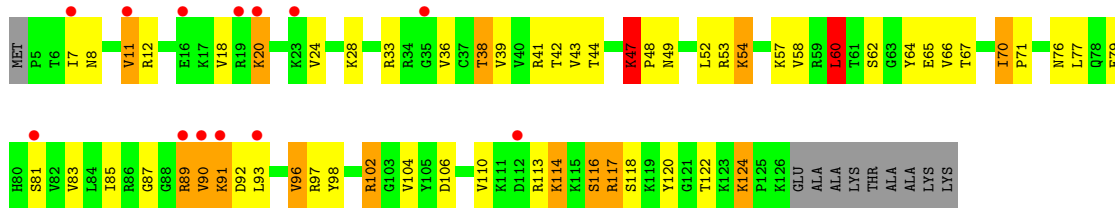


- Molecule 11: 30S ribosomal protein S11

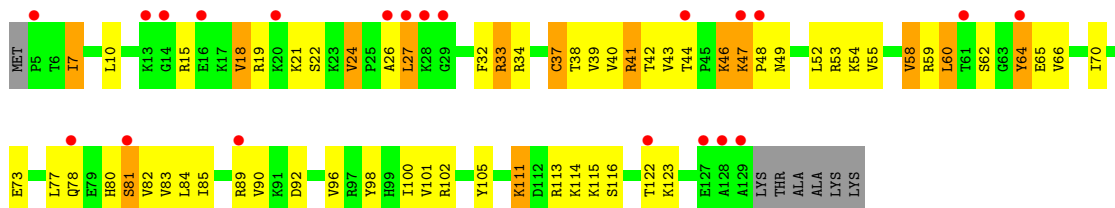


- Molecule 12: 30S ribosomal protein S12

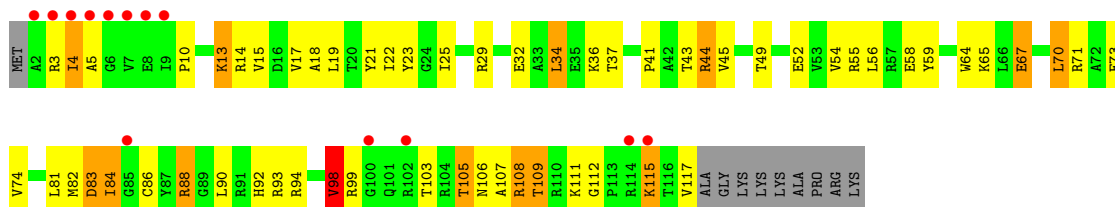
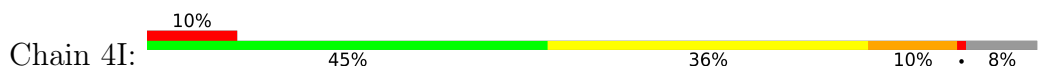




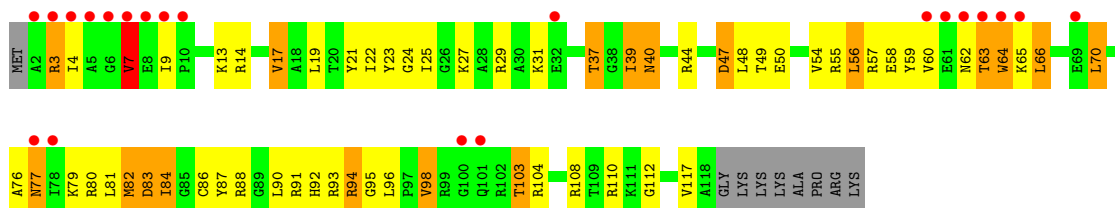
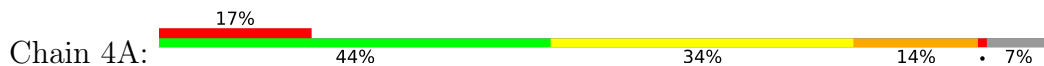
• Molecule 12: 30S ribosomal protein S12



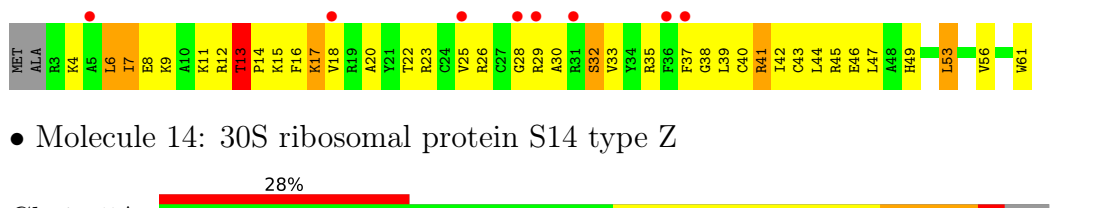
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z

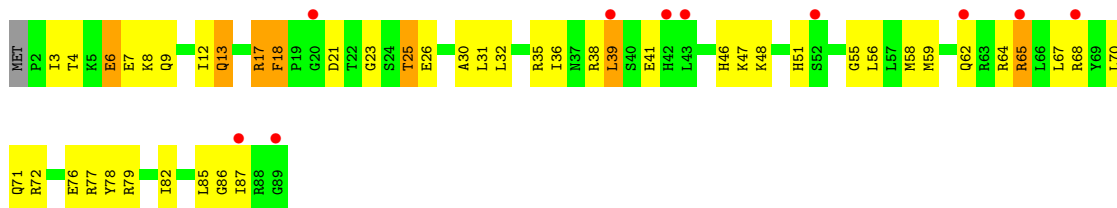


• Molecule 14: 30S ribosomal protein S14 type Z

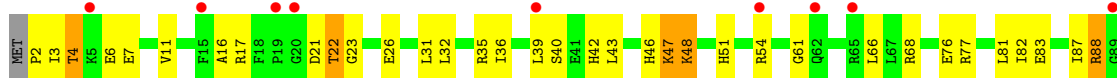




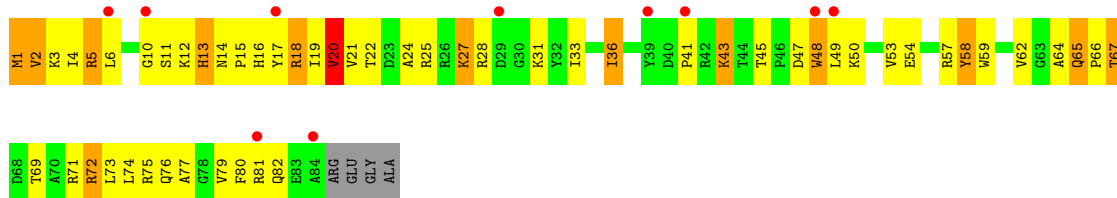
• Molecule 15: 30S ribosomal protein S15



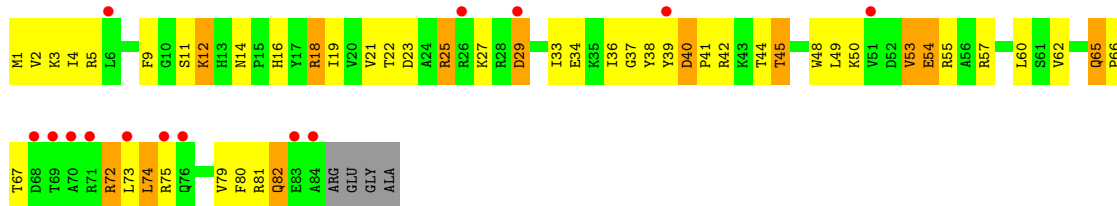
• Molecule 15: 30S ribosomal protein S15



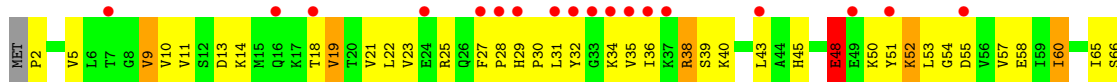
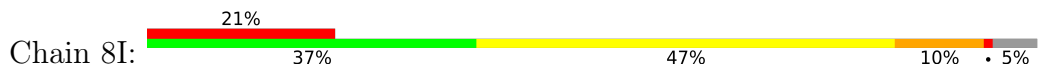
• Molecule 16: 30S ribosomal protein S16

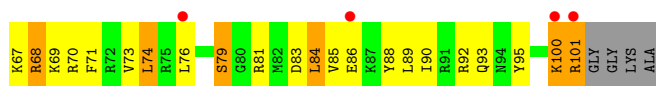


• Molecule 16: 30S ribosomal protein S16

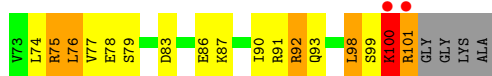
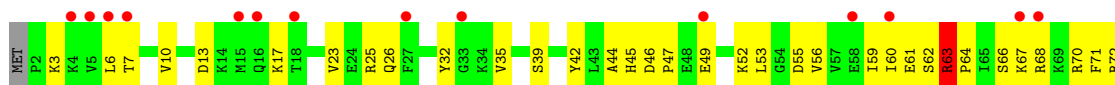


• Molecule 17: 30S ribosomal protein S17

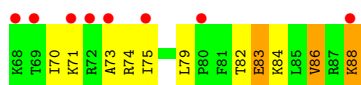
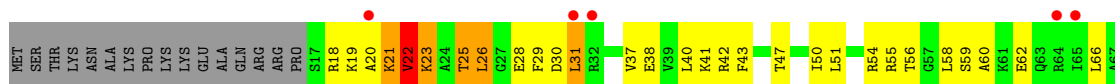




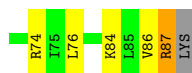
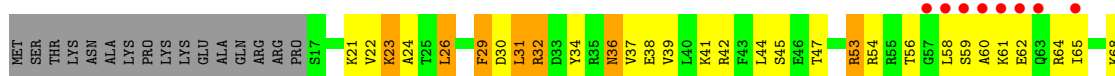
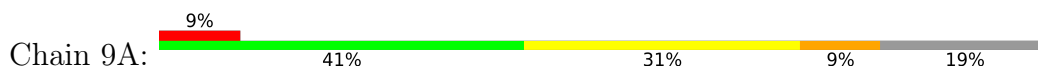
- Molecule 17: 30S ribosomal protein S17



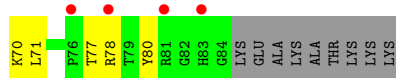
- Molecule 18: 30S ribosomal protein S18



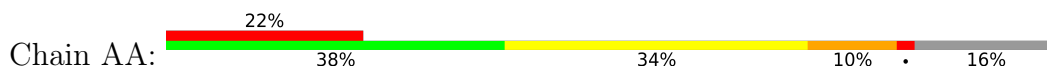
- Molecule 18: 30S ribosomal protein S18

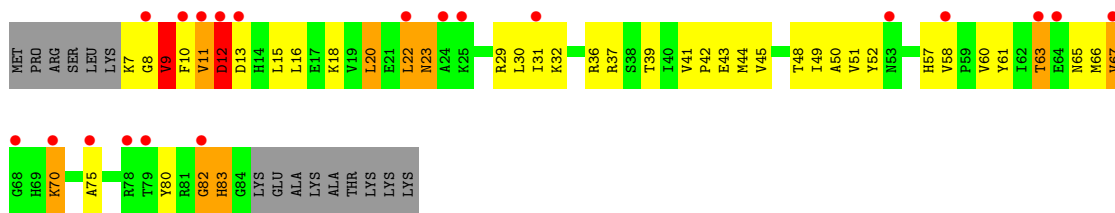


- Molecule 19: 30S ribosomal protein S19

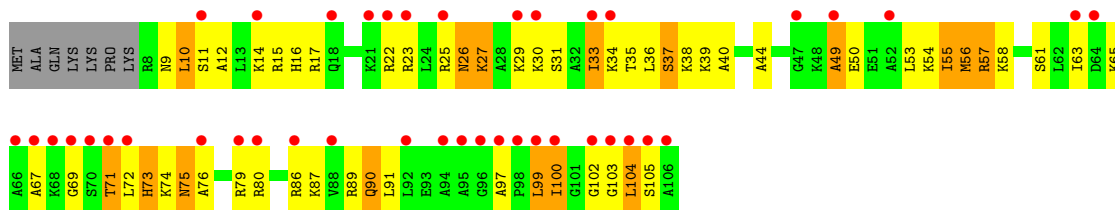


- Molecule 19: 30S ribosomal protein S19

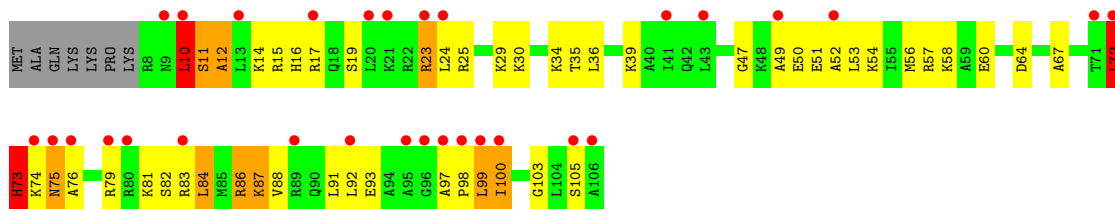




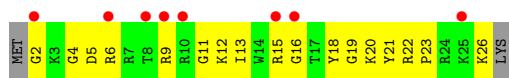
● Molecule 20: 30S ribosomal protein S20



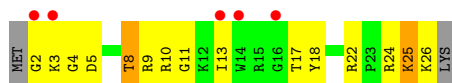
● Molecule 20: 30S ribosomal protein S20



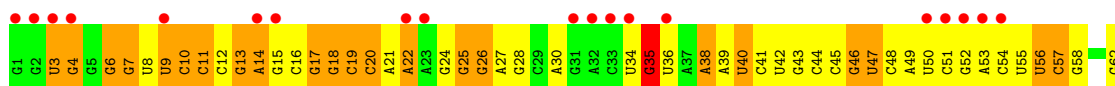
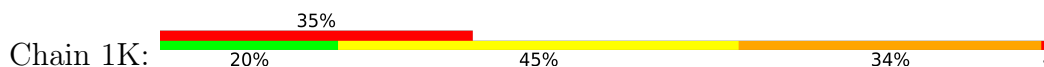
● Molecule 21: 30S ribosomal protein Thx



● Molecule 21: 30S ribosomal protein Thx

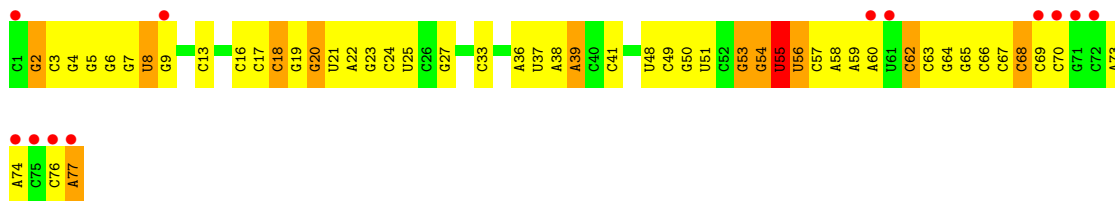


● Molecule 22: tRNA-Tyr

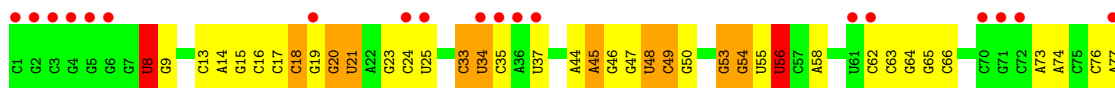




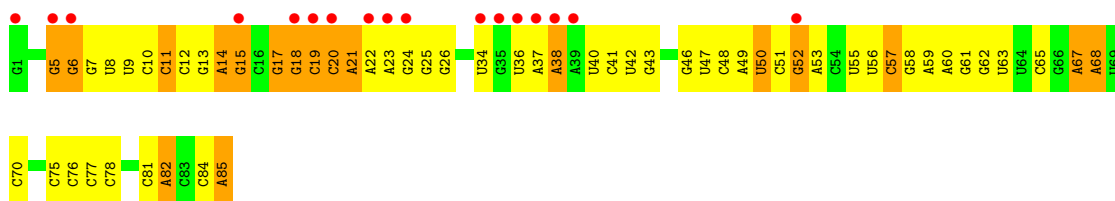
● Molecule 23: tRNA-fMet



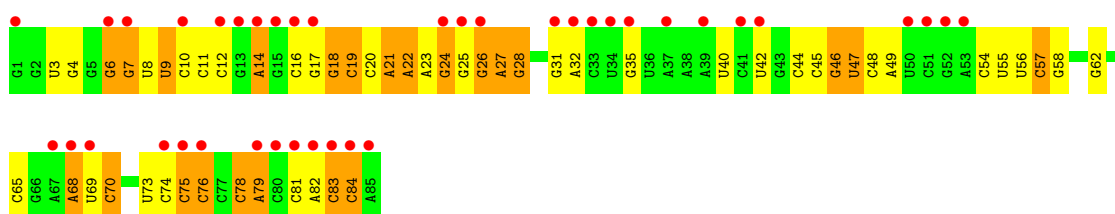
● Molecule 23: tRNA-fMet



● Molecule 24: tRNA-Tyr



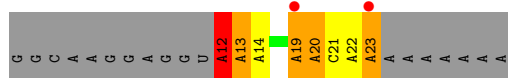
● Molecule 24: tRNA-Tyr



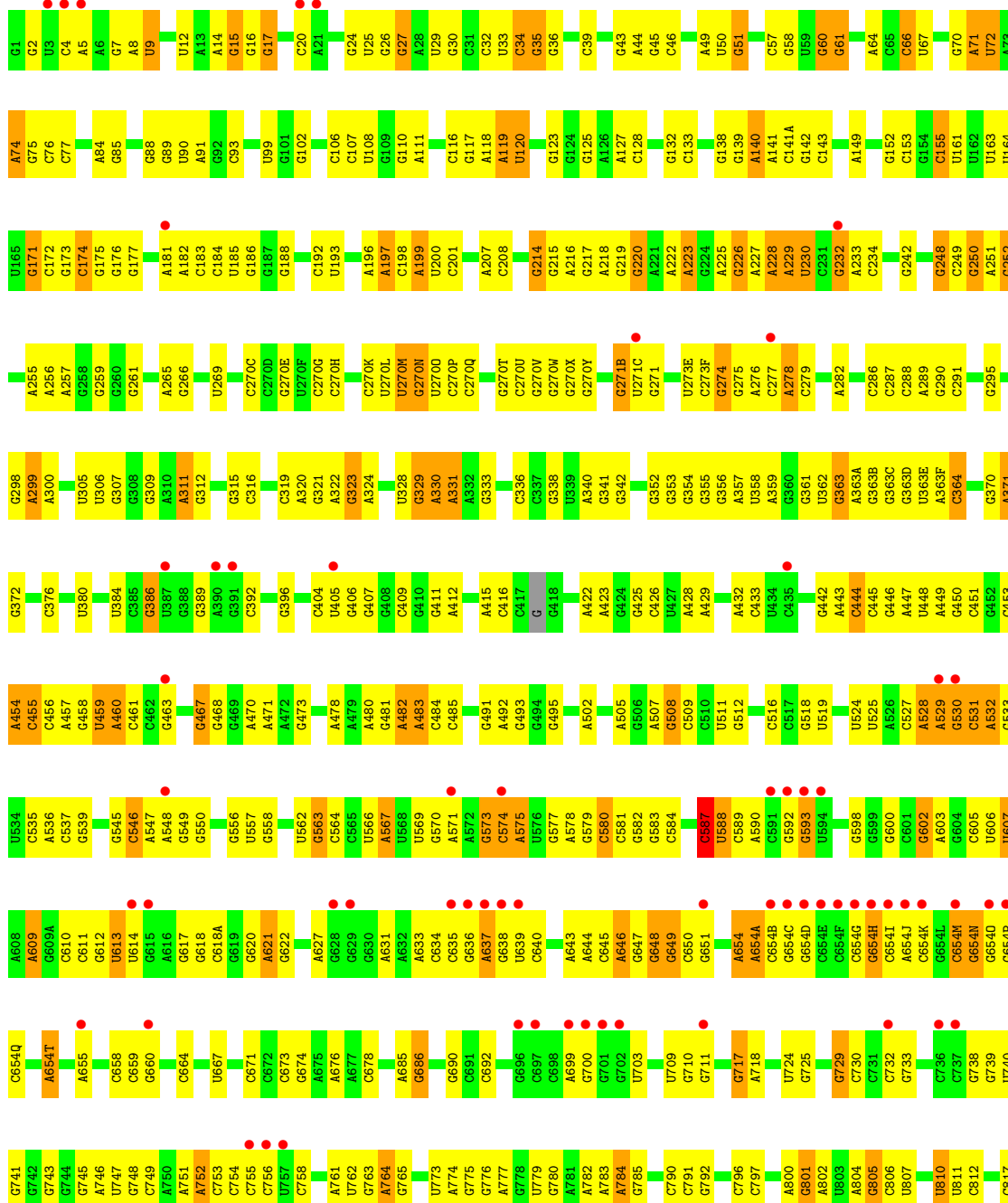
● Molecule 25: mRNA

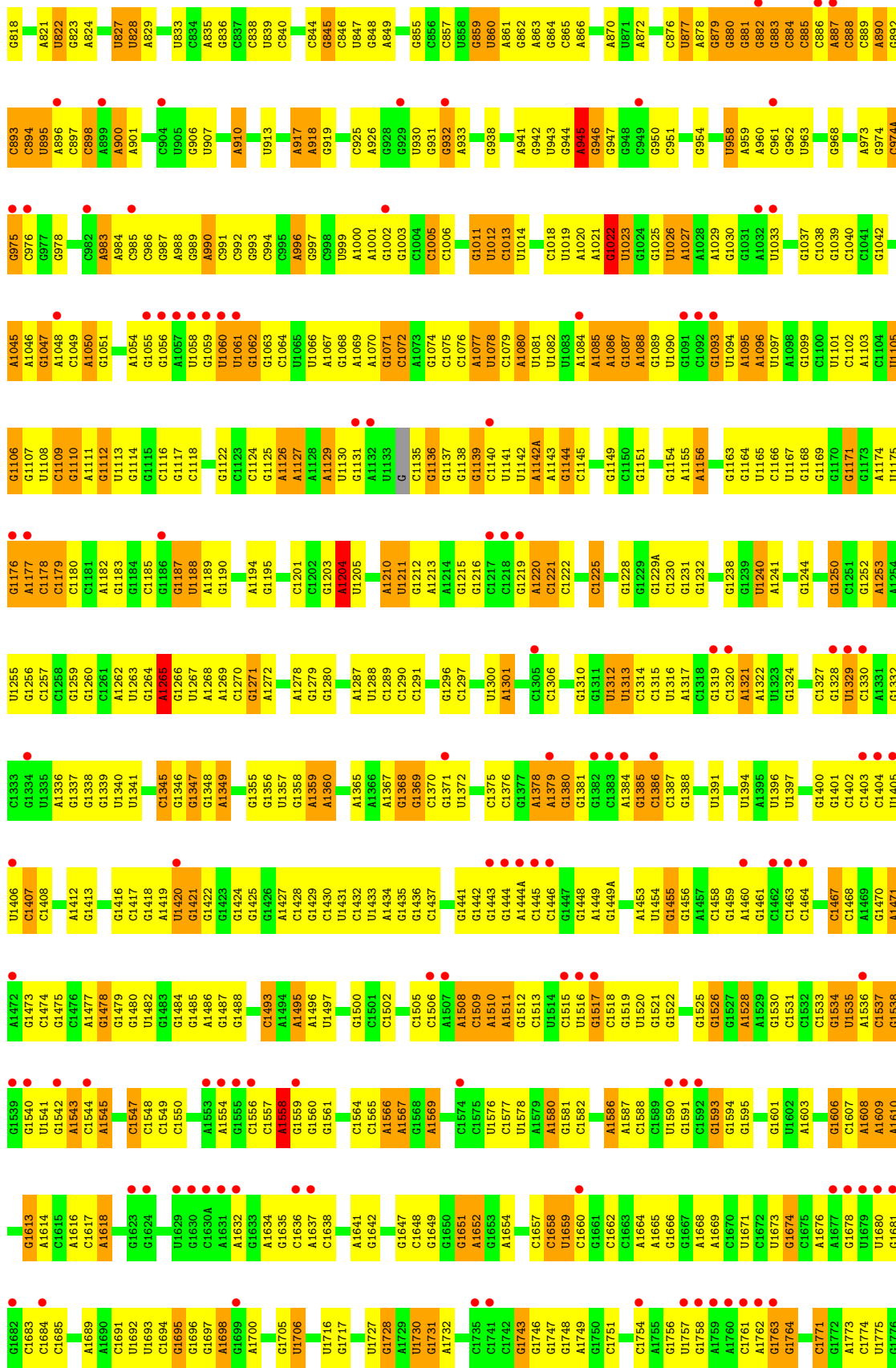


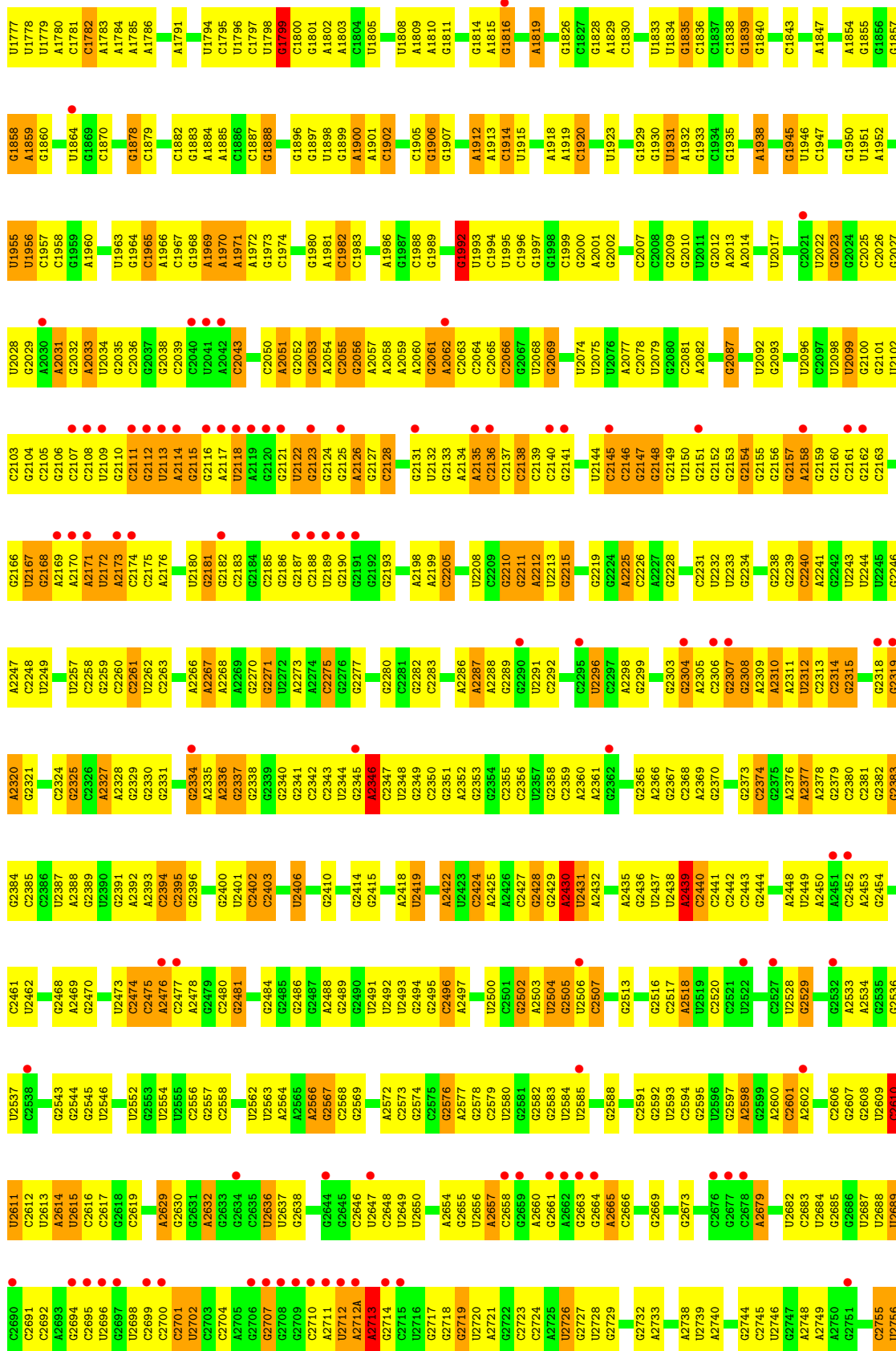
● Molecule 25: mRNA

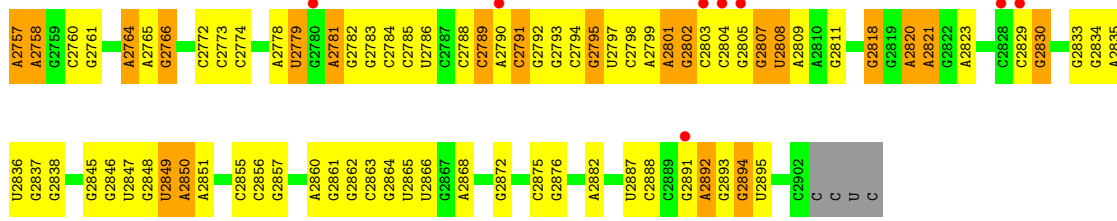


● Molecule 26: 23S ribosomal RNA

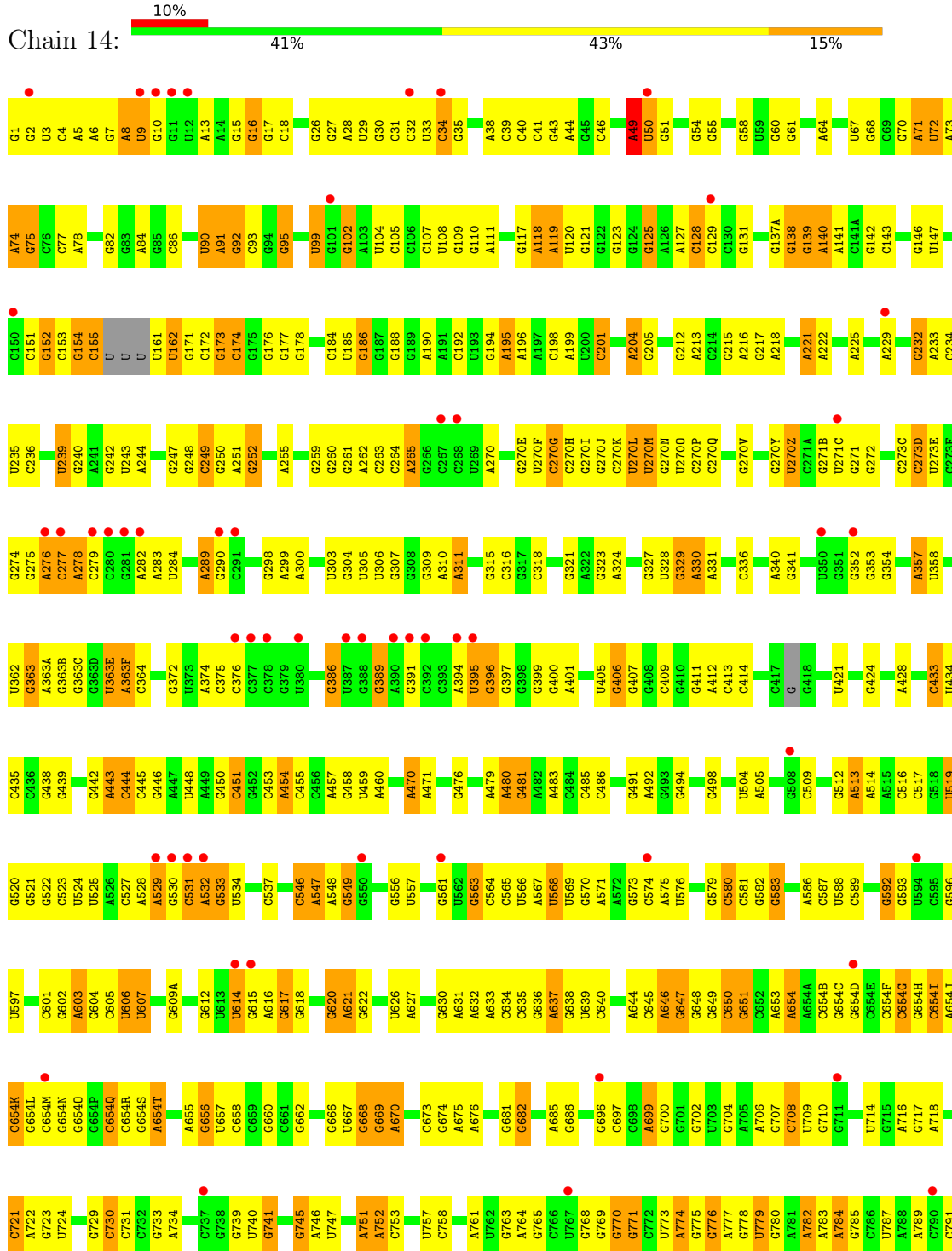


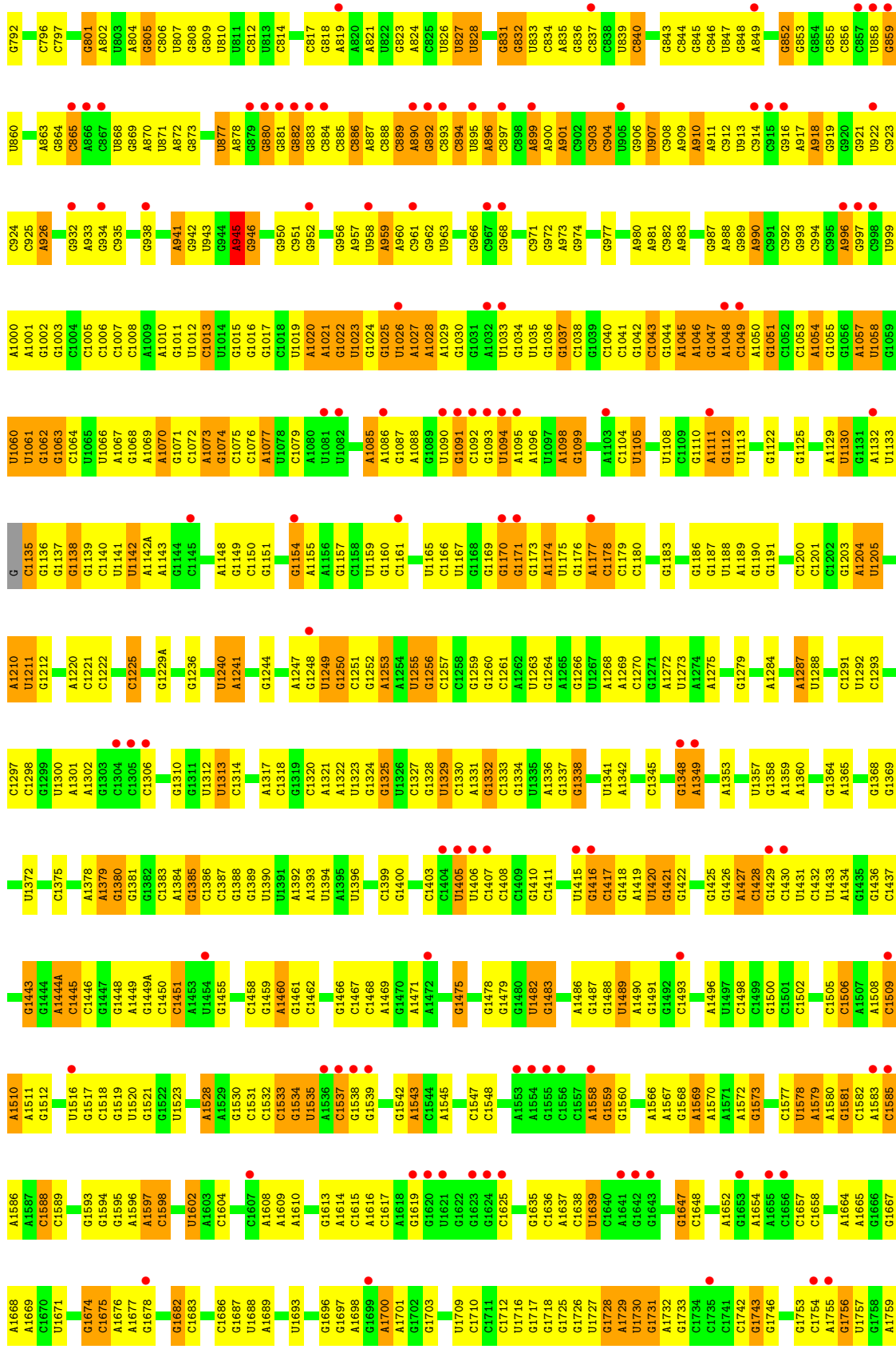


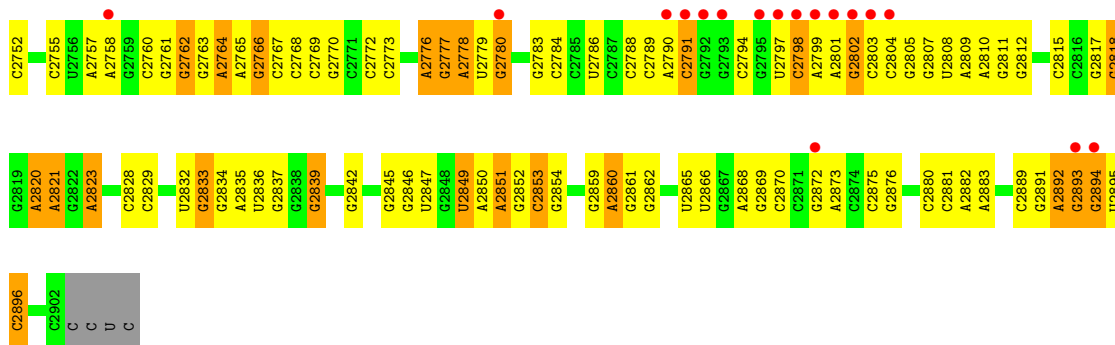




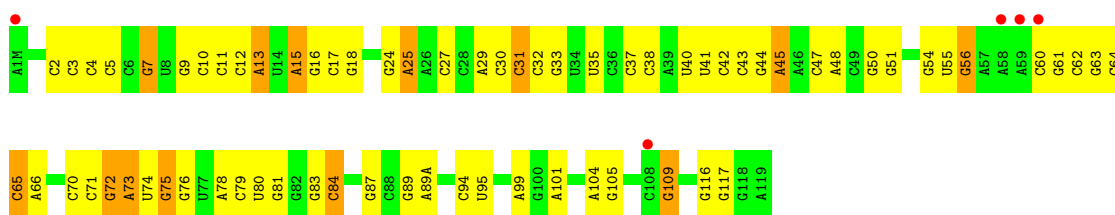
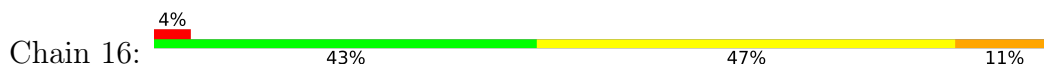
● Molecule 26: 23S ribosomal RNA



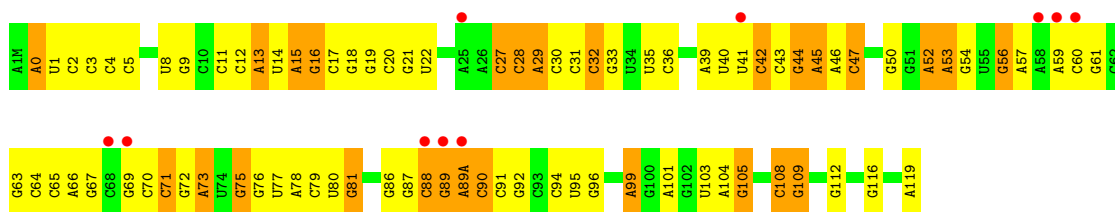




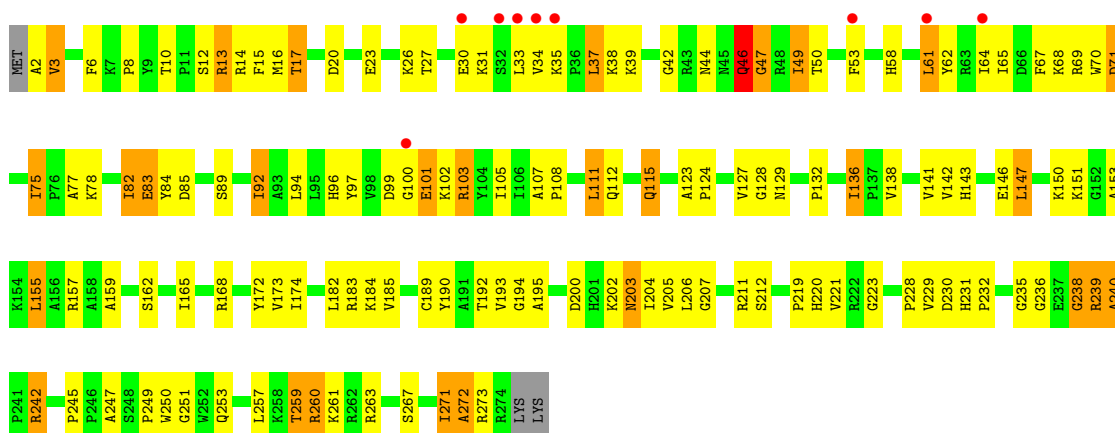
• Molecule 27: 5S ribosomal RNA



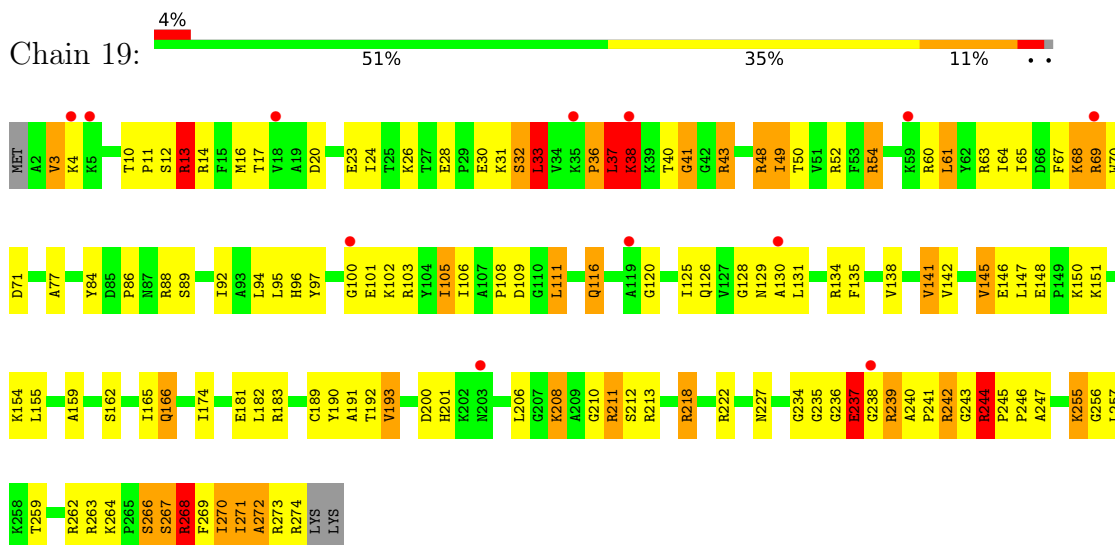
• Molecule 27: 5S ribosomal RNA



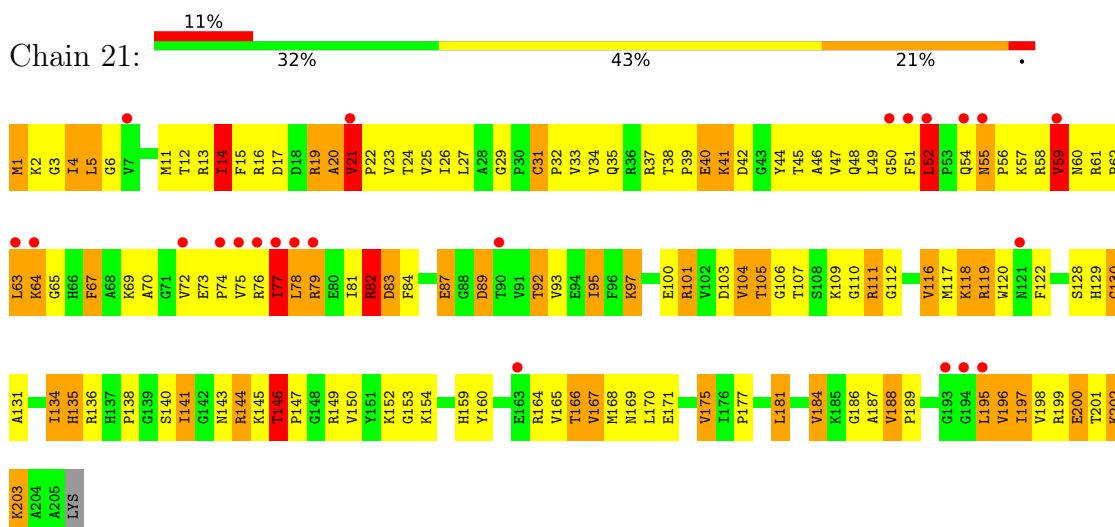
• Molecule 28: 50S ribosomal protein L2



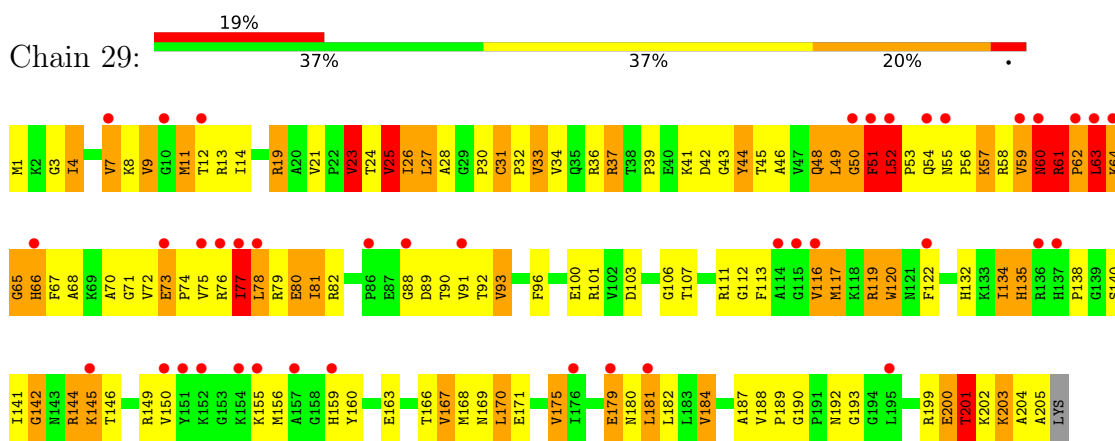
• Molecule 28: 50S ribosomal protein L2



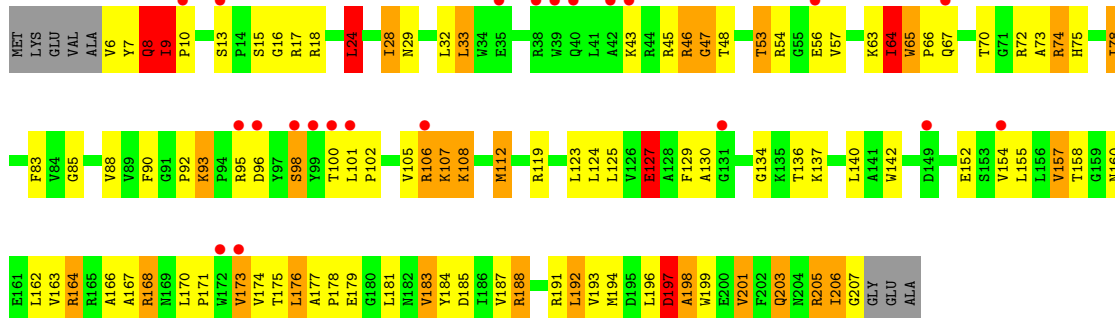
• Molecule 29: 50S ribosomal protein L3



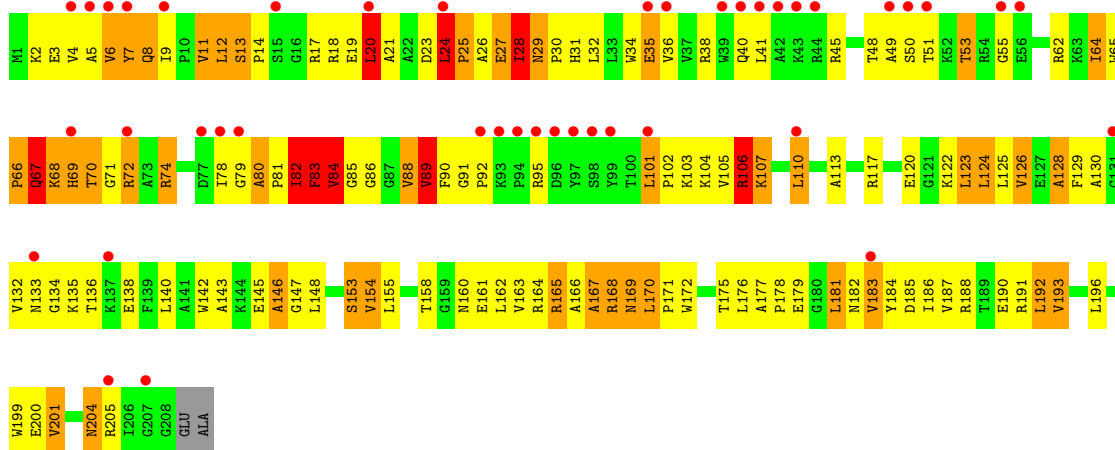
• Molecule 29: 50S ribosomal protein L3



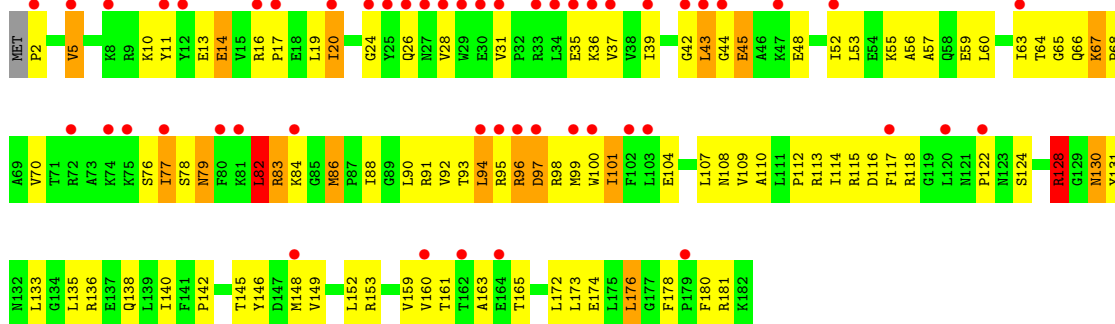
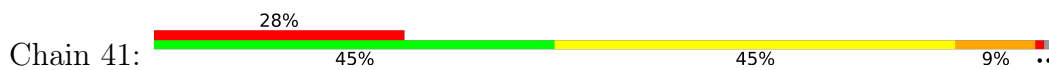
• Molecule 30: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L4

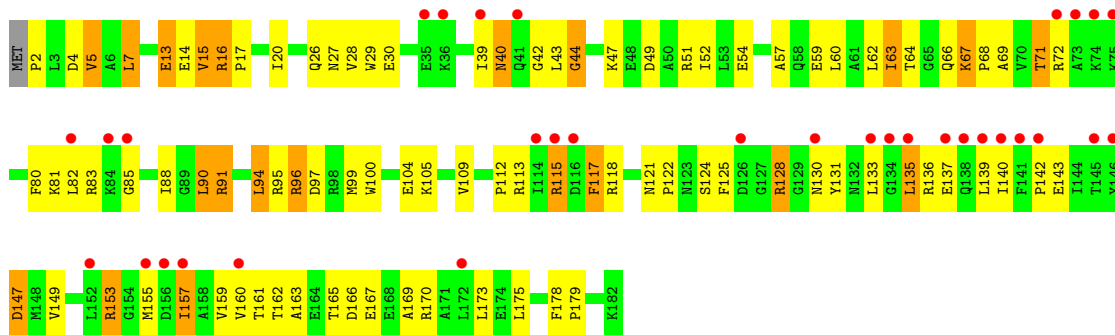


• Molecule 31: 50S ribosomal protein L5

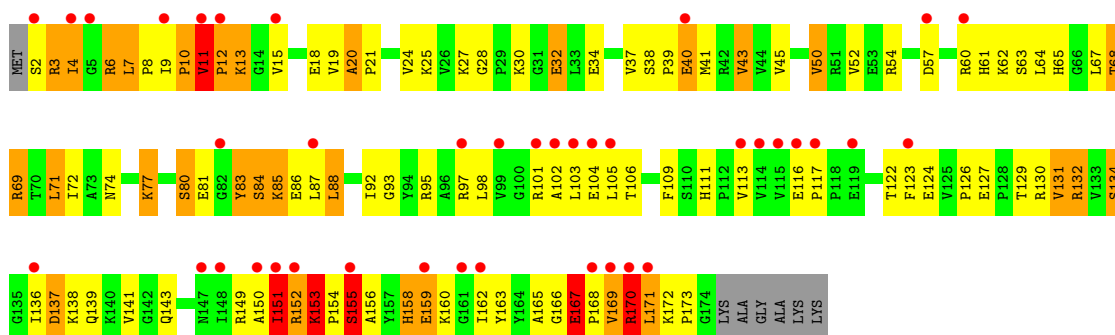


• Molecule 31: 50S ribosomal protein L5

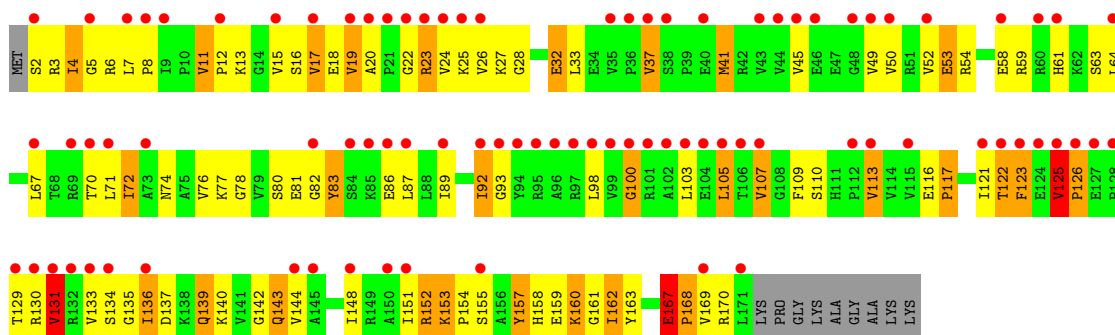
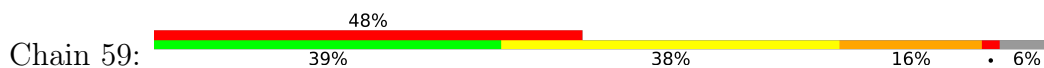




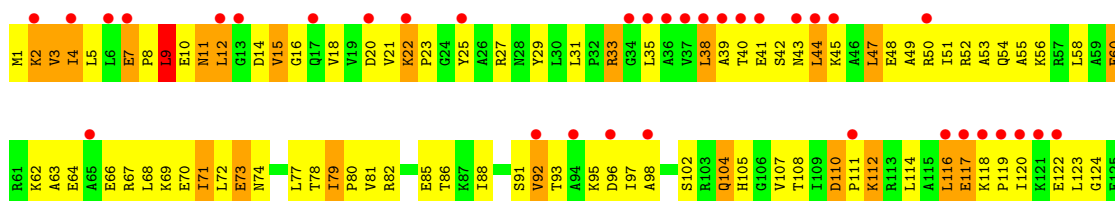
• Molecule 32: 50S ribosomal protein L6

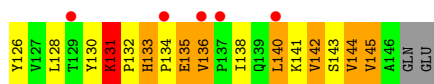


• Molecule 32: 50S ribosomal protein L6

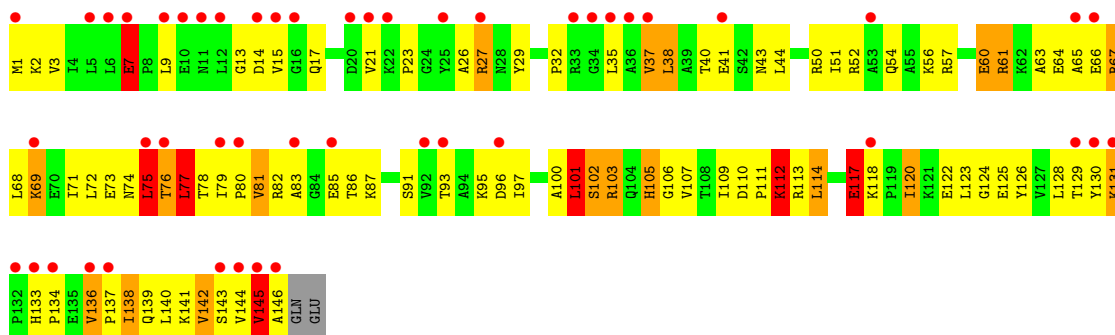


• Molecule 33: 50S ribosomal protein L9

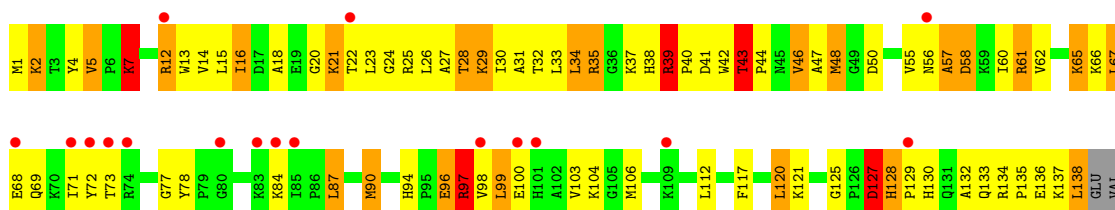




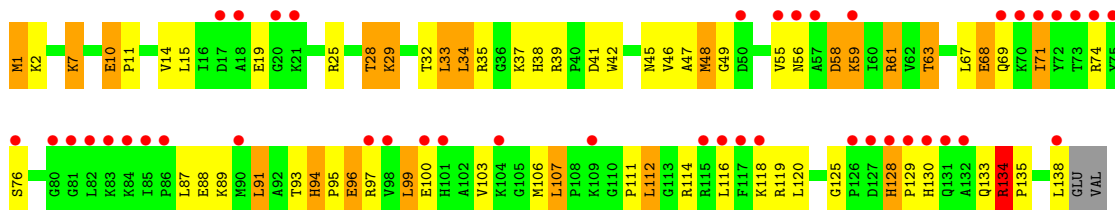
- Molecule 33: 50S ribosomal protein L9



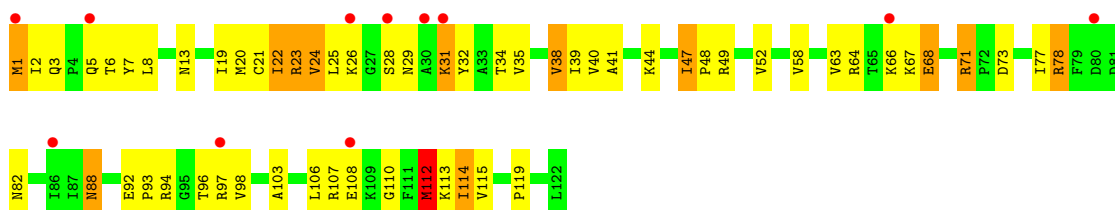
- Molecule 34: 50S ribosomal protein L13



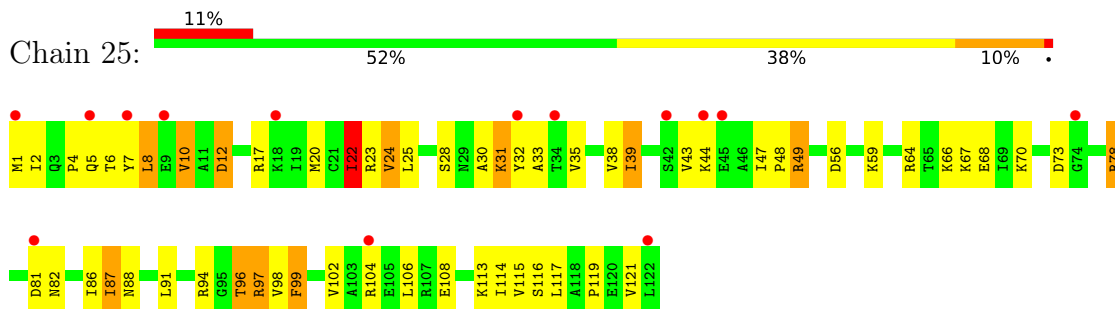
- Molecule 34: 50S ribosomal protein L13



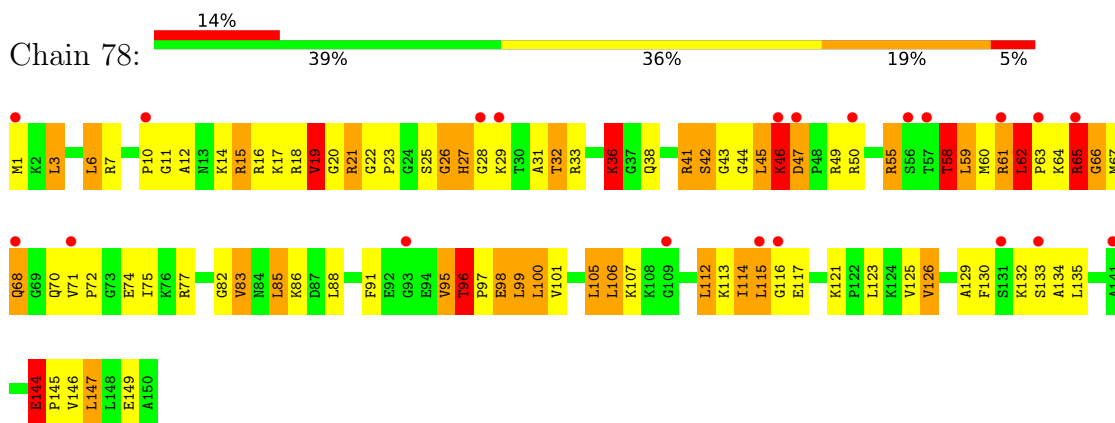
- Molecule 35: 50S ribosomal protein L14



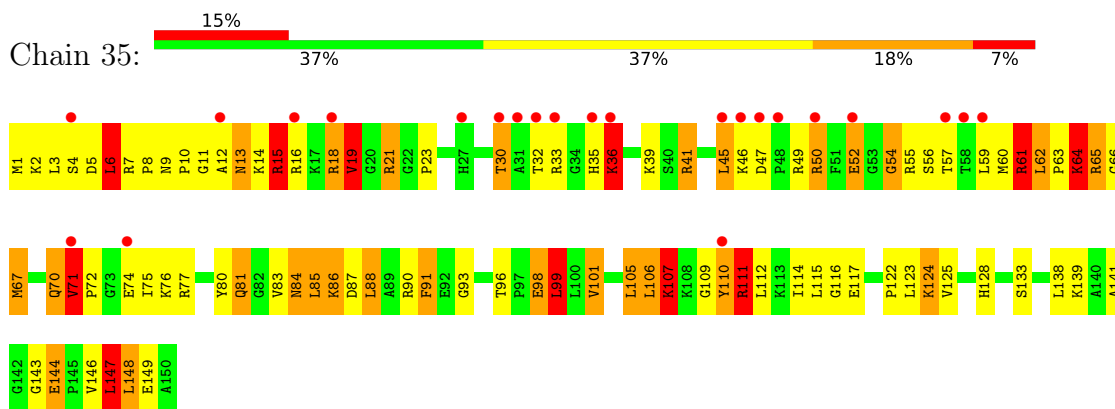
• Molecule 35: 50S ribosomal protein L14



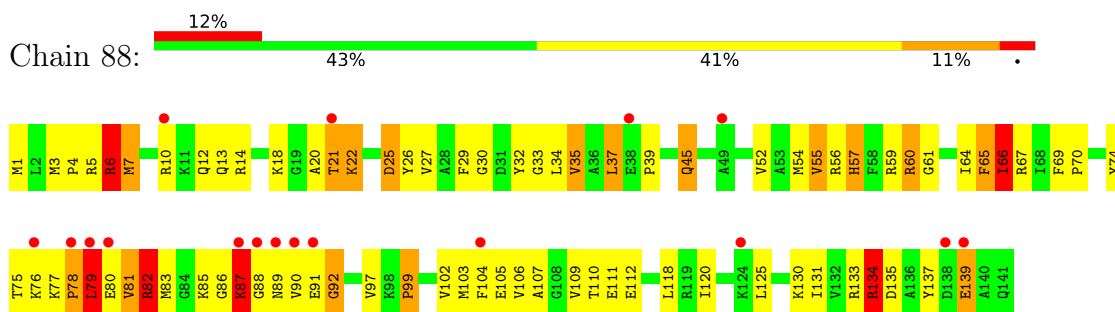
• Molecule 36: 50S ribosomal protein L15



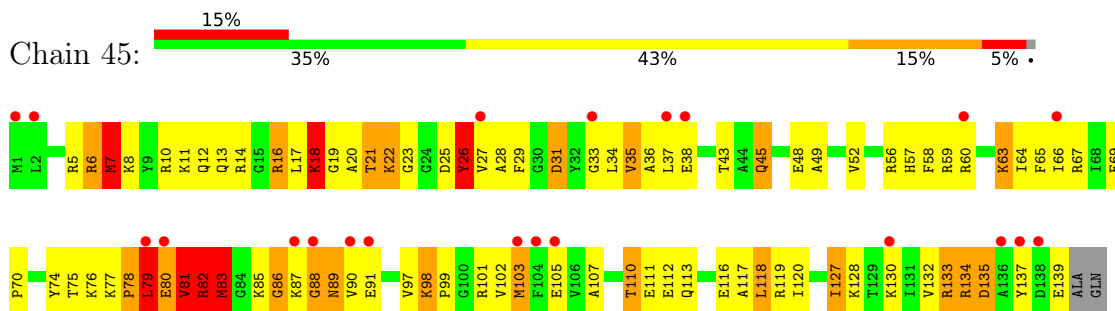
• Molecule 36: 50S ribosomal protein L15



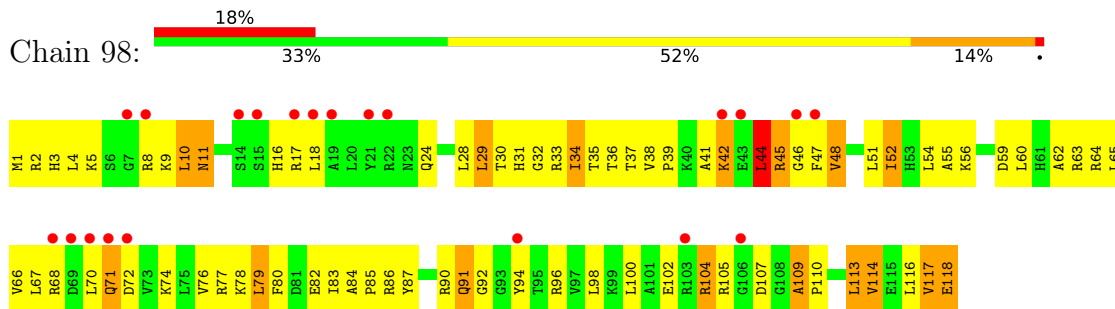
• Molecule 37: 50S ribosomal protein L16



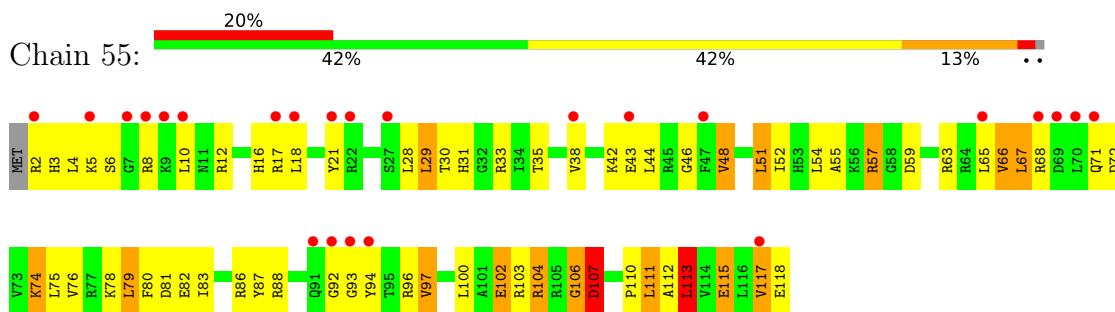
• Molecule 37: 50S ribosomal protein L16



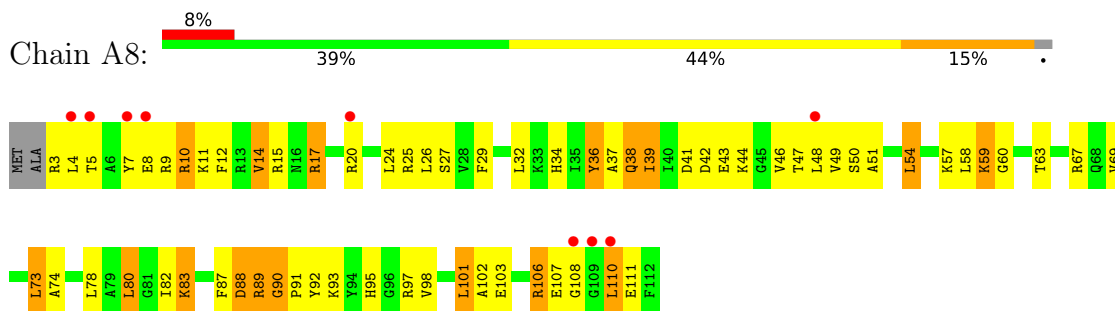
• Molecule 38: 50S ribosomal protein L17



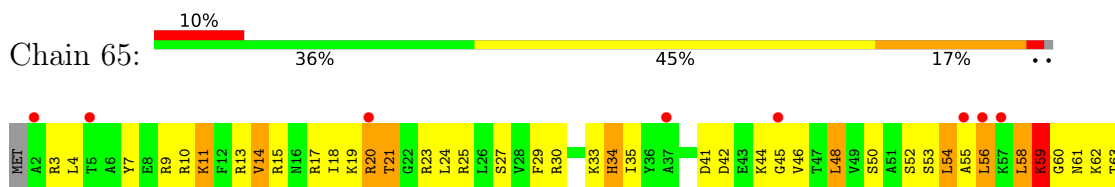
• Molecule 38: 50S ribosomal protein L17

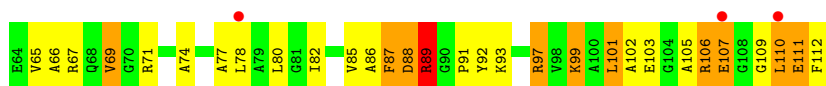


• Molecule 39: 50S ribosomal protein L18

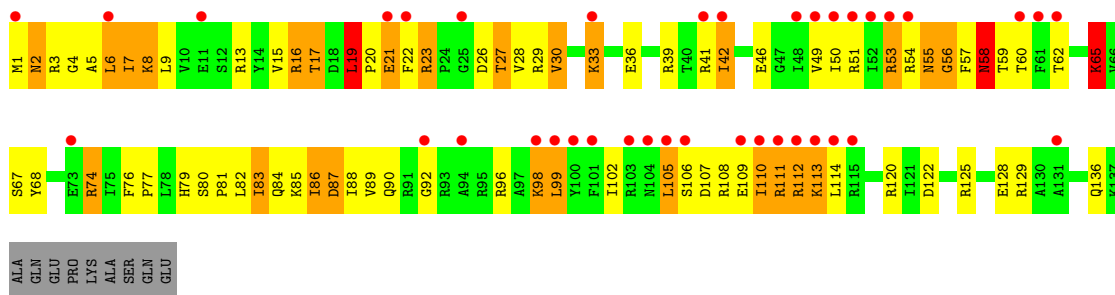


• Molecule 39: 50S ribosomal protein L18

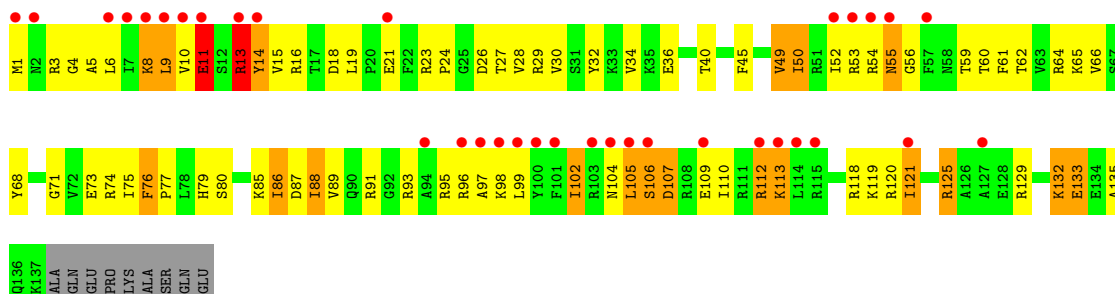




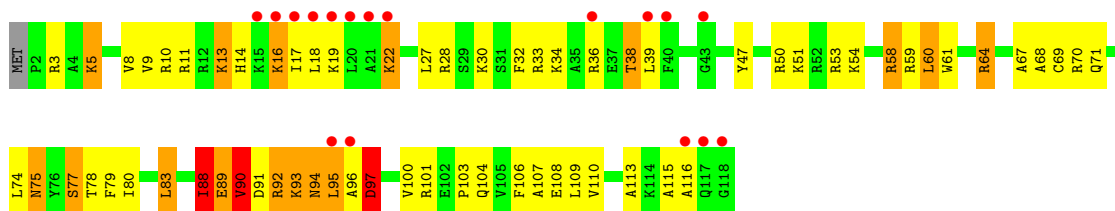
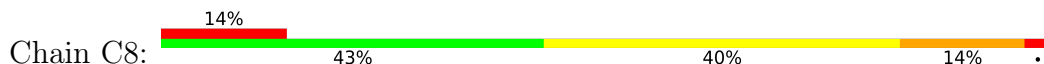
• Molecule 40: 50S ribosomal protein L19



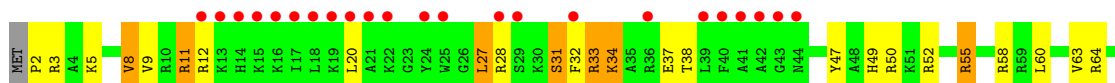
• Molecule 40: 50S ribosomal protein L19

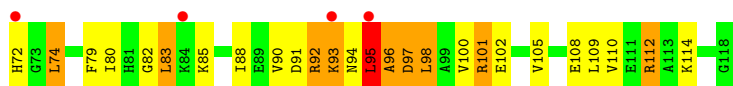


• Molecule 41: 50S ribosomal protein L20

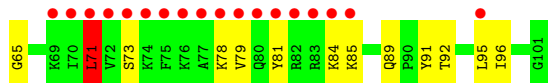
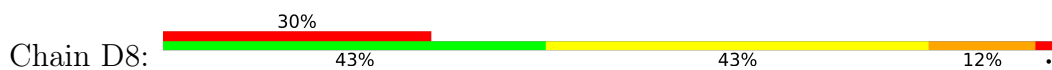


• Molecule 41: 50S ribosomal protein L20

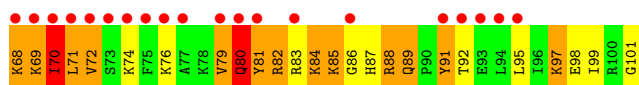
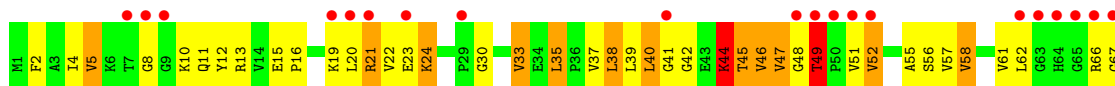




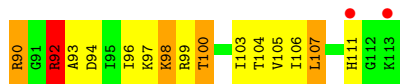
- Molecule 42: 50S ribosomal protein L21



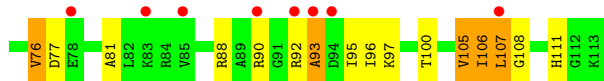
- Molecule 42: 50S ribosomal protein L21



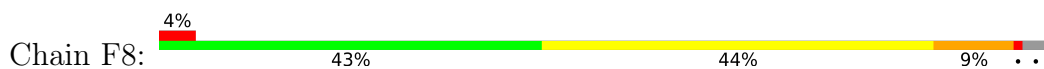
- Molecule 43: 50S ribosomal protein L22

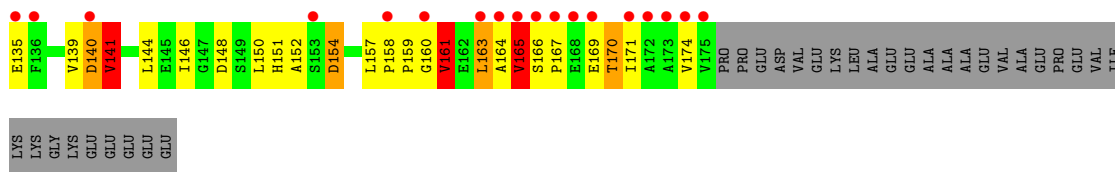


- Molecule 43: 50S ribosomal protein L22

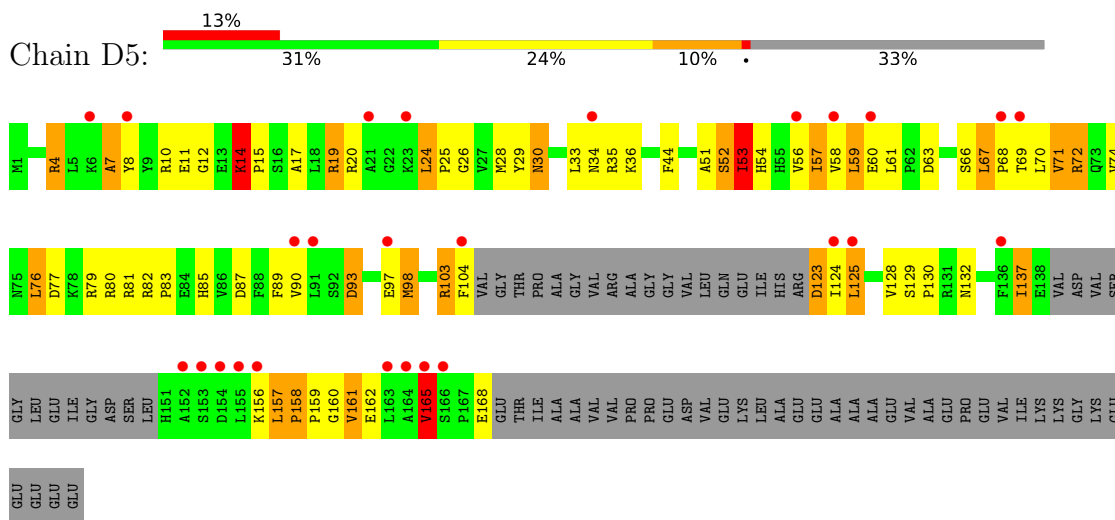


- Molecule 44: 50S ribosomal protein L23

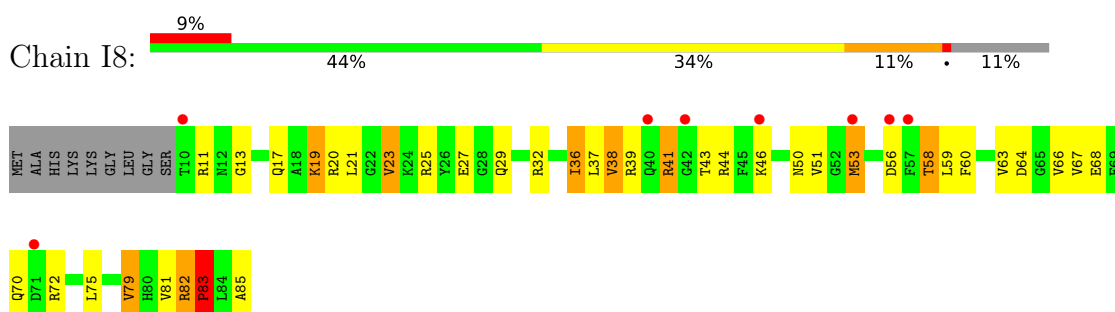




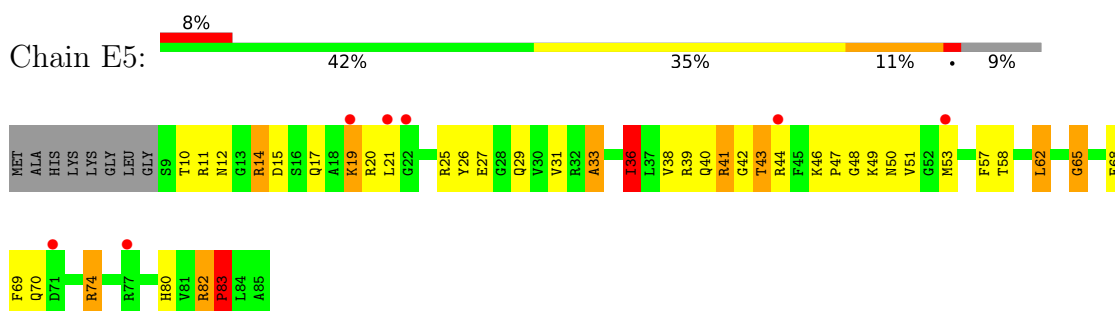
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L27

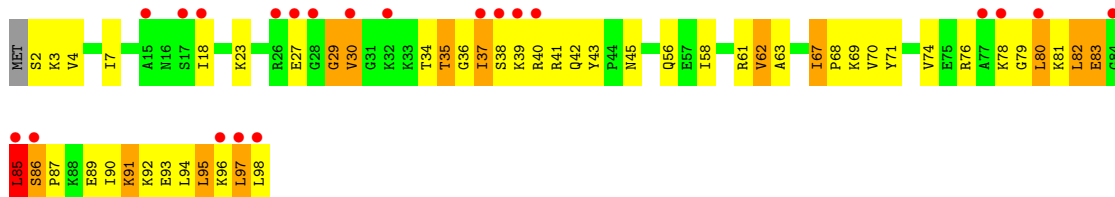


• Molecule 48: 50S ribosomal protein L28

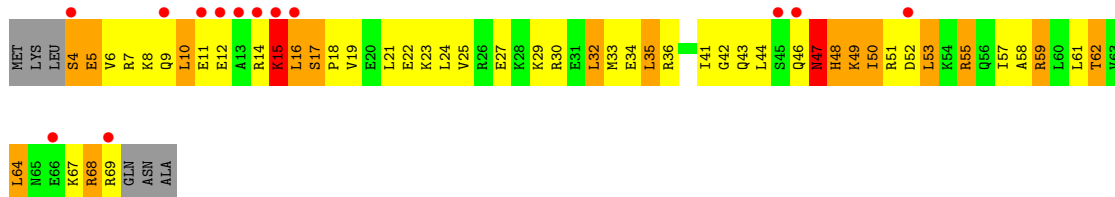
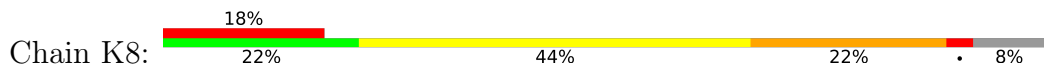




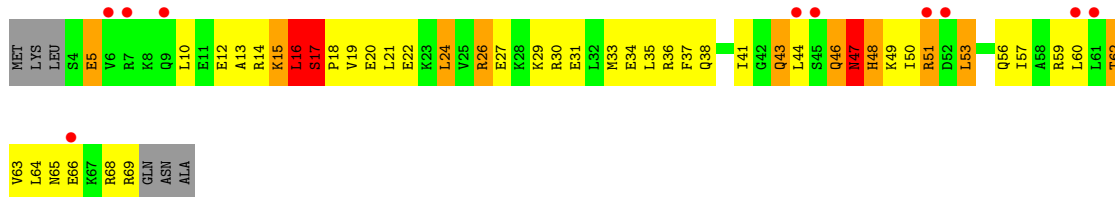
• Molecule 48: 50S ribosomal protein L28



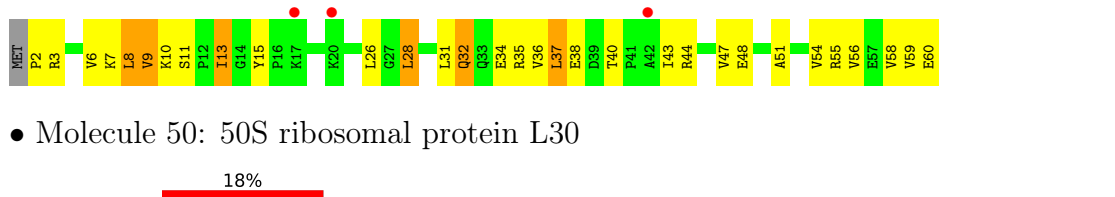
• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29

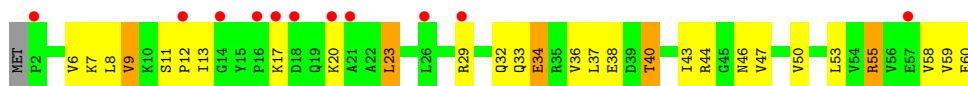


• Molecule 50: 50S ribosomal protein L30

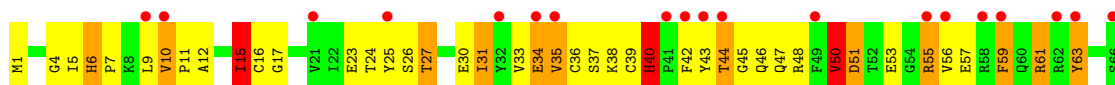


• Molecule 50: 50S ribosomal protein L30



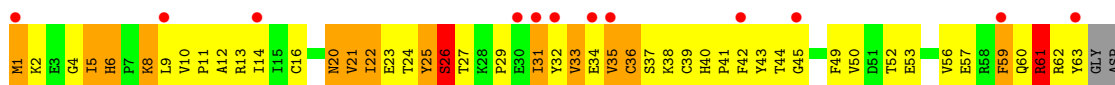
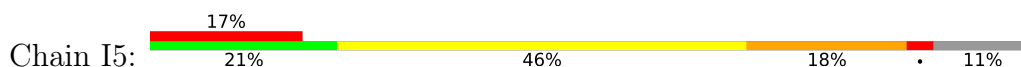


• Molecule 51: 50S ribosomal protein L31



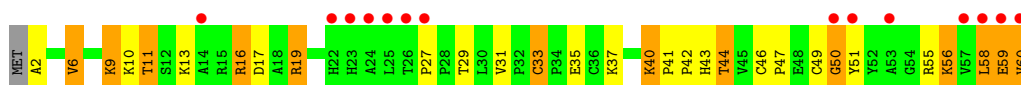
Tyr
Arg
Lys
Gly
Arg

• Molecule 51: 50S ribosomal protein L31

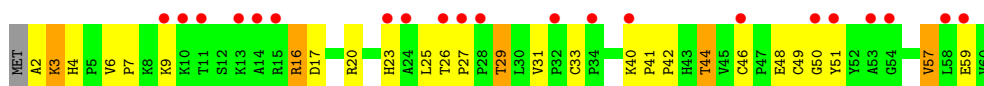


Ser
Tyr
Arg
Lys
Gly
Arg

• Molecule 52: 50S ribosomal protein L32



• Molecule 52: 50S ribosomal protein L32



• Molecule 53: 50S ribosomal protein L34



• Molecule 53: 50S ribosomal protein L34



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 450.90Å 622.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.45 – 3.05 225.45 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (225.45-3.05) 92.8 (225.45-3.05)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.07Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.249 (Not available) , 0.239	Depositor DCC
R_{free} test set	1999 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 179.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299607	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, PAR, PSU, ZN, MG, MIA, 5MU, 4SU, QUO

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	0.42	0/36215	0.67	12/56524 (0.0%)
1	1G	0.37	0/36187	0.61	9/56481 (0.0%)
2	12	0.50	0/1959	1.09	20/2642 (0.8%)
2	1E	0.57	1/1959 (0.1%)	1.08	10/2642 (0.4%)
3	22	0.55	0/1636	1.01	4/2205 (0.2%)
3	2E	0.65	0/1629	1.05	0/2195
4	32	0.62	1/1732 (0.1%)	1.20	18/2318 (0.8%)
4	3E	0.71	0/1732	1.13	8/2318 (0.3%)
5	42	0.61	0/1171	1.04	5/1576 (0.3%)
5	4E	0.69	0/1171	1.10	6/1576 (0.4%)
6	52	0.65	0/855	0.98	3/1154 (0.3%)
6	5E	0.66	0/855	0.98	1/1154 (0.1%)
7	62	0.58	0/1275	1.02	3/1709 (0.2%)
7	6E	0.57	0/1261	1.00	9/1689 (0.5%)
8	72	0.56	0/1127	1.13	3/1517 (0.2%)
8	7E	0.63	0/1135	1.15	9/1527 (0.6%)
9	82	0.53	0/988	1.04	5/1324 (0.4%)
9	8E	0.56	0/1028	1.07	10/1379 (0.7%)
10	1A	0.50	0/814	1.07	5/1095 (0.5%)
10	1I	0.67	0/814	1.04	0/1095
11	2A	0.58	0/888	1.10	3/1198 (0.3%)
11	2I	0.67	0/879	1.17	4/1187 (0.3%)
12	3A	0.74	0/991	1.15	4/1327 (0.3%)
12	3I	0.95	1/972 (0.1%)	1.38	9/1301 (0.7%)
13	4A	0.52	0/943	1.03	6/1265 (0.5%)
13	4I	0.61	0/938	1.05	1/1258 (0.1%)
14	5A	0.57	0/484	0.98	0/643
14	5I	0.77	0/489	1.21	3/650 (0.5%)
15	6A	0.60	0/744	0.99	1/992 (0.1%)
15	6I	0.70	0/744	1.10	5/992 (0.5%)
16	7A	0.76	2/721 (0.3%)	1.14	3/970 (0.3%)
16	7I	0.63	0/721	1.09	5/970 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.63	1/847 (0.1%)	1.04	5/1131 (0.4%)
17	8I	0.65	0/847	1.13	3/1131 (0.3%)
18	9A	0.60	0/586	1.03	1/779 (0.1%)
18	9I	0.62	0/595	1.12	2/790 (0.3%)
19	AA	0.60	0/638	1.14	6/860 (0.7%)
19	AI	0.72	0/680	1.22	5/915 (0.5%)
20	BA	0.64	0/764	1.13	4/1007 (0.4%)
20	BI	0.56	0/764	0.99	1/1007 (0.1%)
21	1B	0.65	0/221	1.05	0/288
21	1F	0.57	0/221	0.99	1/288 (0.3%)
22	1K	0.27	0/1899	0.53	0/2952
23	2K	0.45	1/1747 (0.1%)	0.65	0/2723
23	2L	0.39	1/1747 (0.1%)	0.61	0/2723
24	1L	0.26	0/1996	0.48	0/3108
24	3K	0.24	0/1996	0.46	0/3108
25	4K	0.43	0/319	0.59	0/495
25	4L	0.45	0/294	0.73	1/456 (0.2%)
26	14	0.48	0/70167	0.73	20/109541 (0.0%)
26	1H	0.55	0/70233	0.80	34/109643 (0.0%)
27	16	0.45	0/2928	0.75	0/4568
27	1J	0.40	0/2928	0.67	0/4568
28	11	0.95	2/2170 (0.1%)	1.38	19/2926 (0.6%)
28	19	0.92	2/2170 (0.1%)	1.40	21/2926 (0.7%)
29	21	0.88	1/1601 (0.1%)	1.50	29/2160 (1.3%)
29	29	0.87	1/1601 (0.1%)	1.48	29/2160 (1.3%)
30	31	0.89	0/1620	1.29	19/2194 (0.9%)
30	39	0.78	1/1662 (0.1%)	1.40	22/2249 (1.0%)
31	41	0.65	0/1498	1.13	5/2016 (0.2%)
31	49	0.55	0/1498	1.12	6/2016 (0.3%)
32	51	0.83	0/1346	1.47	21/1821 (1.2%)
32	59	0.58	0/1332	1.26	21/1802 (1.2%)
33	61	0.69	0/1151	1.26	11/1558 (0.7%)
33	69	0.66	1/1151 (0.1%)	1.21	14/1558 (0.9%)
34	15	0.65	0/1131	1.17	8/1525 (0.5%)
34	58	0.76	0/1131	1.22	12/1525 (0.8%)
35	25	0.77	0/942	1.17	2/1269 (0.2%)
35	68	0.84	0/942	1.21	6/1269 (0.5%)
36	35	0.90	2/1161 (0.2%)	1.57	20/1544 (1.3%)
36	78	0.95	1/1161 (0.1%)	1.54	21/1544 (1.4%)
37	45	0.89	2/1128 (0.2%)	1.37	13/1508 (0.9%)
37	88	1.05	5/1142 (0.4%)	1.63	25/1527 (1.6%)
38	55	0.82	0/973	1.18	4/1302 (0.3%)
38	98	0.76	0/981	1.14	3/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	65	0.67	0/891	1.22	3/1187 (0.3%)
39	A8	0.76	0/886	1.21	6/1180 (0.5%)
40	75	0.74	0/1155	1.14	7/1542 (0.5%)
40	B8	0.78	0/1155	1.24	10/1542 (0.6%)
41	85	0.72	0/981	1.12	3/1306 (0.2%)
41	C8	0.87	1/981 (0.1%)	1.21	8/1306 (0.6%)
42	95	0.87	2/789 (0.3%)	1.34	6/1057 (0.6%)
42	D8	0.75	0/789	1.28	9/1057 (0.9%)
43	A5	0.92	0/910	1.20	2/1220 (0.2%)
43	E8	0.83	0/910	1.13	1/1220 (0.1%)
44	B5	0.95	0/739	1.23	4/993 (0.4%)
44	F8	0.87	0/744	1.19	1/1000 (0.1%)
45	C5	0.80	0/807	1.35	7/1076 (0.7%)
45	G8	0.87	0/804	1.36	11/1073 (1.0%)
46	D5	0.59	0/1165	1.27	12/1574 (0.8%)
46	H8	0.65	0/1427	1.20	10/1935 (0.5%)
47	E5	0.78	0/620	1.34	6/827 (0.7%)
47	I8	0.83	0/614	1.30	3/819 (0.4%)
48	F5	0.81	0/769	1.35	8/1022 (0.8%)
48	J8	0.88	0/769	1.22	5/1022 (0.5%)
49	G5	0.67	0/560	1.22	4/741 (0.5%)
49	K8	0.87	0/560	1.31	7/741 (0.9%)
50	H5	0.59	0/473	1.30	4/635 (0.6%)
50	L8	0.73	0/473	1.29	3/635 (0.5%)
51	I5	0.77	0/527	1.29	4/709 (0.6%)
51	M8	0.67	0/545	1.18	4/733 (0.5%)
52	J5	0.82	0/472	1.25	4/639 (0.6%)
52	N8	0.83	0/472	1.33	8/639 (1.3%)
53	L5	0.90	0/399	1.31	2/526 (0.4%)
53	P8	1.10	1/404 (0.2%)	1.25	3/533 (0.6%)
54	M5	1.19	4/502 (0.8%)	1.64	10/661 (1.5%)
54	Q8	1.06	1/494 (0.2%)	1.59	9/649 (1.4%)
55	3L	0.23	0/1970	0.45	0/3065
All	All	0.56	35/322722 (0.0%)	0.87	782/483529 (0.2%)

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
1	13	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	1
2	1E	0	3
4	32	0	2
4	3E	0	1
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	2
14	5A	0	2
19	AA	0	1
19	AI	0	1
20	BA	0	2
26	14	1	0
28	11	0	1
28	19	0	4
29	21	0	5
29	29	0	4
30	39	0	6
31	41	0	1
31	49	0	2
32	51	0	3
32	59	0	1
33	61	0	4
33	69	0	2
34	58	0	1
36	35	0	4
36	78	0	7
37	45	0	8
37	88	0	2
38	55	0	1
38	98	0	1
39	A8	0	1
40	75	0	2
40	B8	0	2
41	85	0	4
41	C8	0	4
42	95	0	1
42	D8	0	2
43	A5	0	1
44	B5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	C5	0	2
45	G8	0	3
46	D5	0	1
46	H8	0	3
47	E5	0	1
47	I8	0	1
48	F5	0	1
48	J8	0	2
49	G5	0	3
49	K8	0	3
51	I5	0	2
51	M8	0	1
52	N8	0	1
54	M5	0	5
54	Q8	0	3
All	All	2	128

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	M5	62	LEU	CA-C	8.05	1.58	1.53
36	78	19	VAL	CA-CB	7.75	1.65	1.54
29	29	135	HIS	CA-C	-7.73	1.45	1.52
2	1E	8	LYS	CA-C	7.65	1.56	1.52
53	P8	5	TRP	NE1-CE2	-7.49	1.29	1.37

The worst 5 of 782 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	88	92	GLY	N-CA-C	16.13	132.21	110.43
8	72	73	ASP	CA-C-N	15.61	135.41	119.64
8	72	73	ASP	C-N-CA	15.61	135.41	119.64
28	19	235	GLY	N-CA-C	15.31	126.49	111.95
28	19	272	ALA	N-CA-C	14.94	131.79	107.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	A	C1'
26	14	945	A	C1'

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
4	3E	29	PRO	Peptide
12	3I	47	LYS	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	32352	0	16325	789	1
1	1G	32327	0	16316	748	3
2	12	1924	0	1975	109	0
2	1E	1924	0	1975	105	0
3	22	1612	0	1677	73	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1763	85	0
4	3E	1702	0	1761	95	0
5	42	1155	0	1213	56	0
5	4E	1155	0	1213	51	0
6	52	842	0	857	34	0
6	5E	842	0	857	38	0
7	62	1256	0	1296	52	0
7	6E	1243	0	1284	51	0
8	72	1107	0	1165	53	0
8	7E	1115	0	1177	58	0
9	82	971	0	1001	59	0
9	8E	1009	0	1037	67	0
10	1A	801	0	849	54	0
10	1I	801	0	849	45	0
11	2A	873	0	894	51	0
11	2I	864	0	881	41	0
12	3A	975	0	1062	40	0
12	3I	956	0	1046	41	0
13	4A	933	0	992	54	0
13	4I	928	0	987	43	0
14	5A	475	0	511	25	0
14	5I	480	0	513	36	0
15	6A	733	0	771	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	733	0	771	30	0
16	7A	705	0	725	41	0
16	7I	705	0	725	52	0
17	8A	834	0	904	40	0
17	8I	834	0	904	56	0
18	9A	581	0	649	35	0
18	9I	590	0	662	30	0
19	AA	624	0	636	34	0
19	AI	665	0	686	40	0
20	BA	762	0	861	32	0
20	BI	762	0	861	53	0
21	1B	217	0	234	13	0
21	1F	217	0	234	11	0
22	1K	1824	0	945	57	0
23	2K	1645	0	841	30	0
23	2L	1645	0	841	33	0
24	1L	1807	0	920	32	0
24	3K	1807	0	920	46	0
25	4K	283	0	143	11	0
25	4L	261	0	132	6	0
26	14	62647	0	31582	1378	1
26	1H	62707	0	31612	1458	1
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	81	0
28	11	2120	0	2197	97	0
28	19	2120	0	2197	91	0
29	21	1568	0	1634	116	0
29	29	1568	0	1634	119	0
30	31	1585	0	1632	89	0
30	39	1627	0	1680	112	0
31	41	1473	0	1535	74	0
31	49	1473	0	1535	64	0
32	51	1321	0	1388	85	0
32	59	1307	0	1382	65	1
33	61	1136	0	1223	67	1
33	69	1136	0	1223	51	0
34	15	1104	0	1180	55	0
34	58	1104	0	1180	84	0
35	25	932	0	996	42	0
35	68	932	0	996	46	0
36	35	1144	0	1228	97	0
36	78	1144	0	1228	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1107	0	1166	77	0
37	88	1121	0	1179	59	0
38	55	959	0	1021	48	0
38	98	967	0	1033	67	0
39	65	881	0	943	63	0
39	A8	876	0	938	48	0
40	75	1141	0	1202	73	0
40	B8	1141	0	1202	66	0
41	85	963	0	1022	44	0
41	C8	963	0	1022	70	0
42	95	778	0	852	69	0
42	D8	778	0	852	41	0
43	A5	899	0	964	28	0
43	E8	899	0	964	32	0
44	B5	725	0	778	37	0
44	F8	730	0	780	33	0
45	C5	794	0	884	53	0
45	G8	791	0	882	54	0
46	D5	1139	0	1163	58	0
46	H8	1397	0	1430	81	0
47	E5	612	0	633	33	0
47	I8	606	0	628	24	0
48	F5	762	0	848	37	0
48	J8	762	0	848	35	0
49	G5	558	0	610	30	0
49	K8	558	0	610	37	0
50	H5	468	0	518	13	0
50	L8	468	0	518	20	0
51	I5	515	0	514	59	0
51	M8	533	0	526	37	0
52	J5	458	0	480	21	0
52	N8	458	0	480	25	0
53	L5	391	0	432	9	0
53	P8	396	0	434	13	0
54	M5	495	0	567	64	0
54	Q8	488	0	560	59	0
55	3L	1814	0	932	51	0
56	11	2	0	0	0	0
56	13	146	0	0	0	0
56	14	391	0	0	0	0
56	16	12	0	0	0	0
56	1G	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	481	0	0	0	0
56	1J	6	0	0	0	0
56	1K	1	0	0	0	0
56	2I	2	0	0	0	0
56	25	1	0	0	0	0
56	29	3	0	0	0	0
56	2K	7	0	0	0	0
56	2L	4	0	0	0	0
56	3I	1	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	4I	1	0	0	0	0
56	45	1	0	0	0	0
56	5E	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	1	0	0	0	0
56	C5	1	0	0	0	0
56	I8	1	0	0	0	0
56	L5	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	13	42	0	45	2	0
57	1G	42	0	45	0	0
58	32	1	0	0	0	0
58	3E	1	0	0	0	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
59	11	10	0	0	1	0
59	13	141	0	0	25	0
59	14	474	0	0	139	0
59	16	11	0	0	2	0
59	19	9	0	0	4	0
59	1G	87	0	0	19	0
59	1H	633	0	0	156	0
59	1I	1	0	0	0	0
59	1J	6	0	0	0	0
59	1K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	5	0	0	3	0
59	29	3	0	0	1	0
59	2K	6	0	0	0	0
59	31	5	0	0	0	0
59	39	5	0	0	0	0
59	3E	1	0	0	0	0
59	3I	2	0	0	0	0
59	4K	3	0	0	0	0
59	55	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	6A	1	0	0	0	0
59	75	1	0	0	0	0
59	78	4	0	0	2	0
59	85	1	0	0	1	0
59	A5	1	0	0	0	0
59	BA	1	0	0	0	0
59	F8	1	0	0	0	0
59	G8	2	0	0	0	0
59	J8	1	0	0	0	0
59	L8	2	0	0	1	0
59	M5	2	0	0	0	0
All	All	299607	0	199932	8690	4

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 18.

The worst 5 of 8690 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)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
4:32:26:CYS:HB3	4:32:31:CYS:SG	1.85	1.17
26:14:2701:C:H3'	26:14:2702:U:H5''	1.31	1.12
26:14:2711:A:OP2	59:14:3464:HOH:O	1.70	1.09
26:1H:229:A:H4'	26:1H:230:U:H5'	1.33	1.08

All (4) 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)
1:13:85:U:O2'	32:59:100:GLY:O[3_555]	1.97	0.23
1:1G:86:U:N3	26:14:275:G:OP2[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.19	0.01
33:61:91:SER:OG	1:1G:368:U:OP1[4_555]	2.19	0.01

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%)	195 (83%)	35 (15%)	5 (2%)	5	21
2	1E	235/256 (92%)	200 (85%)	34 (14%)	1 (0%)	30	57
3	22	204/239 (85%)	184 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	180 (89%)	22 (11%)	1 (0%)	24	52
4	32	206/209 (99%)	181 (88%)	24 (12%)	1 (0%)	24	52
4	3E	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	4E	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	18	45
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
7	6E	148/156 (95%)	140 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	8	28
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	18	45
9	82	118/128 (92%)	105 (89%)	12 (10%)	1 (1%)	16	42
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	115/129 (89%)	104 (90%)	8 (7%)	3 (3%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	114/129 (88%)	101 (89%)	12 (10%)	1 (1%)	14	39
12	3A	123/132 (93%)	101 (82%)	19 (15%)	3 (2%)	4	18
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	42
13	4A	115/126 (91%)	95 (83%)	18 (16%)	2 (2%)	7	25
13	4I	114/126 (90%)	96 (84%)	16 (14%)	2 (2%)	6	24
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	6	24
14	5I	57/61 (93%)	46 (81%)	9 (16%)	2 (4%)	3	13
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	8A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
18	9A	69/88 (78%)	66 (96%)	3 (4%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	9	29
19	AA	76/93 (82%)	62 (82%)	11 (14%)	3 (4%)	2	11
19	AI	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	17
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	12	37
20	BI	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	12	37
21	1B	23/27 (85%)	21 (91%)	1 (4%)	1 (4%)	2	10
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276 (98%)	249 (92%)	18 (7%)	4 (2%)	8	28
28	19	271/276 (98%)	253 (93%)	13 (5%)	5 (2%)	6	24
29	21	203/206 (98%)	161 (79%)	33 (16%)	9 (4%)	2	9
29	29	203/206 (98%)	158 (78%)	36 (18%)	9 (4%)	2	9
30	31	200/210 (95%)	178 (89%)	21 (10%)	1 (0%)	24	52
30	39	206/210 (98%)	161 (78%)	38 (18%)	7 (3%)	3	13
31	41	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7	25
31	49	179/182 (98%)	158 (88%)	20 (11%)	1 (1%)	21	48
32	51	171/180 (95%)	137 (80%)	21 (12%)	13 (8%)	1	3
32	59	168/180 (93%)	128 (76%)	31 (18%)	9 (5%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	61	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	5	21
33	69	144/148 (97%)	113 (78%)	27 (19%)	4 (3%)	4	16
34	15	136/140 (97%)	121 (89%)	14 (10%)	1 (1%)	18	45
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	3	16
35	25	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	42
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	35	148/150 (99%)	113 (76%)	32 (22%)	3 (2%)	6	21
36	78	148/150 (99%)	110 (74%)	30 (20%)	8 (5%)	1	7
37	45	137/141 (97%)	110 (80%)	25 (18%)	2 (2%)	8	28
37	88	139/141 (99%)	107 (77%)	26 (19%)	6 (4%)	2	10
38	55	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	7	25
38	98	116/118 (98%)	106 (91%)	9 (8%)	1 (1%)	14	39
39	65	109/112 (97%)	85 (78%)	22 (20%)	2 (2%)	6	24
39	A8	108/112 (96%)	89 (82%)	18 (17%)	1 (1%)	14	39
40	75	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
40	B8	135/146 (92%)	123 (91%)	12 (9%)	0	100	100
41	85	115/118 (98%)	98 (85%)	17 (15%)	0	100	100
41	C8	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	13
42	95	99/101 (98%)	77 (78%)	18 (18%)	4 (4%)	2	11
42	D8	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	15
43	A5	111/113 (98%)	101 (91%)	7 (6%)	3 (3%)	4	16
43	E8	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
44	B5	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	5	20
44	F8	91/96 (95%)	83 (91%)	6 (7%)	2 (2%)	5	20
45	C5	102/110 (93%)	76 (74%)	24 (24%)	2 (2%)	6	21
45	G8	102/110 (93%)	83 (81%)	13 (13%)	6 (6%)	1	6
46	D5	132/206 (64%)	104 (79%)	24 (18%)	4 (3%)	3	15
46	H8	173/206 (84%)	133 (77%)	33 (19%)	7 (4%)	2	11
47	E5	75/85 (88%)	68 (91%)	5 (7%)	2 (3%)	4	16
47	I8	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	4	16
48	F5	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	5	21
49	G5	64/72 (89%)	60 (94%)	2 (3%)	2 (3%)	3	14
49	K8	64/72 (89%)	59 (92%)	2 (3%)	3 (5%)	2	9
50	H5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	I5	61/71 (86%)	36 (59%)	21 (34%)	4 (7%)	1	5
51	M8	64/71 (90%)	36 (56%)	25 (39%)	3 (5%)	2	9
52	J5	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	24
52	N8	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
53	L5	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
53	P8	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	M5	60/65 (92%)	46 (77%)	11 (18%)	3 (5%)	1	8
54	Q8	59/65 (91%)	52 (88%)	3 (5%)	4 (7%)	1	4
All	All	11183/11946 (94%)	9677 (86%)	1306 (12%)	200 (2%)	6	24

5 of 200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	21	83	ASP
32	51	172	LYS
32	51	173	PRO
36	78	19	VAL

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%)	157 (77%)	48 (23%)	1	3
2	1E	205/220 (93%)	152 (74%)	53 (26%)	0	2
3	22	160/188 (85%)	120 (75%)	40 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2E	159/188 (85%)	119 (75%)	40 (25%)	0	2
4	32	180/181 (99%)	142 (79%)	38 (21%)	1	4
4	3E	180/181 (99%)	136 (76%)	44 (24%)	1	2
5	42	116/123 (94%)	86 (74%)	30 (26%)	0	2
5	4E	116/123 (94%)	92 (79%)	24 (21%)	1	4
6	52	90/90 (100%)	70 (78%)	20 (22%)	1	3
6	5E	90/90 (100%)	70 (78%)	20 (22%)	1	3
7	62	126/127 (99%)	98 (78%)	28 (22%)	1	3
7	6E	126/127 (99%)	99 (79%)	27 (21%)	1	4
8	72	118/119 (99%)	96 (81%)	22 (19%)	1	6
8	7E	119/119 (100%)	86 (72%)	33 (28%)	0	1
9	82	95/99 (96%)	78 (82%)	17 (18%)	2	7
9	8E	98/99 (99%)	74 (76%)	24 (24%)	1	2
10	1A	89/92 (97%)	66 (74%)	23 (26%)	0	2
10	1I	89/92 (97%)	67 (75%)	22 (25%)	1	2
11	2A	89/99 (90%)	68 (76%)	21 (24%)	1	3
11	2I	88/99 (89%)	69 (78%)	19 (22%)	1	4
12	3A	104/109 (95%)	77 (74%)	27 (26%)	0	2
12	3I	103/109 (94%)	81 (79%)	22 (21%)	1	4
13	4A	94/101 (93%)	71 (76%)	23 (24%)	1	2
13	4I	94/101 (93%)	70 (74%)	24 (26%)	0	2
14	5A	48/50 (96%)	35 (73%)	13 (27%)	0	1
14	5I	48/50 (96%)	36 (75%)	12 (25%)	0	2
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	10
15	6I	79/80 (99%)	62 (78%)	17 (22%)	1	4
16	7A	72/74 (97%)	55 (76%)	17 (24%)	1	3
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	95/97 (98%)	78 (82%)	17 (18%)	2	7
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	6
18	9A	62/77 (80%)	45 (73%)	17 (27%)	0	1
18	9I	63/77 (82%)	49 (78%)	14 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AA	67/80 (84%)	52 (78%)	15 (22%)	1	3
19	AI	72/80 (90%)	53 (74%)	19 (26%)	0	1
20	BA	76/82 (93%)	54 (71%)	22 (29%)	0	1
20	BI	76/82 (93%)	54 (71%)	22 (29%)	0	1
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	25
21	1F	20/22 (91%)	18 (90%)	2 (10%)	7	25
28	11	214/218 (98%)	167 (78%)	47 (22%)	1	4
28	19	214/218 (98%)	163 (76%)	51 (24%)	1	3
29	21	165/166 (99%)	117 (71%)	48 (29%)	0	1
29	29	165/166 (99%)	118 (72%)	47 (28%)	0	1
30	31	161/166 (97%)	123 (76%)	38 (24%)	1	3
30	39	165/166 (99%)	117 (71%)	48 (29%)	0	1
31	41	155/156 (99%)	125 (81%)	30 (19%)	1	5
31	49	155/156 (99%)	123 (79%)	32 (21%)	1	4
32	51	142/148 (96%)	98 (69%)	44 (31%)	0	0
32	59	142/148 (96%)	107 (75%)	35 (25%)	1	2
33	61	122/124 (98%)	86 (70%)	36 (30%)	0	1
33	69	122/124 (98%)	84 (69%)	38 (31%)	0	0
34	15	117/119 (98%)	88 (75%)	29 (25%)	1	2
34	58	117/119 (98%)	89 (76%)	28 (24%)	1	3
35	25	100/100 (100%)	74 (74%)	26 (26%)	0	2
35	68	100/100 (100%)	79 (79%)	21 (21%)	1	4
36	35	116/116 (100%)	67 (58%)	49 (42%)	0	0
36	78	116/116 (100%)	77 (66%)	39 (34%)	0	0
37	45	110/111 (99%)	78 (71%)	32 (29%)	0	1
37	88	111/111 (100%)	83 (75%)	28 (25%)	0	2
38	55	100/101 (99%)	71 (71%)	29 (29%)	0	1
38	98	101/101 (100%)	73 (72%)	28 (28%)	0	1
39	65	87/88 (99%)	58 (67%)	29 (33%)	0	0
39	A8	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	75	120/127 (94%)	88 (73%)	32 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	B8	120/127 (94%)	84 (70%)	36 (30%)	0	1
41	85	93/94 (99%)	68 (73%)	25 (27%)	0	1
41	C8	93/94 (99%)	74 (80%)	19 (20%)	1	4
42	95	82/82 (100%)	51 (62%)	31 (38%)	0	0
42	D8	82/82 (100%)	60 (73%)	22 (27%)	0	1
43	A5	92/92 (100%)	68 (74%)	24 (26%)	0	1
43	E8	92/92 (100%)	67 (73%)	25 (27%)	0	1
44	B5	74/78 (95%)	56 (76%)	18 (24%)	1	2
44	F8	74/78 (95%)	57 (77%)	17 (23%)	1	3
45	C5	85/91 (93%)	54 (64%)	31 (36%)	0	0
45	G8	85/91 (93%)	56 (66%)	29 (34%)	0	0
46	D5	127/179 (71%)	99 (78%)	28 (22%)	1	4
46	H8	154/179 (86%)	114 (74%)	40 (26%)	0	2
47	E5	62/67 (92%)	51 (82%)	11 (18%)	2	7
47	I8	61/67 (91%)	47 (77%)	14 (23%)	1	3
48	F5	82/83 (99%)	56 (68%)	26 (32%)	0	0
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	4
49	G5	62/67 (92%)	40 (64%)	22 (36%)	0	0
49	K8	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	H5	51/52 (98%)	38 (74%)	13 (26%)	0	2
50	L8	51/52 (98%)	37 (72%)	14 (28%)	0	1
51	I5	57/63 (90%)	44 (77%)	13 (23%)	1	3
51	M8	59/63 (94%)	43 (73%)	16 (27%)	0	1
52	J5	51/52 (98%)	41 (80%)	10 (20%)	1	5
52	N8	51/52 (98%)	38 (74%)	13 (26%)	0	2
53	L5	38/42 (90%)	30 (79%)	8 (21%)	1	4
53	P8	38/42 (90%)	31 (82%)	7 (18%)	1	7
54	M5	52/55 (94%)	31 (60%)	21 (40%)	0	0
54	Q8	51/55 (93%)	37 (72%)	14 (28%)	0	1
All	All	9444/9894 (96%)	7043 (75%)	2401 (25%)	0	2

5 of 2401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	59	157	TYR
48	F5	37	ILE
34	15	63	THR
32	59	143	GLN
39	65	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
46	H8	30	ASN
35	25	90	GLN
2	12	45	GLN
34	15	69	GLN
41	85	71	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1504/1522 (98%)	381 (25%)	35 (2%)
1	1G	1503/1522 (98%)	362 (24%)	37 (2%)
22	1K	84/85 (98%)	38 (45%)	8 (9%)
23	2K	76/77 (98%)	21 (27%)	3 (3%)
23	2L	76/77 (98%)	17 (22%)	1 (1%)
24	1L	84/85 (98%)	35 (41%)	8 (9%)
24	3K	84/85 (98%)	27 (32%)	4 (4%)
25	4K	11/30 (36%)	4 (36%)	1 (9%)
25	4L	12/30 (40%)	6 (50%)	3 (25%)
26	14	2908/2918 (99%)	763 (26%)	56 (1%)
26	1H	2911/2918 (99%)	727 (24%)	60 (2%)
27	16	121/122 (99%)	20 (16%)	0
27	1J	121/122 (99%)	33 (27%)	3 (2%)
55	3L	84/85 (98%)	34 (40%)	4 (4%)
All	All	9579/9678 (98%)	2468 (25%)	223 (2%)

5 of 2468 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G

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Mol	Chain	Res	Type
1	13	13	U

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	197	A
27	1J	56	G
1	1G	1300	G
26	14	2893	G
26	14	2173	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
24	PSU	1L	40	24	18,21,22	1.27	1 (5%)	21,30,33	1.73	4 (19%)
23	PSU	2L	56	23	18,21,22	1.21	1 (5%)	21,30,33	1.91	2 (9%)
23	4SU	2K	8	23	18,21,22	2.03	4 (22%)	25,30,33	2.77	6 (24%)
23	PSU	2K	56	23	18,21,22	1.27	3 (16%)	21,30,33	1.85	4 (19%)
24	PSU	3K	40	24	18,21,22	1.22	1 (5%)	21,30,33	1.77	3 (14%)
55	MIA	3L	38	55	28,31,32	2.37	5 (17%)	38,44,47	2.86	17 (44%)
23	4SU	2L	8	23	18,21,22	1.86	3 (16%)	25,30,33	2.91	5 (20%)
55	PSU	3L	40	55	18,21,22	1.19	1 (5%)	21,30,33	1.58	3 (14%)
23	OMC	2L	33	23	19,22,23	1.78	4 (21%)	25,31,34	1.23	2 (8%)
22	PSU	1K	64	22	18,21,22	1.27	1 (5%)	21,30,33	1.81	4 (19%)
23	5MU	2L	55	23	19,22,23	3.95	5 (26%)	27,32,35	3.36	9 (33%)
22	QUO	1K	35	22,25	32,35,36	4.73	12 (37%)	36,52,55	4.59	12 (33%)
23	OMC	2K	33	23	19,22,23	1.69	3 (15%)	25,31,34	0.63	0
22	MIA	1K	38	22	28,31,32	2.19	4 (14%)	38,44,47	3.21	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	1K	40	22	18,21,22	1.06	1 (5%)	21,30,33	1.66	4 (19%)
22	5MU	1K	63	22	19,22,23	3.83	5 (26%)	27,32,35	3.15	7 (25%)
23	5MU	2K	55	23	19,22,23	4.00	5 (26%)	27,32,35	3.23	7 (25%)

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
24	PSU	1L	40	24	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
24	PSU	3K	40	24	-	0/7/25/26	0/2/2/2
55	MIA	3L	38	55	-	4/15/33/34	0/3/3/3
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
55	PSU	3L	40	55	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	QUO	1K	35	22,25	-	4/12/43/44	0/4/4/4
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	MIA	1K	38	22	-	3/15/33/34	0/3/3/3
22	PSU	1K	40	22	-	1/7/25/26	0/2/2/2
22	5MU	1K	63	22	-	3/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	2/7/25/26	0/2/2/2

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	35	QUO	C4-N3	15.67	1.70	1.34
23	2K	55	5MU	C2-N1	13.40	1.59	1.38
23	2L	55	5MU	C2-N1	12.84	1.58	1.38
22	1K	63	5MU	C2-N1	12.55	1.58	1.38
22	1K	35	QUO	C6-N1	-12.30	1.15	1.38

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	35	QUO	C5-C4-N3	-17.51	107.42	127.53
22	1K	35	QUO	C1'-N9-C8	-10.76	113.53	125.72
22	1K	38	MIA	C11-S10-C2	-10.60	94.30	102.25
23	2L	55	5MU	C5-C4-N3	10.56	124.50	115.32
22	1K	63	5MU	C5-C4-N3	10.53	124.48	115.32

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	35	QUO	O4'-C4'-C5'-O5'
22	1K	35	QUO	C16-C12-N11-C10
22	1K	38	MIA	N6-C12-C13-C14
22	1K	38	MIA	C12-C13-C14-C15
22	1K	38	MIA	C12-C13-C14-C16

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	56	PSU	1	0
23	2K	8	4SU	1	0
23	2K	56	PSU	1	0
23	2L	8	4SU	1	0
23	2L	33	OMC	6	0
22	1K	64	PSU	1	0
22	1K	35	QUO	5	0
22	1K	38	MIA	7	0
22	1K	40	PSU	2	0
23	2K	55	5MU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1166 ligands modelled in this entry, 1164 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PAR	13	1745	-	44,45,45	0.84	2 (4%)	63,67,67	2.10	17 (26%)
57	PAR	1G	1686	-	44,45,45	0.71	1 (2%)	63,67,67	1.84	11 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	13	1745	-	-	6/18/94/94	0/4/4/4
57	PAR	1G	1686	-	-	5/18/94/94	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1686	PAR	C24-N24	-2.32	1.43	1.47
57	13	1745	PAR	C21-N21	-2.19	1.44	1.47
57	13	1745	PAR	C24-N24	-2.19	1.44	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1G	1686	PAR	C13-O52-C52	-6.92	101.57	117.98
57	13	1745	PAR	C11-O51-C51	5.24	123.95	113.72
57	13	1745	PAR	C14-O54-C54	5.05	123.58	113.72
57	1G	1686	PAR	C11-O51-C51	4.99	123.46	113.72
57	1G	1686	PAR	C14-O54-C54	4.90	123.29	113.72

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1G	1686	PAR	O51-C51-C61-O61
57	1G	1686	PAR	C33-C43-C53-O53
57	1G	1686	PAR	C41-C51-C61-O61
57	1G	1686	PAR	O51-C11-O11-C42

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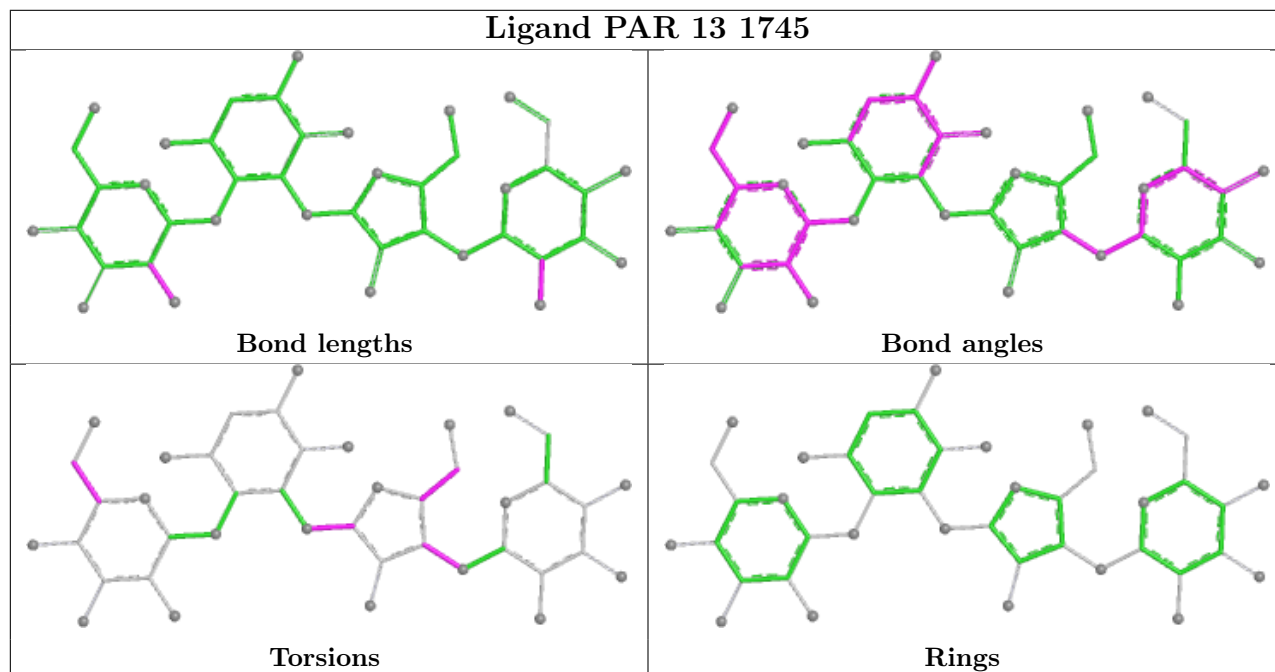
Mol	Chain	Res	Type	Atoms
57	13	1745	PAR	O43-C43-C53-O53

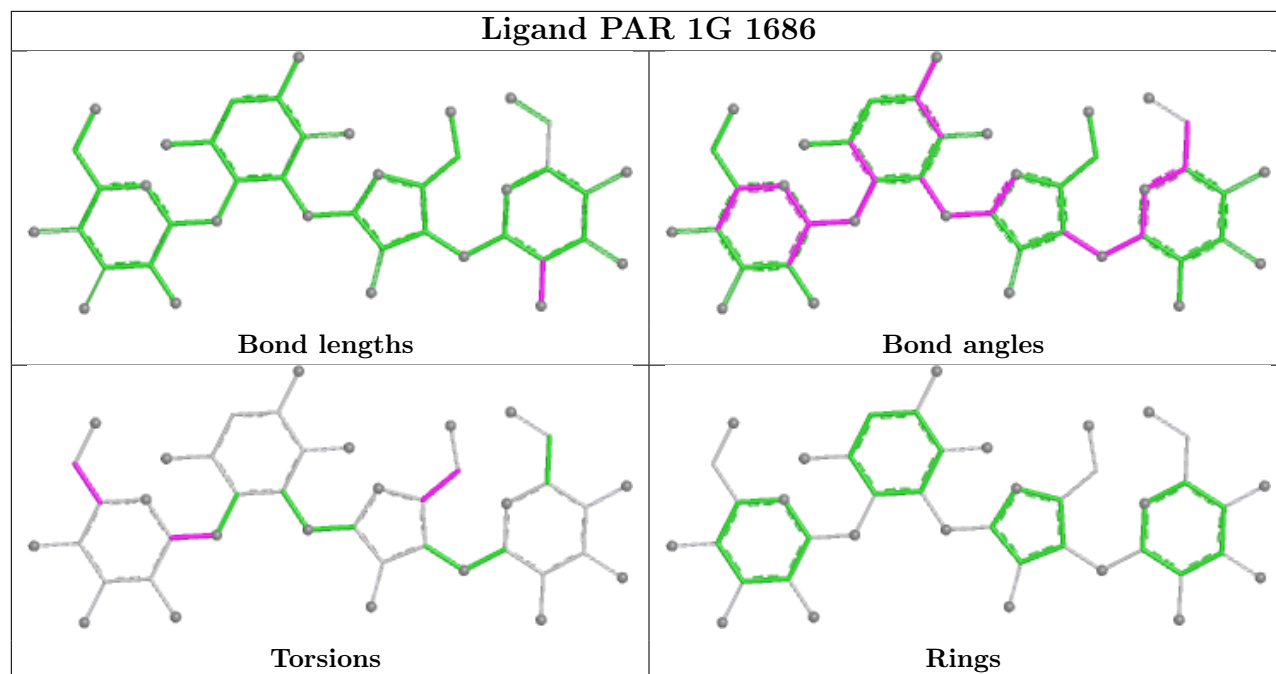
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	13	1745	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	1505/1522 (98%)	0.80	207 (13%) 6 4	53, 96, 178, 280	0
1	1G	1504/1522 (98%)	0.96	248 (16%) 4 2	67, 108, 172, 272	0
2	12	237/256 (92%)	1.60	64 (27%) 1 1	122, 156, 179, 190	0
2	1E	237/256 (92%)	1.20	51 (21%) 2 1	101, 137, 165, 175	0
3	22	206/239 (86%)	1.98	82 (39%) 1 0	114, 132, 162, 173	0
3	2E	205/239 (85%)	0.85	24 (11%) 9 5	81, 103, 132, 138	0
4	32	208/209 (99%)	1.31	45 (21%) 2 1	88, 109, 130, 142	0
4	3E	208/209 (99%)	0.89	35 (16%) 4 2	77, 98, 122, 131	0
5	42	151/162 (93%)	1.36	32 (21%) 2 1	99, 115, 136, 155	0
5	4E	151/162 (93%)	0.82	18 (11%) 9 5	72, 91, 112, 150	0
6	52	101/101 (100%)	0.69	9 (8%) 15 8	78, 94, 114, 144	0
6	5E	101/101 (100%)	0.89	11 (10%) 10 5	75, 94, 115, 132	0
7	62	155/156 (99%)	1.99	43 (27%) 1 1	105, 120, 143, 157	0
7	6E	152/156 (97%)	1.26	25 (16%) 4 2	96, 114, 137, 148	0
8	72	137/138 (99%)	1.14	27 (19%) 3 1	98, 119, 131, 137	0
8	7E	138/138 (100%)	0.79	21 (15%) 5 3	81, 100, 114, 126	0
9	82	122/128 (95%)	2.03	40 (32%) 1 0	102, 149, 166, 170	0
9	8E	127/128 (99%)	1.38	31 (24%) 2 1	81, 135, 158, 168	0
10	1A	99/105 (94%)	1.36	18 (18%) 3 2	111, 148, 164, 171	0
10	1I	99/105 (94%)	1.65	33 (33%) 1 0	73, 128, 159, 161	0
11	2A	117/129 (90%)	1.28	23 (19%) 3 1	81, 103, 120, 147	0
11	2I	116/129 (89%)	1.13	18 (15%) 5 2	72, 98, 120, 150	0
12	3A	125/132 (94%)	1.11	21 (16%) 4 2	78, 96, 129, 157	0
12	3I	122/132 (92%)	0.72	13 (10%) 11 6	61, 71, 97, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	1.65	21 (17%) 3 2	102, 137, 157, 170	0
13	4I	116/126 (92%)	1.02	13 (11%) 10 5	78, 117, 136, 144	0
14	5A	58/61 (95%)	1.72	17 (29%) 1 1	116, 131, 146, 154	0
14	5I	59/61 (96%)	0.72	8 (13%) 7 4	82, 92, 108, 118	0
15	6A	88/89 (98%)	0.66	9 (10%) 12 6	80, 105, 121, 127	0
15	6I	88/89 (98%)	0.67	10 (11%) 10 5	67, 93, 110, 123	0
16	7A	84/88 (95%)	1.11	14 (16%) 4 2	85, 98, 124, 154	0
16	7I	84/88 (95%)	1.06	10 (11%) 9 5	90, 104, 132, 160	0
17	8A	100/105 (95%)	1.11	16 (16%) 5 2	91, 106, 124, 128	0
17	8I	100/105 (95%)	1.33	22 (22%) 2 1	81, 99, 111, 121	0
18	9A	71/88 (80%)	0.93	8 (11%) 10 5	84, 107, 134, 164	0
18	9I	72/88 (81%)	1.14	13 (18%) 3 2	80, 98, 126, 161	0
19	AA	78/93 (83%)	1.49	20 (25%) 1 1	124, 142, 171, 180	0
19	AI	83/93 (89%)	1.45	15 (18%) 3 2	90, 116, 137, 145	0
20	BA	99/106 (93%)	1.28	30 (30%) 1 1	83, 105, 133, 143	0
20	BI	99/106 (93%)	2.04	41 (41%) 0 0	101, 115, 146, 151	0
21	1B	25/27 (92%)	1.57	5 (20%) 3 1	110, 126, 143, 163	0
21	1F	25/27 (92%)	1.54	8 (32%) 1 0	90, 102, 116, 142	0
22	1K	80/85 (94%)	2.61	30 (37%) 1 0	81, 190, 249, 257	0
23	2K	73/77 (94%)	1.20	12 (16%) 4 2	68, 96, 122, 140	0
23	2L	73/77 (94%)	1.47	19 (26%) 1 1	76, 105, 138, 160	0
24	1L	84/85 (98%)	2.79	39 (46%) 0 0	107, 214, 302, 318	0
24	3K	84/85 (98%)	1.48	17 (20%) 3 1	68, 209, 252, 259	0
25	4K	12/30 (40%)	1.15	3 (25%) 2 1	48, 89, 132, 145	1 (8%)
25	4L	12/30 (40%)	0.84	2 (16%) 4 2	85, 117, 155, 188	0
26	14	2909/2918 (99%)	0.49	289 (9%) 13 6	48, 80, 223, 333	0
26	1H	2912/2918 (99%)	0.39	278 (9%) 14 7	38, 71, 216, 270	0
27	16	122/122 (100%)	0.43	5 (4%) 41 22	65, 91, 113, 185	0
27	1J	122/122 (100%)	0.84	10 (8%) 17 9	73, 107, 128, 182	0
28	11	273/276 (98%)	0.15	9 (3%) 49 28	39, 62, 80, 92	0
28	19	273/276 (98%)	0.29	12 (4%) 39 20	42, 70, 88, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	21	205/206 (99%)	0.82	23 (11%) 10 5	48, 85, 125, 137	0
29	29	205/206 (99%)	1.19	40 (19%) 3 1	56, 87, 129, 148	0
30	31	202/210 (96%)	0.69	22 (10%) 10 5	38, 74, 110, 127	0
30	39	208/210 (99%)	1.19	42 (20%) 3 1	54, 95, 146, 178	0
31	41	181/182 (99%)	1.68	51 (28%) 1 1	79, 102, 133, 149	0
31	49	181/182 (99%)	1.12	33 (18%) 3 2	104, 125, 154, 169	0
32	51	173/180 (96%)	1.23	40 (23%) 2 1	79, 102, 115, 151	0
32	59	170/180 (94%)	2.75	86 (50%) 0 0	134, 183, 210, 241	0
33	61	146/148 (98%)	1.55	40 (27%) 1 1	74, 122, 140, 145	0
33	69	146/148 (98%)	1.64	48 (32%) 1 0	77, 118, 142, 146	0
34	15	138/140 (98%)	1.79	43 (31%) 1 1	75, 100, 129, 137	0
34	58	138/140 (98%)	1.10	17 (12%) 8 5	61, 88, 126, 143	0
35	25	122/122 (100%)	0.79	14 (11%) 9 5	61, 84, 102, 110	0
35	68	122/122 (100%)	0.45	11 (9%) 15 8	55, 74, 92, 101	0
36	35	150/150 (100%)	0.87	23 (15%) 5 3	54, 96, 133, 159	0
36	78	150/150 (100%)	0.91	21 (14%) 6 3	45, 81, 111, 152	0
37	45	139/141 (98%)	1.02	21 (15%) 5 3	69, 98, 116, 136	0
37	88	141/141 (100%)	0.81	17 (12%) 8 5	52, 77, 101, 129	0
38	55	117/118 (99%)	1.14	24 (20%) 2 1	56, 75, 92, 108	0
38	98	118/118 (100%)	1.09	21 (17%) 4 2	56, 80, 101, 107	0
39	65	111/112 (99%)	0.86	11 (9%) 13 6	75, 102, 120, 132	0
39	A8	110/112 (98%)	0.59	9 (8%) 17 9	70, 86, 110, 125	0
40	75	137/146 (93%)	1.44	34 (24%) 2 1	75, 91, 148, 185	0
40	B8	137/146 (93%)	1.69	38 (27%) 1 1	70, 89, 136, 159	0
41	85	117/118 (99%)	1.53	27 (23%) 2 1	62, 88, 122, 143	0
41	C8	117/118 (99%)	0.91	17 (14%) 6 3	50, 76, 107, 141	0
42	95	101/101 (100%)	2.19	40 (39%) 1 0	61, 116, 131, 136	0
42	D8	101/101 (100%)	1.92	30 (29%) 1 1	53, 100, 124, 139	0
43	A5	113/113 (100%)	0.69	10 (8%) 15 8	56, 71, 100, 159	0
43	E8	113/113 (100%)	0.55	5 (4%) 39 20	52, 72, 105, 140	0
44	B5	92/96 (95%)	0.44	6 (6%) 25 12	64, 79, 106, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	F8	93/96 (96%)	0.39	4 (4%) 40 21	51, 67, 93, 102	0
45	C5	104/110 (94%)	1.60	36 (34%) 1 0	89, 119, 158, 166	0
45	G8	104/110 (94%)	1.03	14 (13%) 7 4	69, 96, 140, 148	0
46	D5	138/206 (66%)	1.29	26 (18%) 3 2	103, 134, 178, 186	0
46	H8	175/206 (84%)	1.28	36 (20%) 2 1	84, 119, 190, 195	0
47	E5	77/85 (90%)	0.66	7 (9%) 15 8	64, 81, 99, 131	0
47	I8	76/85 (89%)	0.54	8 (10%) 11 6	52, 69, 85, 113	0
48	F5	97/98 (98%)	1.02	21 (21%) 2 1	57, 77, 122, 143	0
48	J8	97/98 (98%)	0.55	9 (9%) 14 7	48, 72, 124, 150	0
49	G5	66/72 (91%)	0.77	10 (15%) 5 3	74, 96, 114, 135	0
49	K8	66/72 (91%)	0.97	13 (19%) 3 1	59, 77, 90, 124	0
50	H5	59/60 (98%)	1.40	11 (18%) 3 2	74, 94, 132, 157	0
50	L8	59/60 (98%)	0.44	3 (5%) 33 17	56, 78, 114, 137	0
51	I5	63/71 (88%)	1.20	12 (19%) 3 1	138, 171, 190, 192	0
51	M8	66/71 (92%)	1.56	19 (28%) 1 1	105, 154, 174, 184	0
52	J5	59/60 (98%)	1.70	21 (35%) 1 0	56, 80, 147, 187	0
52	N8	59/60 (98%)	1.34	14 (23%) 2 1	51, 86, 152, 158	0
53	L5	45/49 (91%)	0.31	3 (6%) 24 12	47, 56, 69, 84	0
53	P8	46/49 (93%)	0.26	3 (6%) 25 12	40, 48, 66, 81	0
54	M5	62/65 (95%)	1.03	14 (22%) 2 1	65, 77, 93, 107	0
54	Q8	61/65 (93%)	0.33	1 (1%) 70 47	56, 66, 80, 98	0
55	3L	83/85 (97%)	1.68	19 (22%) 2 1	72, 217, 260, 269	0
All	All	20954/21624 (96%)	0.92	3312 (15%) 5 2	38, 95, 175, 333	1 (0%)

The worst 5 of 3312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	13	85	U	22.6
32	59	96	ALA	20.5
32	59	99	VAL	18.1
13	4A	6	GLY	17.9
7	62	81	GLY	16.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	5MU	2L	55	21/22	0.76	0.14	101,110,116,118	0
23	5MU	2K	55	21/22	0.80	0.14	88,99,104,112	0
24	PSU	1L	40	20/21	0.81	0.30	99,116,121,124	0
24	PSU	3K	40	20/21	0.83	0.14	106,113,117,119	0
23	PSU	2K	56	20/21	0.84	0.10	93,98,101,113	0
23	PSU	2L	56	20/21	0.84	0.10	101,108,114,119	0
55	PSU	3L	40	20/21	0.84	0.24	110,117,123,123	0
55	MIA	3L	38	29/30	0.88	0.22	102,116,135,141	0
23	4SU	2L	8	20/21	0.89	0.14	99,106,113,117	0
22	PSU	1K	64	20/21	0.90	0.10	106,129,138,140	0
23	OMC	2L	33	21/22	0.90	0.14	86,95,99,102	0
22	5MU	1K	63	21/22	0.92	0.11	106,124,138,141	0
22	QUO	1K	35	32/33	0.92	0.35	67,86,101,111	0
22	PSU	1K	40	20/21	0.92	0.14	78,96,104,105	0
22	MIA	1K	38	29/30	0.94	0.21	67,84,98,112	0
23	4SU	2K	8	20/21	0.94	0.11	83,89,99,107	0
23	OMC	2K	33	21/22	0.95	0.13	70,74,82,85	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1G	1648	1/1	0.14	0.43	121,121,121,121	0
56	MG	14	3254	1/1	0.44	0.36	102,102,102,102	0
56	MG	14	3300	1/1	0.45	0.36	109,109,109,109	0
56	MG	14	3265	1/1	0.47	0.38	121,121,121,121	0
56	MG	14	3148	1/1	0.49	0.56	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	25	201	1/1	0.49	0.42	107,107,107,107	0
56	MG	14	3283	1/1	0.50	0.35	102,102,102,102	0
56	MG	14	3241	1/1	0.53	0.38	91,91,91,91	0
56	MG	1H	3172	1/1	0.53	0.54	84,84,84,84	0
56	MG	1H	3299	1/1	0.54	0.39	82,82,82,82	0
56	MG	3E	301	1/1	0.55	0.21	112,112,112,112	0
56	MG	1G	1636	1/1	0.58	0.38	84,84,84,84	0
56	MG	1H	3296	1/1	0.58	0.34	90,90,90,90	0
56	MG	13	1710	1/1	0.58	0.26	128,128,128,128	0
56	MG	14	3135	1/1	0.59	0.37	78,78,78,78	0
56	MG	1H	3309	1/1	0.59	0.32	98,98,98,98	0
56	MG	1H	3306	1/1	0.60	0.41	86,86,86,86	0
56	MG	1G	1668	1/1	0.60	0.34	82,82,82,82	0
56	MG	14	3298	1/1	0.62	0.53	103,103,103,103	0
56	MG	1H	3325	1/1	0.62	0.32	96,96,96,96	0
56	MG	1H	3322	1/1	0.62	0.39	80,80,80,80	0
56	MG	14	3228	1/1	0.63	0.46	98,98,98,98	0
56	MG	14	3197	1/1	0.63	0.34	89,89,89,89	0
56	MG	1H	3155	1/1	0.64	0.30	74,74,74,74	0
56	MG	14	3198	1/1	0.64	0.37	78,78,78,78	0
56	MG	13	1649	1/1	0.65	0.35	85,85,85,85	0
56	MG	2L	102	1/1	0.65	0.40	79,79,79,79	0
56	MG	C5	201	1/1	0.65	0.23	104,104,104,104	0
56	MG	1H	3217	1/1	0.66	0.35	93,93,93,93	0
56	MG	14	3301	1/1	0.67	0.41	86,86,86,86	0
56	MG	1H	3056	1/1	0.68	0.37	70,70,70,70	0
56	MG	1G	1669	1/1	0.68	0.36	88,88,88,88	0
56	MG	13	1616	1/1	0.68	0.43	93,93,93,93	0
56	MG	14	3025	1/1	0.68	0.35	84,84,84,84	0
56	MG	1G	1652	1/1	0.68	0.37	74,74,74,74	0
56	MG	1G	1654	1/1	0.68	0.39	101,101,101,101	0
56	MG	1H	3333	1/1	0.69	0.24	93,93,93,93	0
56	MG	1H	3349	1/1	0.69	0.47	85,85,85,85	0
56	MG	14	3104	1/1	0.69	0.27	84,84,84,84	0
56	MG	1H	3293	1/1	0.69	0.44	90,90,90,90	0
56	MG	14	3303	1/1	0.69	0.27	101,101,101,101	0
56	MG	1H	3314	1/1	0.69	0.32	90,90,90,90	0
56	MG	14	3149	1/1	0.69	0.26	84,84,84,84	0
56	MG	1H	3075	1/1	0.70	0.42	70,70,70,70	0
56	MG	13	1617	1/1	0.70	0.23	86,86,86,86	0
56	MG	1G	1616	1/1	0.70	0.36	86,86,86,86	0
56	MG	14	3305	1/1	0.70	0.33	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3196	1/1	0.70	0.36	90,90,90,90	0
56	MG	14	3299	1/1	0.70	0.20	70,70,70,70	0
56	MG	13	1615	1/1	0.71	0.43	92,92,92,92	0
56	MG	1J	203	1/1	0.71	0.47	81,81,81,81	0
56	MG	14	3258	1/1	0.71	0.37	73,73,73,73	0
56	MG	1H	3328	1/1	0.71	0.51	91,91,91,91	0
56	MG	13	1707	1/1	0.72	0.47	96,96,96,96	0
56	MG	1H	3182	1/1	0.72	0.32	87,87,87,87	0
56	MG	16	205	1/1	0.72	0.25	77,77,77,77	0
56	MG	1G	1610	1/1	0.72	0.44	77,77,77,77	0
56	MG	13	1690	1/1	0.72	0.25	113,113,113,113	0
56	MG	1J	204	1/1	0.72	0.34	95,95,95,95	0
56	MG	1H	3159	1/1	0.72	0.19	71,71,71,71	0
56	MG	1H	3332	1/1	0.72	0.27	88,88,88,88	0
56	MG	13	1611	1/1	0.73	0.36	70,70,70,70	0
56	MG	14	3133	1/1	0.73	0.23	86,86,86,86	0
56	MG	1H	3117	1/1	0.73	0.41	80,80,80,80	0
56	MG	1G	1664	1/1	0.74	0.37	102,102,102,102	0
56	MG	14	3225	1/1	0.74	0.39	78,78,78,78	0
56	MG	1H	3273	1/1	0.74	0.27	87,87,87,87	0
56	MG	13	1714	1/1	0.74	0.44	99,99,99,99	0
56	MG	14	3284	1/1	0.74	0.29	88,88,88,88	0
56	MG	14	3192	1/1	0.75	0.45	80,80,80,80	0
56	MG	1H	3148	1/1	0.75	0.39	82,82,82,82	0
56	MG	2K	101	1/1	0.75	0.31	79,79,79,79	0
56	MG	2K	102	1/1	0.75	0.40	83,83,83,83	0
56	MG	14	3068	1/1	0.75	0.31	69,69,69,69	0
56	MG	13	1607	1/1	0.75	0.20	77,77,77,77	0
56	MG	14	3122	1/1	0.75	0.41	68,68,68,68	0
56	MG	1H	3300	1/1	0.75	0.21	77,77,77,77	0
56	MG	13	1716	1/1	0.75	0.27	92,92,92,92	0
56	MG	13	1696	1/1	0.75	0.23	116,116,116,116	0
56	MG	1H	3311	1/1	0.75	0.40	78,78,78,78	0
56	MG	13	1703	1/1	0.76	0.25	89,89,89,89	0
56	MG	13	1647	1/1	0.76	0.43	77,77,77,77	0
56	MG	14	3278	1/1	0.76	0.14	98,98,98,98	0
56	MG	1H	3207	1/1	0.76	0.44	73,73,73,73	0
56	MG	14	3161	1/1	0.76	0.25	86,86,86,86	0
56	MG	14	3297	1/1	0.76	0.23	74,74,74,74	0
56	MG	1H	3170	1/1	0.76	0.31	61,61,61,61	0
56	MG	41	201	1/1	0.76	0.32	82,82,82,82	0
56	MG	13	1670	1/1	0.77	0.17	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1G	1625	1/1	0.77	0.36	84,84,84,84	0
56	MG	1G	1626	1/1	0.77	0.40	79,79,79,79	0
56	MG	1G	1635	1/1	0.77	0.29	98,98,98,98	0
56	MG	14	3136	1/1	0.77	0.35	73,73,73,73	0
56	MG	14	3292	1/1	0.77	0.30	82,82,82,82	0
56	MG	2K	104	1/1	0.77	0.30	98,98,98,98	0
56	MG	1G	1647	1/1	0.77	0.32	102,102,102,102	0
56	MG	1H	3257	1/1	0.77	0.34	85,85,85,85	0
56	MG	1H	3121	1/1	0.77	0.29	64,64,64,64	0
56	MG	1H	3342	1/1	0.77	0.44	98,98,98,98	0
56	MG	1H	3283	1/1	0.77	0.27	74,74,74,74	0
56	MG	1H	3356	1/1	0.77	0.25	79,79,79,79	0
56	MG	16	201	1/1	0.77	0.24	78,78,78,78	0
56	MG	13	1712	1/1	0.77	0.34	77,77,77,77	0
56	MG	1H	3316	1/1	0.77	0.33	74,74,74,74	0
56	MG	1H	3149	1/1	0.77	0.31	65,65,65,65	0
56	MG	16	202	1/1	0.78	0.30	59,59,59,59	0
56	MG	1H	3135	1/1	0.78	0.12	54,54,54,54	0
56	MG	16	210	1/1	0.78	0.19	89,89,89,89	0
56	MG	1H	3168	1/1	0.78	0.38	79,79,79,79	0
56	MG	13	1685	1/1	0.78	0.42	91,91,91,91	0
56	MG	1H	3171	1/1	0.78	0.16	79,79,79,79	0
56	MG	1H	3312	1/1	0.78	0.33	78,78,78,78	0
56	MG	13	1631	1/1	0.78	0.38	73,73,73,73	0
56	MG	14	3267	1/1	0.78	0.19	81,81,81,81	0
56	MG	14	3168	1/1	0.78	0.35	71,71,71,71	0
56	MG	1H	3153	1/1	0.78	0.37	64,64,64,64	0
56	MG	13	1694	1/1	0.78	0.23	82,82,82,82	0
58	ZN	G8	201	1/1	0.78	0.18	178,178,178,178	0
56	MG	14	3293	1/1	0.79	0.54	88,88,88,88	0
56	MG	1H	3043	1/1	0.79	0.31	84,84,84,84	0
56	MG	14	3240	1/1	0.79	0.22	77,77,77,77	0
56	MG	1G	1628	1/1	0.79	0.36	77,77,77,77	0
56	MG	1H	3290	1/1	0.79	0.54	84,84,84,84	0
56	MG	1H	3229	1/1	0.79	0.26	95,95,95,95	0
56	MG	14	3140	1/1	0.79	0.44	92,92,92,92	0
56	MG	14	3145	1/1	0.79	0.21	81,81,81,81	0
56	MG	14	3147	1/1	0.79	0.27	78,78,78,78	0
56	MG	14	3220	1/1	0.79	0.24	82,82,82,82	0
56	MG	1H	3282	1/1	0.79	0.30	83,83,83,83	0
56	MG	14	3289	1/1	0.79	0.21	79,79,79,79	0
56	MG	14	3227	1/1	0.79	0.26	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3118	1/1	0.80	0.34	86,86,86,86	0
56	MG	14	3252	1/1	0.80	0.33	96,96,96,96	0
56	MG	1G	1619	1/1	0.80	0.27	84,84,84,84	0
56	MG	13	1656	1/1	0.80	0.23	91,91,91,91	0
56	MG	1H	3335	1/1	0.80	0.14	87,87,87,87	0
56	MG	1H	3280	1/1	0.80	0.32	59,59,59,59	0
56	MG	1H	3348	1/1	0.80	0.41	80,80,80,80	0
56	MG	13	1660	1/1	0.80	0.20	91,91,91,91	0
56	MG	13	1652	1/1	0.80	0.28	80,80,80,80	0
56	MG	13	1708	1/1	0.80	0.28	85,85,85,85	0
56	MG	1H	3163	1/1	0.80	0.45	87,87,87,87	0
56	MG	14	3160	1/1	0.80	0.24	73,73,73,73	0
56	MG	16	204	1/1	0.80	0.31	86,86,86,86	0
56	MG	1H	3295	1/1	0.80	0.27	76,76,76,76	0
56	MG	1H	3032	1/1	0.80	0.32	78,78,78,78	0
56	MG	1H	3326	1/1	0.80	0.25	96,96,96,96	0
56	MG	1G	1607	1/1	0.80	0.24	81,81,81,81	0
56	MG	1H	3246	1/1	0.80	0.22	79,79,79,79	0
56	MG	14	3048	1/1	0.80	0.27	67,67,67,67	0
56	MG	1J	201	1/1	0.80	0.24	87,87,87,87	0
56	MG	13	1719	1/1	0.80	0.29	89,89,89,89	0
56	MG	14	3101	1/1	0.80	0.30	84,84,84,84	0
56	MG	14	3102	1/1	0.80	0.12	49,49,49,49	0
56	MG	14	3235	1/1	0.80	0.32	72,72,72,72	0
56	MG	1G	1618	1/1	0.80	0.19	88,88,88,88	0
56	MG	1H	3201	1/1	0.81	0.22	59,59,59,59	0
56	MG	1H	3310	1/1	0.81	0.25	69,69,69,69	0
56	MG	13	1674	1/1	0.81	0.19	94,94,94,94	0
56	MG	13	1654	1/1	0.81	0.34	75,75,75,75	0
56	MG	13	1623	1/1	0.81	0.44	94,94,94,94	0
56	MG	1G	1615	1/1	0.81	0.31	87,87,87,87	0
56	MG	1H	3112	1/1	0.81	0.22	66,66,66,66	0
56	MG	1H	3254	1/1	0.81	0.15	77,77,77,77	0
56	MG	14	3127	1/1	0.81	0.26	64,64,64,64	0
56	MG	13	1705	1/1	0.81	0.10	94,94,94,94	0
56	MG	1H	3041	1/1	0.81	0.30	87,87,87,87	0
56	MG	1H	3186	1/1	0.81	0.23	83,83,83,83	0
56	MG	14	3139	1/1	0.81	0.25	81,81,81,81	0
56	MG	14	3022	1/1	0.81	0.36	72,72,72,72	0
56	MG	1H	3185	1/1	0.82	0.24	71,71,71,71	0
56	MG	13	1635	1/1	0.82	0.26	59,59,59,59	0
56	MG	14	3132	1/1	0.82	0.41	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	3287	1/1	0.82	0.31	79,79,79,79	0
56	MG	1H	3109	1/1	0.82	0.11	60,60,60,60	0
56	MG	14	3203	1/1	0.82	0.20	55,55,55,55	0
56	MG	1H	3336	1/1	0.82	0.34	79,79,79,79	0
56	MG	14	3224	1/1	0.82	0.14	48,48,48,48	0
56	MG	14	3029	1/1	0.82	0.35	80,80,80,80	0
56	MG	14	3034	1/1	0.82	0.21	86,86,86,86	0
56	MG	14	3042	1/1	0.82	0.27	72,72,72,72	0
56	MG	1G	1650	1/1	0.82	0.18	87,87,87,87	0
56	MG	1H	3158	1/1	0.82	0.26	70,70,70,70	0
56	MG	14	3089	1/1	0.82	0.30	79,79,79,79	0
56	MG	1H	3343	1/1	0.82	0.37	75,75,75,75	0
56	MG	13	1608	1/1	0.82	0.24	71,71,71,71	0
56	MG	1G	1665	1/1	0.82	0.15	94,94,94,94	0
56	MG	13	1609	1/1	0.82	0.28	86,86,86,86	0
56	MG	14	3178	1/1	0.82	0.17	80,80,80,80	0
56	MG	14	3276	1/1	0.82	0.34	76,76,76,76	0
58	ZN	C5	202	1/1	0.82	0.12	192,192,192,192	0
56	MG	13	1651	1/1	0.83	0.26	87,87,87,87	0
56	MG	1H	3259	1/1	0.83	0.26	81,81,81,81	0
56	MG	1H	3223	1/1	0.83	0.28	102,102,102,102	0
56	MG	14	3282	1/1	0.83	0.24	86,86,86,86	0
56	MG	13	1715	1/1	0.83	0.29	83,83,83,83	0
56	MG	14	3217	1/1	0.83	0.22	68,68,68,68	0
56	MG	14	3138	1/1	0.83	0.43	79,79,79,79	0
56	MG	14	3222	1/1	0.83	0.18	83,83,83,83	0
56	MG	1H	3233	1/1	0.83	0.33	53,53,53,53	0
56	MG	1H	3345	1/1	0.83	0.31	60,60,60,60	0
56	MG	14	3226	1/1	0.83	0.36	82,82,82,82	0
56	MG	1G	1614	1/1	0.83	0.37	72,72,72,72	0
56	MG	1H	3234	1/1	0.83	0.25	75,75,75,75	0
56	MG	14	3233	1/1	0.83	0.26	61,61,61,61	0
56	MG	14	3097	1/1	0.83	0.46	59,59,59,59	0
56	MG	1H	3327	1/1	0.83	0.49	79,79,79,79	0
56	MG	1H	3178	1/1	0.83	0.27	63,63,63,63	0
56	MG	14	3242	1/1	0.83	0.23	74,74,74,74	0
56	MG	1H	3363	1/1	0.83	0.36	68,68,68,68	0
56	MG	1H	3329	1/1	0.83	0.33	73,73,73,73	0
56	MG	13	1663	1/1	0.83	0.20	88,88,88,88	0
56	MG	14	3260	1/1	0.83	0.35	85,85,85,85	0
56	MG	14	3261	1/1	0.83	0.39	93,93,93,93	0
56	MG	14	3015	1/1	0.83	0.25	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3183	1/1	0.84	0.26	46,46,46,46	0
56	MG	1K	101	1/1	0.84	0.25	75,75,75,75	0
56	MG	1H	3274	1/1	0.84	0.41	80,80,80,80	0
56	MG	1G	1661	1/1	0.84	0.42	73,73,73,73	0
56	MG	1G	1613	1/1	0.84	0.20	87,87,87,87	0
56	MG	1H	3085	1/1	0.84	0.29	66,66,66,66	0
56	MG	14	3210	1/1	0.84	0.29	71,71,71,71	0
56	MG	14	3285	1/1	0.84	0.35	74,74,74,74	0
56	MG	1H	3225	1/1	0.84	0.30	57,57,57,57	0
56	MG	1H	3175	1/1	0.84	0.37	67,67,67,67	0
56	MG	1H	3134	1/1	0.84	0.32	61,61,61,61	0
56	MG	2L	103	1/1	0.84	0.35	89,89,89,89	0
56	MG	2L	104	1/1	0.84	0.17	65,65,65,65	0
56	MG	1H	3101	1/1	0.84	0.21	62,62,62,62	0
56	MG	1H	3294	1/1	0.84	0.26	47,47,47,47	0
56	MG	1H	3139	1/1	0.84	0.13	66,66,66,66	0
56	MG	14	3028	1/1	0.84	0.36	73,73,73,73	0
56	MG	1H	3167	1/1	0.84	0.23	67,67,67,67	0
56	MG	1H	3053	1/1	0.84	0.51	72,72,72,72	0
56	MG	13	1646	1/1	0.84	0.16	95,95,95,95	0
56	MG	1H	3260	1/1	0.84	0.19	72,72,72,72	0
56	MG	1H	3263	1/1	0.84	0.28	76,76,76,76	0
56	MG	14	3081	1/1	0.84	0.43	52,52,52,52	0
56	MG	88	201	1/1	0.84	0.41	78,78,78,78	0
56	MG	14	3170	1/1	0.84	0.37	79,79,79,79	0
56	MG	14	3091	1/1	0.84	0.14	84,84,84,84	0
56	MG	1H	3248	1/1	0.85	0.45	80,80,80,80	0
56	MG	13	1673	1/1	0.85	0.27	73,73,73,73	0
56	MG	14	3239	1/1	0.85	0.21	76,76,76,76	0
56	MG	1H	3330	1/1	0.85	0.36	67,67,67,67	0
56	MG	1H	3037	1/1	0.85	0.24	62,62,62,62	0
56	MG	1G	1670	1/1	0.85	0.30	77,77,77,77	0
56	MG	1H	3258	1/1	0.85	0.22	63,63,63,63	0
56	MG	14	3253	1/1	0.85	0.18	74,74,74,74	0
56	MG	1H	3210	1/1	0.85	0.34	77,77,77,77	0
56	MG	1H	3076	1/1	0.85	0.19	75,75,75,75	0
56	MG	14	3259	1/1	0.85	0.46	82,82,82,82	0
56	MG	14	3007	1/1	0.85	0.23	48,48,48,48	0
56	MG	14	3010	1/1	0.85	0.36	58,58,58,58	0
56	MG	14	3264	1/1	0.85	0.10	67,67,67,67	0
56	MG	1H	3307	1/1	0.85	0.18	80,80,80,80	0
56	MG	14	3153	1/1	0.85	0.23	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3273	1/1	0.85	0.17	73,73,73,73	0
56	MG	14	3159	1/1	0.85	0.44	73,73,73,73	0
56	MG	1H	3221	1/1	0.85	0.30	80,80,80,80	0
56	MG	1H	3269	1/1	0.85	0.12	62,62,62,62	0
56	MG	14	3163	1/1	0.85	0.27	80,80,80,80	0
56	MG	1H	3127	1/1	0.85	0.37	52,52,52,52	0
56	MG	13	1657	1/1	0.85	0.39	69,69,69,69	0
56	MG	1H	3354	1/1	0.85	0.28	89,89,89,89	0
56	MG	14	3179	1/1	0.85	0.34	64,64,64,64	0
56	MG	14	3290	1/1	0.85	0.13	82,82,82,82	0
56	MG	14	3291	1/1	0.85	0.42	55,55,55,55	0
56	MG	14	3180	1/1	0.85	0.36	71,71,71,71	0
56	MG	1G	1634	1/1	0.85	0.29	76,76,76,76	0
56	MG	14	3294	1/1	0.85	0.26	74,74,74,74	0
56	MG	1H	3313	1/1	0.85	0.44	65,65,65,65	0
56	MG	1H	3358	1/1	0.85	0.24	80,80,80,80	0
56	MG	1G	1640	1/1	0.85	0.29	80,80,80,80	0
56	MG	1G	1646	1/1	0.85	0.46	79,79,79,79	0
56	MG	1H	3276	1/1	0.85	0.22	55,55,55,55	0
56	MG	14	3302	1/1	0.85	0.32	72,72,72,72	0
56	MG	13	1621	1/1	0.85	0.24	74,74,74,74	0
56	MG	14	3304	1/1	0.85	0.26	68,68,68,68	0
56	MG	1H	3106	1/1	0.85	0.23	58,58,58,58	0
56	MG	1H	3028	1/1	0.85	0.26	67,67,67,67	0
56	MG	1G	1653	1/1	0.85	0.24	90,90,90,90	0
56	MG	14	3115	1/1	0.85	0.34	88,88,88,88	0
56	MG	39	301	1/1	0.85	0.09	71,71,71,71	0
56	MG	1H	3240	1/1	0.85	0.33	73,73,73,73	0
56	MG	1G	1659	1/1	0.85	0.38	93,93,93,93	0
56	MG	1H	3199	1/1	0.85	0.29	57,57,57,57	0
56	MG	14	3131	1/1	0.85	0.35	70,70,70,70	0
56	MG	1H	3122	1/1	0.86	0.28	49,49,49,49	0
56	MG	13	1746	1/1	0.86	0.25	72,72,72,72	0
56	MG	1H	3151	1/1	0.86	0.19	66,66,66,66	0
56	MG	14	3117	1/1	0.86	0.43	76,76,76,76	0
56	MG	1H	3323	1/1	0.86	0.31	82,82,82,82	0
56	MG	1H	3227	1/1	0.86	0.26	74,74,74,74	0
56	MG	1H	3228	1/1	0.86	0.36	74,74,74,74	0
56	MG	14	3207	1/1	0.86	0.11	81,81,81,81	0
56	MG	14	3209	1/1	0.86	0.15	74,74,74,74	0
56	MG	1G	1629	1/1	0.86	0.44	79,79,79,79	0
56	MG	1G	1633	1/1	0.86	0.40	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	3297	1/1	0.86	0.44	71,71,71,71	0
56	MG	1H	3198	1/1	0.86	0.34	82,82,82,82	0
56	MG	1H	3270	1/1	0.86	0.17	94,94,94,94	0
56	MG	1H	3152	1/1	0.86	0.22	75,75,75,75	0
56	MG	1H	3331	1/1	0.86	0.28	76,76,76,76	0
56	MG	1H	3128	1/1	0.86	0.37	57,57,57,57	0
56	MG	1H	3275	1/1	0.86	0.42	75,75,75,75	0
56	MG	14	3231	1/1	0.86	0.21	74,74,74,74	0
56	MG	1H	3098	1/1	0.86	0.30	87,87,87,87	0
56	MG	1G	1651	1/1	0.86	0.14	84,84,84,84	0
56	MG	13	1678	1/1	0.86	0.28	74,74,74,74	0
56	MG	14	3069	1/1	0.86	0.30	78,78,78,78	0
56	MG	14	3158	1/1	0.86	0.28	67,67,67,67	0
56	MG	1G	1608	1/1	0.86	0.27	88,88,88,88	0
56	MG	14	3087	1/1	0.86	0.34	62,62,62,62	0
56	MG	1H	3338	1/1	0.86	0.22	60,60,60,60	0
56	MG	1H	3339	1/1	0.86	0.24	88,88,88,88	0
56	MG	14	3166	1/1	0.86	0.32	70,70,70,70	0
56	MG	13	1693	1/1	0.86	0.14	65,65,65,65	0
56	MG	14	3098	1/1	0.86	0.26	54,54,54,54	0
56	MG	14	3100	1/1	0.86	0.23	63,63,63,63	0
56	MG	1H	3219	1/1	0.86	0.14	53,53,53,53	0
56	MG	1H	3036	1/1	0.87	0.26	57,57,57,57	0
56	MG	14	3009	1/1	0.87	0.25	51,51,51,51	0
56	MG	13	1686	1/1	0.87	0.28	69,69,69,69	0
56	MG	1G	1620	1/1	0.87	0.30	78,78,78,78	0
56	MG	1H	3120	1/1	0.87	0.24	60,60,60,60	0
56	MG	13	1743	1/1	0.87	0.14	102,102,102,102	0
56	MG	14	3026	1/1	0.87	0.27	65,65,65,65	0
56	MG	1H	3305	1/1	0.87	0.25	75,75,75,75	0
56	MG	13	1610	1/1	0.87	0.38	72,72,72,72	0
56	MG	14	3031	1/1	0.87	0.32	60,60,60,60	0
56	MG	13	1643	1/1	0.87	0.25	80,80,80,80	0
56	MG	14	3269	1/1	0.87	0.23	59,59,59,59	0
56	MG	14	3272	1/1	0.87	0.36	82,82,82,82	0
56	MG	13	1648	1/1	0.87	0.32	69,69,69,69	0
56	MG	14	3043	1/1	0.87	0.23	67,67,67,67	0
56	MG	1H	3183	1/1	0.87	0.15	66,66,66,66	0
56	MG	14	3280	1/1	0.87	0.41	87,87,87,87	0
56	MG	14	3281	1/1	0.87	0.19	73,73,73,73	0
56	MG	1H	3074	1/1	0.87	0.18	70,70,70,70	0
56	MG	13	1681	1/1	0.87	0.36	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3080	1/1	0.87	0.14	69,69,69,69	0
56	MG	1G	1641	1/1	0.87	0.18	73,73,73,73	0
56	MG	1G	1642	1/1	0.87	0.37	81,81,81,81	0
56	MG	14	3191	1/1	0.87	0.15	57,57,57,57	0
56	MG	1G	1643	1/1	0.87	0.35	88,88,88,88	0
56	MG	1H	3196	1/1	0.87	0.31	68,68,68,68	0
56	MG	1H	3138	1/1	0.87	0.46	66,66,66,66	0
56	MG	13	1697	1/1	0.87	0.28	82,82,82,82	0
56	MG	13	1698	1/1	0.87	0.17	74,74,74,74	0
56	MG	1H	3089	1/1	0.87	0.29	45,45,45,45	0
56	MG	16	208	1/1	0.87	0.34	66,66,66,66	0
56	MG	1H	3093	1/1	0.87	0.15	47,47,47,47	0
56	MG	14	3106	1/1	0.87	0.21	50,50,50,50	0
56	MG	1H	3097	1/1	0.87	0.16	67,67,67,67	0
56	MG	1H	3016	1/1	0.87	0.23	45,45,45,45	0
56	MG	1G	1602	1/1	0.87	0.24	64,64,64,64	0
56	MG	1H	3099	1/1	0.87	0.27	53,53,53,53	0
56	MG	14	3124	1/1	0.87	0.26	63,63,63,63	0
56	MG	1H	3222	1/1	0.87	0.28	80,80,80,80	0
56	MG	1J	202	1/1	0.87	0.40	73,73,73,73	0
56	MG	14	3130	1/1	0.87	0.25	71,71,71,71	0
56	MG	1H	3025	1/1	0.87	0.36	53,53,53,53	0
56	MG	1G	1612	1/1	0.87	0.17	63,63,63,63	0
56	MG	1H	3224	1/1	0.87	0.19	61,61,61,61	0
56	MG	13	1672	1/1	0.87	0.22	91,91,91,91	0
56	MG	13	1717	1/1	0.87	0.18	74,74,74,74	0
56	MG	1H	3110	1/1	0.87	0.13	57,57,57,57	0
56	MG	1H	3008	1/1	0.88	0.20	42,42,42,42	0
56	MG	13	1668	1/1	0.88	0.23	76,76,76,76	0
56	MG	1H	3078	1/1	0.88	0.22	63,63,63,63	0
56	MG	1H	3177	1/1	0.88	0.32	55,55,55,55	0
56	MG	1H	3080	1/1	0.88	0.24	53,53,53,53	0
56	MG	14	3248	1/1	0.88	0.34	76,76,76,76	0
56	MG	14	3014	1/1	0.88	0.28	58,58,58,58	0
56	MG	1H	3347	1/1	0.88	0.35	85,85,85,85	0
56	MG	13	1682	1/1	0.88	0.24	86,86,86,86	0
56	MG	1G	1632	1/1	0.88	0.30	70,70,70,70	0
56	MG	13	1669	1/1	0.88	0.14	76,76,76,76	0
56	MG	1H	3249	1/1	0.88	0.28	85,85,85,85	0
56	MG	1H	3137	1/1	0.88	0.30	49,49,49,49	0
56	MG	1H	3092	1/1	0.88	0.18	50,50,50,50	0
56	MG	1H	3194	1/1	0.88	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3035	1/1	0.88	0.10	54,54,54,54	0
56	MG	1H	3461	1/1	0.88	0.10	108,108,108,108	0
56	MG	13	1622	1/1	0.88	0.28	79,79,79,79	0
56	MG	1H	3035	1/1	0.88	0.32	61,61,61,61	0
56	MG	14	3275	1/1	0.88	0.17	60,60,60,60	0
56	MG	14	3055	1/1	0.88	0.12	64,64,64,64	0
56	MG	13	1632	1/1	0.88	0.30	63,63,63,63	0
56	MG	14	3279	1/1	0.88	0.12	60,60,60,60	0
56	MG	13	1747	1/1	0.88	0.14	64,64,64,64	0
56	MG	14	3078	1/1	0.88	0.32	50,50,50,50	0
56	MG	13	1709	1/1	0.88	0.36	89,89,89,89	0
56	MG	14	3177	1/1	0.88	0.41	72,72,72,72	0
56	MG	13	1644	1/1	0.88	0.41	76,76,76,76	0
56	MG	1H	3213	1/1	0.88	0.24	77,77,77,77	0
56	MG	1H	3050	1/1	0.88	0.24	36,36,36,36	0
56	MG	14	3182	1/1	0.88	0.22	72,72,72,72	0
56	MG	1G	1601	1/1	0.88	0.25	65,65,65,65	0
56	MG	14	3188	1/1	0.88	0.13	56,56,56,56	0
56	MG	14	3094	1/1	0.88	0.24	69,69,69,69	0
56	MG	14	3096	1/1	0.88	0.37	78,78,78,78	0
56	MG	14	3195	1/1	0.88	0.36	65,65,65,65	0
56	MG	1H	3157	1/1	0.88	0.30	72,72,72,72	0
56	MG	1G	1657	1/1	0.88	0.09	126,126,126,126	0
56	MG	1H	3279	1/1	0.88	0.17	73,73,73,73	0
56	MG	13	1645	1/1	0.88	0.22	79,79,79,79	0
56	MG	1G	1663	1/1	0.88	0.07	75,75,75,75	0
56	MG	13	1677	1/1	0.88	0.13	71,71,71,71	0
56	MG	1H	3115	1/1	0.88	0.20	51,51,51,51	0
56	MG	14	3108	1/1	0.88	0.14	76,76,76,76	0
56	MG	14	3109	1/1	0.88	0.13	78,78,78,78	0
56	MG	14	3345	1/1	0.88	0.12	81,81,81,81	0
56	MG	14	3110	1/1	0.88	0.42	64,64,64,64	0
56	MG	14	3112	1/1	0.88	0.16	65,65,65,65	0
56	MG	1H	3284	1/1	0.88	0.09	62,62,62,62	0
56	MG	1H	3116	1/1	0.88	0.17	62,62,62,62	0
56	MG	1H	3059	1/1	0.88	0.12	68,68,68,68	0
56	MG	14	3120	1/1	0.88	0.28	75,75,75,75	0
56	MG	1G	1675	1/1	0.88	0.08	110,110,110,110	0
56	MG	14	3232	1/1	0.88	0.18	62,62,62,62	0
56	MG	13	1634	1/1	0.88	0.34	74,74,74,74	0
56	MG	1H	3236	1/1	0.89	0.35	68,68,68,68	0
56	MG	1H	3239	1/1	0.89	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1H	3298	1/1	0.89	0.23	79,79,79,79	0
56	MG	1H	3058	1/1	0.89	0.21	61,61,61,61	0
56	MG	14	3244	1/1	0.89	0.20	65,65,65,65	0
56	MG	14	3033	1/1	0.89	0.27	64,64,64,64	0
56	MG	14	3249	1/1	0.89	0.32	77,77,77,77	0
56	MG	14	3142	1/1	0.89	0.36	59,59,59,59	0
56	MG	14	3144	1/1	0.89	0.39	79,79,79,79	0
56	MG	1H	3241	1/1	0.89	0.23	65,65,65,65	0
56	MG	14	3255	1/1	0.89	0.12	65,65,65,65	0
56	MG	14	3146	1/1	0.89	0.40	69,69,69,69	0
56	MG	1H	3021	1/1	0.89	0.23	45,45,45,45	0
56	MG	1H	3073	1/1	0.89	0.27	63,63,63,63	0
56	MG	1H	3195	1/1	0.89	0.23	65,65,65,65	0
56	MG	1H	3431	1/1	0.89	0.15	99,99,99,99	0
56	MG	1H	3250	1/1	0.89	0.17	68,68,68,68	0
56	MG	13	1614	1/1	0.89	0.17	79,79,79,79	0
56	MG	1H	3255	1/1	0.89	0.27	76,76,76,76	0
56	MG	1H	3197	1/1	0.89	0.32	66,66,66,66	0
56	MG	1H	3154	1/1	0.89	0.38	74,74,74,74	0
56	MG	13	1606	1/1	0.89	0.19	63,63,63,63	0
56	MG	14	3082	1/1	0.89	0.29	67,67,67,67	0
56	MG	14	3169	1/1	0.89	0.31	77,77,77,77	0
56	MG	13	1601	1/1	0.89	0.25	46,46,46,46	0
56	MG	14	3171	1/1	0.89	0.28	80,80,80,80	0
56	MG	14	3173	1/1	0.89	0.27	62,62,62,62	0
56	MG	14	3088	1/1	0.89	0.33	71,71,71,71	0
56	MG	1H	3206	1/1	0.89	0.32	63,63,63,63	0
56	MG	13	1699	1/1	0.89	0.15	75,75,75,75	0
56	MG	14	3092	1/1	0.89	0.31	41,41,41,41	0
56	MG	13	1700	1/1	0.89	0.31	71,71,71,71	0
56	MG	14	3288	1/1	0.89	0.40	74,74,74,74	0
56	MG	1H	3272	1/1	0.89	0.35	69,69,69,69	0
56	MG	1G	1662	1/1	0.89	0.16	73,73,73,73	0
56	MG	14	3190	1/1	0.89	0.27	85,85,85,85	0
56	MG	1H	3162	1/1	0.89	0.33	68,68,68,68	0
56	MG	13	1702	1/1	0.89	0.18	62,62,62,62	0
56	MG	1G	1609	1/1	0.89	0.49	81,81,81,81	0
56	MG	1H	3125	1/1	0.89	0.19	49,49,49,49	0
56	MG	1H	3038	1/1	0.89	0.23	55,55,55,55	0
56	MG	13	1653	1/1	0.89	0.12	75,75,75,75	0
56	MG	13	1636	1/1	0.89	0.37	66,66,66,66	0
56	MG	2L	101	1/1	0.89	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3046	1/1	0.89	0.32	67,67,67,67	0
56	MG	1H	3005	1/1	0.89	0.24	53,53,53,53	0
56	MG	1H	3051	1/1	0.89	0.18	65,65,65,65	0
56	MG	13	1718	1/1	0.89	0.08	90,90,90,90	0
56	MG	1H	3179	1/1	0.89	0.23	55,55,55,55	0
56	MG	14	3119	1/1	0.89	0.37	69,69,69,69	0
56	MG	1H	3341	1/1	0.89	0.25	67,67,67,67	0
56	MG	1H	3147	1/1	0.89	0.35	68,68,68,68	0
56	MG	13	1602	1/1	0.89	0.14	66,66,66,66	0
56	MG	14	3016	1/1	0.89	0.35	54,54,54,54	0
56	MG	14	3019	1/1	0.89	0.20	74,74,74,74	0
56	MG	1H	3344	1/1	0.89	0.37	87,87,87,87	0
56	MG	14	3024	1/1	0.89	0.35	74,74,74,74	0
56	MG	1G	1631	1/1	0.89	0.28	86,86,86,86	0
56	MG	1G	1658	1/1	0.90	0.40	79,79,79,79	0
56	MG	14	3199	1/1	0.90	0.15	69,69,69,69	0
56	MG	14	3201	1/1	0.90	0.27	72,72,72,72	0
56	MG	14	3274	1/1	0.90	0.13	82,82,82,82	0
56	MG	13	1704	1/1	0.90	0.17	80,80,80,80	0
56	MG	1H	3082	1/1	0.90	0.29	70,70,70,70	0
56	MG	1H	3211	1/1	0.90	0.17	64,64,64,64	0
56	MG	1H	3104	1/1	0.90	0.29	41,41,41,41	0
56	MG	14	3213	1/1	0.90	0.27	85,85,85,85	0
56	MG	P8	101	1/1	0.90	0.19	68,68,68,68	0
56	MG	1H	3215	1/1	0.90	0.15	85,85,85,85	0
56	MG	1H	3142	1/1	0.90	0.21	39,39,39,39	0
56	MG	14	3107	1/1	0.90	0.13	40,40,40,40	0
56	MG	14	3155	1/1	0.90	0.39	75,75,75,75	0
56	MG	1H	3146	1/1	0.90	0.31	75,75,75,75	0
56	MG	1H	3350	1/1	0.90	0.19	67,67,67,67	0
56	MG	13	1667	1/1	0.90	0.15	92,92,92,92	0
56	MG	13	1706	1/1	0.90	0.20	79,79,79,79	0
56	MG	14	3052	1/1	0.90	0.29	62,62,62,62	0
56	MG	14	3116	1/1	0.90	0.27	56,56,56,56	0
56	MG	13	1689	1/1	0.90	0.42	120,120,120,120	0
56	MG	14	3063	1/1	0.90	0.18	66,66,66,66	0
56	MG	14	3296	1/1	0.90	0.23	74,74,74,74	0
56	MG	1H	3359	1/1	0.90	0.43	84,84,84,84	0
56	MG	1H	3042	1/1	0.90	0.29	74,74,74,74	0
56	MG	14	3121	1/1	0.90	0.18	58,58,58,58	0
56	MG	1H	3416	1/1	0.90	0.09	77,77,77,77	0
56	MG	14	3245	1/1	0.90	0.36	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3132	1/1	0.90	0.23	45,45,45,45	0
56	MG	1H	3226	1/1	0.90	0.27	69,69,69,69	0
56	MG	14	3250	1/1	0.90	0.27	74,74,74,74	0
56	MG	14	3129	1/1	0.90	0.15	63,63,63,63	0
56	MG	14	3012	1/1	0.90	0.21	77,77,77,77	0
56	MG	14	3083	1/1	0.90	0.19	60,60,60,60	0
56	MG	14	3184	1/1	0.90	0.24	53,53,53,53	0
56	MG	14	3013	1/1	0.90	0.23	54,54,54,54	0
56	MG	1H	3337	1/1	0.90	0.19	94,94,94,94	0
56	MG	1J	205	1/1	0.90	0.11	82,82,82,82	0
56	MG	14	3134	1/1	0.90	0.29	64,64,64,64	0
56	MG	1H	3133	1/1	0.90	0.27	60,60,60,60	0
56	MG	1H	3077	1/1	0.90	0.24	73,73,73,73	0
56	MG	1G	1656	1/1	0.90	0.28	72,72,72,72	0
56	MG	13	1620	1/1	0.90	0.22	51,51,51,51	0
56	MG	14	3251	1/1	0.91	0.15	48,48,48,48	0
56	MG	1H	3083	1/1	0.91	0.24	69,69,69,69	0
56	MG	1H	3048	1/1	0.91	0.16	48,48,48,48	0
56	MG	1H	3218	1/1	0.91	0.14	61,61,61,61	0
56	MG	1H	3023	1/1	0.91	0.18	51,51,51,51	0
56	MG	1H	3366	1/1	0.91	0.17	74,74,74,74	0
56	MG	14	3176	1/1	0.91	0.19	81,81,81,81	0
56	MG	1H	3319	1/1	0.91	0.39	92,92,92,92	0
56	MG	1H	3024	1/1	0.91	0.27	46,46,46,46	0
56	MG	1H	3180	1/1	0.91	0.16	59,59,59,59	0
56	MG	1H	3480	1/1	0.91	0.22	56,56,56,56	0
56	MG	13	1676	1/1	0.91	0.17	62,62,62,62	0
56	MG	13	1658	1/1	0.91	0.34	70,70,70,70	0
56	MG	14	3270	1/1	0.91	0.22	56,56,56,56	0
56	MG	14	3271	1/1	0.91	0.32	87,87,87,87	0
56	MG	16	203	1/1	0.91	0.20	68,68,68,68	0
56	MG	1H	3030	1/1	0.91	0.25	81,81,81,81	0
56	MG	13	1659	1/1	0.91	0.25	66,66,66,66	0
56	MG	14	3030	1/1	0.91	0.15	55,55,55,55	0
56	MG	1H	3190	1/1	0.91	0.10	67,67,67,67	0
56	MG	1H	3192	1/1	0.91	0.20	72,72,72,72	0
56	MG	11	301	1/1	0.91	0.09	48,48,48,48	0
56	MG	21	301	1/1	0.91	0.18	53,53,53,53	0
56	MG	14	3036	1/1	0.91	0.20	42,42,42,42	0
56	MG	1H	3193	1/1	0.91	0.17	69,69,69,69	0
56	MG	14	3200	1/1	0.91	0.18	66,66,66,66	0
56	MG	2K	103	1/1	0.91	0.39	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1627	1/1	0.91	0.15	62,62,62,62	0
56	MG	1H	3160	1/1	0.91	0.27	56,56,56,56	0
56	MG	14	3208	1/1	0.91	0.08	68,68,68,68	0
56	MG	1H	3237	1/1	0.91	0.32	57,57,57,57	0
56	MG	1G	1603	1/1	0.91	0.20	76,76,76,76	0
56	MG	14	3211	1/1	0.91	0.11	67,67,67,67	0
56	MG	1G	1604	1/1	0.91	0.12	77,77,77,77	0
56	MG	14	3214	1/1	0.91	0.12	65,65,65,65	0
56	MG	1G	1660	1/1	0.91	0.17	74,74,74,74	0
56	MG	14	3076	1/1	0.91	0.14	54,54,54,54	0
56	MG	1H	3161	1/1	0.91	0.18	55,55,55,55	0
56	MG	13	1711	1/1	0.91	0.21	79,79,79,79	0
56	MG	13	1661	1/1	0.91	0.30	54,54,54,54	0
56	MG	1H	3243	1/1	0.91	0.19	69,69,69,69	0
56	MG	1G	1611	1/1	0.91	0.17	72,72,72,72	0
56	MG	14	3085	1/1	0.91	0.29	50,50,50,50	0
56	MG	14	3229	1/1	0.91	0.26	65,65,65,65	0
56	MG	1H	3245	1/1	0.91	0.17	58,58,58,58	0
56	MG	1H	3015	1/1	0.91	0.21	59,59,59,59	0
56	MG	14	3151	1/1	0.91	0.22	72,72,72,72	0
56	MG	1H	3202	1/1	0.91	0.25	66,66,66,66	0
56	MG	13	1642	1/1	0.91	0.41	72,72,72,72	0
56	MG	14	3156	1/1	0.91	0.20	60,60,60,60	0
56	MG	14	3157	1/1	0.91	0.21	88,88,88,88	0
56	MG	1H	3113	1/1	0.91	0.13	41,41,41,41	0
56	MG	1H	3018	1/1	0.91	0.19	52,52,52,52	0
56	MG	13	1633	1/1	0.91	0.24	77,77,77,77	0
56	MG	85	201	1/1	0.91	0.45	69,69,69,69	0
56	MG	1H	3173	1/1	0.91	0.35	52,52,52,52	0
56	MG	14	3006	1/1	0.91	0.17	48,48,48,48	0
56	MG	1H	3214	1/1	0.91	0.32	68,68,68,68	0
56	MG	13	1683	1/1	0.92	0.12	69,69,69,69	0
56	MG	1H	3045	1/1	0.92	0.51	66,66,66,66	0
56	MG	1H	3118	1/1	0.92	0.38	52,52,52,52	0
56	MG	13	1628	1/1	0.92	0.14	48,48,48,48	0
56	MG	13	1638	1/1	0.92	0.17	53,53,53,53	0
56	MG	1H	3084	1/1	0.92	0.40	48,48,48,48	0
56	MG	1H	3242	1/1	0.92	0.15	58,58,58,58	0
56	MG	14	3257	1/1	0.92	0.20	79,79,79,79	0
56	MG	1G	1623	1/1	0.92	0.37	73,73,73,73	0
56	MG	1H	3123	1/1	0.92	0.14	52,52,52,52	0
56	MG	14	3008	1/1	0.92	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3175	1/1	0.92	0.22	56,56,56,56	0
56	MG	1H	3124	1/1	0.92	0.18	52,52,52,52	0
56	MG	13	1655	1/1	0.92	0.23	73,73,73,73	0
56	MG	1H	3360	1/1	0.92	0.36	73,73,73,73	0
56	MG	1H	3361	1/1	0.92	0.16	53,53,53,53	0
56	MG	1H	3247	1/1	0.92	0.40	64,64,64,64	0
56	MG	1H	3204	1/1	0.92	0.39	59,59,59,59	0
56	MG	13	1625	1/1	0.92	0.28	45,45,45,45	0
56	MG	14	3018	1/1	0.92	0.13	68,68,68,68	0
56	MG	14	3111	1/1	0.92	0.22	55,55,55,55	0
56	MG	14	3189	1/1	0.92	0.17	60,60,60,60	0
56	MG	2K	105	1/1	0.92	0.35	78,78,78,78	0
56	MG	1H	3208	1/1	0.92	0.55	78,78,78,78	0
56	MG	14	3023	1/1	0.92	0.29	40,40,40,40	0
56	MG	1H	3129	1/1	0.92	0.09	68,68,68,68	0
56	MG	1H	3054	1/1	0.92	0.17	59,59,59,59	0
56	MG	13	1742	1/1	0.92	0.06	115,115,115,115	0
56	MG	14	3027	1/1	0.92	0.20	70,70,70,70	0
56	MG	1H	3057	1/1	0.92	0.47	57,57,57,57	0
56	MG	1G	1644	1/1	0.92	0.25	70,70,70,70	0
56	MG	14	3286	1/1	0.92	0.35	78,78,78,78	0
56	MG	1H	3034	1/1	0.92	0.22	51,51,51,51	0
56	MG	1H	3216	1/1	0.92	0.23	67,67,67,67	0
56	MG	1H	3266	1/1	0.92	0.14	64,64,64,64	0
56	MG	1H	3174	1/1	0.92	0.30	63,63,63,63	0
56	MG	1H	3100	1/1	0.92	0.18	43,43,43,43	0
56	MG	1H	3176	1/1	0.92	0.24	60,60,60,60	0
56	MG	1H	3220	1/1	0.92	0.30	50,50,50,50	0
56	MG	1H	3007	1/1	0.92	0.22	46,46,46,46	0
56	MG	14	3047	1/1	0.92	0.22	60,60,60,60	0
56	MG	1G	1655	1/1	0.92	0.40	79,79,79,79	0
56	MG	1H	3064	1/1	0.92	0.44	56,56,56,56	0
56	MG	1H	3140	1/1	0.92	0.43	63,63,63,63	0
56	MG	14	3058	1/1	0.92	0.22	61,61,61,61	0
56	MG	14	3141	1/1	0.92	0.15	76,76,76,76	0
56	MG	1H	3334	1/1	0.92	0.17	60,60,60,60	0
56	MG	14	3143	1/1	0.92	0.09	67,67,67,67	0
56	MG	14	3065	1/1	0.92	0.19	46,46,46,46	0
56	MG	14	3067	1/1	0.92	0.14	48,48,48,48	0
56	MG	14	3306	1/1	0.92	0.24	69,69,69,69	0
56	MG	1H	3105	1/1	0.92	0.24	56,56,56,56	0
56	MG	14	3391	1/1	0.92	0.32	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3067	1/1	0.92	0.17	49,49,49,49	0
56	MG	13	1701	1/1	0.92	0.21	80,80,80,80	0
56	MG	14	3234	1/1	0.92	0.25	68,68,68,68	0
56	MG	1H	3012	1/1	0.92	0.30	45,45,45,45	0
56	MG	13	1662	1/1	0.92	0.20	73,73,73,73	0
56	MG	29	303	1/1	0.92	0.36	71,71,71,71	0
56	MG	1H	3288	1/1	0.92	0.08	54,54,54,54	0
56	MG	14	3154	1/1	0.92	0.18	82,82,82,82	0
56	MG	13	1613	1/1	0.92	0.23	71,71,71,71	0
56	MG	1G	1666	1/1	0.92	0.26	74,74,74,74	0
56	MG	14	3084	1/1	0.92	0.20	43,43,43,43	0
56	MG	13	1695	1/1	0.92	0.07	79,79,79,79	0
56	MG	1H	3386	1/1	0.93	0.08	53,53,53,53	0
56	MG	1H	3094	1/1	0.93	0.20	41,41,41,41	0
56	MG	14	3246	1/1	0.93	0.21	66,66,66,66	0
56	MG	14	3247	1/1	0.93	0.17	67,67,67,67	0
56	MG	1H	3062	1/1	0.93	0.29	65,65,65,65	0
56	MG	1G	1630	1/1	0.93	0.10	75,75,75,75	0
56	MG	1H	3063	1/1	0.93	0.31	65,65,65,65	0
56	MG	1H	3244	1/1	0.93	0.16	39,39,39,39	0
56	MG	13	1675	1/1	0.93	0.19	73,73,73,73	0
56	MG	14	3167	1/1	0.93	0.19	59,59,59,59	0
56	MG	13	1666	1/1	0.93	0.23	58,58,58,58	0
56	MG	1H	3289	1/1	0.93	0.07	62,62,62,62	0
56	MG	1H	3068	1/1	0.93	0.23	67,67,67,67	0
56	MG	1G	1638	1/1	0.93	0.21	75,75,75,75	0
56	MG	1H	3291	1/1	0.93	0.15	40,40,40,40	0
56	MG	14	3020	1/1	0.93	0.13	68,68,68,68	0
56	MG	14	3021	1/1	0.93	0.22	55,55,55,55	0
56	MG	16	207	1/1	0.93	0.20	71,71,71,71	0
56	MG	13	1618	1/1	0.93	0.10	58,58,58,58	0
56	MG	14	3266	1/1	0.93	0.14	68,68,68,68	0
56	MG	16	209	1/1	0.93	0.28	56,56,56,56	0
56	MG	1H	3027	1/1	0.93	0.25	32,32,32,32	0
56	MG	16	211	1/1	0.93	0.07	85,85,85,85	0
56	MG	1H	3047	1/1	0.93	0.27	70,70,70,70	0
56	MG	1H	3251	1/1	0.93	0.09	61,61,61,61	0
56	MG	14	3185	1/1	0.93	0.18	52,52,52,52	0
56	MG	14	3186	1/1	0.93	0.29	54,54,54,54	0
56	MG	31	301	1/1	0.93	0.06	56,56,56,56	0
56	MG	1H	3107	1/1	0.93	0.27	65,65,65,65	0
56	MG	78	201	1/1	0.93	0.33	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	5E	201	1/1	0.93	0.08	70,70,70,70	0
56	MG	1H	3049	1/1	0.93	0.19	60,60,60,60	0
56	MG	1H	3010	1/1	0.93	0.20	54,54,54,54	0
56	MG	1H	3301	1/1	0.93	0.14	79,79,79,79	0
56	MG	14	3123	1/1	0.93	0.28	60,60,60,60	0
56	MG	14	3037	1/1	0.93	0.41	61,61,61,61	0
56	MG	14	3125	1/1	0.93	0.30	53,53,53,53	0
56	MG	13	1612	1/1	0.93	0.09	63,63,63,63	0
56	MG	14	3128	1/1	0.93	0.32	58,58,58,58	0
56	MG	1H	3013	1/1	0.93	0.16	31,31,31,31	0
56	MG	14	3205	1/1	0.93	0.43	71,71,71,71	0
56	MG	14	3044	1/1	0.93	0.15	53,53,53,53	0
56	MG	1H	3144	1/1	0.93	0.30	66,66,66,66	0
56	MG	1H	3264	1/1	0.93	0.15	58,58,58,58	0
56	MG	14	3051	1/1	0.93	0.25	78,78,78,78	0
56	MG	1H	3265	1/1	0.93	0.15	54,54,54,54	0
56	MG	14	3212	1/1	0.93	0.19	65,65,65,65	0
56	MG	1H	3014	1/1	0.93	0.23	43,43,43,43	0
56	MG	1H	3353	1/1	0.93	0.27	73,73,73,73	0
56	MG	14	3137	1/1	0.93	0.47	69,69,69,69	0
56	MG	13	1687	1/1	0.93	0.13	70,70,70,70	0
56	MG	14	3064	1/1	0.93	0.16	71,71,71,71	0
56	MG	14	3223	1/1	0.93	0.06	62,62,62,62	0
56	MG	13	1741	1/1	0.93	0.07	110,110,110,110	0
56	MG	13	1679	1/1	0.93	0.17	77,77,77,77	0
56	MG	1H	3209	1/1	0.93	0.35	77,77,77,77	0
56	MG	1H	3238	1/1	0.93	0.34	54,54,54,54	0
56	MG	14	3307	1/1	0.93	0.42	60,60,60,60	0
56	MG	14	3339	1/1	0.93	0.13	94,94,94,94	0
56	MG	14	3072	1/1	0.93	0.19	45,45,45,45	0
56	MG	14	3353	1/1	0.93	0.08	83,83,83,83	0
56	MG	14	3372	1/1	0.93	0.14	84,84,84,84	0
56	MG	14	3376	1/1	0.93	0.09	87,87,87,87	0
56	MG	14	3074	1/1	0.93	0.20	66,66,66,66	0
56	MG	1H	3321	1/1	0.93	0.32	86,86,86,86	0
56	MG	13	1604	1/1	0.93	0.12	68,68,68,68	0
56	MG	1G	1684	1/1	0.93	0.13	122,122,122,122	0
56	MG	1H	3365	1/1	0.93	0.28	64,64,64,64	0
56	MG	1G	1622	1/1	0.93	0.10	72,72,72,72	0
56	MG	14	3236	1/1	0.93	0.14	75,75,75,75	0
56	MG	14	3237	1/1	0.93	0.11	54,54,54,54	0
56	MG	14	3238	1/1	0.93	0.26	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3060	1/1	0.93	0.14	74,74,74,74	0
56	MG	1H	3368	1/1	0.93	0.25	74,74,74,74	0
56	MG	14	3004	1/1	0.93	0.16	46,46,46,46	0
56	MG	14	3086	1/1	0.93	0.20	65,65,65,65	0
56	MG	1H	3091	1/1	0.94	0.14	55,55,55,55	0
56	MG	1H	3165	1/1	0.94	0.16	61,61,61,61	0
56	MG	13	1619	1/1	0.94	0.12	64,64,64,64	0
56	MG	14	3113	1/1	0.94	0.17	42,42,42,42	0
56	MG	14	3114	1/1	0.94	0.20	44,44,44,44	0
56	MG	1H	3070	1/1	0.94	0.12	46,46,46,46	0
56	MG	1H	3292	1/1	0.94	0.21	60,60,60,60	0
56	MG	1H	3256	1/1	0.94	0.34	57,57,57,57	0
56	MG	1H	3405	1/1	0.94	0.15	61,61,61,61	0
56	MG	14	3262	1/1	0.94	0.09	66,66,66,66	0
56	MG	14	3039	1/1	0.94	0.21	38,38,38,38	0
56	MG	14	3040	1/1	0.94	0.27	43,43,43,43	0
56	MG	1H	3141	1/1	0.94	0.32	60,60,60,60	0
56	MG	1H	3200	1/1	0.94	0.12	59,59,59,59	0
56	MG	14	3193	1/1	0.94	0.19	59,59,59,59	0
56	MG	1H	3444	1/1	0.94	0.08	59,59,59,59	0
56	MG	14	3045	1/1	0.94	0.21	57,57,57,57	0
56	MG	1G	1617	1/1	0.94	0.07	80,80,80,80	0
56	MG	1H	3454	1/1	0.94	0.11	98,98,98,98	0
56	MG	14	3049	1/1	0.94	0.30	54,54,54,54	0
56	MG	14	3050	1/1	0.94	0.17	63,63,63,63	0
56	MG	13	1639	1/1	0.94	0.18	56,56,56,56	0
56	MG	14	3202	1/1	0.94	0.10	55,55,55,55	0
56	MG	1G	1667	1/1	0.94	0.17	80,80,80,80	0
56	MG	14	3204	1/1	0.94	0.15	51,51,51,51	0
56	MG	1H	3477	1/1	0.94	0.08	106,106,106,106	0
56	MG	14	3206	1/1	0.94	0.22	48,48,48,48	0
56	MG	1G	1621	1/1	0.94	0.24	81,81,81,81	0
56	MG	14	3060	1/1	0.94	0.14	48,48,48,48	0
56	MG	1H	3119	1/1	0.94	0.25	52,52,52,52	0
56	MG	1H	3145	1/1	0.94	0.21	49,49,49,49	0
56	MG	1G	1680	1/1	0.94	0.12	94,94,94,94	0
56	MG	1G	1624	1/1	0.94	0.23	63,63,63,63	0
56	MG	1G	1685	1/1	0.94	0.07	111,111,111,111	0
56	MG	1G	1687	1/1	0.94	0.18	81,81,81,81	0
56	MG	14	3215	1/1	0.94	0.16	50,50,50,50	0
56	MG	1H	3006	1/1	0.94	0.21	49,49,49,49	0
56	MG	13	1691	1/1	0.94	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3221	1/1	0.94	0.11	58,58,58,58	0
56	MG	14	3295	1/1	0.94	0.10	64,64,64,64	0
56	MG	13	1684	1/1	0.94	0.27	62,62,62,62	0
56	MG	1H	3304	1/1	0.94	0.20	69,69,69,69	0
56	MG	14	3003	1/1	0.94	0.20	54,54,54,54	0
56	MG	16	206	1/1	0.94	0.42	60,60,60,60	0
56	MG	1H	3340	1/1	0.94	0.15	74,74,74,74	0
56	MG	1H	3026	1/1	0.94	0.17	53,53,53,53	0
56	MG	3I	201	1/1	0.94	0.17	58,58,58,58	0
56	MG	1H	3102	1/1	0.94	0.13	60,60,60,60	0
56	MG	14	3230	1/1	0.94	0.19	73,73,73,73	0
56	MG	1H	3079	1/1	0.94	0.21	45,45,45,45	0
56	MG	13	1650	1/1	0.94	0.17	68,68,68,68	0
56	MG	1G	1637	1/1	0.94	0.15	81,81,81,81	0
56	MG	11	302	1/1	0.94	0.16	42,42,42,42	0
56	MG	1G	1639	1/1	0.94	0.23	85,85,85,85	0
56	MG	1H	3081	1/1	0.94	0.18	61,61,61,61	0
56	MG	1H	3130	1/1	0.94	0.07	54,54,54,54	0
56	MG	13	1720	1/1	0.94	0.08	62,62,62,62	0
56	MG	13	1605	1/1	0.94	0.21	67,67,67,67	0
56	MG	1H	3281	1/1	0.94	0.09	74,74,74,74	0
56	MG	L8	101	1/1	0.94	0.09	70,70,70,70	0
56	MG	1H	3317	1/1	0.94	0.30	61,61,61,61	0
56	MG	14	3243	1/1	0.94	0.20	72,72,72,72	0
56	MG	13	1630	1/1	0.94	0.15	43,43,43,43	0
56	MG	14	3103	1/1	0.94	0.15	67,67,67,67	0
56	MG	1G	1649	1/1	0.94	0.17	72,72,72,72	0
56	MG	14	3105	1/1	0.94	0.18	47,47,47,47	0
56	MG	1H	3066	1/1	0.94	0.10	67,67,67,67	0
56	MG	13	1688	1/1	0.94	0.21	77,77,77,77	0
56	MG	L5	101	1/1	0.94	0.13	73,73,73,73	0
56	MG	1H	3287	1/1	0.94	0.17	50,50,50,50	0
56	MG	1G	1606	1/1	0.94	0.30	79,79,79,79	0
56	MG	13	1728	1/1	0.95	0.07	85,85,85,85	0
56	MG	1G	1679	1/1	0.95	0.09	90,90,90,90	0
56	MG	1H	3465	1/1	0.95	0.10	94,94,94,94	0
56	MG	1G	1681	1/1	0.95	0.08	110,110,110,110	0
56	MG	1H	3468	1/1	0.95	0.10	71,71,71,71	0
56	MG	14	3054	1/1	0.95	0.44	74,74,74,74	0
56	MG	14	3263	1/1	0.95	0.24	71,71,71,71	0
56	MG	1H	3040	1/1	0.95	0.09	49,49,49,49	0
56	MG	14	3056	1/1	0.95	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3126	1/1	0.95	0.24	66,66,66,66	0
56	MG	14	3057	1/1	0.95	0.20	68,68,68,68	0
56	MG	13	1730	1/1	0.95	0.07	86,86,86,86	0
56	MG	1H	3166	1/1	0.95	0.20	72,72,72,72	0
56	MG	1H	3143	1/1	0.95	0.08	49,49,49,49	0
56	MG	13	1692	1/1	0.95	0.11	79,79,79,79	0
56	MG	13	1680	1/1	0.95	0.30	69,69,69,69	0
56	MG	13	1624	1/1	0.95	0.25	48,48,48,48	0
56	MG	1H	3103	1/1	0.95	0.15	30,30,30,30	0
56	MG	1H	3346	1/1	0.95	0.28	73,73,73,73	0
56	MG	14	3277	1/1	0.95	0.29	66,66,66,66	0
56	MG	14	3070	1/1	0.95	0.13	39,39,39,39	0
56	MG	1H	3315	1/1	0.95	0.08	66,66,66,66	0
56	MG	14	3073	1/1	0.95	0.07	80,80,80,80	0
56	MG	13	1626	1/1	0.95	0.30	68,68,68,68	0
56	MG	14	3075	1/1	0.95	0.13	53,53,53,53	0
56	MG	1H	3253	1/1	0.95	0.09	78,78,78,78	0
56	MG	14	3077	1/1	0.95	0.23	68,68,68,68	0
56	MG	1H	3318	1/1	0.95	0.22	56,56,56,56	0
56	MG	14	3216	1/1	0.95	0.39	83,83,83,83	0
56	MG	14	3079	1/1	0.95	0.17	57,57,57,57	0
56	MG	14	3218	1/1	0.95	0.28	77,77,77,77	0
56	MG	14	3219	1/1	0.95	0.31	56,56,56,56	0
56	MG	14	3011	1/1	0.95	0.17	43,43,43,43	0
56	MG	1H	3351	1/1	0.95	0.18	70,70,70,70	0
56	MG	1H	3029	1/1	0.95	0.38	73,73,73,73	0
56	MG	1H	3320	1/1	0.95	0.08	91,91,91,91	0
56	MG	1H	3355	1/1	0.95	0.19	60,60,60,60	0
56	MG	13	1629	1/1	0.95	0.19	46,46,46,46	0
56	MG	14	3017	1/1	0.95	0.25	49,49,49,49	0
56	MG	1H	3357	1/1	0.95	0.29	62,62,62,62	0
56	MG	1H	3002	1/1	0.95	0.13	40,40,40,40	0
56	MG	1H	3205	1/1	0.95	0.18	62,62,62,62	0
56	MG	1H	3087	1/1	0.95	0.22	43,43,43,43	0
56	MG	1H	3232	1/1	0.95	0.27	43,43,43,43	0
56	MG	1H	3362	1/1	0.95	0.06	69,69,69,69	0
56	MG	1H	3088	1/1	0.95	0.38	73,73,73,73	0
56	MG	1H	3364	1/1	0.95	0.09	68,68,68,68	0
56	MG	13	1640	1/1	0.95	0.14	75,75,75,75	0
56	MG	14	3164	1/1	0.95	0.49	64,64,64,64	0
56	MG	14	3099	1/1	0.95	0.15	46,46,46,46	0
56	MG	1H	3019	1/1	0.95	0.16	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3367	1/1	0.95	0.12	66,66,66,66	0
56	MG	14	3349	1/1	0.95	0.09	63,63,63,63	0
56	MG	1H	3114	1/1	0.95	0.16	48,48,48,48	0
56	MG	1H	3052	1/1	0.95	0.16	46,46,46,46	0
56	MG	1H	3393	1/1	0.95	0.09	65,65,65,65	0
56	MG	14	3377	1/1	0.95	0.09	96,96,96,96	0
56	MG	14	3379	1/1	0.95	0.08	72,72,72,72	0
56	MG	14	3380	1/1	0.95	0.11	93,93,93,93	0
56	MG	1H	3396	1/1	0.95	0.07	57,57,57,57	0
56	MG	1H	3212	1/1	0.95	0.18	63,63,63,63	0
56	MG	1H	3409	1/1	0.95	0.10	53,53,53,53	0
56	MG	13	1641	1/1	0.95	0.19	59,59,59,59	0
56	MG	1H	3427	1/1	0.95	0.10	76,76,76,76	0
56	MG	1H	3271	1/1	0.95	0.31	65,65,65,65	0
56	MG	29	301	1/1	0.95	0.13	44,44,44,44	0
56	MG	1H	3303	1/1	0.95	0.24	65,65,65,65	0
56	MG	1H	3451	1/1	0.95	0.09	46,46,46,46	0
56	MG	1H	3453	1/1	0.95	0.09	76,76,76,76	0
56	MG	1H	3022	1/1	0.95	0.20	53,53,53,53	0
56	MG	1H	3456	1/1	0.95	0.08	92,92,92,92	0
56	MG	14	3046	1/1	0.95	0.28	53,53,53,53	0
57	PAR	1G	1686	42/42	0.95	0.10	69,76,87,91	0
56	MG	1G	1672	1/1	0.95	0.07	78,78,78,78	0
56	MG	14	3256	1/1	0.95	0.08	66,66,66,66	0
56	MG	1H	3003	1/1	0.96	0.15	35,35,35,35	0
56	MG	I8	101	1/1	0.96	0.27	53,53,53,53	0
56	MG	14	3005	1/1	0.96	0.24	53,53,53,53	0
56	MG	1H	3424	1/1	0.96	0.07	58,58,58,58	0
56	MG	1H	3235	1/1	0.96	0.11	38,38,38,38	0
56	MG	1H	3191	1/1	0.96	0.08	75,75,75,75	0
56	MG	1G	1645	1/1	0.96	0.18	73,73,73,73	0
56	MG	1H	3433	1/1	0.96	0.07	83,83,83,83	0
56	MG	1H	3435	1/1	0.96	0.07	90,90,90,90	0
56	MG	14	3172	1/1	0.96	0.36	69,69,69,69	0
56	MG	1H	3437	1/1	0.96	0.07	59,59,59,59	0
56	MG	14	3174	1/1	0.96	0.26	66,66,66,66	0
56	MG	14	3066	1/1	0.96	0.13	49,49,49,49	0
56	MG	1H	3438	1/1	0.96	0.10	54,54,54,54	0
56	MG	1H	3004	1/1	0.96	0.37	47,47,47,47	0
56	MG	1H	3446	1/1	0.96	0.08	78,78,78,78	0
56	MG	13	1671	1/1	0.96	0.04	98,98,98,98	0
56	MG	1H	3169	1/1	0.96	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3181	1/1	0.96	0.10	55,55,55,55	0
56	MG	1H	3095	1/1	0.96	0.35	49,49,49,49	0
56	MG	1H	3352	1/1	0.96	0.19	61,61,61,61	0
56	MG	1H	3457	1/1	0.96	0.06	92,92,92,92	0
56	MG	1H	3324	1/1	0.96	0.11	87,87,87,87	0
56	MG	1H	3267	1/1	0.96	0.18	60,60,60,60	0
56	MG	1H	3096	1/1	0.96	0.23	54,54,54,54	0
56	MG	1H	3473	1/1	0.96	0.06	73,73,73,73	0
56	MG	13	1665	1/1	0.96	0.10	67,67,67,67	0
56	MG	1H	3478	1/1	0.96	0.11	102,102,102,102	0
56	MG	13	1664	1/1	0.96	0.07	59,59,59,59	0
56	MG	1H	3481	1/1	0.96	0.06	77,77,77,77	0
56	MG	14	3194	1/1	0.96	0.05	52,52,52,52	0
56	MG	14	3315	1/1	0.96	0.07	68,68,68,68	0
56	MG	14	3332	1/1	0.96	0.10	73,73,73,73	0
56	MG	1H	3017	1/1	0.96	0.11	41,41,41,41	0
56	MG	14	3342	1/1	0.96	0.06	74,74,74,74	0
56	MG	2K	107	1/1	0.96	0.15	59,59,59,59	0
56	MG	1H	3055	1/1	0.96	0.08	61,61,61,61	0
56	MG	1H	3071	1/1	0.96	0.22	53,53,53,53	0
56	MG	14	3359	1/1	0.96	0.06	87,87,87,87	0
56	MG	14	3366	1/1	0.96	0.09	66,66,66,66	0
56	MG	14	3367	1/1	0.96	0.09	70,70,70,70	0
56	MG	1H	3203	1/1	0.96	0.31	80,80,80,80	0
56	MG	1G	1627	1/1	0.96	0.25	57,57,57,57	0
56	MG	14	3090	1/1	0.96	0.16	52,52,52,52	0
56	MG	1H	3009	1/1	0.96	0.20	43,43,43,43	0
56	MG	1H	3031	1/1	0.96	0.22	71,71,71,71	0
56	MG	14	3389	1/1	0.96	0.06	97,97,97,97	0
56	MG	14	3093	1/1	0.96	0.30	48,48,48,48	0
56	MG	1G	1677	1/1	0.96	0.16	104,104,104,104	0
56	MG	14	3095	1/1	0.96	0.31	56,56,56,56	0
56	MG	1H	3308	1/1	0.96	0.20	65,65,65,65	0
56	MG	14	3041	1/1	0.96	0.25	39,39,39,39	0
56	MG	13	1713	1/1	0.96	0.10	70,70,70,70	0
56	MG	1H	3090	1/1	0.96	0.10	44,44,44,44	0
56	MG	29	302	1/1	0.96	0.11	65,65,65,65	0
56	MG	14	3152	1/1	0.96	0.08	67,67,67,67	0
56	MG	1H	3011	1/1	0.96	0.15	48,48,48,48	0
56	MG	1H	3385	1/1	0.96	0.07	54,54,54,54	0
56	MG	1H	3231	1/1	0.96	0.09	31,31,31,31	0
56	MG	1H	3285	1/1	0.96	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1H	3286	1/1	0.96	0.27	70,70,70,70	0
57	PAR	13	1745	42/42	0.96	0.08	57,66,72,75	0
56	MG	1H	3164	1/1	0.96	0.11	52,52,52,52	0
56	MG	1H	3126	1/1	0.96	0.36	60,60,60,60	0
56	MG	14	3001	1/1	0.96	0.15	53,53,53,53	0
56	MG	1H	3061	1/1	0.97	0.08	48,48,48,48	0
56	MG	1H	3150	1/1	0.97	0.10	59,59,59,59	0
56	MG	1H	3458	1/1	0.97	0.07	84,84,84,84	0
56	MG	14	3032	1/1	0.97	0.18	65,65,65,65	0
56	MG	14	3165	1/1	0.97	0.34	58,58,58,58	0
56	MG	1G	1683	1/1	0.97	0.09	104,104,104,104	0
56	MG	1H	3302	1/1	0.97	0.07	59,59,59,59	0
56	MG	1H	3462	1/1	0.97	0.08	92,92,92,92	0
56	MG	1G	1605	1/1	0.97	0.11	74,74,74,74	0
56	MG	1H	3464	1/1	0.97	0.05	92,92,92,92	0
56	MG	1H	3370	1/1	0.97	0.07	54,54,54,54	0
56	MG	14	3308	1/1	0.97	0.06	46,46,46,46	0
56	MG	14	3314	1/1	0.97	0.07	55,55,55,55	0
56	MG	1H	3371	1/1	0.97	0.07	46,46,46,46	0
56	MG	14	3325	1/1	0.97	0.06	63,63,63,63	0
56	MG	14	3331	1/1	0.97	0.12	70,70,70,70	0
56	MG	1H	3379	1/1	0.97	0.07	46,46,46,46	0
56	MG	1H	3475	1/1	0.97	0.06	79,79,79,79	0
56	MG	14	3341	1/1	0.97	0.05	48,48,48,48	0
56	MG	14	3002	1/1	0.97	0.11	43,43,43,43	0
56	MG	1H	3383	1/1	0.97	0.06	52,52,52,52	0
56	MG	13	1733	1/1	0.97	0.05	73,73,73,73	0
56	MG	14	3352	1/1	0.97	0.07	84,84,84,84	0
56	MG	13	1603	1/1	0.97	0.14	58,58,58,58	0
56	MG	1H	3181	1/1	0.97	0.13	54,54,54,54	0
56	MG	14	3365	1/1	0.97	0.05	85,85,85,85	0
56	MG	13	1729	1/1	0.97	0.07	97,97,97,97	0
56	MG	1H	3261	1/1	0.97	0.12	61,61,61,61	0
56	MG	14	3369	1/1	0.97	0.05	97,97,97,97	0
56	MG	14	3370	1/1	0.97	0.05	68,68,68,68	0
56	MG	1H	3065	1/1	0.97	0.16	54,54,54,54	0
56	MG	14	3375	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3184	1/1	0.97	0.06	45,45,45,45	0
56	MG	1H	3420	1/1	0.97	0.06	48,48,48,48	0
56	MG	1H	3421	1/1	0.97	0.06	57,57,57,57	0
56	MG	1H	3422	1/1	0.97	0.06	54,54,54,54	0
56	MG	14	3385	1/1	0.97	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3387	1/1	0.97	0.05	97,97,97,97	0
56	MG	14	3187	1/1	0.97	0.12	53,53,53,53	0
56	MG	1H	3086	1/1	0.97	0.25	66,66,66,66	0
56	MG	1H	3156	1/1	0.97	0.05	54,54,54,54	0
56	MG	1H	3187	1/1	0.97	0.37	56,56,56,56	0
56	MG	1H	3188	1/1	0.97	0.09	60,60,60,60	0
56	MG	14	3061	1/1	0.97	0.12	50,50,50,50	0
56	MG	14	3062	1/1	0.97	0.07	56,56,56,56	0
56	MG	16	212	1/1	0.97	0.05	73,73,73,73	0
56	MG	1H	3189	1/1	0.97	0.30	63,63,63,63	0
56	MG	14	3150	1/1	0.97	0.29	51,51,51,51	0
56	MG	13	1724	1/1	0.97	0.10	78,78,78,78	0
56	MG	1H	3131	1/1	0.97	0.35	67,67,67,67	0
56	MG	45	201	1/1	0.97	0.04	50,50,50,50	0
56	MG	21	302	1/1	0.97	0.11	66,66,66,66	0
56	MG	1H	3443	1/1	0.97	0.06	58,58,58,58	0
56	MG	1H	3044	1/1	0.97	0.06	51,51,51,51	0
56	MG	1H	3001	1/1	0.97	0.09	49,49,49,49	0
56	MG	1H	3111	1/1	0.97	0.15	43,43,43,43	0
58	ZN	3E	302	1/1	0.97	0.23	89,89,89,89	0
56	MG	1H	3039	1/1	0.97	0.09	47,47,47,47	0
56	MG	1H	3278	1/1	0.97	0.15	76,76,76,76	0
56	MG	1H	3448	1/1	0.98	0.13	88,88,88,88	0
56	MG	1H	3449	1/1	0.98	0.04	72,72,72,72	0
56	MG	1H	3450	1/1	0.98	0.08	67,67,67,67	0
56	MG	14	3053	1/1	0.98	0.18	52,52,52,52	0
56	MG	1H	3378	1/1	0.98	0.05	55,55,55,55	0
56	MG	14	3310	1/1	0.98	0.04	50,50,50,50	0
56	MG	13	1722	1/1	0.98	0.05	76,76,76,76	0
56	MG	1H	3382	1/1	0.98	0.06	45,45,45,45	0
56	MG	14	3323	1/1	0.98	0.05	55,55,55,55	0
56	MG	1H	3072	1/1	0.98	0.06	43,43,43,43	0
56	MG	14	3326	1/1	0.98	0.06	65,65,65,65	0
56	MG	14	3327	1/1	0.98	0.05	58,58,58,58	0
56	MG	1H	3384	1/1	0.98	0.07	57,57,57,57	0
56	MG	14	3059	1/1	0.98	0.28	52,52,52,52	0
56	MG	14	3336	1/1	0.98	0.04	52,52,52,52	0
56	MG	14	3338	1/1	0.98	0.05	53,53,53,53	0
56	MG	13	1637	1/1	0.98	0.41	61,61,61,61	0
56	MG	14	3340	1/1	0.98	0.05	59,59,59,59	0
56	MG	1H	3459	1/1	0.98	0.10	77,77,77,77	0
56	MG	14	3162	1/1	0.98	0.04	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3343	1/1	0.98	0.06	46,46,46,46	0
56	MG	13	1726	1/1	0.98	0.05	77,77,77,77	0
56	MG	14	3348	1/1	0.98	0.13	54,54,54,54	0
56	MG	1H	3390	1/1	0.98	0.05	66,66,66,66	0
56	MG	14	3350	1/1	0.98	0.08	83,83,83,83	0
56	MG	1H	3392	1/1	0.98	0.07	64,64,64,64	0
56	MG	14	3268	1/1	0.98	0.30	57,57,57,57	0
56	MG	14	3358	1/1	0.98	0.14	77,77,77,77	0
56	MG	13	1734	1/1	0.98	0.04	86,86,86,86	0
56	MG	14	3362	1/1	0.98	0.05	69,69,69,69	0
56	MG	1H	3467	1/1	0.98	0.04	75,75,75,75	0
56	MG	1H	3394	1/1	0.98	0.05	57,57,57,57	0
56	MG	1H	3469	1/1	0.98	0.07	90,90,90,90	0
56	MG	1H	3268	1/1	0.98	0.14	46,46,46,46	0
56	MG	1H	3474	1/1	0.98	0.07	64,64,64,64	0
56	MG	14	3371	1/1	0.98	0.04	56,56,56,56	0
56	MG	14	3071	1/1	0.98	0.09	61,61,61,61	0
56	MG	14	3373	1/1	0.98	0.05	69,69,69,69	0
56	MG	14	3374	1/1	0.98	0.10	76,76,76,76	0
56	MG	1H	3398	1/1	0.98	0.08	55,55,55,55	0
56	MG	1H	3399	1/1	0.98	0.05	47,47,47,47	0
56	MG	1H	3402	1/1	0.98	0.08	48,48,48,48	0
56	MG	14	3378	1/1	0.98	0.04	79,79,79,79	0
56	MG	2K	106	1/1	0.98	0.05	84,84,84,84	0
56	MG	1H	3406	1/1	0.98	0.04	45,45,45,45	0
56	MG	14	3381	1/1	0.98	0.06	62,62,62,62	0
56	MG	14	3383	1/1	0.98	0.05	86,86,86,86	0
56	MG	13	1736	1/1	0.98	0.04	73,73,73,73	0
56	MG	13	1738	1/1	0.98	0.05	72,72,72,72	0
56	MG	1H	3033	1/1	0.98	0.08	67,67,67,67	0
56	MG	13	1739	1/1	0.98	0.10	73,73,73,73	0
56	MG	13	1740	1/1	0.98	0.08	88,88,88,88	0
56	MG	1G	1671	1/1	0.98	0.07	73,73,73,73	0
56	MG	1H	3136	1/1	0.98	0.05	41,41,41,41	0
56	MG	1G	1673	1/1	0.98	0.05	74,74,74,74	0
56	MG	1H	3426	1/1	0.98	0.04	59,59,59,59	0
56	MG	1J	206	1/1	0.98	0.04	73,73,73,73	0
56	MG	1H	3108	1/1	0.98	0.18	34,34,34,34	0
56	MG	1H	3429	1/1	0.98	0.05	40,40,40,40	0
56	MG	1H	3277	1/1	0.98	0.11	70,70,70,70	0
56	MG	1H	3069	1/1	0.98	0.07	44,44,44,44	0
56	MG	1G	1682	1/1	0.98	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	35	201	1/1	0.98	0.17	60,60,60,60	0
56	MG	1H	3434	1/1	0.98	0.10	75,75,75,75	0
56	MG	1H	3369	1/1	0.98	0.05	45,45,45,45	0
56	MG	13	1721	1/1	0.98	0.13	90,90,90,90	0
56	MG	1H	3262	1/1	0.98	0.34	56,56,56,56	0
56	MG	1H	3439	1/1	0.98	0.07	69,69,69,69	0
56	MG	1H	3373	1/1	0.98	0.09	45,45,45,45	0
56	MG	1H	3375	1/1	0.98	0.04	37,37,37,37	0
56	MG	1H	3445	1/1	0.98	0.04	52,52,52,52	0
58	ZN	32	301	1/1	0.98	0.23	96,96,96,96	0
56	MG	1H	3377	1/1	0.98	0.05	44,44,44,44	0
56	MG	1H	3479	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3334	1/1	0.99	0.03	79,79,79,79	0
56	MG	14	3335	1/1	0.99	0.05	55,55,55,55	0
56	MG	1H	3395	1/1	0.99	0.04	45,45,45,45	0
56	MG	14	3337	1/1	0.99	0.03	55,55,55,55	0
56	MG	13	1732	1/1	0.99	0.05	62,62,62,62	0
56	MG	1H	3436	1/1	0.99	0.04	60,60,60,60	0
56	MG	1H	3397	1/1	0.99	0.06	66,66,66,66	0
56	MG	13	1737	1/1	0.99	0.04	62,62,62,62	0
56	MG	13	1723	1/1	0.99	0.12	86,86,86,86	0
56	MG	1H	3440	1/1	0.99	0.06	61,61,61,61	0
56	MG	14	3344	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3441	1/1	0.99	0.11	86,86,86,86	0
56	MG	14	3346	1/1	0.99	0.06	59,59,59,59	0
56	MG	14	3347	1/1	0.99	0.12	56,56,56,56	0
56	MG	1G	1674	1/1	0.99	0.04	70,70,70,70	0
56	MG	1H	3442	1/1	0.99	0.03	42,42,42,42	0
56	MG	1G	1676	1/1	0.99	0.03	75,75,75,75	0
56	MG	1H	3401	1/1	0.99	0.05	64,64,64,64	0
56	MG	1G	1678	1/1	0.99	0.11	98,98,98,98	0
56	MG	14	3354	1/1	0.99	0.04	71,71,71,71	0
56	MG	14	3355	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3381	1/1	0.99	0.08	40,40,40,40	0
56	MG	14	3038	1/1	0.99	0.12	34,34,34,34	0
56	MG	14	3360	1/1	0.99	0.04	63,63,63,63	0
56	MG	14	3361	1/1	0.99	0.04	60,60,60,60	0
56	MG	1H	3403	1/1	0.99	0.04	43,43,43,43	0
56	MG	14	3363	1/1	0.99	0.07	74,74,74,74	0
56	MG	14	3364	1/1	0.99	0.02	75,75,75,75	0
56	MG	13	1744	1/1	0.99	0.06	95,95,95,95	0
56	MG	1H	3447	1/1	0.99	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3252	1/1	0.99	0.12	49,49,49,49	0
56	MG	14	3368	1/1	0.99	0.03	53,53,53,53	0
56	MG	1H	3407	1/1	0.99	0.04	57,57,57,57	0
56	MG	13	1731	1/1	0.99	0.05	94,94,94,94	0
56	MG	1H	3410	1/1	0.99	0.06	46,46,46,46	0
56	MG	1H	3452	1/1	0.99	0.04	49,49,49,49	0
56	MG	1H	3412	1/1	0.99	0.03	32,32,32,32	0
56	MG	1H	3415	1/1	0.99	0.17	68,68,68,68	0
56	MG	13	1735	1/1	0.99	0.03	71,71,71,71	0
56	MG	1H	3417	1/1	0.99	0.10	61,61,61,61	0
56	MG	1H	3418	1/1	0.99	0.07	42,42,42,42	0
56	MG	1H	3372	1/1	0.99	0.05	37,37,37,37	0
56	MG	1H	3460	1/1	0.99	0.03	55,55,55,55	0
56	MG	1H	3387	1/1	0.99	0.02	54,54,54,54	0
56	MG	1H	3388	1/1	0.99	0.05	64,64,64,64	0
56	MG	14	3382	1/1	0.99	0.05	69,69,69,69	0
56	MG	1H	3463	1/1	0.99	0.14	101,101,101,101	0
56	MG	14	3384	1/1	0.99	0.03	62,62,62,62	0
56	MG	1H	3389	1/1	0.99	0.04	68,68,68,68	0
56	MG	14	3386	1/1	0.99	0.10	60,60,60,60	0
56	MG	1H	3425	1/1	0.99	0.03	67,67,67,67	0
56	MG	14	3388	1/1	0.99	0.04	88,88,88,88	0
56	MG	1H	3466	1/1	0.99	0.03	56,56,56,56	0
56	MG	14	3390	1/1	0.99	0.11	90,90,90,90	0
56	MG	1H	3230	1/1	0.99	0.09	37,37,37,37	0
56	MG	1H	3391	1/1	0.99	0.05	71,71,71,71	0
56	MG	1H	3428	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3470	1/1	0.99	0.05	106,106,106,106	0
56	MG	14	3309	1/1	0.99	0.10	58,58,58,58	0
56	MG	1H	3471	1/1	0.99	0.13	68,68,68,68	0
56	MG	14	3312	1/1	0.99	0.03	67,67,67,67	0
56	MG	1H	3472	1/1	0.99	0.06	56,56,56,56	0
56	MG	1H	3374	1/1	0.99	0.05	50,50,50,50	0
56	MG	14	3316	1/1	0.99	0.04	49,49,49,49	0
56	MG	14	3317	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3318	1/1	0.99	0.04	57,57,57,57	0
56	MG	14	3319	1/1	0.99	0.03	62,62,62,62	0
56	MG	14	3320	1/1	0.99	0.04	60,60,60,60	0
56	MG	14	3321	1/1	0.99	0.03	62,62,62,62	0
56	MG	14	3322	1/1	0.99	0.10	77,77,77,77	0
56	MG	1H	3430	1/1	0.99	0.05	76,76,76,76	0
56	MG	1H	3020	1/1	0.99	0.12	47,47,47,47	0

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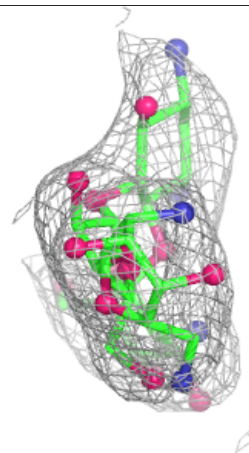
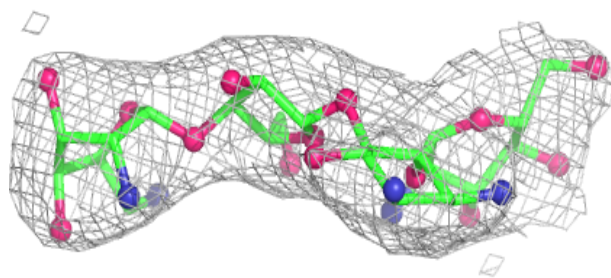
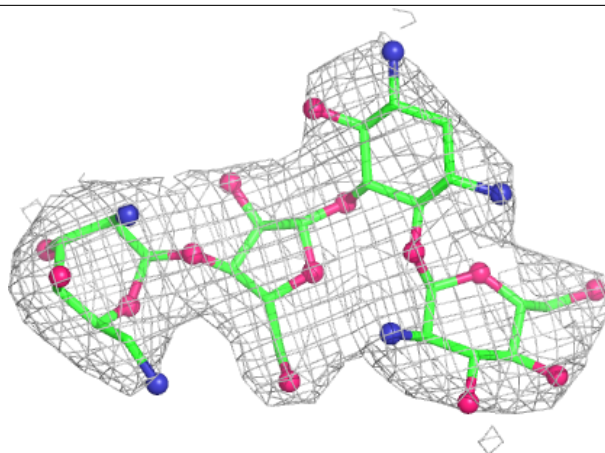
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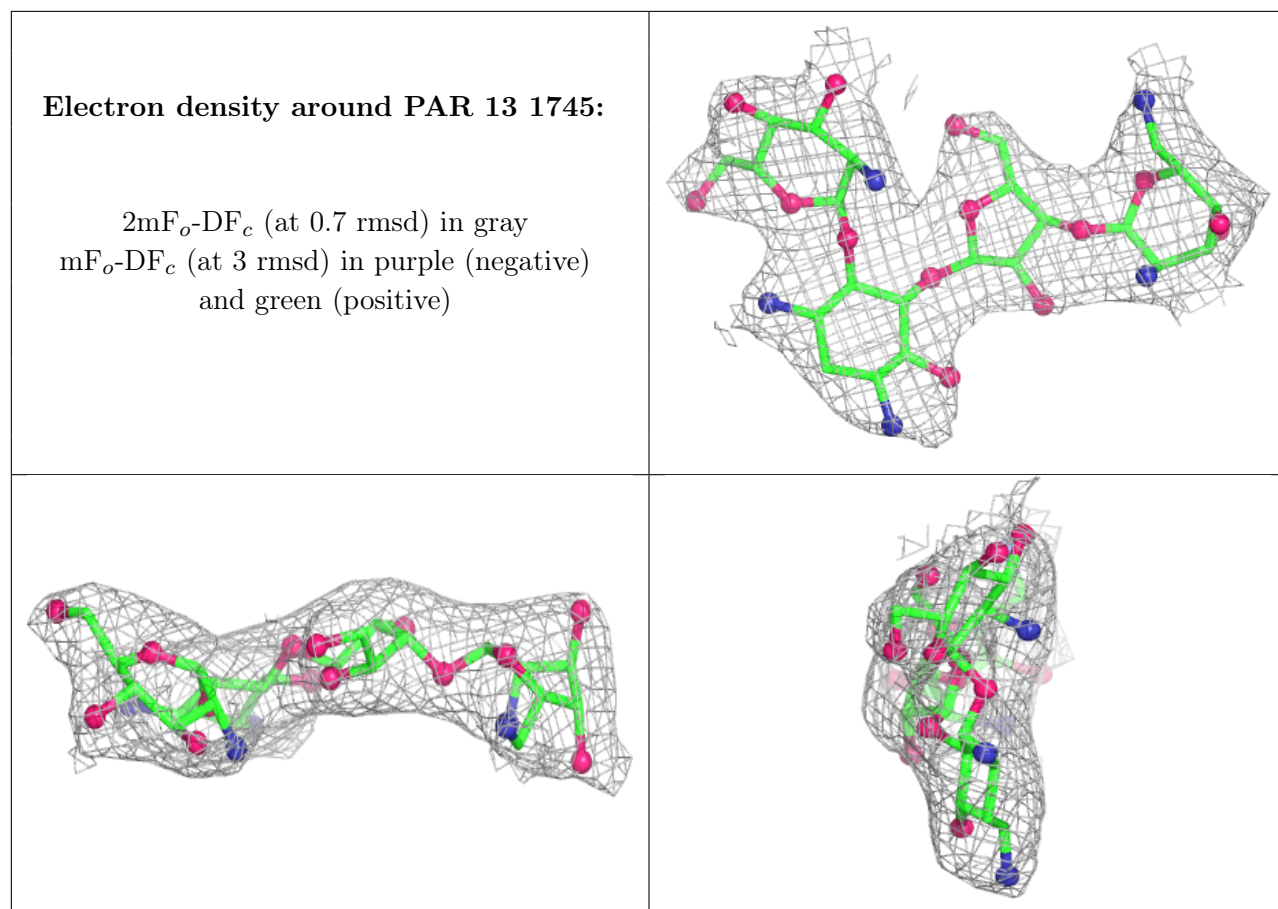
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3476	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3432	1/1	0.99	0.08	65,65,65,65	0
58	ZN	5I	101	1/1	0.99	0.04	88,88,88,88	0
56	MG	14	3329	1/1	0.99	0.04	45,45,45,45	0
56	MG	14	3330	1/1	0.99	0.04	48,48,48,48	0
58	ZN	5A	101	1/1	0.99	0.04	121,121,121,121	0
56	MG	1H	3376	1/1	0.99	0.02	36,36,36,36	0
56	MG	14	3356	1/1	1.00	0.02	72,72,72,72	0
56	MG	14	3357	1/1	1.00	0.12	62,62,62,62	0
56	MG	1H	3423	1/1	1.00	0.05	44,44,44,44	0
56	MG	1H	3413	1/1	1.00	0.10	44,44,44,44	0
56	MG	1H	3414	1/1	1.00	0.05	53,53,53,53	0
56	MG	14	3324	1/1	1.00	0.04	52,52,52,52	0
56	MG	13	1725	1/1	1.00	0.05	62,62,62,62	0
56	MG	14	3311	1/1	1.00	0.05	51,51,51,51	0
56	MG	1H	3380	1/1	1.00	0.02	41,41,41,41	0
56	MG	14	3328	1/1	1.00	0.04	62,62,62,62	0
56	MG	14	3313	1/1	1.00	0.03	50,50,50,50	0
56	MG	1H	3408	1/1	1.00	0.03	47,47,47,47	0
56	MG	13	1727	1/1	1.00	0.05	76,76,76,76	0
56	MG	1H	3419	1/1	1.00	0.04	37,37,37,37	0
56	MG	14	3333	1/1	1.00	0.04	58,58,58,58	0
56	MG	14	3351	1/1	1.00	0.14	43,43,43,43	0
56	MG	1H	3404	1/1	1.00	0.03	45,45,45,45	0
56	MG	1H	3411	1/1	1.00	0.08	53,53,53,53	0
56	MG	1H	3455	1/1	1.00	0.01	57,57,57,57	0
56	MG	1H	3400	1/1	1.00	0.05	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR 1G 1686:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.