



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 10:34 am BST

PDB ID : 5E7K
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and cognate tRNA^{Lys} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-10-12
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

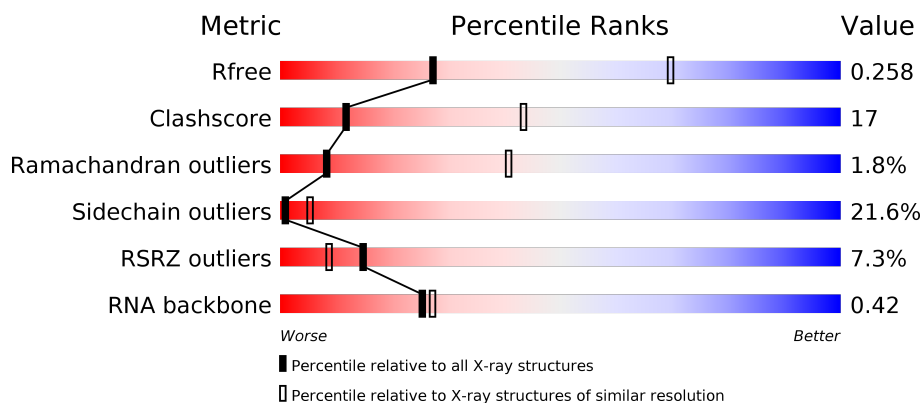
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



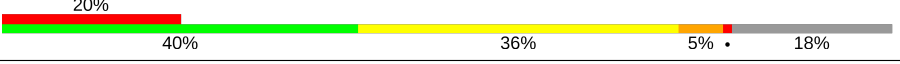
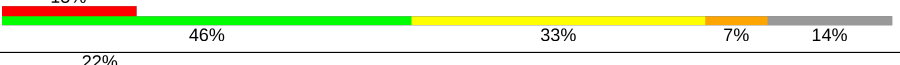
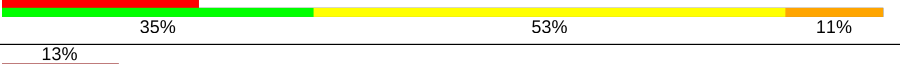


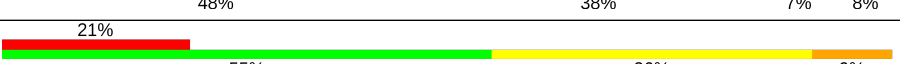

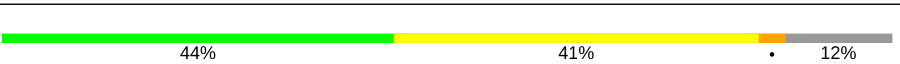


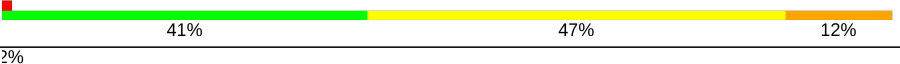
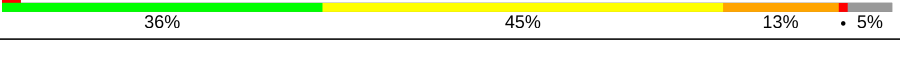

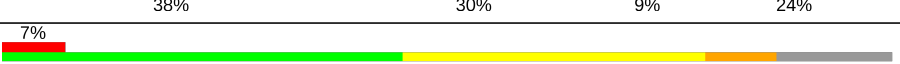

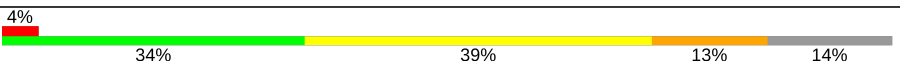


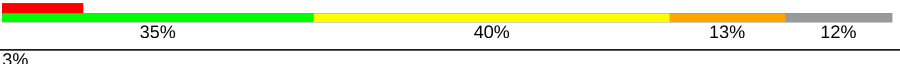


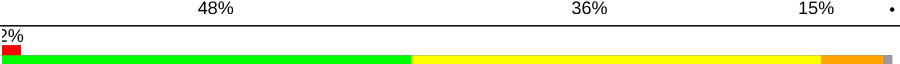



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	


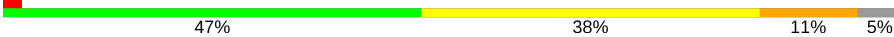
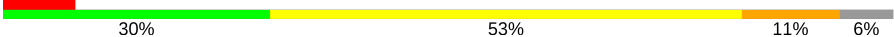


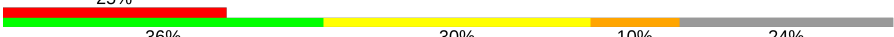
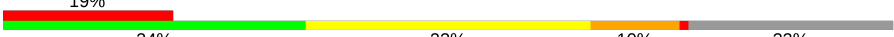
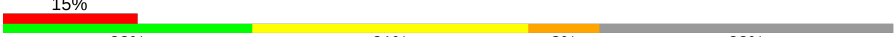
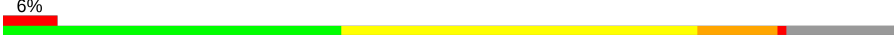

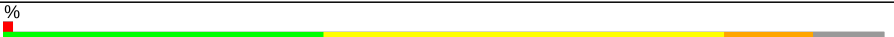


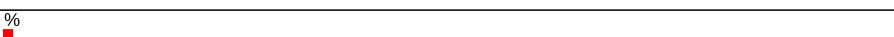

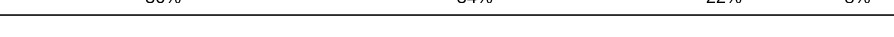




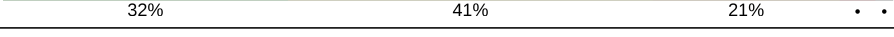
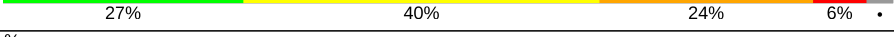
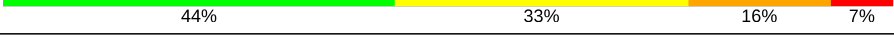
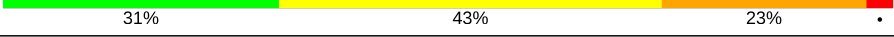

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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	75	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	71	229	
28	79	229	

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Mol	Chain	Length	Quality of chain
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	

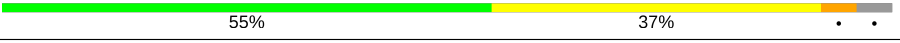

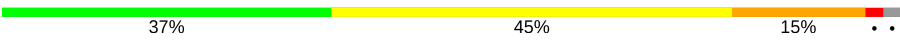
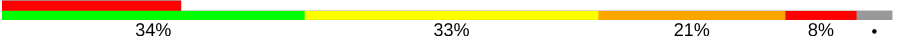
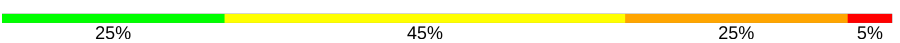
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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Mol	Chain	Length	Quality of chain
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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
58	MG	13	1603	-	-	-	X
58	MG	13	1630	-	-	-	X
58	MG	13	1641	-	-	-	X
58	MG	13	1644	-	-	-	X
58	MG	13	1653	-	-	-	X
58	MG	13	1659	-	-	-	X
58	MG	13	1672	-	-	-	X
58	MG	13	1689	-	-	-	X
58	MG	13	1694	-	-	-	X
58	MG	13	1695	-	-	-	X
58	MG	13	1704	-	-	-	X
58	MG	14	3017	-	-	-	X
58	MG	14	3018	-	-	-	X
58	MG	14	3019	-	-	-	X
58	MG	14	3029	-	-	-	X
58	MG	14	3034	-	-	-	X
58	MG	14	3037	-	-	-	X
58	MG	14	3052	-	-	-	X
58	MG	14	3068	-	-	-	X
58	MG	14	3073	-	-	-	X
58	MG	14	3080	-	-	-	X
58	MG	14	3085	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3108	-	-	-	X
58	MG	14	3117	-	-	-	X
58	MG	14	3129	-	-	-	X
58	MG	14	3144	-	-	-	X
58	MG	14	3150	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3153	-	-	-	X
58	MG	14	3155	-	-	-	X
58	MG	14	3181	-	-	-	X
58	MG	14	3182	-	-	-	X
58	MG	14	3183	-	-	-	X
58	MG	14	3185	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3188	-	-	-	X
58	MG	14	3190	-	-	-	X
58	MG	14	3191	-	-	-	X
58	MG	14	3227	-	-	-	X
58	MG	14	3229	-	-	-	X
58	MG	14	3234	-	-	-	X
58	MG	14	3243	-	-	-	X
58	MG	14	3250	-	-	-	X
58	MG	14	3251	-	-	-	X
58	MG	14	3257	-	-	-	X
58	MG	14	3259	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3261	-	-	-	X
58	MG	14	3264	-	-	-	X
58	MG	14	3265	-	-	-	X
58	MG	14	3268	-	-	-	X
58	MG	14	3269	-	-	-	X
58	MG	14	3280	-	-	-	X
58	MG	14	3282	-	-	-	X
58	MG	14	3288	-	-	-	X
58	MG	14	3293	-	-	-	X
58	MG	14	3297	-	-	-	X
58	MG	14	3302	-	-	-	X
58	MG	14	3304	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	14	3313	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1604	-	-	-	X
58	MG	1G	1649	-	-	-	X
58	MG	1G	1666	-	-	-	X
58	MG	1G	1672	-	-	-	X
58	MG	1H	3016	-	-	-	X
58	MG	1H	3024	-	-	-	X
58	MG	1H	3031	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3032	-	-	-	X
58	MG	1H	3033	-	-	-	X
58	MG	1H	3035	-	-	-	X
58	MG	1H	3036	-	-	-	X
58	MG	1H	3043	-	-	-	X
58	MG	1H	3087	-	-	-	X
58	MG	1H	3122	-	-	-	X
58	MG	1H	3142	-	-	-	X
58	MG	1H	3154	-	-	-	X
58	MG	1H	3167	-	-	-	X
58	MG	1H	3171	-	-	-	X
58	MG	1H	3175	-	-	-	X
58	MG	1H	3180	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3201	-	-	-	X
58	MG	1H	3207	-	-	-	X
58	MG	1H	3224	-	-	-	X
58	MG	1H	3228	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3268	-	-	-	X
58	MG	1H	3278	-	-	-	X
58	MG	1H	3279	-	-	-	X
58	MG	1H	3282	-	-	-	X
58	MG	1H	3284	-	-	-	X
58	MG	1H	3285	-	-	-	X
58	MG	1H	3288	-	-	-	X
58	MG	1H	3301	-	-	-	X
58	MG	1H	3309	-	-	-	X
58	MG	1H	3315	-	-	-	X
58	MG	1H	3324	-	-	-	X
58	MG	1H	3327	-	-	-	X
58	MG	1H	3328	-	-	-	X
58	MG	1H	3331	-	-	-	X
58	MG	1H	3342	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	2K	102	-	-	-	X
58	MG	2K	103	-	-	-	X
58	MG	2L	102	-	-	-	X
58	MG	E5	101	-	-	-	X
59	SF4	32	301	-	-	X	-

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 294444 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	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	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	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	126	Total	C	N	O		0	0	0
			1000	634	196	170				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	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	23	Total	C	N	O		0	0	0
			199	122	48	29				
21	1B	22	Total	C	N	O		0	0	0
			188	116	44	28				

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	71	Total	C	N	O	P	S	0	0	0
			1520	681	264	503	71	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1K	?	-	G	deletion	GB 836716955

- 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
			1646	735	297	536	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	18	Total	C	N	O	P	0	0	0
			397	178	84	117	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total	C	N	O	P	0	0	0
			61028	27159	11418	19618	2833			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	79	57	Total	C	N	O	0	0	0
			456	283	91	82			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1458	931	266	257	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	73	Total	C	N	O		0	0	0
			568	356	116	96				

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	S	0	0	0
			881	556	176	149				
40	65	110	Total	C	N	O	S	0	0	0
			876	553	175	148				

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	105	Total	C	N	O	S	0	0	0
			796	513	150	128	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
47	D5	132	Total	C	N	O	S	0	0	0
			1074	691	193	188	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			568	352	115	100	1			
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			
51	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 56 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	73	Total	C	N	O	P	S	0	0
			1563	700	271	518	73	1		

- Molecule 57 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	76	Total	C	N	O	P		0	0
			1612	722	281	534	75			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	98	1	Total	Mg	0	0
			1	1		
58	45	2	Total	Mg	0	0
			2	2		
58	P8	1	Total	Mg	0	0
			1	1		
58	13	132	Total	Mg	0	0
			132	132		
58	1J	5	Total	Mg	0	0
			5	5		
58	1E	1	Total	Mg	0	0
			1	1		
58	35	3	Total	Mg	0	0
			3	3		
58	16	9	Total	Mg	0	0
			9	9		
58	25	1	Total	Mg	0	0
			1	1		
58	3K	1	Total	Mg	0	0
			1	1		
58	21	2	Total	Mg	0	0
			2	2		
58	2K	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Q8	1	Total 1	Mg 1	0	0
58	L8	1	Total 1	Mg 1	0	0
58	I8	3	Total 3	Mg 3	0	0
58	5E	1	Total 1	Mg 1	0	0
58	29	4	Total 4	Mg 4	0	0
58	78	1	Total 1	Mg 1	0	0
58	J8	1	Total 1	Mg 1	0	0
58	39	1	Total 1	Mg 1	0	0
58	1G	90	Total 90	Mg 90	0	0
58	1H	467	Total 467	Mg 467	0	0
58	E5	1	Total 1	Mg 1	0	0
58	88	1	Total 1	Mg 1	0	0
58	14	399	Total 399	Mg 399	0	0
58	55	1	Total 1	Mg 1	0	0
58	6A	1	Total 1	Mg 1	0	0
58	1K	1	Total 1	Mg 1	0	0
58	41	1	Total 1	Mg 1	0	0
58	2L	2	Total 2	Mg 2	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C5	1	Total	Zn	0	0
			1	1		
60	5A	1	Total	Zn	0	0
			1	1		
60	G8	1	Total	Zn	0	0
			1	1		
60	5I	1	Total	Zn	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	126	Total	O	0	0
			126	126		
61	3I	2	Total	O	0	0
			2	2		
61	5I	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	2	Total 2	O 2	0	0
61	1H	629	Total 629	O 629	0	0
61	16	29	Total 29	O 29	0	0
61	11	7	Total 7	O 7	0	0
61	21	4	Total 4	O 4	0	0
61	31	9	Total 9	O 9	0	0
61	58	2	Total 2	O 2	0	0
61	78	7	Total 7	O 7	0	0
61	88	1	Total 1	O 1	0	0
61	B8	1	Total 1	O 1	0	0
61	E8	2	Total 2	O 2	0	0
61	F8	1	Total 1	O 1	0	0
61	G8	1	Total 1	O 1	0	0
61	I8	3	Total 3	O 3	0	0
61	L8	2	Total 2	O 2	0	0
61	1G	78	Total 78	O 78	0	0
61	32	1	Total 1	O 1	0	0
61	5A	2	Total 2	O 2	0	0
61	14	417	Total 417	O 417	0	0

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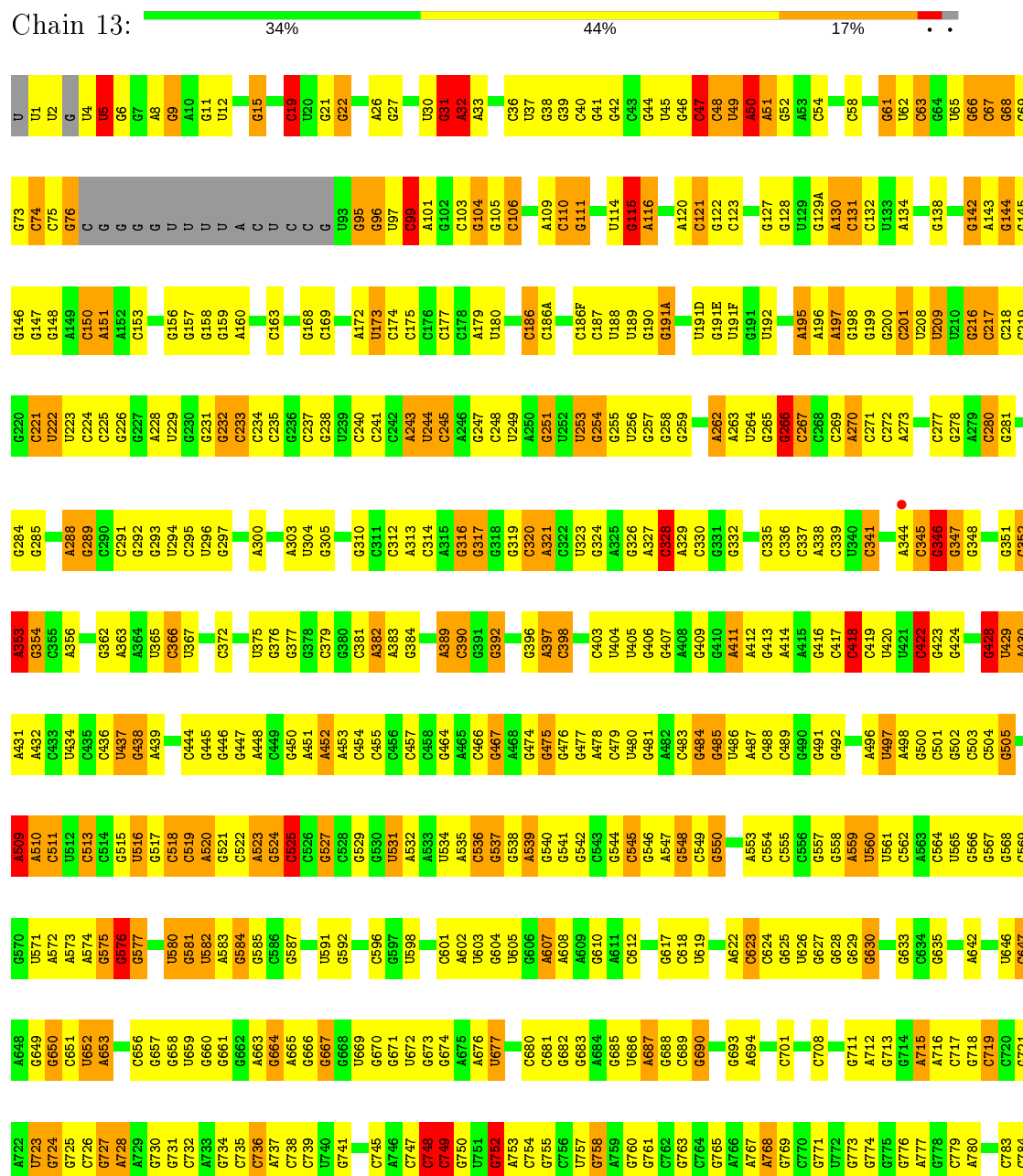
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1J	6	Total 6	O 6	0	0
61	19	8	Total 8	O 8	0	0
61	29	2	Total 2	O 2	0	0
61	39	5	Total 5	O 5	0	0
61	35	1	Total 1	O 1	0	0
61	55	1	Total 1	O 1	0	0
61	A5	1	Total 1	O 1	0	0
61	H5	2	Total 2	O 2	0	0

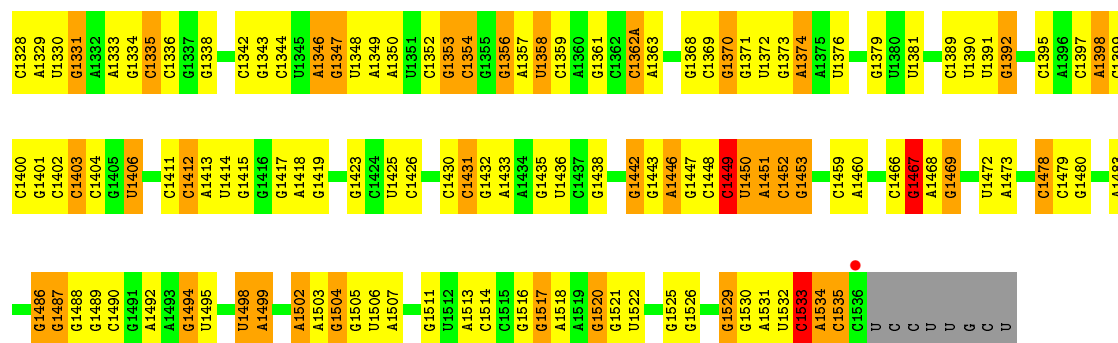
3 Residue-property plots

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

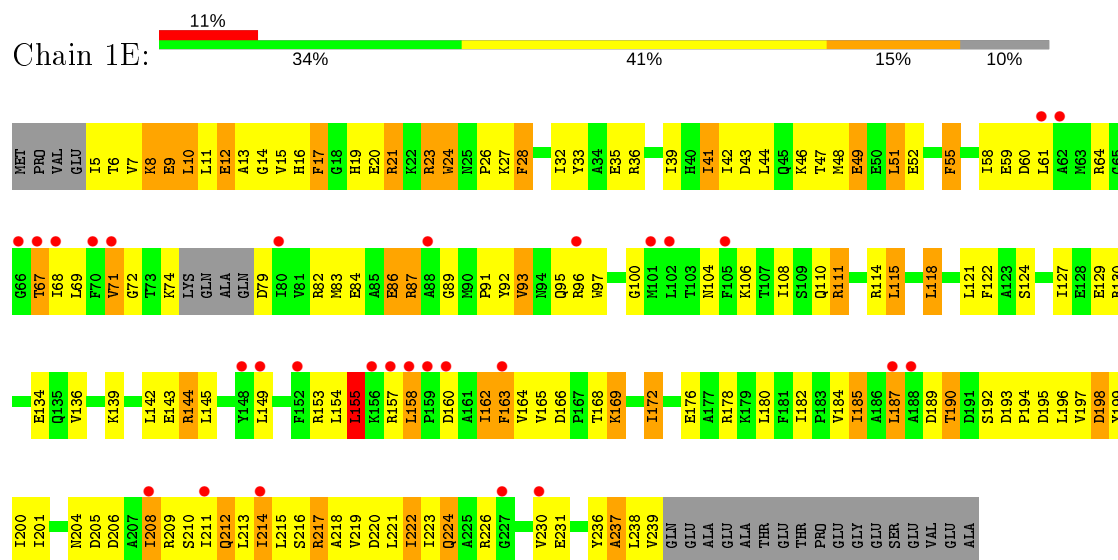
• Molecule 1: 16S rRNA



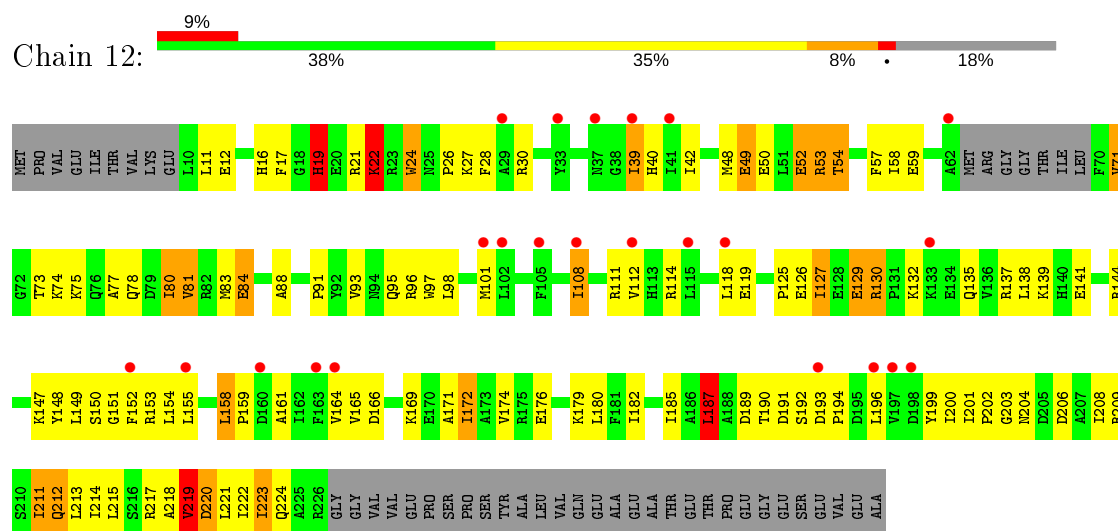
G1267	G1200	U1135	G1061	U999	G933	G851	A768	G674	G600	A532	C449	G377	G297	G220
A1268	A1201	U1136	U1062	A1000	C934	G852	G769	A675	C601	A533	G450	G378	A298	C221
A1269	G1202	C1137	C1063	G1001	A935	G853	G770	A676	A602	U534	A451	G394	G299	U222
C1270	C1203	G1138	G1064	G1002	C936	G854	G771	U677	U603	A452	A453	G301	U223	U230
G1271	A1204	G1139	U1065	G1003	A937	G855	U772	G681	G604	C536	A454	U387	G301	C224
G1272	U1205	G1140	C1066	A1004	A938	C856	G775	G682	U605	G537	C455	U388	C225	C226
G1273	G1206	G1141	A1067	A1005	G942	C857	G776	G683	G606	G538	C456	A389	G309	G227
A1274	G1207	G1142	G1068	C1006	G943	G858	A777	G684	A608	A539	C457	C390	G310	A228
G1275	C1208	G1143	C1069	A1007	G944	A859	G778	G685	A609	G540	C458	G391	C311	G229
G1276	C1209	G1144	U1070	G1008	A945	G860	A730	G686	G610	G541	G464	A393	C312	U230
G1277	C1210	C1145	U1071	C1009	A946	G861	A731	G687	G613	G542	A465	A394	G316	G230
U1278	U1211	A1146	G1072	G1010	G947	C862	A781	A687	C613	G546	C466	G395	G317	C235
A1279	U1212	C1147	U1073	G1011	G948	G863	A782	G688	A614	A547	G467	C396	G321	G236
A1280	A1213	U1148	C1076	A1014	A949	A864	C783	C689	C615	G548	A468	A397	A321	C237
U1281	C1214	C1149	U1077	A1015	U950	A865	C784	G690	G616	C549	G474	C398	G324	C240
A1282	G1215	U1150	G1078	A1016	G951	G866	A787	G691	G617	G550	G475	C401	G325	C241
G1283	G1216	A1151	U1079	G1017	G952	C868	G791	A694	C618	U551	G484	U404	G326	C242
C1284	C1217	G1152	A1080	G1018	G953	G869	A792	C701	C620	U552	G485	U405	A327	A243
A1285	C1218	C1153	G1081	U1020	U955	A872	A793	A702	A621	C555	G486	G406	A328	U244
A1286	U1219	G1154	U1082	G1021	U956	A873	A794	A703	G625	A559	A487	G407	A329	C245
A1288	G1220	G1155	U1084	G1022	U957	A874	G800	A706	U626	U561	C488	A408	G332	A246
A1289	G1221	G1156	U1085	G1023	A958	C874	A707	G707	G627	C562	C489	A409	G333	G247
A1290	G1222	A1157	U1086	G1024	A959	C875	A802	C708	G628	C563	G490	G410	C334	A250
G1291	U1223	G1158	A1092	U1025	U960	C879	A803	G718	G629	C564	G491	A411	C335	G251
G1292	G1224	U1159	A1093	G1026	U961	C880	U801	C719	G630	U565	G492	A412	C336	U252
U1293	A1225	G1160	G1094	C1027	C962	C882	A802	C720	G631	G566	U497	A413	C337	U253
G1294	G1226	C1161	U1095	C1028	G963	G885	U803	G718	G632	G567	A415	A414	G338	G254
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G1297	G1237	G1164	C1100	G1030	C967	G887	A807	U723	C634	G570	C501	G416	C341	G257
A1298	A1238	A1169	A1101	G1031	A968	A892	C808	G724	G635	A571	G502	G416	C342	G258
A1299	C1239	A1170	C1103	A1032	A969	A893	C811	G725	C643	A572	C503	U420	C343	U261
U1301	U1240	G1171	G1104	G1032A	C970	G894	C812	G726	G644	A573	G504	U421	G350	A262
A1302	G1241	C1172	A1105	G1032B	G971	G895	U813	C726	G645	G575	G505	G422	G351	A263
C1303	G1242	G1173	C1106	G1033	G972	C896	A814	G731	U646	G576	C507	G423	C352	U264
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A1306	A1245	A1176	C1109	C1037	A975	U905	C817	C736	G649	U580	A510	G426	C355	G267
U1307	C1246	G1177	A1110	G1038	G976	G906	G818	C739	G650	G581	C511	U427	C356	C267
G1308	U1247	G1178	A1111	C1039	A977	G907	A819	C739	G651	U582	C512	U428	A356	C271
A1309	A1248	A1179	C1112	U1040	A978	A908	U820	U740	C651	U583	C513	U429	A357	C272
G1310	C1249	G1180	C1113	A1041	C979	A909	U821	G741	U652	A584	C514	A430	A360	G276
G1311	A1250	G1181	C1114	G1042	C980	A913	C826	C748	G654	G585	G515	A431	G361	G277
G1312	A1251	G1182	C1115	C1043	U982	A914	U827	C749	A655	G586	U516	A432	A362	C277
C1313	G1252	A1183	C1116	G1047	C983	A915	A828	G750	G660	G587	G517	U433	A363	C280
C1314	C1253	G1184	C1117	G1048	C984	G916	G829	G751	G661	G588	C518	U434	A364	G281
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G1316	A1255	A1188	C1050	C1051	A986	U920	C834	A753	G664	C590	A520	G438	U367	U287
C1317	U1257	G1189	G1052	C1052	U991	U921	U835	C754	A665	U591	G521	A439	C370	A288
A1318	G1258	A1190	U1053	G1053	U992	G922	G836	G755	G666	G592	C522	A440	G371	G289
A1319	C1259	A1191	C1054	G1054	G993	A923	G837	C756	G667	G593	A523	C442	C372	C290
C1320	C1260	G1192	G127	C1054	A994	G924	G838	U757	G668	G594	C443	C443	C373	C291
C1321	G1261	C1193	U1055	A1055	U995	G925	U841	G758	U669	G595	G527	C444	A372	G292
G1322	A1262	U1194	C1128	U1056	C995	G926	C842	A759	G670	C596	G528	C445	A373	C293
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A1324	G1264	G1196	C1130	U1058	U997	G928	C844	A761	G672	U598	G530	G447	U375	C295
C1325	C1265	G1197	G1133	C1059	G998	G929	C845	A762	G673	C599	U531	G448	G376	U296
C1326	G1266	U1199	G1134	C1060	C998A	C932	C846	G765	G673	C599	U531	G448	G376	U296



• Molecule 2: 30S ribosomal protein S2

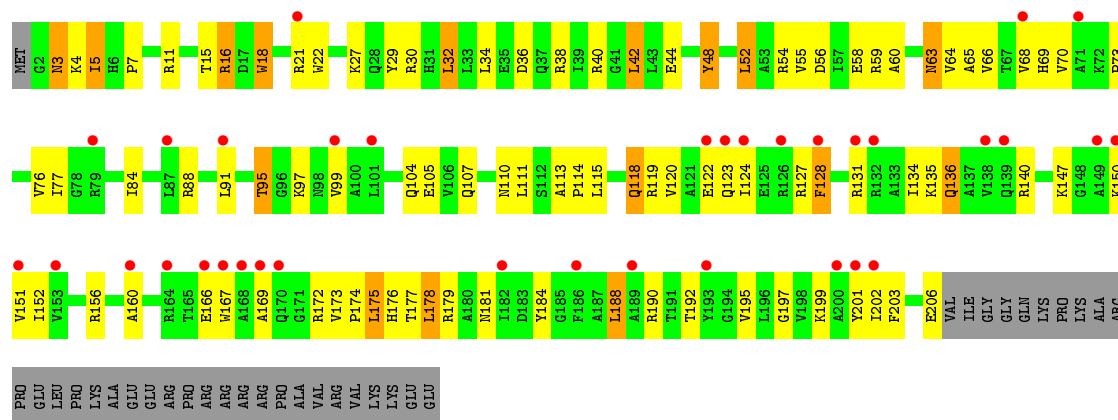


• Molecule 2: 30S ribosomal protein S2

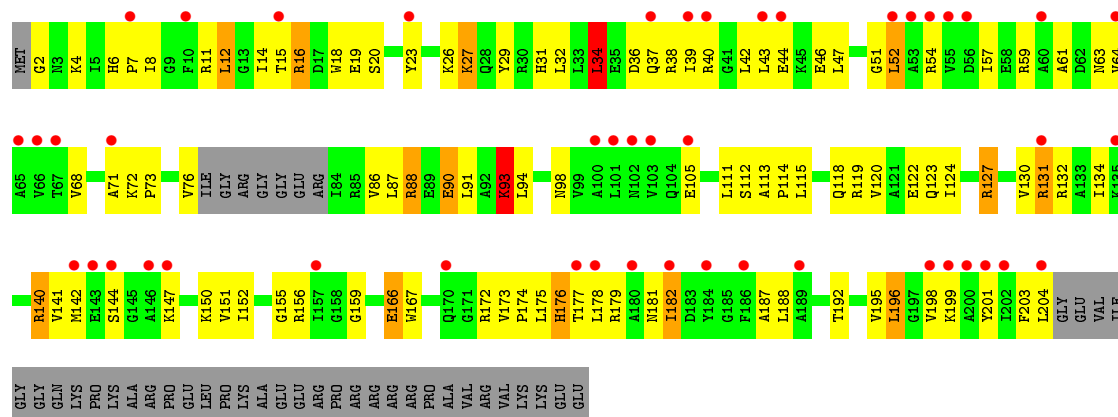
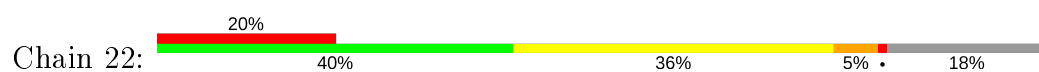


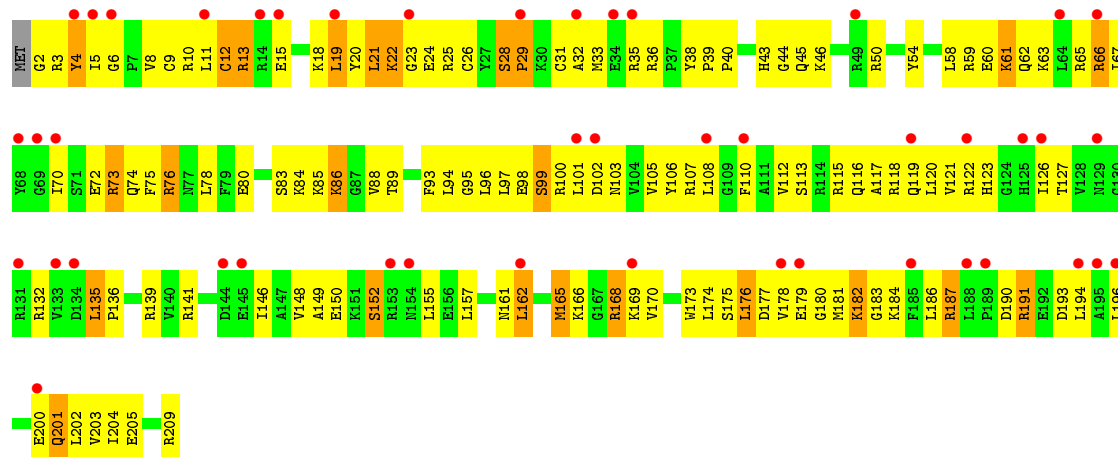
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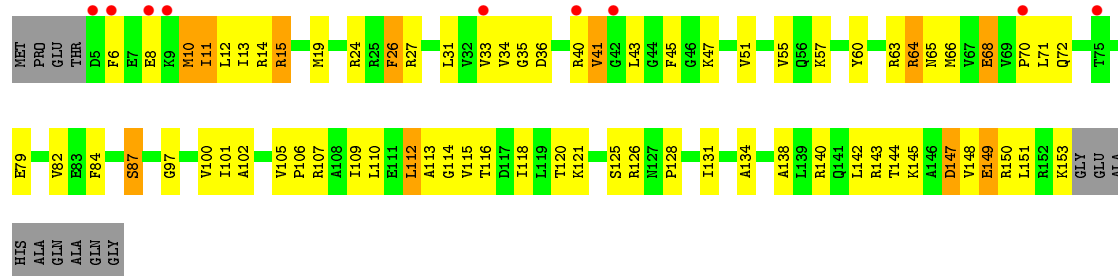


• Molecule 3: 30S ribosomal protein S3

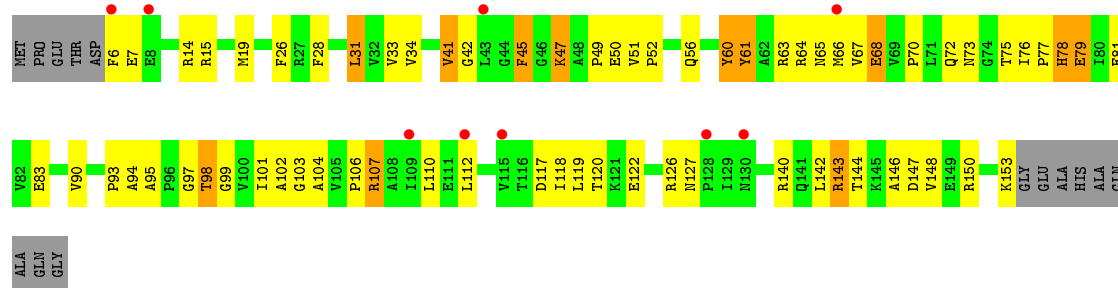




• Molecule 5: 30S ribosomal protein S5

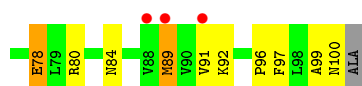


• Molecule 5: 30S ribosomal protein S5

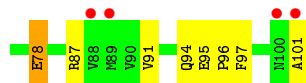
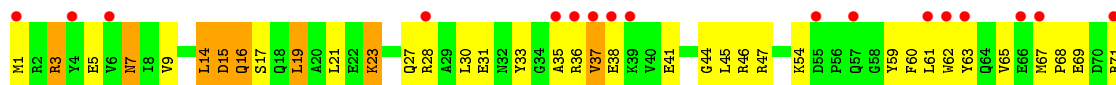


• Molecule 6: 30S ribosomal protein S6

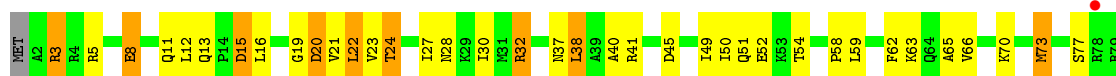




- Molecule 6: 30S ribosomal protein S6



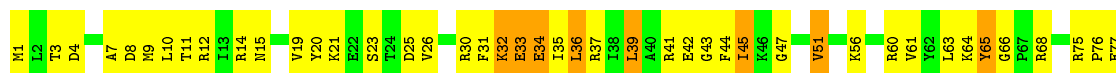
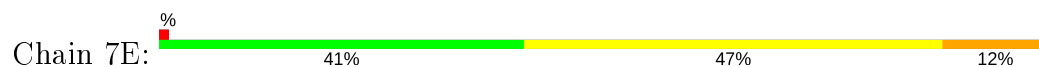
- Molecule 7: 30S ribosomal protein S7



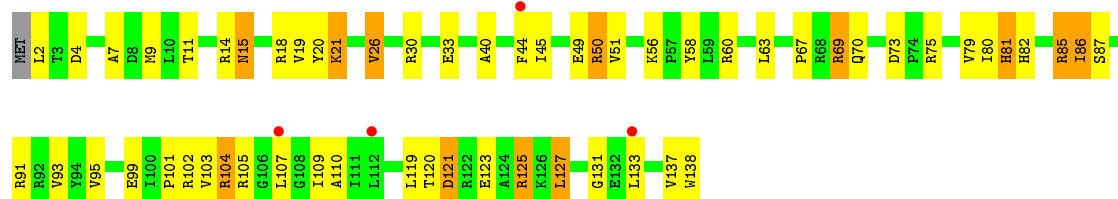
- Molecule 7: 30S ribosomal protein S7



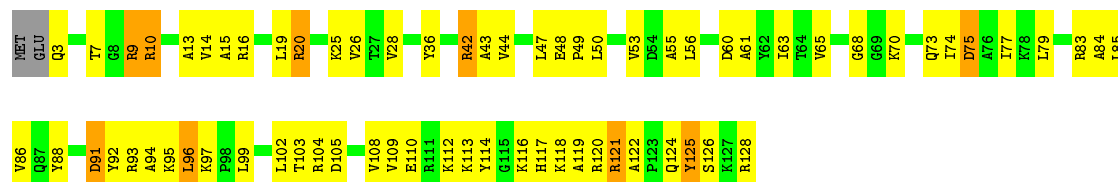
- Molecule 8: 30S ribosomal protein S8



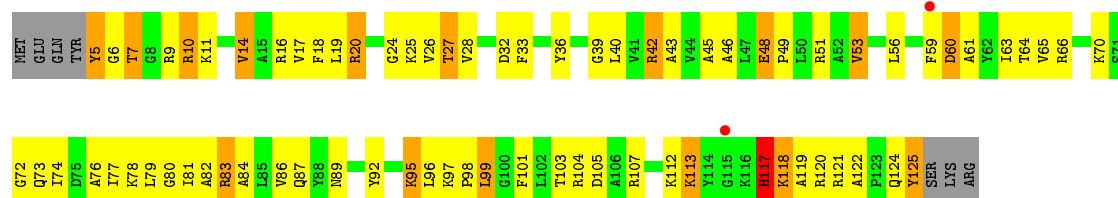
- Molecule 8: 30S ribosomal protein S8



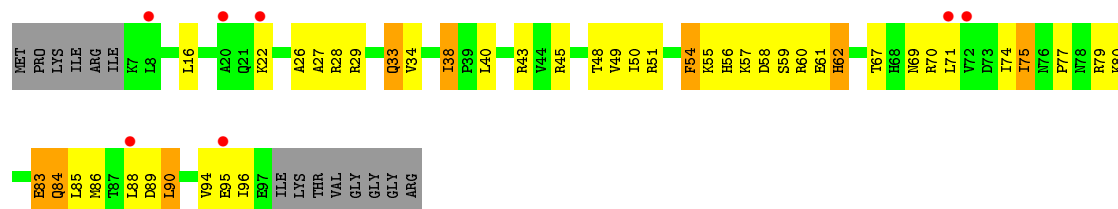
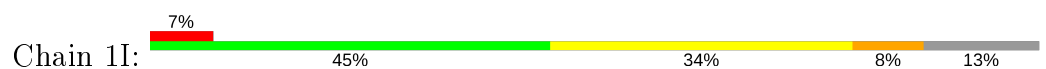
• Molecule 9: 30S ribosomal protein S9



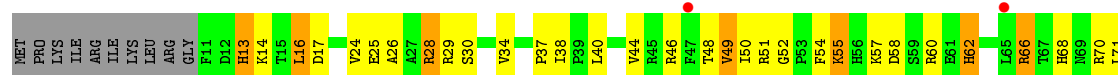
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

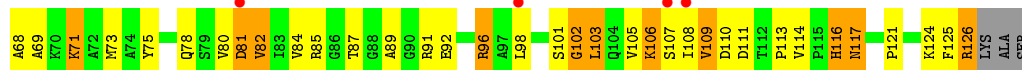
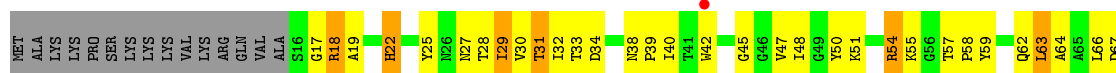


• Molecule 10: 30S ribosomal protein S10

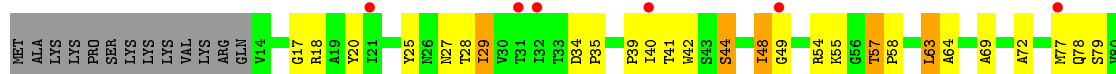




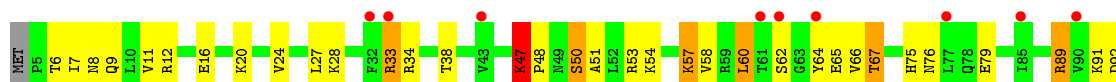
- Molecule 11: 30S ribosomal protein S11



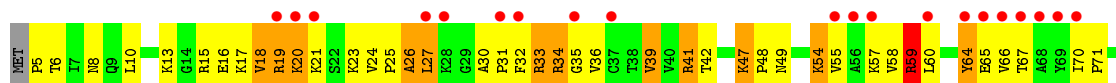
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

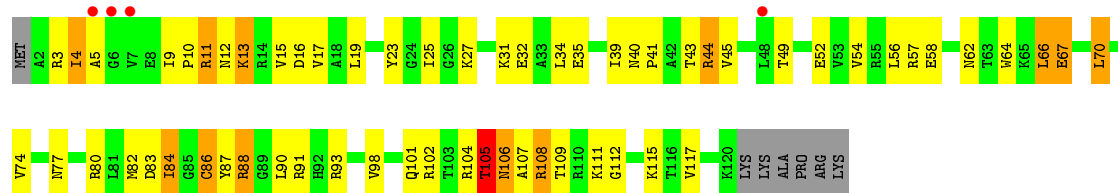


- Molecule 12: 30S ribosomal protein S12

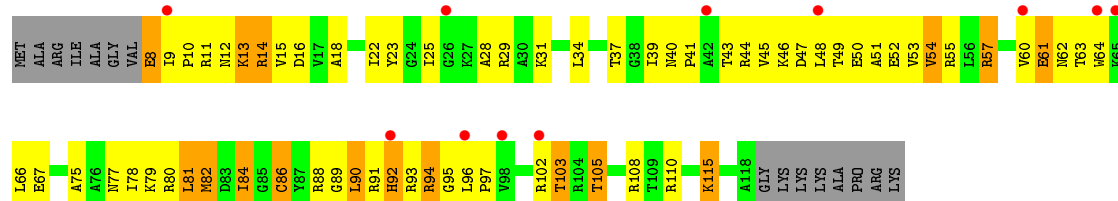


- Molecule 13: 30S ribosomal protein S13

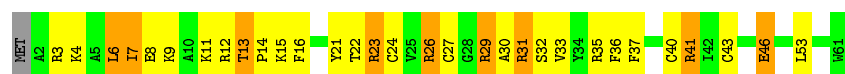




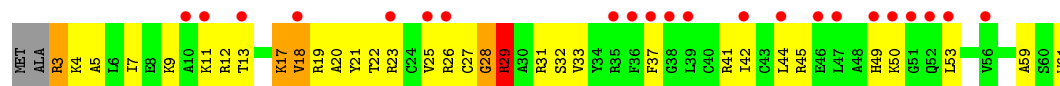
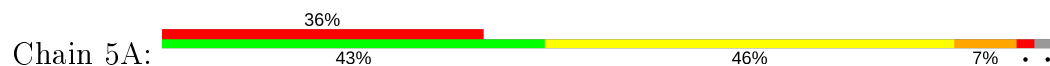
- Molecule 13: 30S ribosomal protein S13



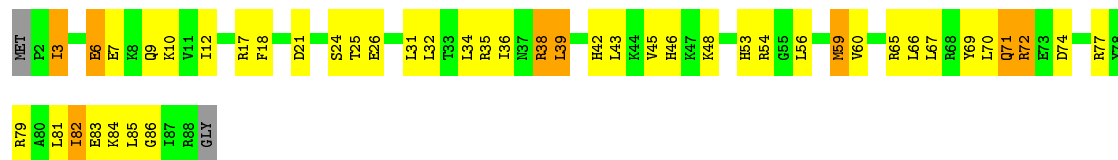
- Molecule 14: 30S ribosomal protein S14 type Z



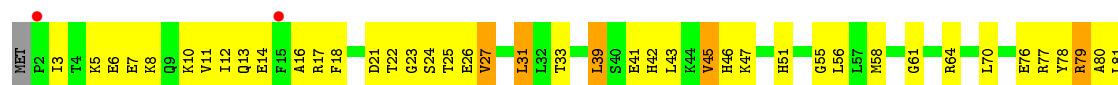
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

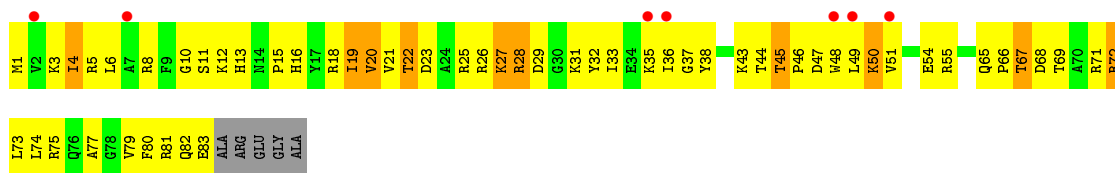


- Molecule 15: 30S ribosomal protein S15

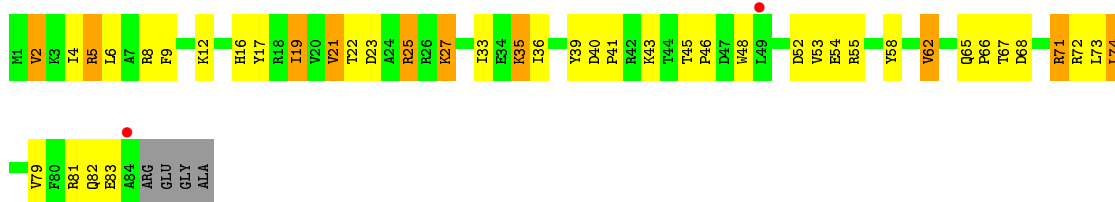




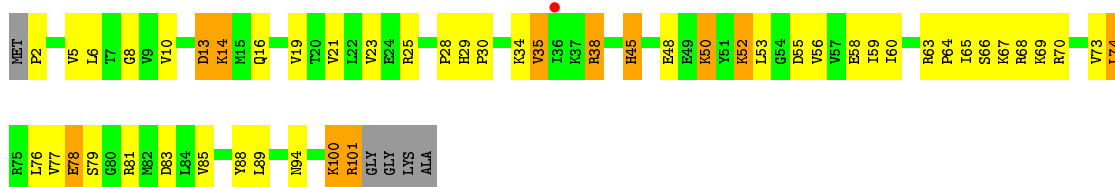
- Molecule 16: 30S ribosomal protein S16



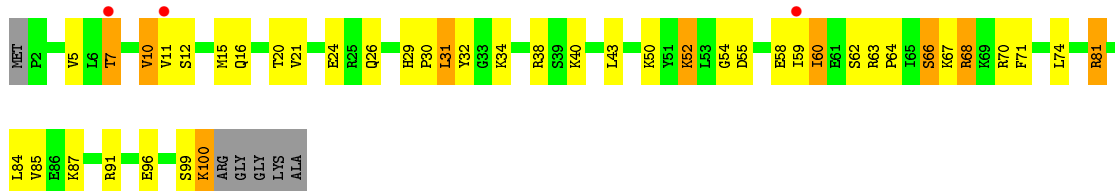
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

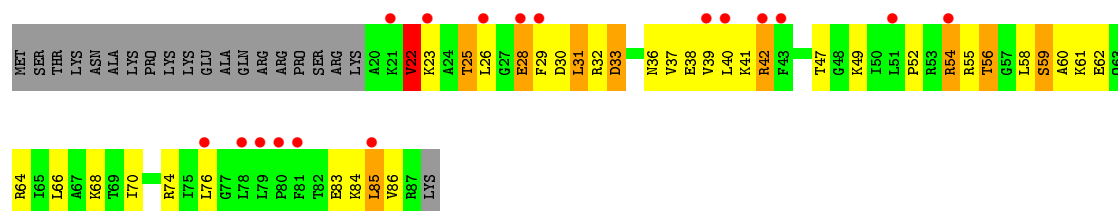


- Molecule 17: 30S ribosomal protein S17

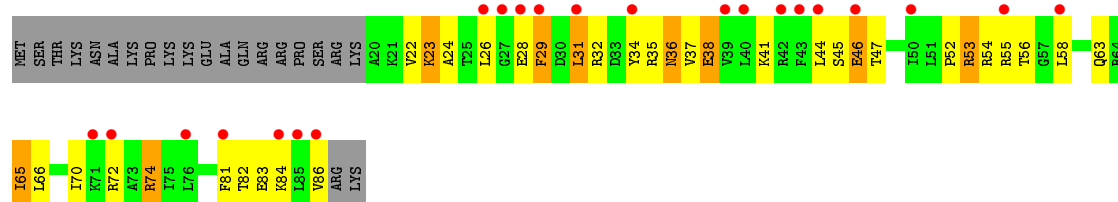


- Molecule 18: 30S ribosomal protein S18

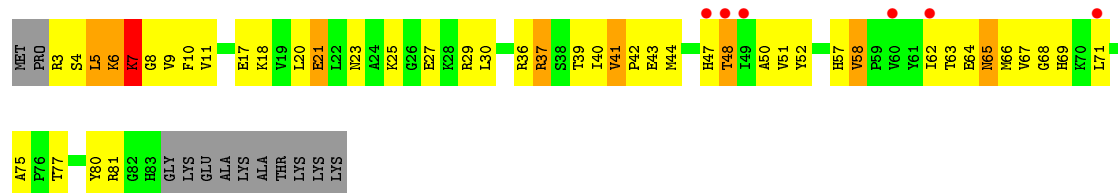




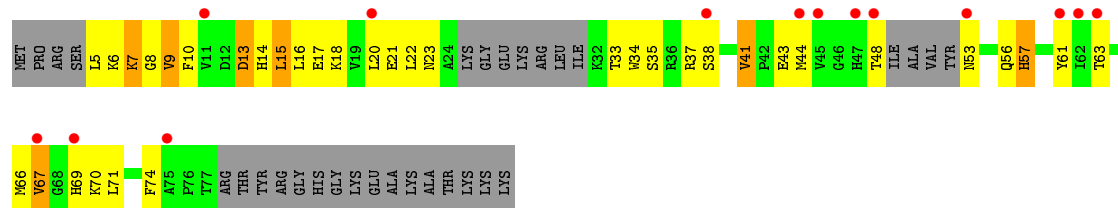
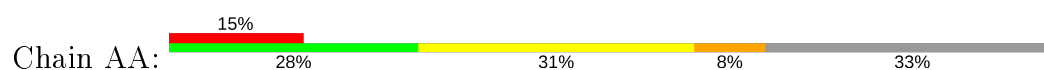
• Molecule 18: 30S ribosomal protein S18



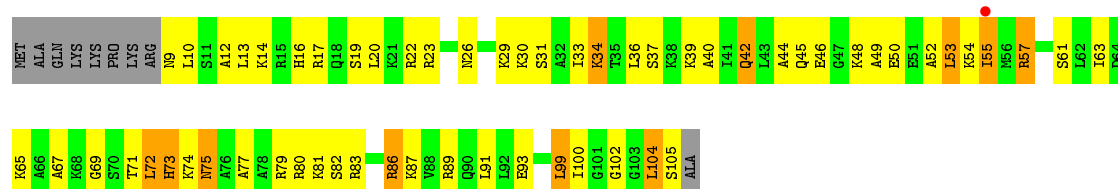
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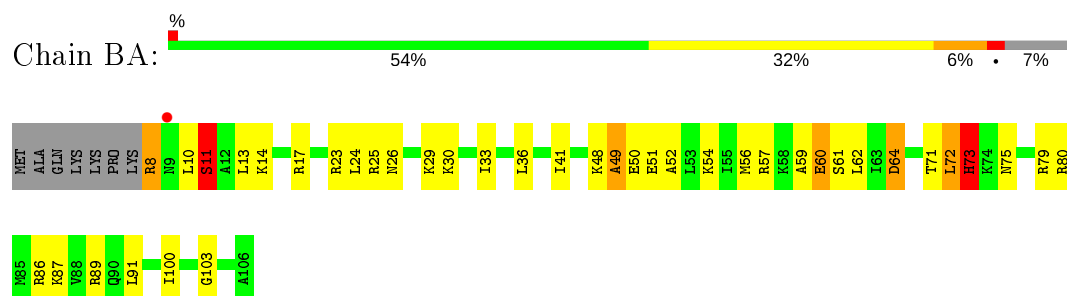
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



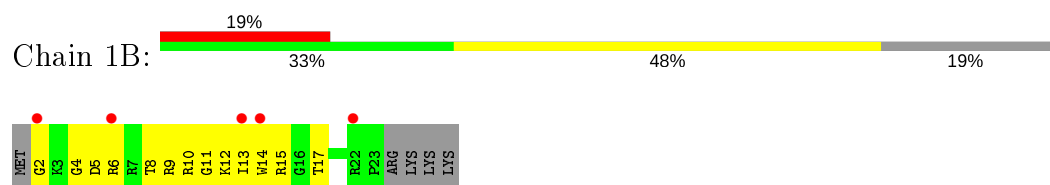
- Molecule 20: 30S ribosomal protein S20



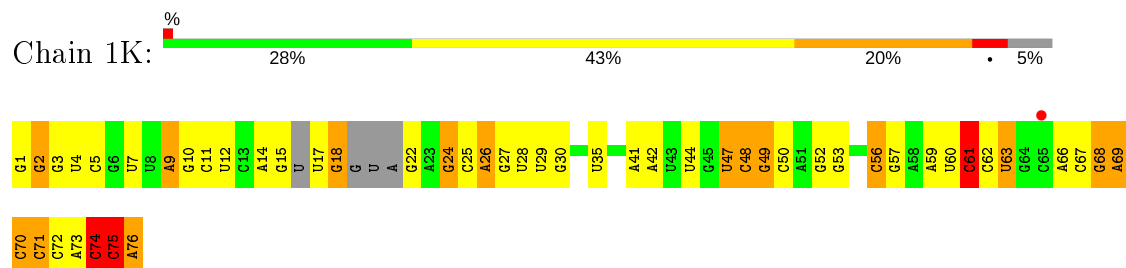
- Molecule 21: 30S ribosomal protein Thx



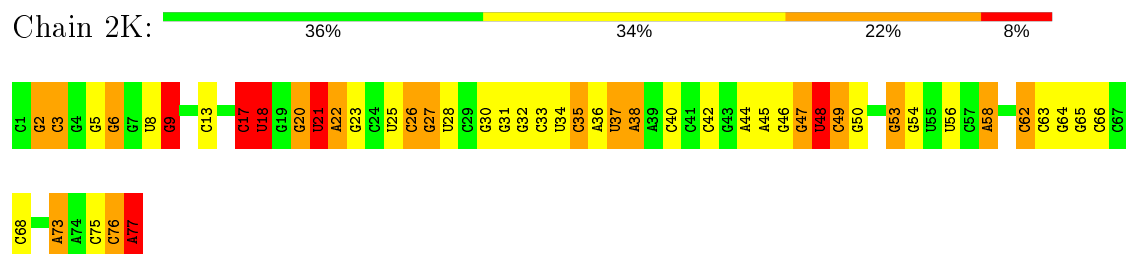
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA^{Lys}

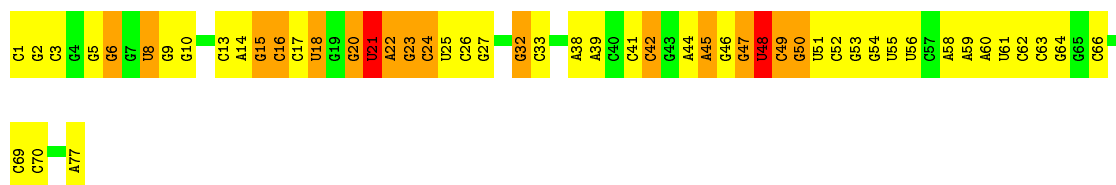


- Molecule 23: tRNA^{fMet}

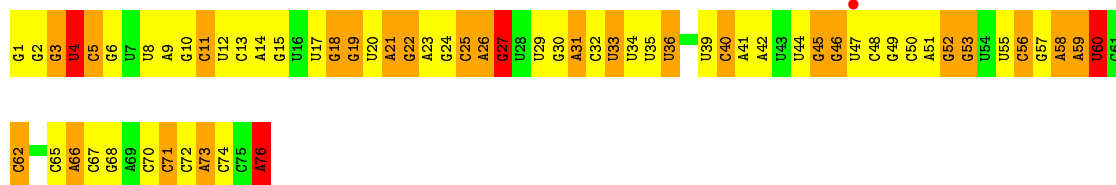
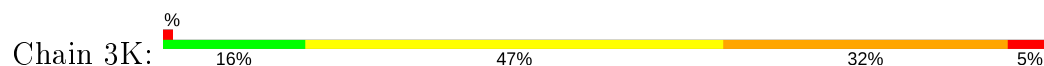


- Molecule 23: tRNA^{fMet}





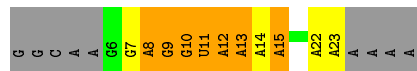
• Molecule 24: tRNA^{Lys}



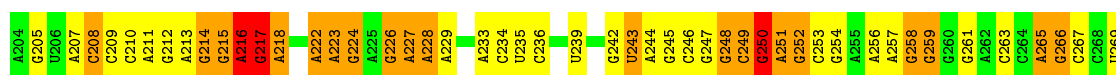
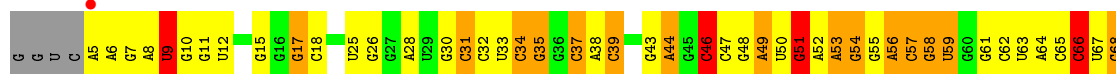
• Molecule 25: mRNA



• Molecule 25: mRNA

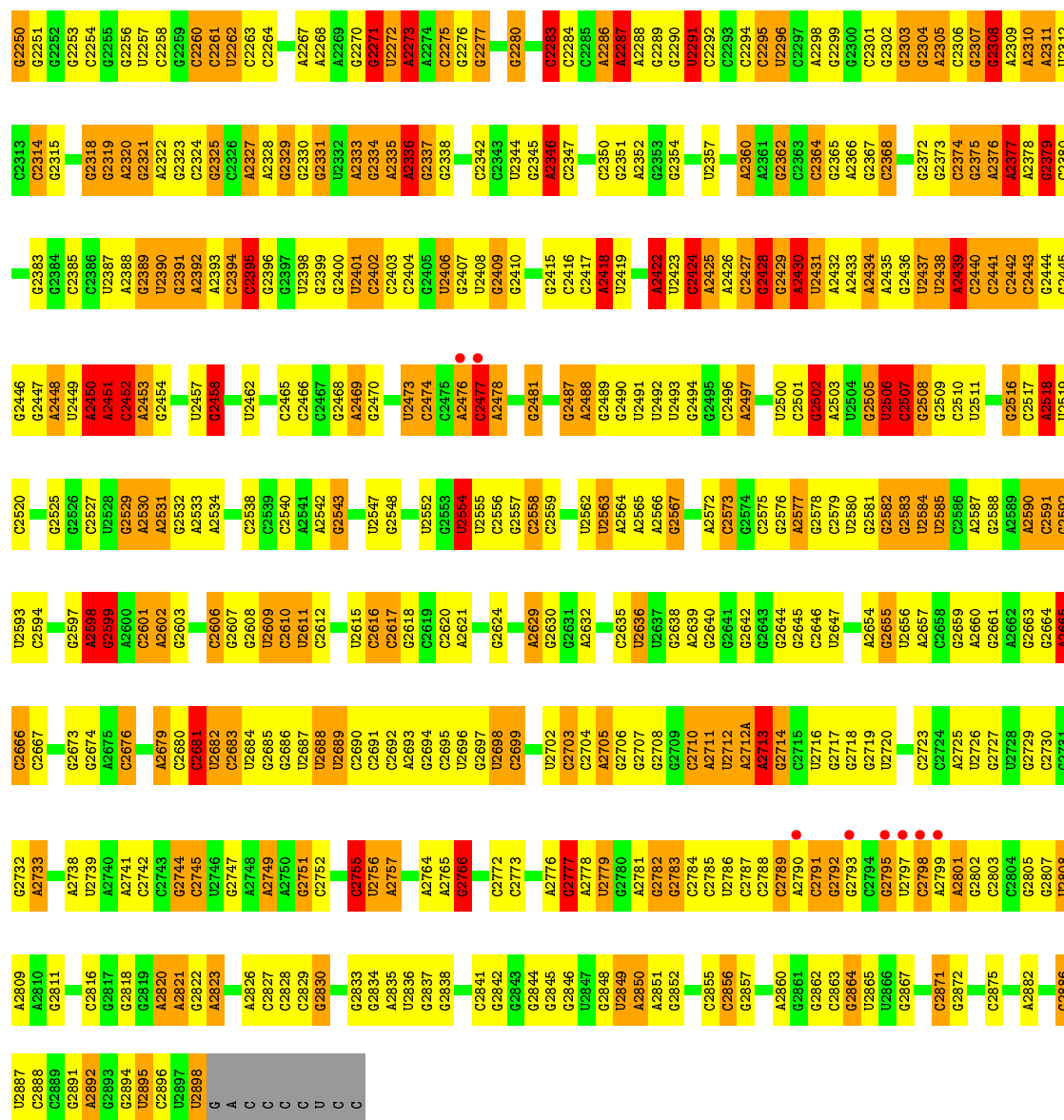


• Molecule 26: 23S rRNA

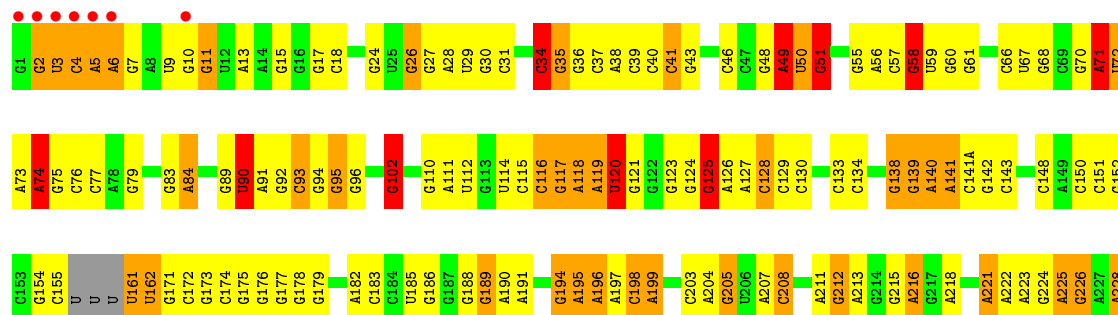


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G1229	G1157	G1026	C961	C997	U828	G763	G700	C	G595	C	A454	C385	G315
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G1246	A1176	G1040	A973	A909	G837	A774	G710	C	G605	G535	U464	U395	A324
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G1248	C1171	G1042	C974A	A911	U839	G776	U714	C654N	U607	C537	A466	G397	G329
G1249	U1178	C1043	A980	C912	C840	A777	U715	A654T	G617	C543	G467	G398	G330
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A1261	G1190	G	C991	C927	G856	A789	G726	C665	G625	G556	A480	C413	G344
A1262	G1191	U	C992	A928	C857	C790	G727	C666	G626	G559	A481	C414	A345
A1263	G1192	U	C993	G928	C858	G791	G728	U667	G627	G562	A482	C415	A346
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A1268	G1197	U	G1002	G933	G862	C796	G733	C672	A632	U568	A492	C426	G354
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A1270	U1199	A	C1004	G935	G864	G	G736	C674	G634	G570	G494	A428	G356
A1271	C1200	A	C1005	G936	C865	U800	G737	A675	C635	A571	G495	A429	A357
A1272	G1201	G	C1006	A941	C866	A801	C738	G676	G636	G572	G496	G430	G363
A1273	U1273	G	C1007	G942	C867	A802	G739	C677	G637	G573	U431	U431	A363A
A1274	U1274	C	C1008	U943	C868	A803	G740	C678	G638	G574	G500	A432	G363B
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A1276	G1206	G	A1010	A945	G870	C806	G742	C680	G640	U576	A502	U434	G363D
A1277	G1207	U	G1011	G946	G871	U807	G743	C681	C641	G577	A503	C435	U363E
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A1281	G1216	U	U1015	C950	C	U813	G747	C685	G647	G582	A507	G442	C365
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A2173	C2111	A2042	U1976	G1904	A1821	G1758	U1673	A1614	G1552	G1487	A1419	G1355	U1294
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C2177	A2114	G2045	C1979	C1909	G1824	A1761	A1676	C1617	C1555	A1490	G1423	A1359	A1298
G2178	G2115	G2046	G1980	C1909	A1825	A1762	A1677	A1618	C1556	G1491	G1424	A1360	G1299
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G2187	G2126	A2057	G1989	C1920	U1834	A1773	C1686	G1627	C1565	C1502	U1432	G1369	A1308
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G2193	G2131	A2062	G1999	A1928	G1842	U1779	C1694	A1632	A1508	U1508	U1438	C1375	C1315
A2198	U2132	C2063	C1999	G1929	G1843	A1780	G1695	G1633	C1572	C1509	A1439	G1376	U1316
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A2225	C2147	A2082	G2018	U1946	C1870	C1795	U1709	G1648	C1588	G1524	G1456	A1393	C1330
C2226	G2148	G2083	A2019	C1947	A1871	U1796	C1710	G1649	C1589	G1525	U1394	A1394	A1331
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C2231	G2152	U2086	U2022	G1950	C1879	G1799	C1726	A1652	C1592	A1528	G1461	U1397	G1334
U2232	G2153	G2087	G2023	U1955	C1879	C1800	G1727	G1653	G1593	C1532	C1462	C1398	U1335
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A2241	G2162	G2101	G2032	A1966	C1895	A1809	C1741	C1662	U1602	G1540	A1471	C1407	G1344
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U2243	C2103	C2103	U2034	G1968	G1897	A1812	A1749	A1664	C1604	C1544	C1476	G1409	G1346
U2244	G2104	G2105	G2035	A1969	G1897	A1813	A1749	A1665	C1605	A1545	A1477	A1412	G1347
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G2246	G2167	G2107	G2037	A1971	G1899	G1816	G1753	G1667	C1607	C1547	G1479	G1414	C1350
C2247	A2169	C2107	U2038	A1972	A1900	G1817	G1754	A1668	A1608	C1548	U1480	U1415	G1351
C2248	A2170	G1973	C2039	A1973	A1901	U1818	A1755	A1669	A1609	C1549	U1482	G1416	U1352
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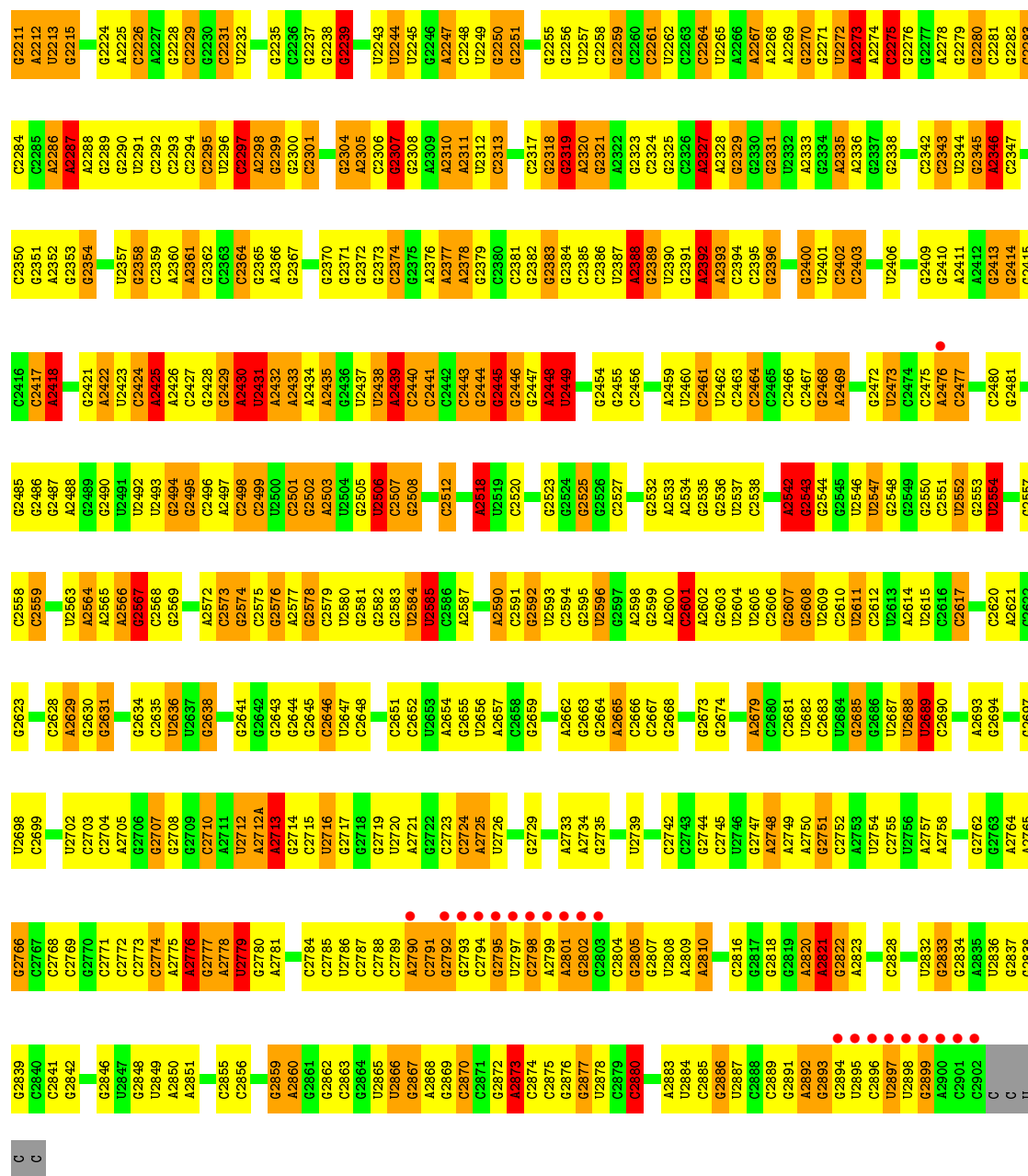


• Molecule 26: 23S rRNA

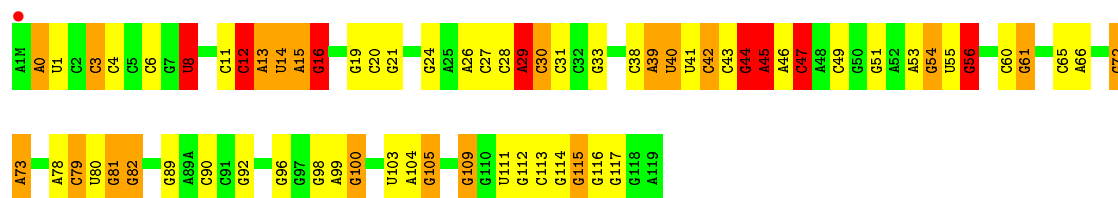
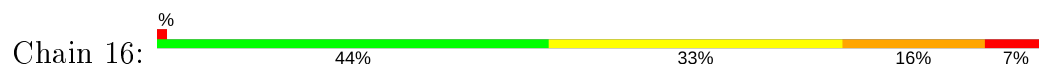


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G1154	A1087	U1026	A959	C997	G832	C766	U694	A654	C587	G520	G450	G363C	C277	A233
A1155	A1027	A1027	A960	C998	U833	G695	G695	A654A	U588	G521	C451	G363C	C279	C234
G1156	A1028	A1028	A961	A899	C834	G771	G696	G654B	C589	G522	C452	G370	A283	U235
A1157	A1029	A1029	A962	A900	A835	G772	G697	G654C	A590	C523	C453	G371	U284	C236
G1158	G1030	G1030	U963	A901	G836	U773	C698	G654D	C591	U524	A454	G372	A288	U243
U1159	G1031	G1031	G902	C902	C837	A774	A699	C	C595	A526	C455	G373	U239	
G1160	C1032	A1032	C903	C903	C838	G775	G700	C	C596	A527	C456	U372	G247	
C1161	U1033	U1033	C904	C904	U839	A776	G704	C	G596	C527	A457	U373	G248	
G1164	G1034	G1034	U905	C940	C840	A777	A705	G	U597	A528	G458	C374	G240	
U1165	U1035	U1035	G906	A841	A841	G778	A706	A	G598	A529	U459	C375	A241	
G1166	A1036	A1036	U907	G842	G842	U779	A707	C	G599	G530	A460	U380	G242	
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G1168	C1038	C1038	A909	A909	A782	A781	C708	G	C601	A532	G462	U382	G247	
G1169	G1039	G1039	A910	A910	U709	A782	U709	C	G602	G533	G463	U383	G248	
C1170	G1040	G1040	A911	A911	C946	A783	G717	G	A603	U534	G468	U384	A299	
G1171	C1041	C1041	C912	C912	U847	A784	A718	G	G604	C535	C469	U385	A300	
G1173	U1042	U1042	U913	U913	G848	G785	G719	C	C605	A536	A470	G386	G301	
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G1175	G1044	G1044	U915	U915	U851	U787	C721	A654R	A608	G540	A472	G388	U303	
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G1177	A	A	A917	A917	G855	A722	A722	G	G609A	C542		C392	U305	
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G1181	A1050	A1050	G921	G921	G859	G726	G726	U657	G615	A548	A481	G396	G309	
A1182	G1051	G1051	U922	U922	U860	A727	A727	C658	G616	G549	A482	G397	A311	
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G1194	U1063	U1063	C935	C935	A872	G739	G739	A670	G630	C564	A494	C419	A337	
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U1198	G1003	G1003	U937	U937	C876	G741	G741	G674	A632	U566	A496	C421	A339	
U1199	U1004	U1004	G938	G938	A878	G742	G742	A675	A633	U569	A497	C422	A340	
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G1205	C1072	C1072	G944	G944	C	G748	G748	G681	U639	C575	A506	C428	A346	
U1206	U1012	U1012	A945	A945	G	C749	C749	G682	C640	U576	A507	C429	A347	
U1207	C1013	C1013	G946	G946	C	A816	A750	G683	C641	U577	A508	C430	A348	
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U1212	U1017	U1017	C951	C951	C	A820	C753	G687	C645	C580	U512	C434	A352	
G1213	C1018	C1018	G952	G952	C	G823	C754	C688	A646	C581	A513	C435	A353	
A1214	U1019	U1019	A953	A953	A	A824	G760	U689	A647	C582	A514	C436	A354	
G1215	A1020	A1020	G954	G954	C	C825	A761	A690	G647	C583	A515	C437	A355	
U1216	U1021	U1021	C955	C955	G	U826	U762	A691	C650	C584	A516	C438	A356	
G1217	G1022	G1022	G956	G956	C	U827	G763	C691			A517	C439	A357	
	U1023	U1023				U828					A518	C440	A358	
											A519	C441	A359	
											A520	C442	A360	
											A521	C443	A361	
											A522	C444	A362	
											A523	C445	A363	
											A524	C446	A364	
											A525	C447	A365	
											A526	C448	A366	
											A527	C449	A367	
											A528	C450	A368	
											A529	C451	A369	
											A530	C452	A370	
											A531	C453	A371	
											A532	C454	A372	
											A533	C455	A373	
											A534	C456	A374	
											A535	C457	A375	
											A536	C458	A376	
											A537	C459	A377	
											A538	C460	A378	
											A539	C461	A379	
											A540	C462	A380	
											A541	C463	A381	
											A542	C464	A382	
											A543	C465	A383	
											A544	C466	A384	
											A545	C467	A385	
											A546	C468	A386	
											A547	C469	A387	
											A548	C470	A388	
											A549	C471	A389	
											A550	C472	A390	
											A551	C473	A391	
											A552	C474	A392	
											A553	C475	A393	
											A554	C476	A394	
											A555	C477	A395	
											A556	C478	A396	
											A557	C479	A397	
											A558	C480	A398	
											A559	C481	A399	
											A560	C482	A400	
											A561	C483	A401	
											A562	C484	A402	
											A563	C485	A403	
											A564	C486	A404	
											A565	C487	A405	
											A566	C488	A406	
											A567	C489	A407	
											A568	C490	A408	
											A569	C491	A409	
											A570	C492	A410	
											A571	C493	A411	
											A572	C494	A412	
											A573	C495	A413	
											A574	C496	A414	
											A575	C497	A415	
											A576	C498	A416	
											A577	C499	A417	
		</												





• Molecule 27: 5S rRNA

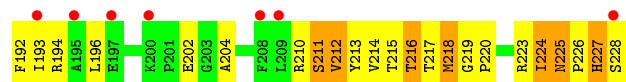
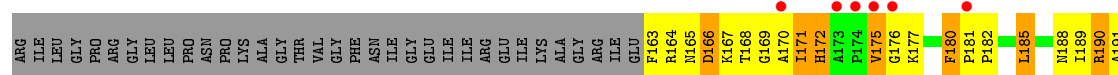
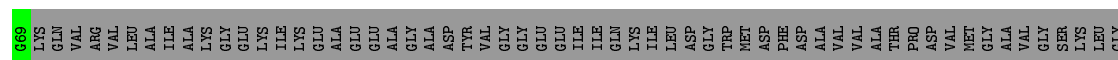
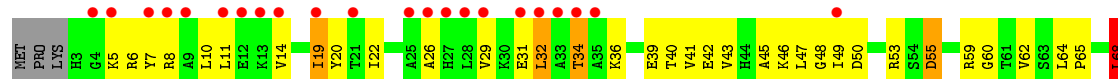
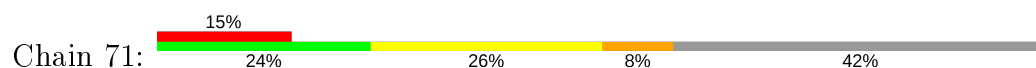


• Molecule 27: 5S rRNA

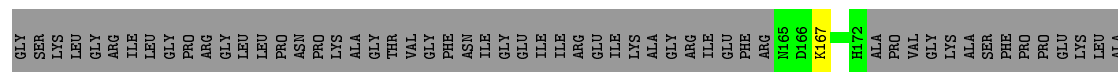
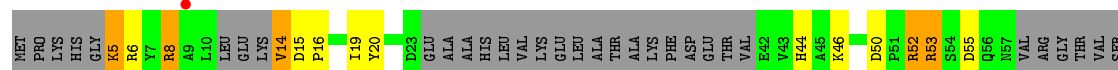




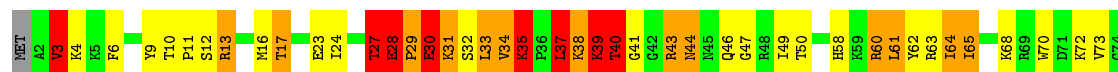
• Molecule 28: 50S ribosomal protein L1

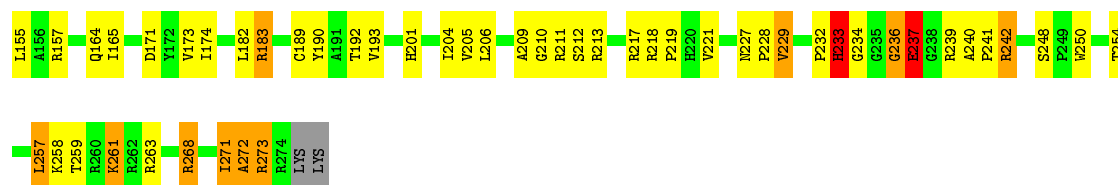


• Molecule 28: 50S ribosomal protein L1

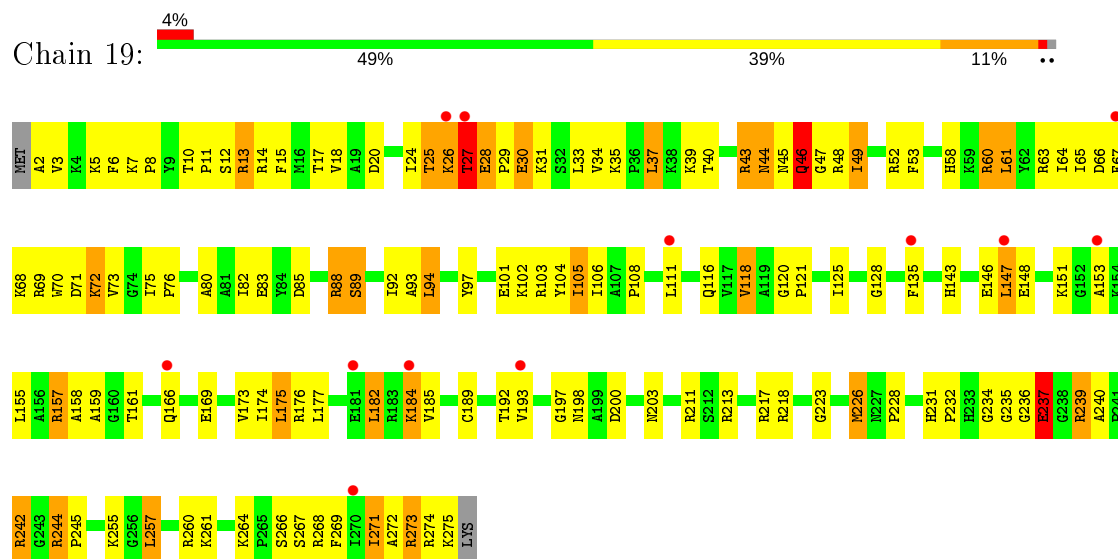


• Molecule 29: 50S ribosomal protein L2

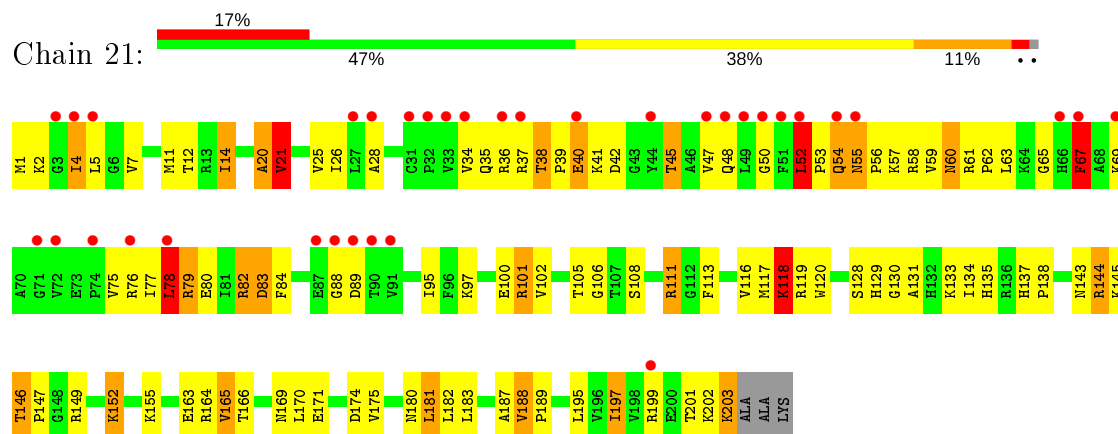




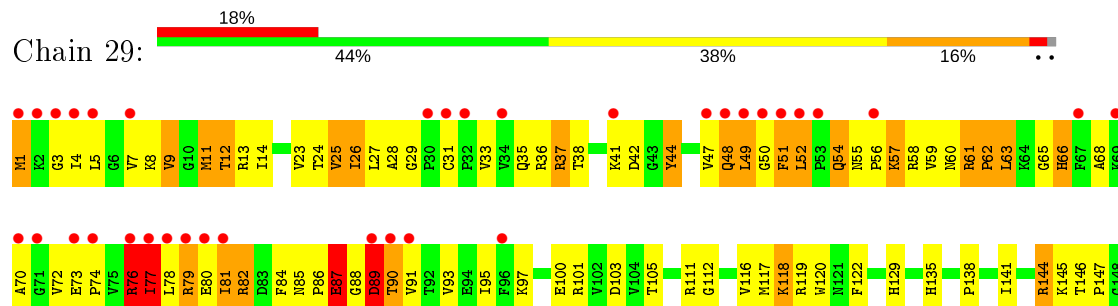
• Molecule 29: 50S ribosomal protein L2



• Molecule 30: 50S ribosomal protein L3

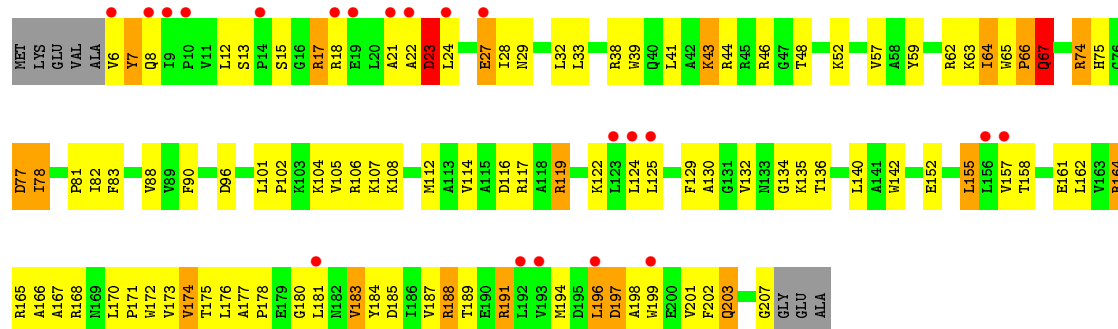


• Molecule 30: 50S ribosomal protein L3

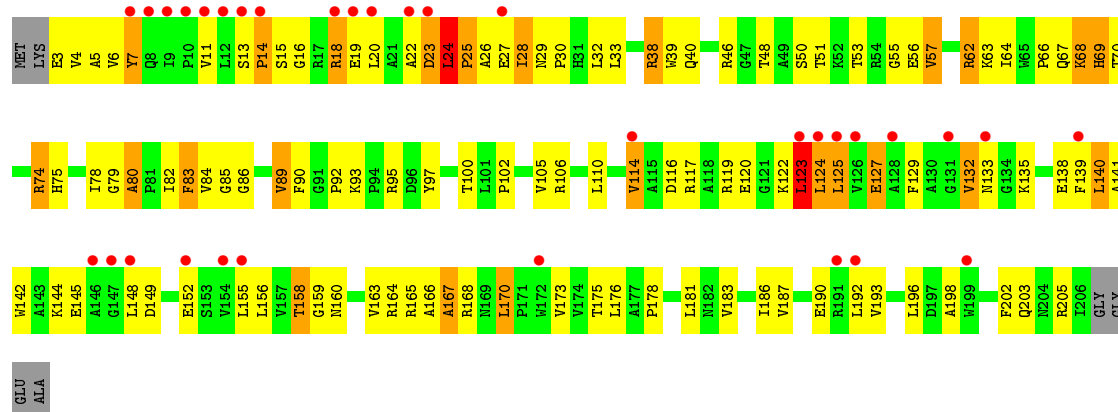
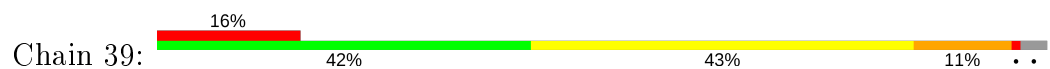




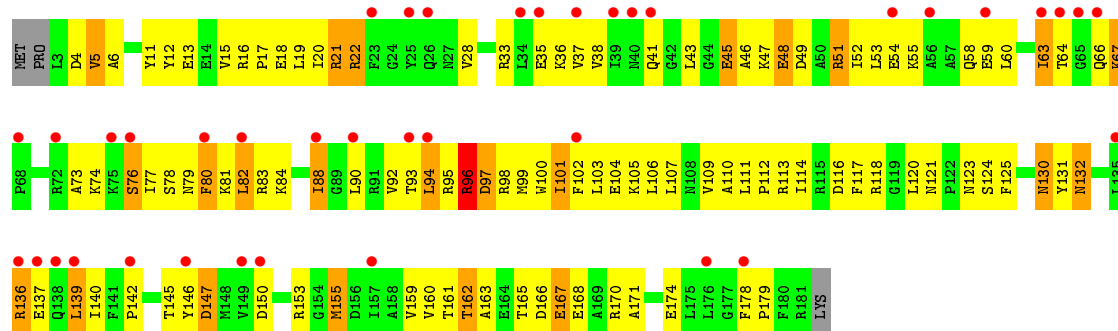
• Molecule 31: 50S ribosomal protein L4



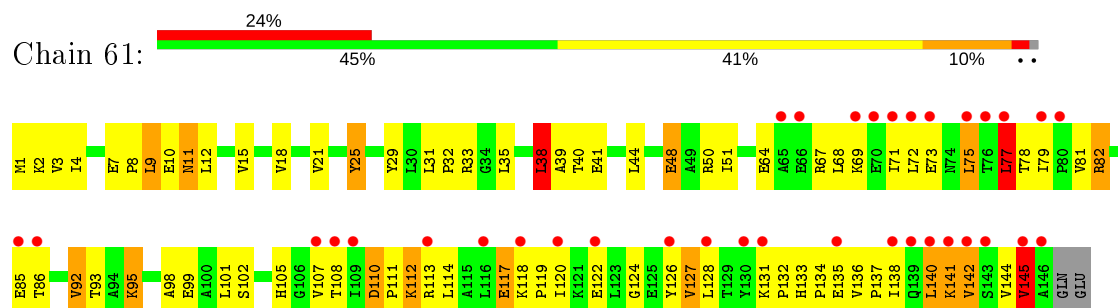
• Molecule 31: 50S ribosomal protein L4



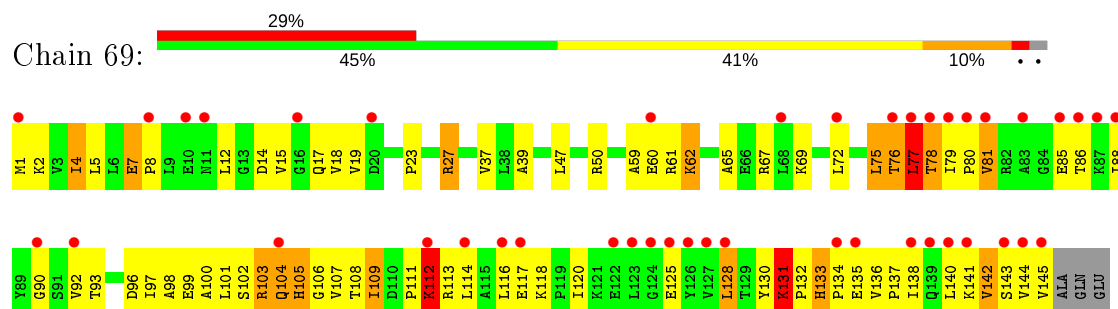
• Molecule 32: 50S ribosomal protein L5



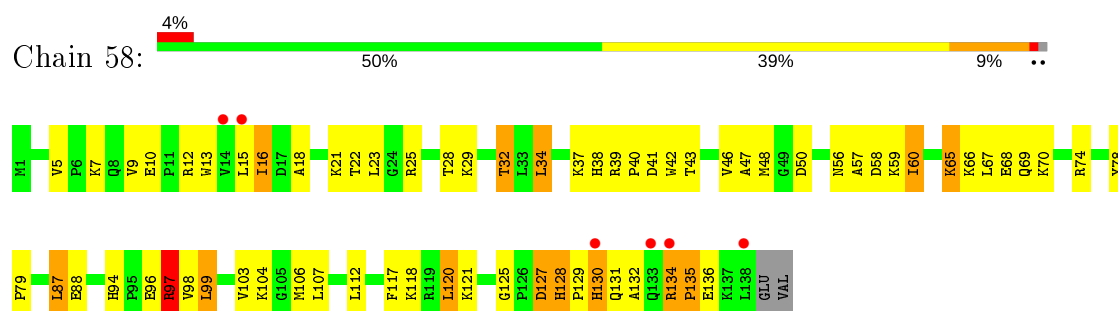
• Molecule 32: 50S ribosomal protein L5



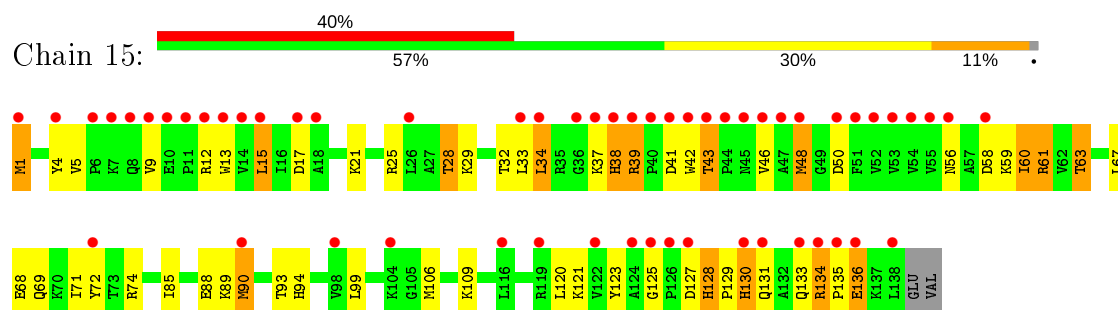
- Molecule 34: 50S ribosomal protein L9



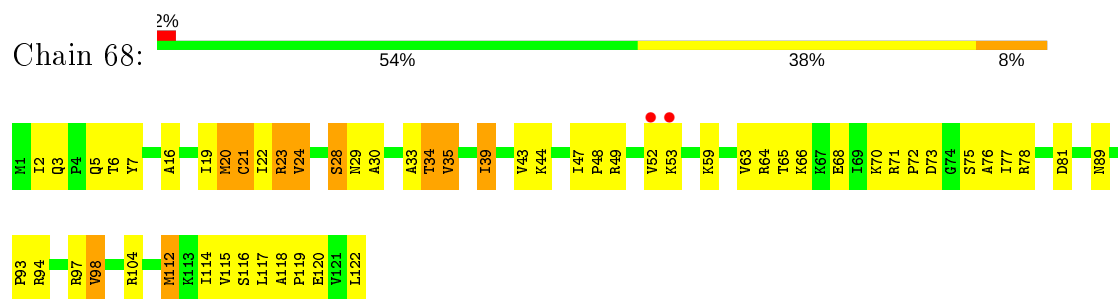
- Molecule 35: 50S ribosomal protein L13



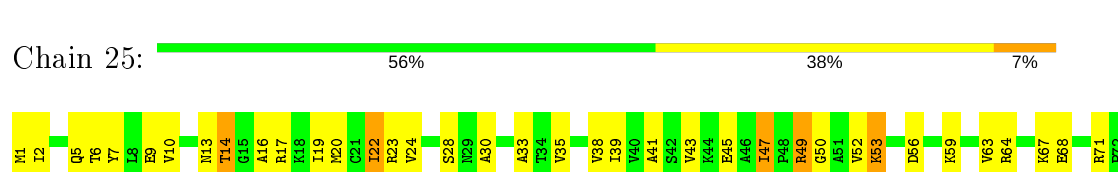
- Molecule 35: 50S ribosomal protein L13

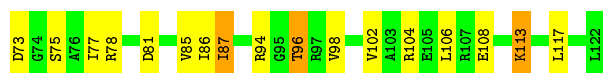


- Molecule 36: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L14

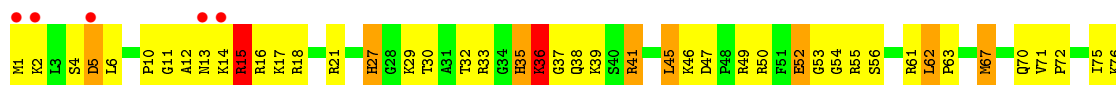




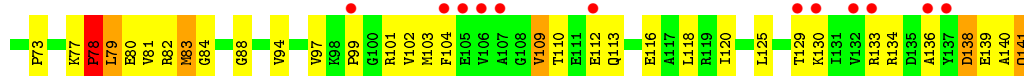
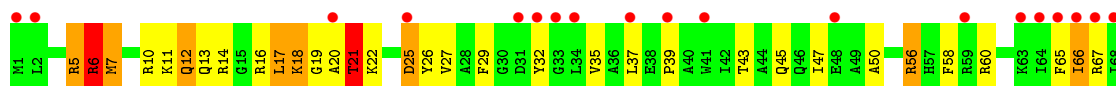
- Molecule 37: 50S ribosomal protein L15



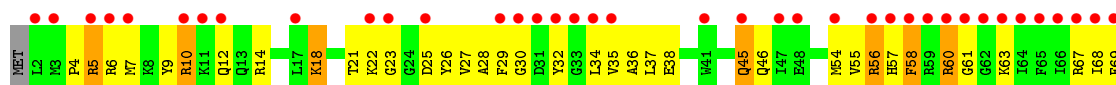
- Molecule 37: 50S ribosomal protein L15

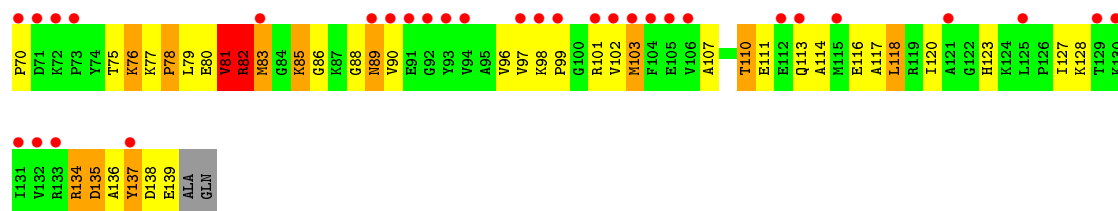


- Molecule 38: 50S ribosomal protein L16

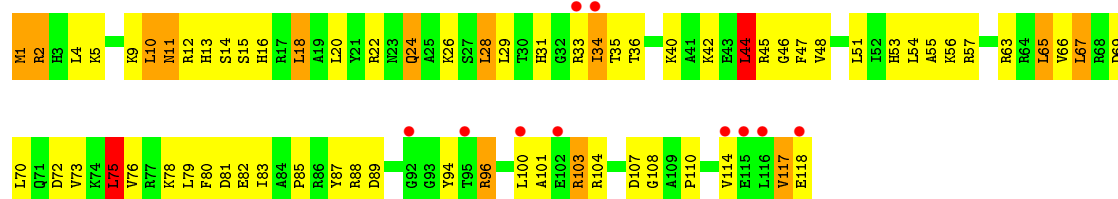
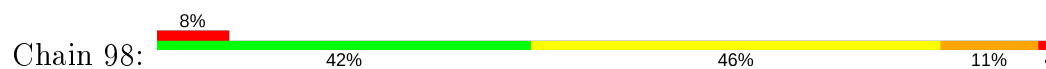


- Molecule 38: 50S ribosomal protein L16

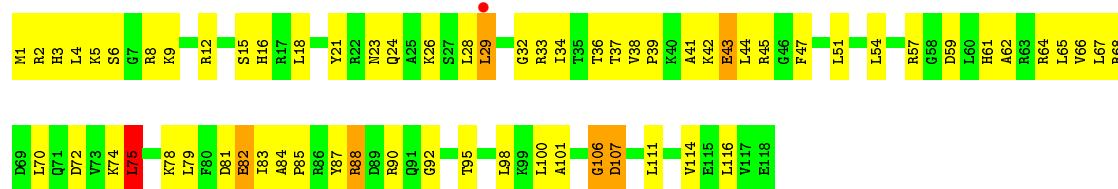
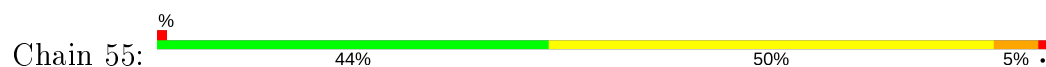




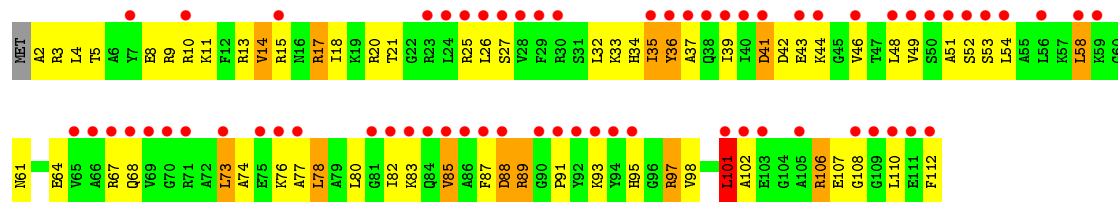
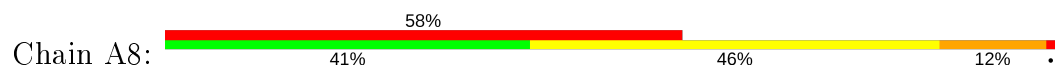
• Molecule 39: 50S ribosomal protein L17



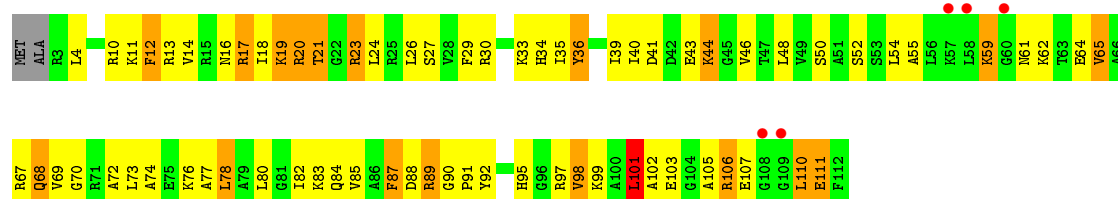
• Molecule 39: 50S ribosomal protein L17



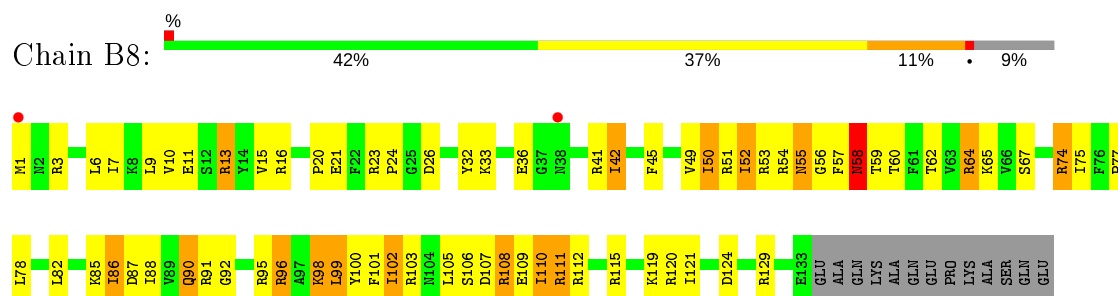
• Molecule 40: 50S ribosomal protein L18



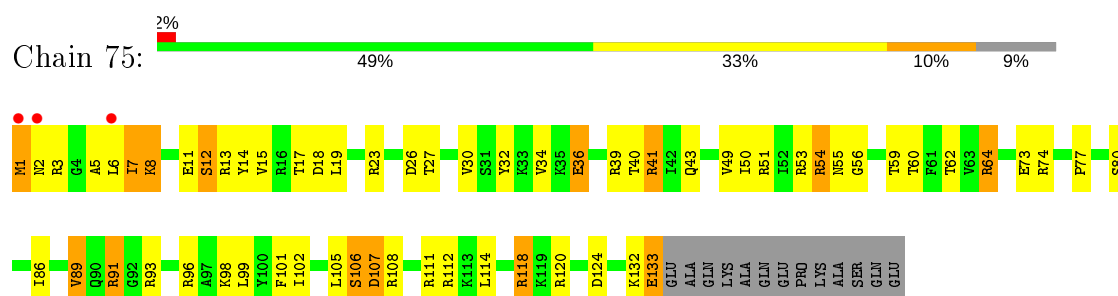
• Molecule 40: 50S ribosomal protein L18



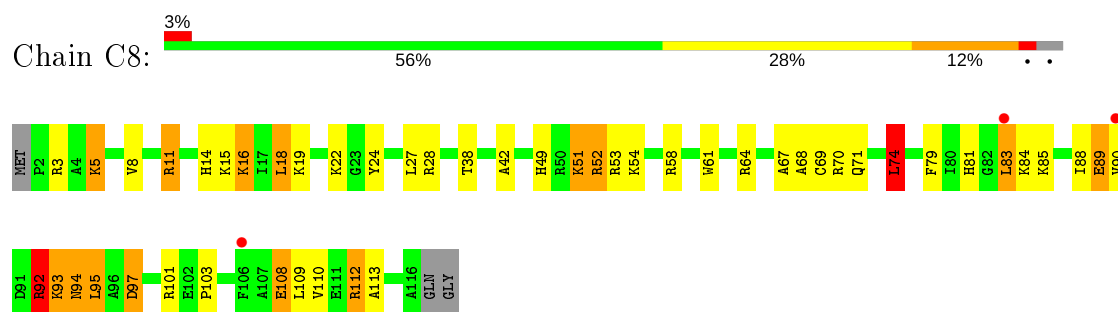
- Molecule 41: 50S ribosomal protein L19



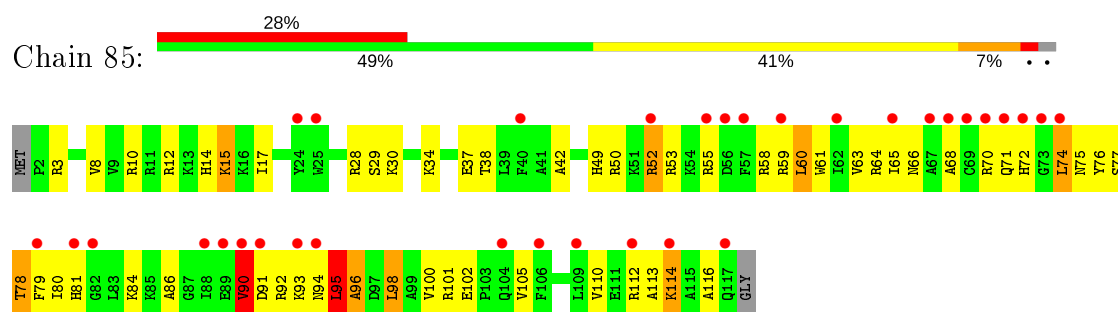
- Molecule 41: 50S ribosomal protein L19



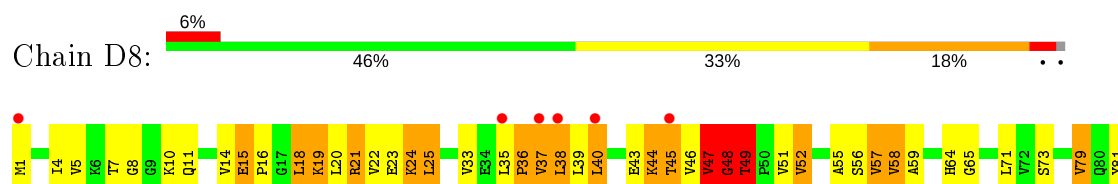
- Molecule 42: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L20

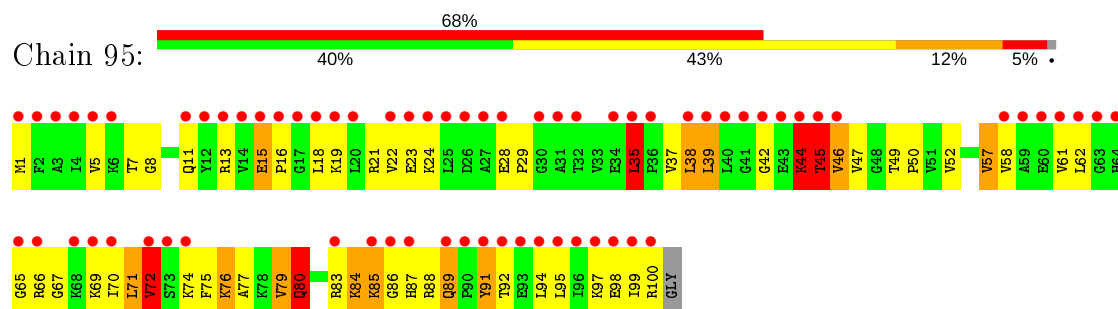


- Molecule 43: 50S ribosomal protein L21

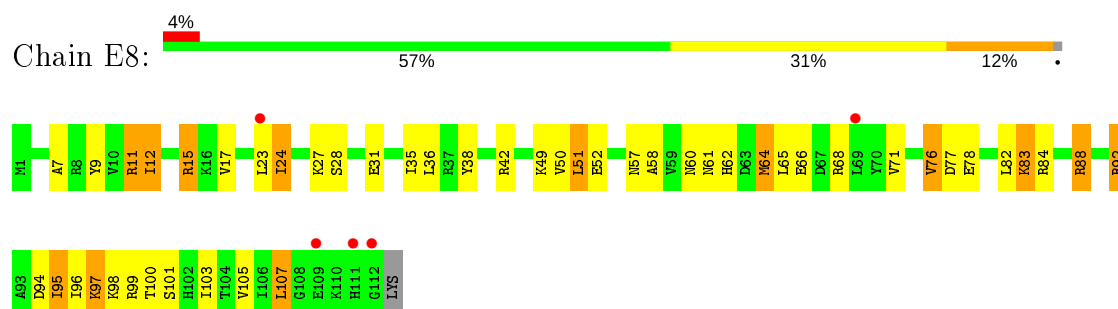




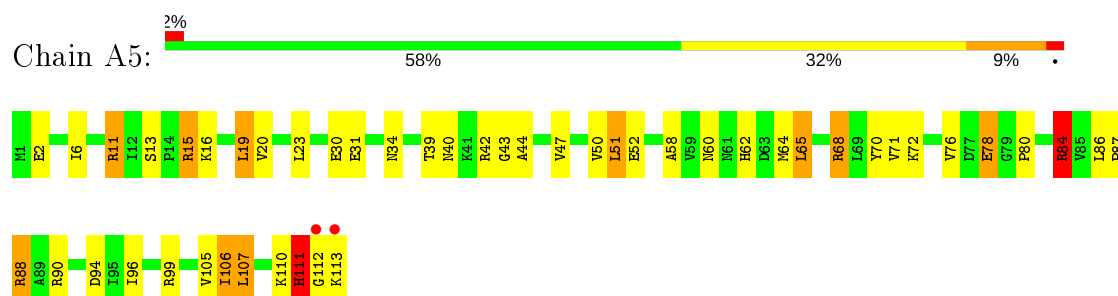
- Molecule 43: 50S ribosomal protein L21



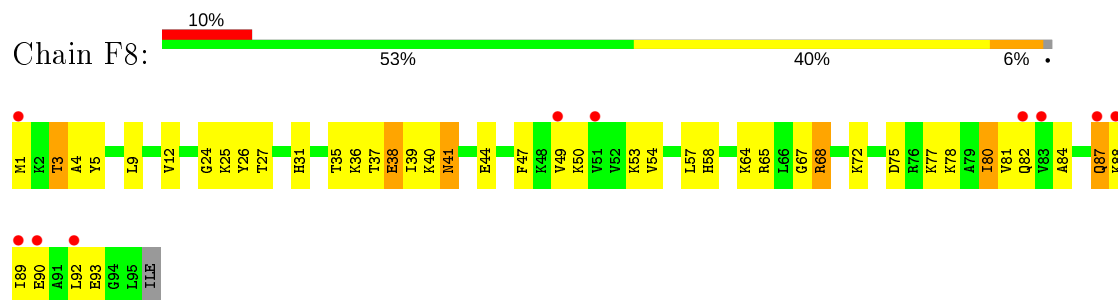
- Molecule 44: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L22

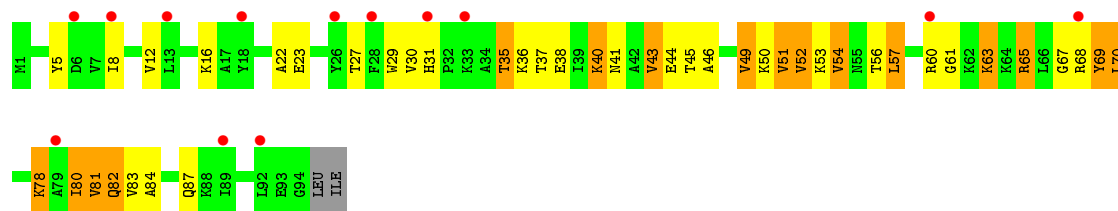


- Molecule 45: 50S ribosomal protein L23



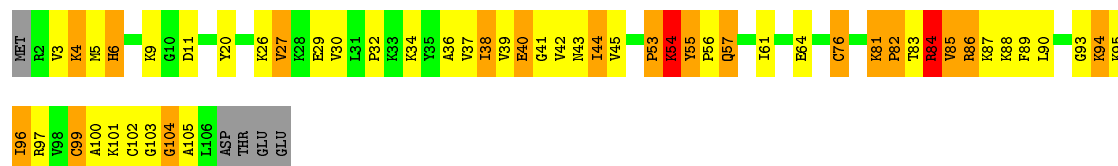
- Molecule 45: 50S ribosomal protein L23





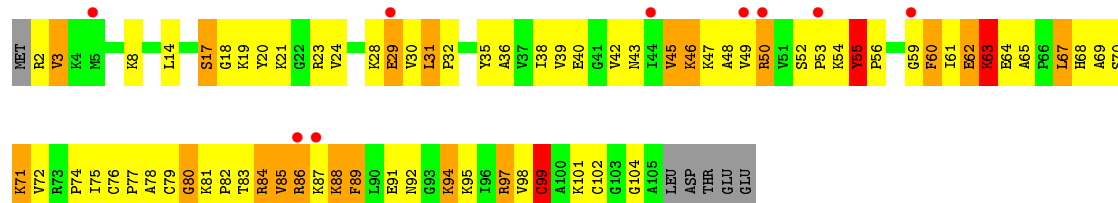
• Molecule 46: 50S ribosomal protein L24

Chain G8: 47% 30% 16% 5%



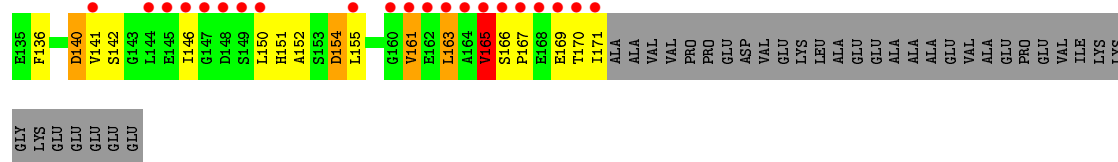
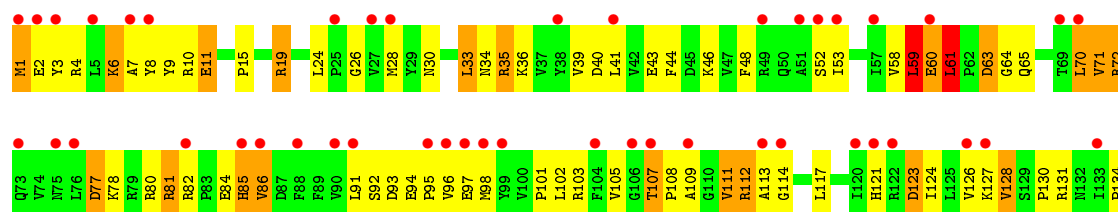
• Molecule 46: 50S ribosomal protein L24

Chain C5: 8% 28% 46% 17% 5%



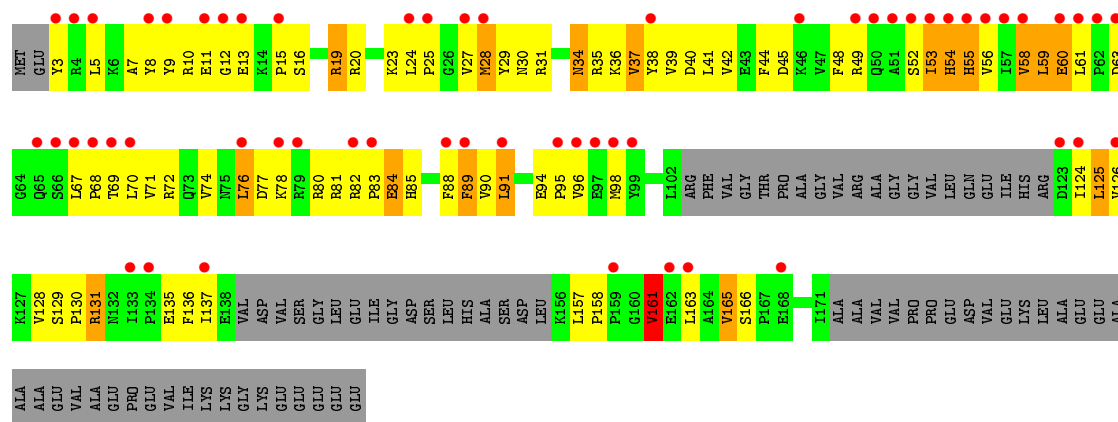
• Molecule 47: 50S ribosomal protein L25

Chain H8: 32% 37% 33% 12% 17%

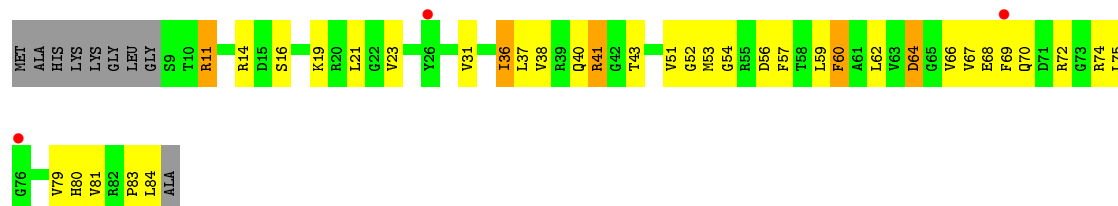


• Molecule 47: 50S ribosomal protein L25

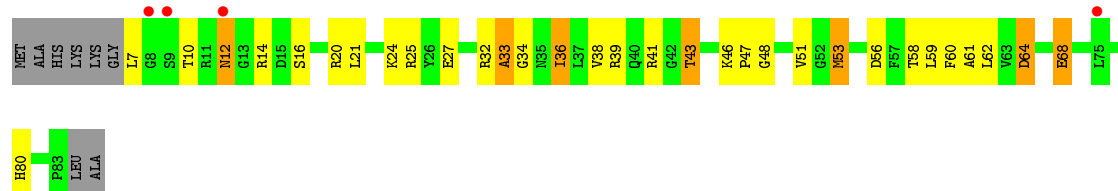
Chain D5: 28% 23% 32% 8% 36%



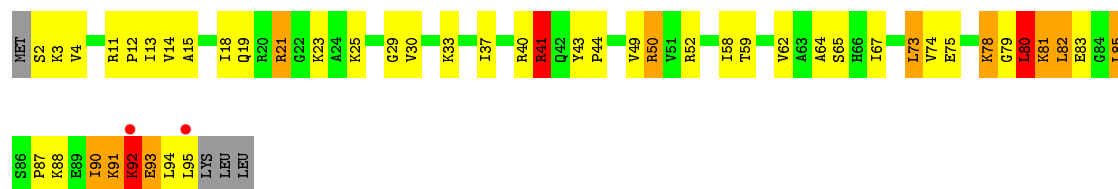
• Molecule 48: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L27

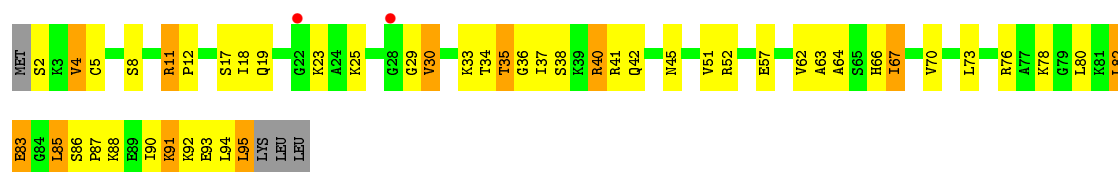


• Molecule 49: 50S ribosomal protein L28

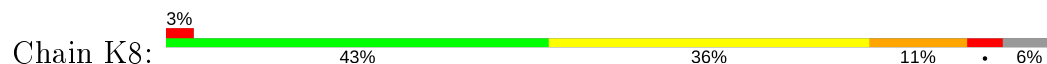


• Molecule 49: 50S ribosomal protein L28

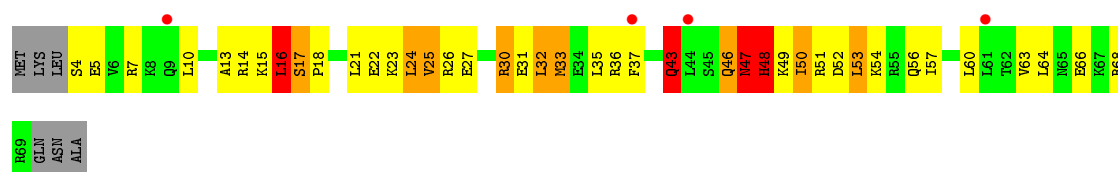




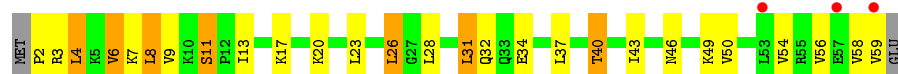
- Molecule 50: 50S ribosomal protein L29



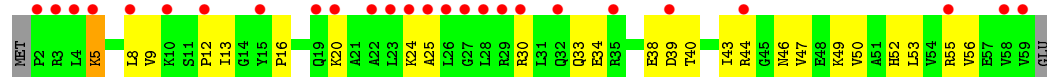
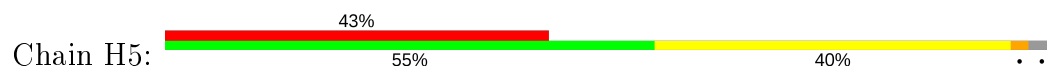
- Molecule 50: 50S ribosomal protein L29



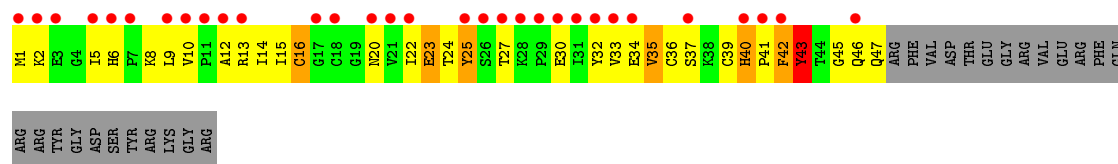
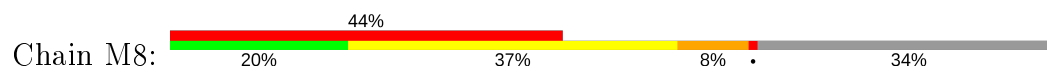
- Molecule 51: 50S ribosomal protein L30



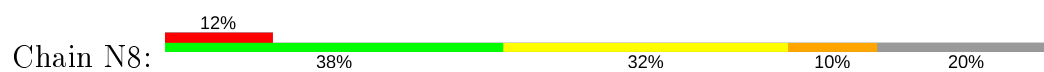
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L34



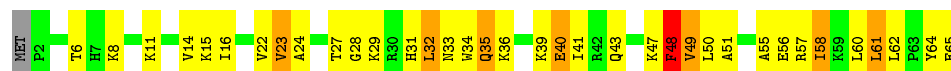
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35

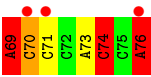


- Molecule 55: 50S ribosomal protein L35

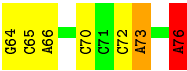
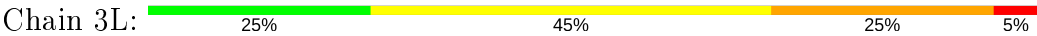


- Molecule 56: tRNA^{Lys}





● Molecule 57: tRNA^{Lys}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.50Å 450.10Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.72 – 3.20 173.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.72-3.20) 93.8 (173.72-3.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.258 0.192 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	294444	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

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

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, U8U, G7M, SF4, MG, 4SU, T6A, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.75	5/35994 (0.0%)	1.39	368/56171 (0.7%)
1	1G	0.64	1/36258 (0.0%)	1.26	191/56589 (0.3%)
2	12	0.44	0/1752	0.74	1/2360 (0.0%)
2	1E	0.46	0/1908	0.74	4/2573 (0.2%)
3	22	0.40	0/1564	0.64	1/2109 (0.0%)
3	2E	0.49	0/1629	0.67	0/2195
4	32	0.48	0/1732	0.74	1/2318 (0.0%)
4	3E	0.52	0/1728	0.74	1/2313 (0.0%)
5	42	0.45	0/1150	0.69	0/1548
5	4E	0.53	0/1158	0.71	0/1559
6	52	0.51	0/855	0.68	0/1154
6	5E	0.57	0/850	0.72	0/1147
7	62	0.43	0/1122	0.65	0/1500
7	6E	0.43	0/1259	0.59	0/1686
8	72	0.41	0/1127	0.65	0/1517
8	7E	0.47	0/1135	0.74	1/1527 (0.1%)
9	82	0.42	0/971	0.71	0/1304
9	8E	0.44	0/1019	0.66	0/1367
10	1A	0.42	0/658	0.60	0/885
10	1I	0.51	0/747	0.75	1/1006 (0.1%)
11	2A	0.45	0/850	0.63	0/1150
11	2I	0.49	0/838	0.69	0/1133
12	3A	0.55	0/972	0.83	2/1301 (0.2%)
12	3I	0.72	0/972	0.87	0/1301
13	4A	0.42	0/903	0.72	1/1211 (0.1%)
13	4I	0.53	0/952	0.73	0/1277
14	5A	0.47	0/495	0.72	1/657 (0.2%)
14	5I	0.62	0/500	0.75	0/664
15	6A	0.44	0/744	0.59	0/992
15	6I	0.52	0/740	0.71	0/987
16	7A	0.49	0/721	0.74	0/970
16	7I	0.47	0/716	0.73	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.45	0/836	0.64	0/1117
17	8I	0.52	0/847	0.70	0/1131
18	9A	0.46	0/549	0.70	0/732
18	9I	0.53	0/554	0.77	0/739
19	AA	0.44	0/490	0.70	0/662
19	AI	0.53	0/668	0.79	0/899
20	BA	0.43	0/764	0.73	0/1007
20	BI	0.43	0/748	0.65	1/986 (0.1%)
21	1B	0.47	0/192	0.70	0/252
21	1F	0.52	0/203	0.68	0/266
22	1K	0.66	0/1565	1.29	14/2429 (0.6%)
23	2K	0.84	1/1721 (0.1%)	1.50	32/2682 (1.2%)
23	2L	0.66	1/1721 (0.1%)	1.24	10/2682 (0.4%)
24	3K	0.67	0/1799	1.31	17/2801 (0.6%)
25	4K	0.91	0/473	1.34	1/737 (0.1%)
25	4L	0.67	0/448	1.13	0/698
26	14	0.90	57/69023 (0.1%)	1.59	1407/107740 (1.3%)
26	1H	1.06	113/68351 (0.2%)	1.80	2304/106700 (2.2%)
27	16	0.84	0/2928	1.55	47/4568 (1.0%)
27	1J	0.70	0/2928	1.36	28/4568 (0.6%)
28	71	0.46	0/1055	0.72	1/1425 (0.1%)
28	79	0.43	0/459	0.90	3/608 (0.5%)
29	11	0.82	2/2170 (0.1%)	1.01	7/2926 (0.2%)
29	19	0.71	1/2175 (0.0%)	0.93	3/2933 (0.1%)
30	21	0.67	0/1591	0.96	2/2146 (0.1%)
30	29	0.63	0/1596	0.92	2/2153 (0.1%)
31	31	0.73	1/1620 (0.1%)	0.91	1/2194 (0.0%)
31	39	0.62	0/1637	0.90	3/2218 (0.1%)
32	41	0.52	0/1481	0.78	1/1994 (0.1%)
32	49	0.43	0/1482	0.68	0/1994
33	51	0.68	0/1337	1.00	9/1809 (0.5%)
33	59	0.46	0/577	0.88	2/776 (0.3%)
34	61	0.52	0/1151	0.80	2/1558 (0.1%)
34	69	0.46	0/1146	0.77	3/1551 (0.2%)
35	15	0.46	0/1131	0.68	0/1525
35	58	0.60	0/1131	0.82	0/1525
36	25	0.58	0/942	0.74	0/1269
36	68	0.67	0/942	0.81	0/1269
37	35	0.61	0/1139	0.98	2/1514 (0.1%)
37	78	0.70	0/1139	1.12	8/1514 (0.5%)
38	45	0.69	0/1120	0.97	4/1498 (0.3%)
38	88	0.78	0/1134	0.98	2/1519 (0.1%)
39	55	0.64	0/981	0.85	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	98	0.56	0/981	0.85	1/1312 (0.1%)
40	65	0.51	0/886	0.86	3/1180 (0.3%)
40	A8	0.63	0/891	0.85	1/1187 (0.1%)
41	75	0.56	0/1123	0.72	0/1500
41	B8	0.66	0/1123	0.82	0/1500
42	85	0.59	0/977	0.75	1/1301 (0.1%)
42	C8	0.67	0/968	0.82	1/1289 (0.1%)
43	95	0.70	0/785	0.87	1/1052 (0.1%)
43	D8	0.58	0/785	0.90	4/1052 (0.4%)
44	A5	0.62	0/910	0.84	1/1220 (0.1%)
44	E8	0.66	0/901	0.87	0/1209
45	B5	0.68	0/749	0.79	0/1007
45	F8	0.76	0/757	0.87	0/1017
46	C5	0.63	0/807	0.93	2/1076 (0.2%)
46	G8	0.82	1/809 (0.1%)	1.08	4/1080 (0.4%)
47	D5	0.51	0/1098	0.73	0/1487
47	H8	0.53	0/1403	0.81	1/1901 (0.1%)
48	E5	0.57	0/616	0.84	0/821
48	I8	0.76	0/614	0.94	0/819
49	F5	0.66	0/744	0.88	1/989 (0.1%)
49	J8	0.73	0/744	0.93	4/989 (0.4%)
50	G5	0.59	0/560	0.82	2/741 (0.3%)
50	K8	0.72	0/570	0.97	0/755
51	H5	0.49	0/464	0.66	0/623
51	L8	0.63	0/464	0.84	0/623
52	M8	0.53	0/375	0.95	2/507 (0.4%)
53	J5	0.61	0/448	0.81	0/606
53	N8	0.69	1/381 (0.3%)	0.86	0/516
54	L5	0.69	0/409	0.89	0/540
54	P8	0.85	0/409	1.07	2/540 (0.4%)
55	M5	0.75	0/524	1.00	3/691 (0.4%)
55	Q8	0.79	0/524	1.17	4/691 (0.6%)
56	1L	0.61	1/1613 (0.1%)	1.18	11/2504 (0.4%)
57	3L	0.65	0/1733	1.28	14/2699 (0.5%)
All	All	0.81	185/317108 (0.1%)	1.41	4553/475084 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	13	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	4
2	1E	0	4
3	22	0	2
4	32	0	1
4	3E	0	1
9	82	0	1
9	8E	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	1
13	4A	0	2
13	4I	0	3
14	5A	0	1
18	9I	0	1
19	AI	0	2
20	BA	0	2
28	71	0	3
29	11	0	4
29	19	0	4
30	21	0	5
30	29	0	5
31	31	0	4
31	39	0	7
32	41	0	1
32	49	0	1
33	51	0	6
34	61	0	4
34	69	0	2
37	35	0	3
37	78	0	5
38	45	0	6
38	88	0	1
39	55	0	1
39	98	0	1
40	65	0	1
41	75	0	1
41	B8	0	1
42	85	0	4
42	C8	0	2
43	95	0	2
43	D8	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	A5	0	2
45	B5	0	1
45	F8	0	2
46	C5	0	3
46	G8	0	7
47	D5	0	2
47	H8	0	4
49	J8	0	2
50	G5	0	4
50	K8	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	1
All	All	1	141

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-11.99	1.30	1.37
26	1H	2430	A	N9-C4	-11.47	1.30	1.37
26	1H	783	A	N3-C4	-11.40	1.28	1.34
26	14	2430	A	N9-C4	-10.71	1.31	1.37
26	14	528	A	N9-C4	-10.24	1.31	1.37

The worst 5 of 4553 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-19.34	114.40	126.00
26	1H	783	A	C8-N9-C4	-17.08	98.97	105.80
26	14	2518	A	N1-C6-N6	17.07	128.84	118.60
26	1H	676	A	C2-N3-C4	-16.88	102.16	110.60
26	14	774	A	C2-N3-C4	-16.75	102.23	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	A	C1'

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	9	GLU	Peptide
4	3E	193	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16233	755	0
1	1G	32391	0	16353	749	0
2	12	1721	0	1758	101	0
2	1E	1874	0	1926	103	0
3	22	1541	0	1606	69	0
3	2E	1605	0	1668	58	0
4	32	1702	0	1765	110	0
4	3E	1698	0	1761	83	0
5	42	1134	0	1200	45	0
5	4E	1142	0	1204	62	0
6	52	842	0	857	30	0
6	5E	837	0	852	35	0
7	62	1110	0	1163	49	0
7	6E	1242	0	1286	44	0
8	72	1107	0	1165	39	0
8	7E	1115	0	1177	58	0
9	82	953	0	983	70	0
9	8E	1000	0	1031	58	0
10	1A	646	0	662	33	0
10	1I	734	0	761	43	0
11	2A	835	0	847	31	0
11	2I	823	0	833	49	0
12	3A	956	0	1046	56	0
12	3I	956	0	1046	33	0
13	4A	893	0	946	61	0
13	4I	942	0	997	53	0
14	5A	486	0	525	25	0
14	5I	491	0	529	26	0
15	6A	733	0	771	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	29	0
16	7A	705	0	725	29	0
16	7I	700	0	720	47	0
17	8A	823	0	891	35	0
17	8I	834	0	904	42	0
18	9A	544	0	605	26	0
18	9I	549	0	607	36	0
19	AA	481	0	468	32	0
19	AI	654	0	675	44	0
20	BA	762	0	861	32	0
20	BI	746	0	843	49	0
21	1B	188	0	195	13	0
21	1F	199	0	208	5	0
22	1K	1520	0	778	41	0
23	2K	1646	0	843	30	0
23	2L	1646	0	843	40	0
24	3K	1611	0	817	48	0
25	4K	419	0	208	6	0
25	4L	397	0	197	12	0
26	14	61630	0	31073	1315	0
26	1H	61028	0	30763	1351	0
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	65	0
28	71	1033	0	1048	77	0
28	79	456	0	460	22	0
29	11	2120	0	2197	131	0
29	19	2125	0	2199	104	0
30	21	1558	0	1624	83	0
30	29	1563	0	1629	117	0
31	31	1585	0	1632	89	0
31	39	1602	0	1649	80	0
32	41	1457	0	1514	94	0
32	49	1458	0	1516	59	0
33	51	1312	0	1384	66	0
33	59	568	0	595	48	0
34	61	1136	0	1223	57	0
34	69	1131	0	1218	48	0
35	15	1104	0	1180	38	0
35	58	1104	0	1180	54	0
36	25	932	0	996	36	0
36	68	932	0	996	42	0
37	35	1122	0	1206	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	78	1122	0	1206	94	0
38	45	1099	0	1154	79	0
38	88	1113	0	1157	51	0
39	55	967	0	1033	49	0
39	98	967	0	1033	49	0
40	65	876	0	938	65	0
40	A8	881	0	943	52	0
41	75	1109	0	1170	55	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	53	0
42	C8	950	0	1011	52	0
43	95	774	0	849	63	0
43	D8	774	0	849	43	0
44	A5	899	0	964	28	0
44	E8	890	0	951	25	0
45	B5	735	0	785	35	0
45	F8	743	0	794	36	0
46	C5	794	0	886	68	0
46	G8	796	0	886	45	0
47	D5	1074	0	1086	53	0
47	H8	1373	0	1402	59	0
48	E5	608	0	622	26	0
48	I8	606	0	625	30	0
49	F5	737	0	813	32	0
49	J8	737	0	813	39	0
50	G5	558	0	610	33	0
50	K8	568	0	614	36	0
51	H5	459	0	512	10	0
51	L8	459	0	512	18	0
52	M8	366	0	370	37	0
53	J5	434	0	454	22	0
53	N8	369	0	388	22	0
54	L5	401	0	436	14	0
54	P8	401	0	436	14	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1563	0	799	42	0
57	3L	1612	0	819	41	0
58	13	132	0	0	0	0
58	14	399	0	0	0	0
58	16	9	0	0	0	0
58	1E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1G	90	0	0	0	0
58	1H	467	0	0	0	0
58	1J	5	0	0	0	0
58	1K	1	0	0	0	0
58	2I	2	0	0	0	0
58	25	1	0	0	0	0
58	29	4	0	0	0	0
58	2K	3	0	0	0	0
58	2L	2	0	0	0	0
58	35	3	0	0	0	0
58	39	1	0	0	0	0
58	3K	1	0	0	0	0
58	4I	1	0	0	0	0
58	45	2	0	0	0	0
58	55	1	0	0	0	0
58	5E	1	0	0	0	0
58	6A	1	0	0	0	0
58	78	1	0	0	0	0
58	88	1	0	0	0	0
58	98	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	3	0	0	0	0
58	J8	1	0	0	0	0
58	L8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	2	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	1I	7	0	0	5	0
61	13	126	0	0	21	0
61	14	417	0	0	73	0
61	16	29	0	0	6	0
61	19	8	0	0	1	0
61	1G	78	0	0	9	0
61	1H	629	0	0	101	0
61	1J	6	0	0	1	0
61	1K	8	0	0	0	0
61	2I	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	2	0	0	0	0
61	31	9	0	0	0	0
61	32	1	0	0	0	0
61	35	1	0	0	0	0
61	39	5	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	4K	2	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	2	0	0	0	0
61	5I	2	0	0	0	0
61	78	7	0	0	2	0
61	88	1	0	0	0	0
61	A5	1	0	0	0	0
61	B8	1	0	0	0	0
61	E8	2	0	0	0	0
61	F8	1	0	0	0	0
61	G8	1	0	0	0	0
61	H5	2	0	0	1	0
61	I8	3	0	0	1	0
61	L8	2	0	0	1	0
All	All	294444	0	196318	8229	0

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

The worst 5 of 8229 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)
46:G8:100:ALA:HB1	46:G8:101:LYS:HG2	1.34	1.09
55:M5:48:PHE:HB2	55:M5:49:VAL:HG22	1.31	1.07
26:14:161:U:H5'	26:14:171:G:H21	1.18	1.06
26:1H:2711:A:OP2	61:1H:3501:HOH:O	1.73	1.05
26:14:2002:G:N7	61:14:3505:HOH:O	1.91	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	206/256 (80%)	168 (82%)	31 (15%)	7 (3%)	3	24
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12	47
3	22	192/239 (80%)	169 (88%)	22 (12%)	1 (0%)	29	67
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29	67
4	3E	205/209 (98%)	188 (92%)	14 (7%)	3 (2%)	10	44
5	42	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22	61
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	22	61
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22	61
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	22	61
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22	61
9	82	119/128 (93%)	107 (90%)	11 (9%)	1 (1%)	19	58
9	8E	124/128 (97%)	104 (84%)	19 (15%)	1 (1%)	19	58
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	89/105 (85%)	83 (93%)	6 (7%)	0	100	100
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	8	41
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	17	56
12	3A	120/132 (91%)	102 (85%)	13 (11%)	5 (4%)	3	20
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	58
13	4A	109/126 (86%)	95 (87%)	13 (12%)	1 (1%)	17	56
13	4I	117/126 (93%)	97 (83%)	19 (16%)	1 (1%)	17	56
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	24
15	6A	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	2 (3%)	1 (2%)	10	44
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	44
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	3	23
19	AI	79/93 (85%)	67 (85%)	10 (13%)	2 (2%)	5	32
20	BA	97/106 (92%)	80 (82%)	15 (16%)	2 (2%)	7	37
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	119 (92%)	10 (8%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	243 (90%)	17 (6%)	11 (4%)	3	21
29	19	272/276 (99%)	241 (89%)	25 (9%)	6 (2%)	6	35
30	21	201/206 (98%)	157 (78%)	36 (18%)	8 (4%)	3	21
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	21
31	31	200/210 (95%)	175 (88%)	25 (12%)	0	100	100
31	39	202/210 (96%)	157 (78%)	36 (18%)	9 (4%)	2	18
32	41	177/182 (97%)	155 (88%)	19 (11%)	3 (2%)	9	42
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	14	51
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	12
33	59	67/180 (37%)	50 (75%)	14 (21%)	3 (4%)	2	18
34	61	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	11	46
34	69	143/148 (97%)	116 (81%)	26 (18%)	1 (1%)	22	61
35	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	61
35	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
36	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	35	145/150 (97%)	114 (79%)	29 (20%)	2 (1%)	11	46
37	78	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3	24
38	45	136/141 (96%)	112 (82%)	21 (15%)	3 (2%)	6	35
38	88	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	23
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	56
39	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	17	56
40	65	108/112 (96%)	86 (80%)	20 (18%)	2 (2%)	8	39
40	A8	109/112 (97%)	92 (84%)	14 (13%)	3 (3%)	5	29
41	75	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
41	B8	131/146 (90%)	119 (91%)	12 (9%)	0	100	100
42	85	114/118 (97%)	101 (89%)	11 (10%)	2 (2%)	8	41
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	30
43	95	98/101 (97%)	77 (79%)	14 (14%)	7 (7%)	1	8
43	D8	98/101 (97%)	87 (89%)	6 (6%)	5 (5%)	2	15
44	A5	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	17	56
44	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	4 (4%)	3 (3%)	4	25
45	F8	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	51
46	C5	102/110 (93%)	75 (74%)	17 (17%)	10 (10%)	0	3
46	G8	103/110 (94%)	86 (84%)	13 (13%)	4 (4%)	3	22
47	D5	126/206 (61%)	100 (79%)	21 (17%)	5 (4%)	3	21
47	H8	169/206 (82%)	136 (80%)	25 (15%)	8 (5%)	2	17
48	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	12	47
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	85 (92%)	6 (6%)	1 (1%)	14	51
49	J8	92/98 (94%)	83 (90%)	8 (9%)	1 (1%)	14	51
50	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	4	26
50	K8	66/72 (92%)	58 (88%)	5 (8%)	3 (4%)	2	18
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	M8	45/71 (63%)	29 (64%)	15 (33%)	1 (2%)	6	35
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	P8	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
55	M5	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	26
55	Q8	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	17
All	All	10973/12333 (89%)	9576 (87%)	1201 (11%)	196 (2%)	8	41

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	13	THR
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	154 (85%)	28 (15%)	2	13
2	1E	200/220 (91%)	143 (72%)	57 (28%)	0	1
3	22	154/188 (82%)	123 (80%)	31 (20%)	1	6
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	5
4	32	180/181 (99%)	143 (79%)	37 (21%)	1	6
4	3E	180/181 (99%)	137 (76%)	43 (24%)	0	3
5	42	114/123 (93%)	91 (80%)	23 (20%)	1	6
5	4E	115/123 (94%)	98 (85%)	17 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	6
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1	8
7	62	114/127 (90%)	95 (83%)	19 (17%)	2	10
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1	8
8	72	118/119 (99%)	98 (83%)	20 (17%)	2	10
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	92/99 (93%)	71 (77%)	21 (23%)	1	4
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	6
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	1
10	1I	81/92 (88%)	65 (80%)	16 (20%)	1	7
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	9
11	2I	84/99 (85%)	61 (73%)	23 (27%)	0	1
12	3A	103/109 (94%)	81 (79%)	22 (21%)	1	5
12	3I	103/109 (94%)	87 (84%)	16 (16%)	2	12
13	4A	91/101 (90%)	70 (77%)	21 (23%)	1	3
13	4I	94/101 (93%)	75 (80%)	19 (20%)	1	6
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1	4
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	13
15	6I	79/80 (99%)	62 (78%)	17 (22%)	1	5
16	7A	72/74 (97%)	52 (72%)	20 (28%)	0	1
16	7I	72/74 (97%)	51 (71%)	21 (29%)	0	1
17	8A	94/97 (97%)	79 (84%)	15 (16%)	2	11
17	8I	95/97 (98%)	79 (83%)	16 (17%)	2	10
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0	1
18	9I	58/77 (75%)	44 (76%)	14 (24%)	0	3
19	AA	52/80 (65%)	40 (77%)	12 (23%)	1	3
19	AI	71/80 (89%)	58 (82%)	13 (18%)	1	8
20	BA	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	BI	75/82 (92%)	59 (79%)	16 (21%)	1	5
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1F	18/22 (82%)	17 (94%)	1 (6%)	21	57
28	71	109/181 (60%)	87 (80%)	22 (20%)	1	6
28	79	48/181 (26%)	38 (79%)	10 (21%)	1	6
29	11	214/218 (98%)	161 (75%)	53 (25%)	0	2
29	19	214/218 (98%)	169 (79%)	45 (21%)	1	6
30	21	165/166 (99%)	128 (78%)	37 (22%)	1	4
30	29	165/166 (99%)	126 (76%)	39 (24%)	1	3
31	31	161/166 (97%)	126 (78%)	35 (22%)	1	5
31	39	163/166 (98%)	130 (80%)	33 (20%)	1	6
32	41	153/156 (98%)	121 (79%)	32 (21%)	1	6
32	49	153/156 (98%)	125 (82%)	28 (18%)	1	8
33	51	142/148 (96%)	109 (77%)	33 (23%)	1	3
33	59	59/148 (40%)	50 (85%)	9 (15%)	2	13
34	61	122/124 (98%)	95 (78%)	27 (22%)	1	4
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	117/119 (98%)	87 (74%)	30 (26%)	0	2
35	58	117/119 (98%)	90 (77%)	27 (23%)	1	3
36	25	100/100 (100%)	82 (82%)	18 (18%)	1	9
36	68	100/100 (100%)	85 (85%)	15 (15%)	3	14
37	35	114/116 (98%)	78 (68%)	36 (32%)	0	0
37	78	114/116 (98%)	80 (70%)	34 (30%)	0	1
38	45	109/111 (98%)	89 (82%)	20 (18%)	1	8
38	88	109/111 (98%)	87 (80%)	22 (20%)	1	6
39	55	101/101 (100%)	83 (82%)	18 (18%)	2	9
39	98	101/101 (100%)	76 (75%)	25 (25%)	0	2
40	65	87/88 (99%)	64 (74%)	23 (26%)	0	2
40	A8	87/88 (99%)	67 (77%)	20 (23%)	1	3
41	75	117/127 (92%)	91 (78%)	26 (22%)	1	4
41	B8	117/127 (92%)	87 (74%)	30 (26%)	0	2
42	85	93/94 (99%)	83 (89%)	10 (11%)	6	27
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	95	82/82 (100%)	61 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	59 (72%)	23 (28%)	0	1
44	A5	92/92 (100%)	73 (79%)	19 (21%)	1	6
44	E8	91/92 (99%)	65 (71%)	26 (29%)	0	1
45	B5	74/78 (95%)	52 (70%)	22 (30%)	0	1
45	F8	75/78 (96%)	64 (85%)	11 (15%)	3	14
46	C5	85/91 (93%)	60 (71%)	25 (29%)	0	1
46	G8	85/91 (93%)	70 (82%)	15 (18%)	2	9
47	D5	118/179 (66%)	93 (79%)	25 (21%)	1	5
47	H8	152/179 (85%)	113 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	4	19
48	I8	61/67 (91%)	51 (84%)	10 (16%)	2	11
49	F5	79/83 (95%)	61 (77%)	18 (23%)	1	4
49	J8	79/83 (95%)	60 (76%)	19 (24%)	0	3
50	G5	62/67 (92%)	47 (76%)	15 (24%)	0	2
50	K8	62/67 (92%)	44 (71%)	18 (29%)	0	1
51	H5	50/52 (96%)	40 (80%)	10 (20%)	1	6
51	L8	50/52 (96%)	38 (76%)	12 (24%)	0	3
52	M8	42/63 (67%)	31 (74%)	11 (26%)	0	2
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	8
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	6
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4	19
54	P8	38/42 (90%)	34 (90%)	4 (10%)	7	28
55	M5	54/55 (98%)	44 (82%)	10 (18%)	1	8
55	Q8	54/55 (98%)	39 (72%)	15 (28%)	0	1
All	All	9277/10193 (91%)	7277 (78%)	2000 (22%)	1	5

5 of 2000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	F8	68	ARG
3	22	198	VAL
44	A5	88	ARG

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Mol	Chain	Res	Type
47	H8	35	ARG
51	L8	11	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
8	72	15	ASN
10	1A	13	HIS
41	75	2	ASN
9	82	87	GLN
10	1A	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	361 (24%)	29 (1%)
1	1G	1506/1522 (98%)	367 (24%)	27 (1%)
22	1K	67/75 (89%)	27 (40%)	2 (2%)
23	2K	76/77 (98%)	22 (28%)	1 (1%)
23	2L	76/77 (98%)	14 (18%)	2 (2%)
24	3K	75/76 (98%)	42 (56%)	4 (5%)
25	4K	18/27 (66%)	12 (66%)	2 (11%)
25	4L	17/27 (62%)	9 (52%)	0
26	14	2853/2917 (97%)	731 (25%)	38 (1%)
26	1H	2829/2917 (96%)	722 (25%)	50 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	1 (0%)
56	1L	69/76 (90%)	27 (39%)	4 (5%)
57	3L	75/76 (98%)	35 (46%)	1 (1%)
All	All	9396/9633 (97%)	2428 (25%)	162 (1%)

5 of 2428 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	9	G
1	13	15	G

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	1980	G
1	1G	80	G
26	14	2238	G
26	1H	2035	G
26	1H	2448	A

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

23 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
56	PSU	1L	39	56	17,21,22	1.10	2 (11%)	20,30,33	3.28	6 (30%)
56	T6A	1L	37	56	24,34,35	2.57	5 (20%)	24,49,52	2.52	7 (29%)
23	PSU	2K	56	23	17,21,22	1.13	2 (11%)	20,30,33	2.92	6 (30%)
23	OMC	2K	33	23	15,22,23	2.23	4 (26%)	17,31,34	1.50	2 (11%)
23	OMC	2L	33	23	15,22,23	2.15	4 (26%)	17,31,34	1.61	3 (17%)
23	4SU	2L	8	23	14,21,22	3.25	2 (14%)	15,30,33	0.85	1 (6%)
22	5MU	1K	54	22	15,22,23	2.12	3 (20%)	16,32,35	1.87	2 (12%)
57	5MU	3L	54	57	15,22,23	2.31	3 (20%)	16,32,35	1.92	2 (12%)
22	PSU	1K	39	22	17,21,22	1.07	1 (5%)	20,30,33	3.21	5 (25%)
23	G7M	2K	47	23	20,26,27	5.37	7 (35%)	20,39,42	1.86	4 (20%)
57	PSU	3L	39	57	17,21,22	1.12	2 (11%)	20,30,33	3.39	5 (25%)
22	T6A	1K	37	22	24,34,35	2.43	5 (20%)	24,49,52	2.14	5 (20%)
56	U8U	1L	34	25,56	17,24,25	2.70	4 (23%)	19,34,37	1.64	3 (15%)
22	PSU	1K	55	22	17,21,22	1.04	1 (5%)	20,30,33	3.69	5 (25%)
22	U8U	1K	34	25,22	17,24,25	2.51	4 (23%)	19,34,37	1.71	3 (15%)
23	5MU	2K	55	23	15,22,23	2.21	3 (20%)	16,32,35	1.94	2 (12%)
23	G7M	2L	47	23	20,26,27	5.49	7 (35%)	20,39,42	1.98	5 (25%)
56	PSU	1L	55	56	17,21,22	1.15	2 (11%)	20,30,33	3.43	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PSU	3L	55	57	17,21,22	1.06	2 (11%)	20,30,33	3.22	8 (40%)
23	5MU	2L	55	23	15,22,23	2.17	3 (20%)	16,32,35	1.90	2 (12%)
56	5MU	1L	54	56	15,22,23	2.15	3 (20%)	16,32,35	1.72	2 (12%)
23	PSU	2L	56	23	17,21,22	1.16	1 (5%)	20,30,33	3.11	5 (25%)
23	4SU	2K	8	23	14,21,22	3.23	2 (14%)	15,30,33	1.42	2 (13%)

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
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
56	T6A	1L	37	56	-	5/15/41/42	0/3/3/3
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
23	OMC	2L	33	23	-	0/7/27/28	0/2/2/2
23	4SU	2L	8	23	-	0/5/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
57	5MU	3L	54	57	-	0/5/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	3/3/25/26	0/3/3/3
57	PSU	3L	39	57	-	2/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	3/15/41/42	0/3/3/3
56	U8U	1L	34	25,56	-	2/7/28/29	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	2/7/28/29	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/3/25/26	0/3/3/3
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
57	PSU	3L	55	57	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/5/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	17.58	1.65	1.33
23	2K	47	G7M	C8-N7	17.37	1.65	1.33
23	2L	47	G7M	C5-C4	-11.32	1.24	1.39
23	2K	47	G7M	C5-C4	-10.96	1.24	1.39
23	2K	8	4SU	C5-C4	9.76	1.49	1.38

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	55	PSU	N1-C2-N3	-12.20	118.73	128.43
56	1L	55	PSU	N1-C2-N3	-11.68	119.15	128.43
57	3L	39	PSU	N1-C2-N3	-11.66	119.16	128.43
56	1L	39	PSU	N1-C2-N3	-11.25	119.49	128.43
22	1K	39	PSU	N1-C2-N3	-11.23	119.50	128.43

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C13-C12-C14-O14
57	3L	39	PSU	C3'-C4'-C5'-O5'
56	1L	34	U8U	O4'-C4'-C5'-O5'
23	2K	56	PSU	O4'-C4'-C5'-O5'
57	3L	39	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	56	PSU	1	0
23	2K	33	OMC	2	0
23	2L	33	OMC	1	0
23	2L	8	4SU	2	0
23	2K	47	G7M	1	0
57	3L	39	PSU	1	0
56	1L	34	U8U	2	0
23	2L	47	G7M	2	0
56	1L	55	PSU	1	0
57	3L	55	PSU	1	0
23	2L	55	5MU	1	0
23	2L	56	PSU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1144 ligands modelled in this entry, 1142 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	$\# Z > 2$
59	SF4	32	301	-	0,12,12	0.00	-	-		
59	SF4	3E	301	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	32	301	-	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	301	SF4	2	0
59	3E	301	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1496/1522 (98%)	-0.66	1 (0%) 95 95	62, 109, 164, 193	0
1	1G	1507/1522 (99%)	-0.64	2 (0%) 95 95	80, 127, 170, 197	0
2	12	210/256 (82%)	0.46	23 (10%) 5 3	127, 152, 162, 177	0
2	1E	231/256 (90%)	0.62	29 (12%) 3 2	117, 141, 159, 166	0
3	22	196/239 (82%)	1.21	47 (23%) 0 0	129, 143, 156, 164	0
3	2E	205/239 (85%)	0.92	35 (17%) 1 1	94, 114, 136, 145	0
4	32	208/209 (99%)	1.20	45 (21%) 0 1	108, 128, 145, 152	0
4	3E	207/209 (99%)	0.82	27 (13%) 3 2	92, 114, 134, 139	0
5	42	148/162 (91%)	0.60	9 (6%) 21 12	114, 129, 143, 152	0
5	4E	149/162 (91%)	0.53	9 (6%) 21 12	89, 108, 124, 140	0
6	52	101/101 (100%)	1.28	21 (20%) 1 1	95, 111, 129, 137	0
6	5E	100/101 (99%)	0.77	11 (11%) 5 3	87, 107, 126, 136	0
7	62	138/156 (88%)	-0.42	0 100 100	121, 134, 144, 148	0
7	6E	154/156 (98%)	-0.23	2 (1%) 77 65	109, 125, 148, 166	0
8	72	137/138 (99%)	0.07	4 (2%) 51 36	111, 133, 142, 145	0
8	7E	138/138 (100%)	-0.05	1 (0%) 87 81	97, 117, 128, 138	0
9	82	121/128 (94%)	-0.34	2 (1%) 70 57	117, 149, 158, 163	0
9	8E	126/128 (98%)	-0.44	0 100 100	96, 135, 152, 157	0
10	1A	80/105 (76%)	0.04	2 (2%) 57 43	129, 146, 156, 161	0
10	1I	91/105 (86%)	0.47	7 (7%) 13 7	87, 129, 159, 165	0
11	2A	113/129 (87%)	0.76	13 (11%) 4 3	94, 117, 130, 138	0
11	2I	111/129 (86%)	0.35	5 (4%) 33 21	85, 113, 127, 142	0
12	3A	122/132 (92%)	1.10	28 (22%) 0 0	89, 107, 130, 146	0
12	3I	122/132 (92%)	1.08	16 (13%) 3 2	73, 82, 106, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.72	11 (9%) 7 4	125, 145, 156, 160	0
13	4I	119/126 (94%)	0.18	4 (3%) 45 29	93, 123, 136, 147	0
14	5A	59/61 (96%)	1.75	22 (37%) 0 0	134, 143, 153, 154	0
14	5I	60/61 (98%)	-0.16	0 100 100	92, 103, 118, 131	0
15	6A	88/89 (98%)	0.30	2 (2%) 60 47	96, 119, 135, 139	0
15	6I	87/89 (97%)	-0.07	0 100 100	88, 104, 122, 127	0
16	7A	84/88 (95%)	0.19	2 (2%) 59 44	102, 117, 135, 152	0
16	7I	83/88 (94%)	0.53	7 (8%) 11 6	110, 119, 143, 150	0
17	8A	99/105 (94%)	0.19	3 (3%) 50 34	105, 120, 132, 133	0
17	8I	100/105 (95%)	0.32	1 (1%) 82 72	98, 114, 124, 126	0
18	9A	67/88 (76%)	1.36	22 (32%) 0 0	106, 121, 135, 142	0
18	9I	68/88 (77%)	1.17	17 (25%) 0 0	94, 109, 133, 136	0
19	AA	62/93 (66%)	1.29	14 (22%) 0 0	134, 149, 156, 158	0
19	AI	81/93 (87%)	0.54	6 (7%) 14 8	102, 122, 138, 151	0
20	BA	99/106 (93%)	-0.19	1 (1%) 82 72	100, 118, 141, 152	0
20	BI	97/106 (91%)	-0.10	1 (1%) 82 72	112, 125, 148, 157	0
21	1B	22/27 (81%)	1.15	5 (22%) 0 0	129, 137, 145, 148	0
21	1F	23/27 (85%)	-0.33	0 100 100	94, 112, 118, 122	0
22	1K	66/75 (88%)	0.07	1 (1%) 73 61	85, 153, 177, 183	0
23	2K	72/77 (93%)	-0.44	0 100 100	77, 104, 132, 146	0
23	2L	72/77 (93%)	-0.30	0 100 100	85, 122, 151, 162	0
24	3K	76/76 (100%)	-0.28	1 (1%) 77 65	79, 178, 191, 196	0
25	4K	19/27 (70%)	-0.20	1 (5%) 26 14	79, 152, 184, 184	0
25	4L	18/27 (66%)	0.10	0 100 100	101, 161, 187, 187	0
26	14	2861/2917 (98%)	-0.36	35 (1%) 79 67	55, 92, 180, 204	0
26	1H	2833/2917 (97%)	-0.42	13 (0%) 91 86	49, 79, 168, 203	0
27	16	122/122 (100%)	-0.12	1 (0%) 86 78	74, 98, 119, 179	0
27	1J	122/122 (100%)	-0.73	0 100 100	93, 125, 145, 177	0
28	71	133/229 (58%)	1.28	35 (26%) 0 0	143, 174, 185, 189	0
28	79	57/229 (24%)	-0.24	1 (1%) 68 55	140, 165, 176, 179	0
29	11	273/276 (98%)	-0.20	0 100 100	48, 71, 89, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.53	12 (4%) 34 21	58, 82, 101, 117	0
30	21	203/206 (98%)	0.81	35 (17%) 1 1	55, 93, 139, 153	0
30	29	204/206 (99%)	0.63	38 (18%) 1 1	60, 99, 134, 144	0
31	31	202/210 (96%)	0.39	21 (10%) 6 4	54, 85, 118, 142	0
31	39	204/210 (97%)	0.79	33 (16%) 1 1	62, 111, 151, 168	0
32	41	179/182 (98%)	1.18	39 (21%) 0 0	85, 107, 140, 156	0
32	49	179/182 (98%)	0.97	41 (22%) 0 0	122, 139, 155, 171	0
33	51	171/180 (95%)	0.46	9 (5%) 26 14	89, 110, 127, 139	0
33	59	73/180 (40%)	0.25	8 (10%) 5 3	136, 154, 165, 177	0
34	61	146/148 (98%)	1.08	35 (23%) 0 0	83, 130, 143, 150	0
34	69	145/148 (97%)	1.35	43 (29%) 0 0	93, 129, 147, 152	0
35	15	138/140 (98%)	1.92	56 (40%) 0 0	86, 114, 139, 155	0
35	58	138/140 (98%)	0.27	6 (4%) 35 22	68, 97, 130, 145	0
36	25	122/122 (100%)	0.04	0 100 100	77, 94, 114, 120	0
36	68	122/122 (100%)	0.03	2 (1%) 72 59	64, 81, 99, 104	0
37	35	147/150 (98%)	0.31	8 (5%) 25 14	65, 111, 138, 144	0
37	78	147/150 (98%)	0.05	3 (2%) 65 51	53, 88, 113, 120	0
38	45	138/141 (97%)	2.27	69 (50%) 0 0	78, 108, 128, 142	0
38	88	141/141 (100%)	1.23	31 (21%) 0 0	63, 83, 108, 129	0
39	55	118/118 (100%)	-0.03	1 (0%) 86 78	69, 86, 108, 127	0
39	98	118/118 (100%)	0.49	10 (8%) 10 6	67, 90, 109, 122	0
40	65	110/112 (98%)	0.34	5 (4%) 33 21	92, 117, 135, 142	0
40	A8	111/112 (99%)	2.42	65 (58%) 0 0	71, 93, 115, 123	0
41	75	133/146 (91%)	-0.35	3 (2%) 60 47	87, 101, 129, 141	0
41	B8	133/146 (91%)	-0.43	2 (1%) 73 61	78, 98, 133, 149	0
42	85	116/118 (98%)	1.37	33 (28%) 0 0	73, 100, 132, 138	0
42	C8	115/118 (97%)	-0.16	3 (2%) 56 40	59, 86, 114, 118	0
43	95	100/101 (99%)	2.98	69 (69%) 0 0	69, 121, 139, 153	0
43	D8	100/101 (99%)	0.14	6 (6%) 21 12	62, 106, 126, 144	0
44	A5	113/113 (100%)	0.01	2 (1%) 68 55	68, 82, 112, 158	0
44	E8	112/113 (99%)	0.36	5 (4%) 33 21	63, 79, 106, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	0.94	13 (13%) 2 2	77, 91, 118, 128	0
45	F8	95/96 (98%)	0.67	10 (10%) 6 3	60, 76, 104, 118	0
46	C5	104/110 (94%)	0.44	9 (8%) 10 5	91, 122, 149, 154	0
46	G8	105/110 (95%)	-0.23	0 100 100	75, 101, 131, 139	0
47	D5	132/206 (64%)	1.81	58 (43%) 0 0	115, 135, 150, 158	0
47	H8	171/206 (83%)	1.74	66 (38%) 0 0	90, 122, 167, 172	0
48	E5	77/85 (90%)	0.12	4 (5%) 27 15	72, 94, 111, 131	0
48	I8	76/85 (89%)	0.49	3 (3%) 39 25	61, 75, 90, 102	0
49	F5	94/98 (95%)	0.15	2 (2%) 63 49	67, 88, 121, 136	0
49	J8	94/98 (95%)	0.10	2 (2%) 63 49	62, 77, 120, 122	0
50	G5	66/72 (91%)	0.52	4 (6%) 21 12	87, 108, 126, 145	0
50	K8	68/72 (94%)	0.15	2 (2%) 51 36	68, 84, 102, 124	0
51	H5	58/60 (96%)	1.89	26 (44%) 0 0	81, 106, 128, 135	0
51	L8	58/60 (96%)	0.37	3 (5%) 27 15	63, 85, 115, 127	0
52	M8	47/71 (66%)	2.74	31 (65%) 0 0	109, 143, 158, 163	0
53	J5	56/60 (93%)	-0.11	0 100 100	66, 86, 141, 148	0
53	N8	48/60 (80%)	0.41	7 (14%) 2 1	56, 84, 140, 142	0
54	L5	47/49 (95%)	0.14	2 (4%) 35 22	58, 66, 85, 91	0
54	P8	47/49 (95%)	-0.44	0 100 100	52, 57, 77, 88	0
55	M5	64/65 (98%)	0.14	0 100 100	76, 85, 101, 117	0
55	Q8	64/65 (98%)	0.15	0 100 100	61, 71, 88, 99	0
56	1L	68/76 (89%)	1.09	15 (22%) 0 0	118, 173, 181, 188	0
57	3L	73/76 (96%)	-0.60	0 100 100	87, 172, 185, 190	0
All	All	20602/21966 (93%)	0.11	1495 (7%) 15 9	48, 107, 162, 204	0

The worst 5 of 1495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2899	G	12.6
26	14	2901	C	10.8
26	14	2799	A	10.4
26	14	2902	C	9.9
43	95	45	THR	9.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
57	PSU	3L	55	20/21	0.83	0.08	166,169,175,175	0
56	PSU	1L	55	20/21	0.87	0.30	134,150,156,159	0
57	5MU	3L	54	21/22	0.87	0.09	162,169,172,173	0
56	PSU	1L	39	20/21	0.88	0.18	105,127,133,134	0
23	PSU	2L	56	20/21	0.88	0.12	116,129,133,137	0
22	PSU	1K	55	20/21	0.90	0.17	109,120,133,134	0
57	PSU	3L	39	20/21	0.91	0.13	153,162,166,168	0
56	U8U	1L	34	23/24	0.91	0.18	110,126,134,138	0
23	4SU	2L	8	20/21	0.91	0.17	112,125,130,135	0
23	4SU	2K	8	20/21	0.92	0.17	93,98,102,106	0
56	T6A	1L	37	32/33	0.93	0.18	102,120,127,130	0
23	G7M	2L	47	24/25	0.93	0.12	129,137,150,151	0
23	G7M	2K	47	24/25	0.94	0.12	104,115,129,135	0
23	5MU	2L	55	21/22	0.94	0.13	128,133,141,143	0
22	5MU	1K	54	21/22	0.94	0.22	114,122,134,142	0
23	PSU	2K	56	20/21	0.94	0.14	104,113,121,127	0
22	PSU	1K	39	20/21	0.95	0.15	79,98,105,108	0
56	5MU	1L	54	21/22	0.95	0.25	138,147,154,155	0
23	5MU	2K	55	21/22	0.96	0.12	112,118,125,127	0
23	OMC	2L	33	21/22	0.96	0.15	109,114,117,125	0
22	T6A	1K	37	32/33	0.96	0.16	76,86,103,106	0
22	U8U	1K	34	23/24	0.96	0.15	78,88,93,105	0
23	OMC	2K	33	21/22	0.97	0.14	82,87,92,96	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
58	MG	13	1698	1/1	0.08	0.21	138,138,138,138	0
58	MG	13	1699	1/1	0.28	0.31	94,94,94,94	0
58	MG	14	3303	1/1	0.32	0.18	106,106,106,106	0
58	MG	14	3282	1/1	0.32	0.42	109,109,109,109	0
58	MG	13	1603	1/1	0.33	0.47	92,92,92,92	0
58	MG	1H	3016	1/1	0.34	0.56	75,75,75,75	0
58	MG	1H	3297	1/1	0.39	0.24	99,99,99,99	0
58	MG	14	3258	1/1	0.41	0.38	92,92,92,92	0
58	MG	14	3311	1/1	0.42	0.36	100,100,100,100	0
58	MG	1H	3219	1/1	0.43	0.37	103,103,103,103	0
58	MG	1G	1638	1/1	0.44	0.30	93,93,93,93	0
58	MG	14	3108	1/1	0.46	0.73	92,92,92,92	0
58	MG	1H	3283	1/1	0.48	0.24	92,92,92,92	0
58	MG	13	1697	1/1	0.49	0.22	92,92,92,92	0
58	MG	14	3224	1/1	0.51	0.38	90,90,90,90	0
58	MG	1H	3152	1/1	0.51	0.34	100,100,100,100	0
58	MG	1G	1664	1/1	0.51	0.30	100,100,100,100	0
58	MG	2K	102	1/1	0.52	0.69	94,94,94,94	0
58	MG	13	1700	1/1	0.52	0.33	94,94,94,94	0
58	MG	14	3034	1/1	0.52	0.97	88,88,88,88	0
58	MG	39	301	1/1	0.52	0.21	96,96,96,96	0
58	MG	14	3399	1/1	0.53	0.28	107,107,107,107	0
58	MG	13	1653	1/1	0.54	0.41	72,72,72,72	0
58	MG	1H	3249	1/1	0.54	0.37	80,80,80,80	0
58	MG	13	1672	1/1	0.54	0.45	109,109,109,109	0
58	MG	13	1696	1/1	0.55	0.32	92,92,92,92	0
58	MG	14	3037	1/1	0.56	0.46	106,106,106,106	0
58	MG	1H	3171	1/1	0.56	0.43	83,83,83,83	0
58	MG	1H	3284	1/1	0.56	0.48	81,81,81,81	0
58	MG	1H	3036	1/1	0.56	0.74	100,100,100,100	0
58	MG	1H	3309	1/1	0.56	0.51	90,90,90,90	0
58	MG	14	3294	1/1	0.57	0.26	87,87,87,87	0
58	MG	14	3304	1/1	0.58	0.71	92,92,92,92	0
58	MG	13	1688	1/1	0.58	0.34	101,101,101,101	0
58	MG	1H	3035	1/1	0.59	0.45	83,83,83,83	0
58	MG	1H	3279	1/1	0.59	0.49	67,67,67,67	0
58	MG	25	201	1/1	0.59	0.34	102,102,102,102	0
58	MG	14	3316	1/1	0.60	0.35	122,122,122,122	0
58	MG	1H	3336	1/1	0.60	0.24	104,104,104,104	0
58	MG	14	3184	1/1	0.60	0.24	98,98,98,98	0
58	MG	14	3283	1/1	0.60	0.32	69,69,69,69	0
58	MG	14	3197	1/1	0.61	0.34	116,116,116,116	0
58	MG	14	3180	1/1	0.61	0.30	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3185	1/1	0.61	0.51	82,82,82,82	0
58	MG	14	3191	1/1	0.61	0.58	96,96,96,96	0
58	MG	14	3190	1/1	0.61	0.58	86,86,86,86	0
58	MG	1H	3164	1/1	0.61	0.21	64,64,64,64	0
58	MG	14	3229	1/1	0.61	0.76	88,88,88,88	0
58	MG	14	3140	1/1	0.62	0.33	82,82,82,82	0
58	MG	1H	3024	1/1	0.62	0.69	82,82,82,82	0
58	MG	14	3129	1/1	0.62	0.69	73,73,73,73	0
58	MG	1H	3331	1/1	0.62	0.62	73,73,73,73	0
58	MG	1H	3264	1/1	0.62	0.18	76,76,76,76	0
58	MG	1G	1603	1/1	0.62	0.59	102,102,102,102	0
58	MG	13	1605	1/1	0.62	0.24	76,76,76,76	0
58	MG	1H	3278	1/1	0.62	0.48	95,95,95,95	0
58	MG	14	3017	1/1	0.62	0.51	90,90,90,90	0
58	MG	14	3068	1/1	0.63	0.65	100,100,100,100	0
58	MG	1H	3160	1/1	0.63	0.28	72,72,72,72	0
58	MG	14	3269	1/1	0.63	0.50	88,88,88,88	0
58	MG	1G	1646	1/1	0.63	0.24	100,100,100,100	0
58	MG	1G	1635	1/1	0.63	0.28	107,107,107,107	0
58	MG	1G	1616	1/1	0.63	0.31	87,87,87,87	0
58	MG	14	3089	1/1	0.64	0.88	79,79,79,79	0
58	MG	13	1630	1/1	0.64	0.48	80,80,80,80	0
58	MG	14	3085	1/1	0.64	0.47	67,67,67,67	0
58	MG	14	3302	1/1	0.64	0.46	66,66,66,66	0
58	MG	1H	3285	1/1	0.65	0.47	68,68,68,68	0
58	MG	14	3261	1/1	0.65	0.49	77,77,77,77	0
58	MG	14	3153	1/1	0.66	0.44	89,89,89,89	0
58	MG	1E	301	1/1	0.66	0.20	106,106,106,106	0
58	MG	14	3026	1/1	0.66	0.34	89,89,89,89	0
58	MG	1J	203	1/1	0.66	0.23	103,103,103,103	0
58	MG	14	3275	1/1	0.67	0.37	91,91,91,91	0
58	MG	1H	3194	1/1	0.67	0.40	84,84,84,84	0
58	MG	1H	3167	1/1	0.67	0.54	93,93,93,93	0
58	MG	35	202	1/1	0.67	0.24	87,87,87,87	0
58	MG	1H	3207	1/1	0.67	0.48	84,84,84,84	0
58	MG	14	3264	1/1	0.67	0.57	85,85,85,85	0
58	MG	14	3277	1/1	0.67	0.34	85,85,85,85	0
58	MG	1H	3122	1/1	0.68	0.63	79,79,79,79	0
58	MG	2L	102	1/1	0.68	0.64	83,83,83,83	0
58	MG	14	3227	1/1	0.68	0.44	76,76,76,76	0
58	MG	13	1695	1/1	0.68	0.43	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3292	1/1	0.68	0.30	77,77,77,77	0
58	MG	1H	3253	1/1	0.68	0.37	66,66,66,66	0
58	MG	1H	3254	1/1	0.68	0.57	99,99,99,99	0
58	MG	14	3135	1/1	0.68	0.24	95,95,95,95	0
58	MG	14	3262	1/1	0.68	0.34	96,96,96,96	0
58	MG	14	3392	1/1	0.68	0.06	128,128,128,128	0
58	MG	1H	3459	1/1	0.69	0.06	106,106,106,106	0
58	MG	1H	3079	1/1	0.69	0.38	79,79,79,79	0
58	MG	13	1632	1/1	0.69	0.40	107,107,107,107	0
58	MG	14	3186	1/1	0.69	0.45	82,82,82,82	0
58	MG	1H	3293	1/1	0.69	0.35	84,84,84,84	0
58	MG	14	3308	1/1	0.69	0.70	106,106,106,106	0
58	MG	1H	3277	1/1	0.70	0.32	68,68,68,68	0
58	MG	14	3257	1/1	0.70	1.14	86,86,86,86	0
58	MG	1H	3305	1/1	0.70	0.39	67,67,67,67	0
58	MG	1G	1648	1/1	0.70	0.32	117,117,117,117	0
58	MG	1H	3314	1/1	0.70	0.30	85,85,85,85	0
58	MG	1G	1649	1/1	0.70	0.41	83,83,83,83	0
58	MG	1H	3306	1/1	0.70	0.31	91,91,91,91	0
58	MG	14	3030	1/1	0.70	0.39	86,86,86,86	0
58	MG	1H	3178	1/1	0.70	0.38	71,71,71,71	0
58	MG	1H	3301	1/1	0.70	0.44	84,84,84,84	0
58	MG	13	1646	1/1	0.70	0.29	75,75,75,75	0
58	MG	14	3295	1/1	0.71	0.20	85,85,85,85	0
58	MG	14	3255	1/1	0.71	0.25	78,78,78,78	0
58	MG	14	3313	1/1	0.71	0.49	92,92,92,92	0
58	MG	14	3259	1/1	0.71	0.75	98,98,98,98	0
58	MG	1H	3328	1/1	0.71	0.58	80,80,80,80	0
58	MG	1H	3217	1/1	0.71	0.34	71,71,71,71	0
58	MG	13	1728	1/1	0.71	0.11	118,118,118,118	0
58	MG	16	204	1/1	0.71	0.32	73,73,73,73	0
58	MG	1H	3251	1/1	0.71	0.39	71,71,71,71	0
58	MG	1H	3315	1/1	0.71	0.53	76,76,76,76	0
58	MG	1H	3302	1/1	0.71	0.22	92,92,92,92	0
58	MG	13	1705	1/1	0.71	0.35	90,90,90,90	0
58	MG	1H	3324	1/1	0.72	0.57	89,89,89,89	0
58	MG	13	1656	1/1	0.72	0.15	103,103,103,103	0
58	MG	14	3058	1/1	0.72	0.18	84,84,84,84	0
58	MG	13	1659	1/1	0.72	0.62	97,97,97,97	0
58	MG	E5	101	1/1	0.72	0.47	89,89,89,89	0
58	MG	1H	3224	1/1	0.72	0.58	73,73,73,73	0
58	MG	1J	201	1/1	0.72	0.30	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3231	1/1	0.72	0.34	86,86,86,86	0
58	MG	1H	3368	1/1	0.72	0.24	74,74,74,74	0
58	MG	13	1641	1/1	0.73	0.44	93,93,93,93	0
58	MG	1H	3180	1/1	0.73	0.43	75,75,75,75	0
58	MG	1H	3139	1/1	0.73	0.36	71,71,71,71	0
58	MG	14	3155	1/1	0.73	0.71	64,64,64,64	0
58	MG	14	3234	1/1	0.73	0.89	70,70,70,70	0
58	MG	1H	3101	1/1	0.73	0.26	59,59,59,59	0
58	MG	1H	3032	1/1	0.73	0.49	79,79,79,79	0
58	MG	1H	3288	1/1	0.74	0.87	93,93,93,93	0
58	MG	14	3181	1/1	0.74	0.41	89,89,89,89	0
58	MG	1H	3222	1/1	0.74	0.33	98,98,98,98	0
58	MG	14	3143	1/1	0.74	0.30	102,102,102,102	0
58	MG	14	3300	1/1	0.74	0.24	117,117,117,117	0
58	MG	14	3019	1/1	0.74	0.67	90,90,90,90	0
58	MG	29	301	1/1	0.74	0.34	77,77,77,77	0
58	MG	14	3260	1/1	0.74	0.78	72,72,72,72	0
58	MG	1H	3342	1/1	0.74	0.63	92,92,92,92	0
58	MG	13	1689	1/1	0.74	0.52	107,107,107,107	0
58	MG	14	3251	1/1	0.74	0.50	69,69,69,69	0
58	MG	14	3194	1/1	0.74	0.34	81,81,81,81	0
58	MG	1H	3031	1/1	0.75	0.53	76,76,76,76	0
58	MG	14	3250	1/1	0.75	0.41	78,78,78,78	0
58	MG	1H	3228	1/1	0.75	0.45	83,83,83,83	0
58	MG	1H	3080	1/1	0.75	0.21	65,65,65,65	0
58	MG	14	3144	1/1	0.75	0.41	71,71,71,71	0
58	MG	1H	3457	1/1	0.75	0.06	141,141,141,141	0
58	MG	2K	103	1/1	0.75	0.42	114,114,114,114	0
58	MG	18	101	1/1	0.75	0.32	73,73,73,73	0
58	MG	1H	3154	1/1	0.76	0.54	84,84,84,84	0
58	MG	14	3052	1/1	0.76	0.50	113,113,113,113	0
58	MG	35	203	1/1	0.76	0.24	75,75,75,75	0
58	MG	1H	3291	1/1	0.76	0.31	73,73,73,73	0
58	MG	1H	3197	1/1	0.76	0.63	80,80,80,80	0
58	MG	14	3288	1/1	0.76	0.74	86,86,86,86	0
58	MG	14	3147	1/1	0.76	0.23	95,95,95,95	0
58	MG	13	1681	1/1	0.76	0.19	116,116,116,116	0
58	MG	1H	3043	1/1	0.76	0.76	81,81,81,81	0
58	MG	1H	3247	1/1	0.76	0.21	81,81,81,81	0
58	MG	1H	3313	1/1	0.76	0.26	98,98,98,98	0
58	MG	1H	3199	1/1	0.76	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3310	1/1	0.76	0.23	114,114,114,114	0
58	MG	1G	1666	1/1	0.76	0.50	84,84,84,84	0
58	MG	13	1662	1/1	0.76	0.36	118,118,118,118	0
58	MG	14	3188	1/1	0.76	0.56	88,88,88,88	0
58	MG	1H	3142	1/1	0.77	0.45	68,68,68,68	0
58	MG	14	3117	1/1	0.77	0.44	81,81,81,81	0
58	MG	1G	1672	1/1	0.77	0.43	99,99,99,99	0
58	MG	1H	3087	1/1	0.77	0.57	70,70,70,70	0
58	MG	14	3290	1/1	0.77	0.22	92,92,92,92	0
58	MG	13	1621	1/1	0.77	0.21	90,90,90,90	0
58	MG	14	3301	1/1	0.77	0.21	109,109,109,109	0
58	MG	14	3345	1/1	0.77	0.10	90,90,90,90	0
58	MG	29	302	1/1	0.77	0.45	65,65,65,65	0
58	MG	1H	3296	1/1	0.77	0.22	57,57,57,57	0
58	MG	1H	3136	1/1	0.77	0.34	49,49,49,49	0
58	MG	14	3268	1/1	0.77	0.41	94,94,94,94	0
58	MG	14	3291	1/1	0.77	0.35	87,87,87,87	0
58	MG	14	3293	1/1	0.77	0.51	91,91,91,91	0
58	MG	1G	1604	1/1	0.78	0.44	87,87,87,87	0
58	MG	14	3247	1/1	0.78	0.28	67,67,67,67	0
58	MG	1H	3439	1/1	0.78	0.07	99,99,99,99	0
58	MG	14	3265	1/1	0.78	0.52	98,98,98,98	0
58	MG	14	3029	1/1	0.78	0.72	78,78,78,78	0
58	MG	13	1706	1/1	0.78	0.39	109,109,109,109	0
58	MG	1H	3271	1/1	0.78	0.39	76,76,76,76	0
58	MG	13	1644	1/1	0.78	0.43	96,96,96,96	0
58	MG	35	201	1/1	0.78	0.26	74,74,74,74	0
58	MG	1G	1643	1/1	0.78	0.24	132,132,132,132	0
58	MG	1H	3263	1/1	0.78	0.25	76,76,76,76	0
58	MG	1H	3364	1/1	0.78	0.10	98,98,98,98	0
58	MG	14	3183	1/1	0.78	0.77	79,79,79,79	0
58	MG	14	3073	1/1	0.78	1.32	83,83,83,83	0
58	MG	14	3306	1/1	0.78	0.29	88,88,88,88	0
58	MG	1H	3201	1/1	0.78	0.69	92,92,92,92	0
58	MG	1H	3327	1/1	0.78	0.79	82,82,82,82	0
58	MG	1H	3175	1/1	0.78	0.53	65,65,65,65	0
58	MG	1H	3022	1/1	0.78	0.39	62,62,62,62	0
58	MG	14	3243	1/1	0.79	0.47	81,81,81,81	0
58	MG	14	3280	1/1	0.79	0.91	86,86,86,86	0
58	MG	1G	1618	1/1	0.79	0.33	109,109,109,109	0
58	MG	14	3353	1/1	0.79	0.09	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3253	1/1	0.79	0.26	94,94,94,94	0
58	MG	1H	3083	1/1	0.79	0.33	67,67,67,67	0
58	MG	1G	1606	1/1	0.79	0.22	88,88,88,88	0
58	MG	14	3018	1/1	0.79	0.61	72,72,72,72	0
58	MG	13	1694	1/1	0.79	0.55	64,64,64,64	0
58	MG	14	3252	1/1	0.79	0.39	84,84,84,84	0
58	MG	14	3182	1/1	0.79	0.74	75,75,75,75	0
58	MG	16	209	1/1	0.79	0.10	100,100,100,100	0
58	MG	1G	1680	1/1	0.79	0.06	140,140,140,140	0
58	MG	1H	3414	1/1	0.79	0.19	80,80,80,80	0
58	MG	1H	3045	1/1	0.79	0.33	82,82,82,82	0
58	MG	14	3187	1/1	0.80	0.45	80,80,80,80	0
58	MG	13	1679	1/1	0.80	0.28	100,100,100,100	0
58	MG	1G	1678	1/1	0.80	0.06	128,128,128,128	0
58	MG	1H	3196	1/1	0.80	0.44	83,83,83,83	0
58	MG	1H	3033	1/1	0.80	0.58	88,88,88,88	0
58	MG	1J	204	1/1	0.80	0.27	101,101,101,101	0
58	MG	1G	1667	1/1	0.80	0.28	109,109,109,109	0
58	MG	14	3297	1/1	0.80	0.69	70,70,70,70	0
58	MG	1H	3205	1/1	0.80	0.19	81,81,81,81	0
58	MG	14	3080	1/1	0.80	0.46	82,82,82,82	0
58	MG	1H	3298	1/1	0.80	0.35	74,74,74,74	0
58	MG	1H	3021	1/1	0.80	0.30	83,83,83,83	0
58	MG	14	3179	1/1	0.80	0.24	60,60,60,60	0
58	MG	1H	3268	1/1	0.80	0.42	85,85,85,85	0
58	MG	13	1704	1/1	0.80	0.41	82,82,82,82	0
58	MG	13	1675	1/1	0.80	0.30	73,73,73,73	0
58	MG	14	3023	1/1	0.80	0.29	83,83,83,83	0
58	MG	14	3221	1/1	0.80	0.20	69,69,69,69	0
58	MG	1H	3282	1/1	0.80	0.60	88,88,88,88	0
58	MG	14	3292	1/1	0.80	0.14	113,113,113,113	0
58	MG	1H	3173	1/1	0.80	0.47	84,84,84,84	0
58	MG	14	3391	1/1	0.80	0.13	104,104,104,104	0
58	MG	14	3150	1/1	0.80	0.40	87,87,87,87	0
58	MG	13	1678	1/1	0.80	0.27	93,93,93,93	0
58	MG	1H	3019	1/1	0.81	0.49	92,92,92,92	0
58	MG	14	3146	1/1	0.81	0.43	57,57,57,57	0
58	MG	1H	3179	1/1	0.81	0.35	83,83,83,83	0
58	MG	1H	3209	1/1	0.81	0.42	90,90,90,90	0
58	MG	1H	3097	1/1	0.81	0.44	71,71,71,71	0
58	MG	13	1637	1/1	0.81	0.38	56,56,56,56	0
58	MG	14	3228	1/1	0.81	0.17	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	98	201	1/1	0.81	0.41	72,72,72,72	0
58	MG	1H	3307	1/1	0.81	0.52	94,94,94,94	0
58	MG	1H	3441	1/1	0.81	0.13	89,89,89,89	0
58	MG	16	205	1/1	0.81	0.11	81,81,81,81	0
58	MG	1H	3246	1/1	0.81	0.23	54,54,54,54	0
58	MG	14	3170	1/1	0.81	0.37	83,83,83,83	0
58	MG	1G	1657	1/1	0.81	0.36	92,92,92,92	0
58	MG	14	3395	1/1	0.81	0.10	103,103,103,103	0
58	MG	1G	1686	1/1	0.81	0.08	125,125,125,125	0
58	MG	1H	3337	1/1	0.81	0.22	89,89,89,89	0
58	MG	14	3271	1/1	0.81	0.21	81,81,81,81	0
58	MG	13	1661	1/1	0.81	0.48	103,103,103,103	0
58	MG	1G	1679	1/1	0.81	0.11	119,119,119,119	0
58	MG	1G	1663	1/1	0.81	0.10	94,94,94,94	0
58	MG	14	3245	1/1	0.81	0.47	77,77,77,77	0
58	MG	P8	101	1/1	0.81	0.58	77,77,77,77	0
58	MG	13	1670	1/1	0.81	0.19	97,97,97,97	0
58	MG	14	3177	1/1	0.81	0.46	72,72,72,72	0
58	MG	1G	1659	1/1	0.81	0.18	142,142,142,142	0
58	MG	16	203	1/1	0.81	0.14	90,90,90,90	0
58	MG	1G	1615	1/1	0.82	0.23	125,125,125,125	0
58	MG	13	1685	1/1	0.82	0.24	121,121,121,121	0
58	MG	14	3059	1/1	0.82	0.32	86,86,86,86	0
58	MG	14	3060	1/1	0.82	0.23	73,73,73,73	0
58	MG	1H	3438	1/1	0.82	0.11	83,83,83,83	0
58	MG	1H	3413	1/1	0.82	0.08	102,102,102,102	0
58	MG	14	3074	1/1	0.82	0.81	79,79,79,79	0
58	MG	78	201	1/1	0.82	0.36	70,70,70,70	0
58	MG	1G	1684	1/1	0.82	0.11	109,109,109,109	0
58	MG	1H	3151	1/1	0.82	0.20	55,55,55,55	0
58	MG	1H	3280	1/1	0.82	0.33	77,77,77,77	0
58	MG	3K	101	1/1	0.82	0.34	162,162,162,162	0
58	MG	1H	3128	1/1	0.82	0.22	62,62,62,62	0
58	MG	1G	1636	1/1	0.82	0.32	101,101,101,101	0
58	MG	14	3393	1/1	0.82	0.06	127,127,127,127	0
58	MG	14	3222	1/1	0.82	0.23	97,97,97,97	0
58	MG	1J	202	1/1	0.82	0.27	95,95,95,95	0
58	MG	13	1682	1/1	0.82	0.45	88,88,88,88	0
58	MG	1G	1668	1/1	0.82	0.36	116,116,116,116	0
58	MG	14	3109	1/1	0.82	0.38	73,73,73,73	0
58	MG	14	3193	1/1	0.82	0.40	77,77,77,77	0
58	MG	14	3125	1/1	0.82	0.75	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1668	1/1	0.83	0.09	90,90,90,90	0
58	MG	13	1604	1/1	0.83	0.27	87,87,87,87	0
58	MG	1G	1620	1/1	0.83	0.31	82,82,82,82	0
58	MG	1H	3341	1/1	0.83	0.21	79,79,79,79	0
58	MG	1G	1630	1/1	0.83	0.41	103,103,103,103	0
58	MG	1G	1609	1/1	0.83	0.18	94,94,94,94	0
58	MG	1G	1650	1/1	0.83	0.30	114,114,114,114	0
58	MG	13	1650	1/1	0.83	0.30	94,94,94,94	0
58	MG	14	3012	1/1	0.83	0.81	80,80,80,80	0
58	MG	6A	101	1/1	0.83	0.26	93,93,93,93	0
58	MG	14	3201	1/1	0.83	0.27	59,59,59,59	0
58	MG	13	1715	1/1	0.83	0.10	109,109,109,109	0
58	MG	1H	3338	1/1	0.83	0.37	65,65,65,65	0
58	MG	13	1634	1/1	0.83	1.02	93,93,93,93	0
58	MG	1H	3137	1/1	0.83	0.61	88,88,88,88	0
58	MG	14	3273	1/1	0.83	0.46	101,101,101,101	0
58	MG	21	302	1/1	0.83	0.33	77,77,77,77	0
58	MG	1H	3190	1/1	0.83	0.32	73,73,73,73	0
58	MG	1H	3287	1/1	0.83	0.29	104,104,104,104	0
58	MG	14	3107	1/1	0.83	0.51	77,77,77,77	0
58	MG	1H	3262	1/1	0.83	0.37	94,94,94,94	0
58	MG	1H	3159	1/1	0.83	0.42	67,67,67,67	0
58	MG	13	1669	1/1	0.83	0.30	68,68,68,68	0
58	MG	14	3238	1/1	0.83	0.33	99,99,99,99	0
58	MG	1H	3018	1/1	0.83	0.55	71,71,71,71	0
58	MG	14	3022	1/1	0.83	0.38	64,64,64,64	0
58	MG	14	3236	1/1	0.83	0.51	89,89,89,89	0
58	MG	14	3230	1/1	0.83	0.41	64,64,64,64	0
58	MG	13	1708	1/1	0.83	0.13	89,89,89,89	0
58	MG	1H	3335	1/1	0.83	0.68	74,74,74,74	0
58	MG	1H	3233	1/1	0.84	0.59	62,62,62,62	0
58	MG	14	3248	1/1	0.84	0.21	79,79,79,79	0
58	MG	1H	3125	1/1	0.84	0.50	69,69,69,69	0
58	MG	14	3278	1/1	0.84	0.34	75,75,75,75	0
58	MG	14	3256	1/1	0.84	0.54	83,83,83,83	0
58	MG	14	3067	1/1	0.84	0.31	87,87,87,87	0
58	MG	14	3363	1/1	0.84	0.19	72,72,72,72	0
58	MG	1H	3226	1/1	0.84	0.38	85,85,85,85	0
58	MG	14	3237	1/1	0.84	0.37	83,83,83,83	0
58	MG	1H	3316	1/1	0.84	0.88	92,92,92,92	0
58	MG	1H	3089	1/1	0.84	0.44	59,59,59,59	0
58	MG	1H	3184	1/1	0.84	0.26	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	5E	201	1/1	0.84	0.26	89,89,89,89	0
58	MG	14	3021	1/1	0.84	0.45	52,52,52,52	0
58	MG	1H	3308	1/1	0.84	0.51	90,90,90,90	0
58	MG	14	3027	1/1	0.84	0.39	96,96,96,96	0
58	MG	29	304	1/1	0.84	0.22	81,81,81,81	0
58	MG	1H	3187	1/1	0.84	0.25	69,69,69,69	0
58	MG	14	3309	1/1	0.85	0.44	110,110,110,110	0
58	MG	1H	3213	1/1	0.85	0.38	74,74,74,74	0
58	MG	1H	3130	1/1	0.85	0.32	74,74,74,74	0
58	MG	14	3205	1/1	0.85	0.34	96,96,96,96	0
58	MG	1H	3322	1/1	0.85	0.65	81,81,81,81	0
58	MG	1H	3463	1/1	0.85	0.08	112,112,112,112	0
58	MG	1H	3096	1/1	0.85	0.33	60,60,60,60	0
58	MG	41	201	1/1	0.85	0.07	78,78,78,78	0
58	MG	1H	3071	1/1	0.85	0.38	61,61,61,61	0
58	MG	1H	3072	1/1	0.85	0.30	77,77,77,77	0
58	MG	1H	3332	1/1	0.85	0.32	74,74,74,74	0
58	MG	1G	1633	1/1	0.85	0.31	98,98,98,98	0
58	MG	13	1703	1/1	0.85	0.78	77,77,77,77	0
58	MG	1G	1665	1/1	0.85	0.26	113,113,113,113	0
58	MG	1H	3108	1/1	0.85	0.33	74,74,74,74	0
58	MG	1H	3252	1/1	0.85	0.50	66,66,66,66	0
58	MG	1G	1637	1/1	0.85	0.55	87,87,87,87	0
58	MG	1H	3193	1/1	0.85	0.50	73,73,73,73	0
58	MG	14	3061	1/1	0.85	0.12	81,81,81,81	0
58	MG	1H	3227	1/1	0.85	0.68	85,85,85,85	0
58	MG	1H	3422	1/1	0.85	0.16	112,112,112,112	0
58	MG	1H	3020	1/1	0.85	0.32	66,66,66,66	0
58	MG	14	3266	1/1	0.85	0.53	85,85,85,85	0
58	MG	1H	3157	1/1	0.86	0.47	73,73,73,73	0
58	MG	14	3296	1/1	0.86	0.41	84,84,84,84	0
58	MG	1G	1619	1/1	0.86	0.21	101,101,101,101	0
58	MG	13	1647	1/1	0.86	0.23	89,89,89,89	0
58	MG	1H	3203	1/1	0.86	0.37	79,79,79,79	0
58	MG	1G	1671	1/1	0.86	0.38	88,88,88,88	0
58	MG	1H	3015	1/1	0.86	0.27	63,63,63,63	0
58	MG	1H	3206	1/1	0.86	0.35	77,77,77,77	0
58	MG	1G	1634	1/1	0.86	0.29	112,112,112,112	0
58	MG	1H	3216	1/1	0.86	0.40	67,67,67,67	0
58	MG	1H	3426	1/1	0.86	0.13	58,58,58,58	0
58	MG	1G	1641	1/1	0.86	0.34	113,113,113,113	0
58	MG	1H	3276	1/1	0.86	0.68	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	55	201	1/1	0.86	0.30	74,74,74,74	0
58	MG	1H	3188	1/1	0.86	0.38	73,73,73,73	0
58	MG	14	3163	1/1	0.86	0.27	90,90,90,90	0
58	MG	1H	3234	1/1	0.86	0.08	66,66,66,66	0
58	MG	1H	3329	1/1	0.86	0.77	81,81,81,81	0
58	MG	14	3013	1/1	0.86	0.23	78,78,78,78	0
58	MG	1H	3141	1/1	0.86	0.40	61,61,61,61	0
58	MG	1H	3126	1/1	0.86	0.23	58,58,58,58	0
58	MG	13	1692	1/1	0.86	0.16	122,122,122,122	0
58	MG	13	1707	1/1	0.86	0.15	76,76,76,76	0
58	MG	1H	3242	1/1	0.86	0.36	52,52,52,52	0
58	MG	13	1606	1/1	0.86	0.46	94,94,94,94	0
58	MG	14	3199	1/1	0.86	0.50	69,69,69,69	0
58	MG	1H	3321	1/1	0.86	0.25	67,67,67,67	0
58	MG	14	3118	1/1	0.86	0.45	69,69,69,69	0
58	MG	1H	3185	1/1	0.86	0.40	95,95,95,95	0
58	MG	1H	3303	1/1	0.86	0.77	78,78,78,78	0
58	MG	1G	1654	1/1	0.86	0.53	83,83,83,83	0
58	MG	1H	3340	1/1	0.86	0.50	78,78,78,78	0
58	MG	1H	3290	1/1	0.86	0.22	70,70,70,70	0
58	MG	1H	3376	1/1	0.87	0.23	76,76,76,76	0
58	MG	1H	3182	1/1	0.87	0.20	78,78,78,78	0
58	MG	14	3084	1/1	0.87	0.56	80,80,80,80	0
58	MG	1H	3158	1/1	0.87	0.49	74,74,74,74	0
58	MG	1H	3135	1/1	0.87	0.12	65,65,65,65	0
58	MG	1H	3445	1/1	0.87	0.07	110,110,110,110	0
58	MG	14	3169	1/1	0.87	0.40	58,58,58,58	0
58	MG	14	3274	1/1	0.87	0.15	76,76,76,76	0
58	MG	1H	3258	1/1	0.87	0.27	59,59,59,59	0
58	MG	1G	1662	1/1	0.87	0.68	72,72,72,72	0
58	MG	14	3272	1/1	0.87	0.38	76,76,76,76	0
58	MG	1H	3168	1/1	0.87	0.38	69,69,69,69	0
58	MG	1H	3452	1/1	0.87	0.13	104,104,104,104	0
58	MG	14	3281	1/1	0.87	0.38	86,86,86,86	0
58	MG	1H	3281	1/1	0.87	0.20	88,88,88,88	0
58	MG	1J	205	1/1	0.87	0.09	101,101,101,101	0
58	MG	13	1680	1/1	0.87	0.28	96,96,96,96	0
58	MG	14	3263	1/1	0.87	0.24	75,75,75,75	0
58	MG	1H	3186	1/1	0.87	0.34	75,75,75,75	0
58	MG	14	3211	1/1	0.87	0.37	91,91,91,91	0
58	MG	14	3284	1/1	0.87	0.78	78,78,78,78	0
58	MG	13	1639	1/1	0.87	0.56	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	16	202	1/1	0.87	0.25	64,64,64,64	0
58	MG	14	3246	1/1	0.87	0.22	69,69,69,69	0
58	MG	1H	3326	1/1	0.87	0.56	83,83,83,83	0
58	MG	14	3154	1/1	0.87	0.25	69,69,69,69	0
58	MG	14	3131	1/1	0.87	0.33	95,95,95,95	0
58	MG	13	1686	1/1	0.87	0.50	76,76,76,76	0
58	MG	1H	3176	1/1	0.87	0.46	76,76,76,76	0
58	MG	1K	101	1/1	0.87	0.09	145,145,145,145	0
58	MG	1H	3066	1/1	0.87	0.33	59,59,59,59	0
58	MG	1H	3156	1/1	0.87	0.31	67,67,67,67	0
58	MG	1H	3333	1/1	0.88	0.34	100,100,100,100	0
58	MG	1H	3144	1/1	0.88	0.40	77,77,77,77	0
58	MG	1H	3041	1/1	0.88	0.22	76,76,76,76	0
58	MG	1G	1628	1/1	0.88	0.44	95,95,95,95	0
58	MG	13	1677	1/1	0.88	0.16	104,104,104,104	0
58	MG	14	3386	1/1	0.88	0.16	90,90,90,90	0
58	MG	14	3100	1/1	0.88	0.38	76,76,76,76	0
58	MG	14	3232	1/1	0.88	0.21	81,81,81,81	0
58	MG	13	1608	1/1	0.88	0.75	90,90,90,90	0
58	MG	14	3055	1/1	0.88	0.10	81,81,81,81	0
58	MG	1H	3323	1/1	0.88	0.45	80,80,80,80	0
58	MG	1H	3170	1/1	0.88	0.46	65,65,65,65	0
58	MG	14	3364	1/1	0.88	0.16	85,85,85,85	0
58	MG	14	3032	1/1	0.88	0.45	75,75,75,75	0
58	MG	1H	3140	1/1	0.88	0.27	58,58,58,58	0
58	MG	Q8	101	1/1	0.88	0.33	70,70,70,70	0
58	MG	14	3286	1/1	0.88	0.38	80,80,80,80	0
58	MG	1H	3269	1/1	0.88	0.32	65,65,65,65	0
58	MG	I8	102	1/1	0.88	0.24	70,70,70,70	0
58	MG	13	1624	1/1	0.88	0.23	103,103,103,103	0
58	MG	14	3299	1/1	0.88	0.20	98,98,98,98	0
58	MG	1G	1613	1/1	0.88	0.21	98,98,98,98	0
58	MG	1H	3320	1/1	0.88	0.46	77,77,77,77	0
58	MG	1G	1677	1/1	0.88	0.12	96,96,96,96	0
58	MG	1H	3286	1/1	0.88	0.32	94,94,94,94	0
58	MG	1H	3467	1/1	0.88	0.10	84,84,84,84	0
58	MG	L8	101	1/1	0.88	0.62	84,84,84,84	0
58	MG	1H	3334	1/1	0.89	0.30	76,76,76,76	0
58	MG	1G	1689	1/1	0.89	0.17	121,121,121,121	0
58	MG	14	3220	1/1	0.89	0.43	76,76,76,76	0
58	MG	1H	3325	1/1	0.89	0.44	71,71,71,71	0
58	MG	13	1687	1/1	0.89	0.27	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3285	1/1	0.89	0.25	68,68,68,68	0
58	MG	1G	1647	1/1	0.89	0.80	83,83,83,83	0
58	MG	14	3104	1/1	0.89	0.65	86,86,86,86	0
58	MG	13	1652	1/1	0.89	0.24	99,99,99,99	0
58	MG	1H	3232	1/1	0.89	0.17	52,52,52,52	0
58	MG	14	3160	1/1	0.89	0.37	72,72,72,72	0
58	MG	14	3090	1/1	0.89	0.29	74,74,74,74	0
58	MG	1H	3221	1/1	0.89	0.40	89,89,89,89	0
58	MG	14	3126	1/1	0.89	0.39	67,67,67,67	0
58	MG	13	1691	1/1	0.89	0.48	90,90,90,90	0
58	MG	13	1620	1/1	0.89	0.28	73,73,73,73	0
58	MG	14	3307	1/1	0.89	0.48	101,101,101,101	0
58	MG	1H	3353	1/1	0.89	0.16	57,57,57,57	0
58	MG	1H	3417	1/1	0.89	0.22	94,94,94,94	0
58	MG	14	3287	1/1	0.89	0.22	82,82,82,82	0
58	MG	1H	3388	1/1	0.89	0.07	77,77,77,77	0
58	MG	1H	3042	1/1	0.89	0.85	90,90,90,90	0
58	MG	1H	3419	1/1	0.89	0.06	101,101,101,101	0
58	MG	14	3203	1/1	0.89	0.34	56,56,56,56	0
58	MG	1G	1631	1/1	0.89	0.25	96,96,96,96	0
58	MG	14	3324	1/1	0.89	0.06	99,99,99,99	0
58	MG	14	3244	1/1	0.89	0.59	70,70,70,70	0
58	MG	1H	3131	1/1	0.89	0.56	73,73,73,73	0
58	MG	14	3195	1/1	0.89	0.37	68,68,68,68	0
58	MG	1G	1622	1/1	0.89	1.19	92,92,92,92	0
58	MG	14	3024	1/1	0.89	0.57	77,77,77,77	0
58	MG	14	3007	1/1	0.89	0.48	54,54,54,54	0
58	MG	14	3025	1/1	0.90	0.62	84,84,84,84	0
58	MG	14	3111	1/1	0.90	0.14	81,81,81,81	0
58	MG	13	1655	1/1	0.90	0.46	87,87,87,87	0
58	MG	13	1631	1/1	0.90	0.37	93,93,93,93	0
58	MG	1H	3063	1/1	0.90	0.13	78,78,78,78	0
58	MG	13	1702	1/1	0.90	0.27	98,98,98,98	0
58	MG	14	3028	1/1	0.90	0.25	69,69,69,69	0
58	MG	1H	3119	1/1	0.90	0.20	69,69,69,69	0
58	MG	14	3325	1/1	0.90	0.14	63,63,63,63	0
58	MG	14	3096	1/1	0.90	0.34	73,73,73,73	0
58	MG	1H	3238	1/1	0.90	0.14	65,65,65,65	0
58	MG	14	3212	1/1	0.90	0.39	70,70,70,70	0
58	MG	14	3312	1/1	0.90	0.54	80,80,80,80	0
58	MG	14	3033	1/1	0.90	0.26	77,77,77,77	0
58	MG	1H	3009	1/1	0.90	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3319	1/1	0.90	0.52	110,110,110,110	0
58	MG	14	3389	1/1	0.90	0.09	102,102,102,102	0
58	MG	45	201	1/1	0.90	0.16	108,108,108,108	0
58	MG	14	3157	1/1	0.90	0.25	57,57,57,57	0
58	MG	14	3149	1/1	0.90	0.54	73,73,73,73	0
58	MG	1G	1639	1/1	0.90	0.51	74,74,74,74	0
58	MG	1G	1661	1/1	0.90	0.23	123,123,123,123	0
58	MG	14	3168	1/1	0.90	0.53	106,106,106,106	0
58	MG	1H	3027	1/1	0.90	0.32	81,81,81,81	0
58	MG	1H	3034	1/1	0.90	0.45	80,80,80,80	0
58	MG	1G	1687	1/1	0.90	0.06	139,139,139,139	0
58	MG	1H	3003	1/1	0.90	0.26	64,64,64,64	0
58	MG	14	3204	1/1	0.90	0.19	77,77,77,77	0
58	MG	14	3200	1/1	0.90	0.46	74,74,74,74	0
58	MG	14	3172	1/1	0.90	0.70	70,70,70,70	0
58	MG	14	3176	1/1	0.90	0.47	79,79,79,79	0
58	MG	1H	3155	1/1	0.90	0.34	74,74,74,74	0
58	MG	1H	3464	1/1	0.90	0.14	107,107,107,107	0
58	MG	1G	1640	1/1	0.90	0.48	87,87,87,87	0
58	MG	14	3333	1/1	0.90	0.17	74,74,74,74	0
58	MG	1H	3200	1/1	0.90	0.49	81,81,81,81	0
58	MG	1H	3085	1/1	0.90	0.42	63,63,63,63	0
58	MG	1H	3267	1/1	0.90	0.49	73,73,73,73	0
58	MG	1H	3362	1/1	0.90	0.11	53,53,53,53	0
58	MG	14	3035	1/1	0.90	0.22	93,93,93,93	0
58	MG	1H	3039	1/1	0.90	0.32	68,68,68,68	0
58	MG	14	3378	1/1	0.90	0.07	100,100,100,100	0
58	MG	1H	3272	1/1	0.90	0.18	64,64,64,64	0
58	MG	13	1651	1/1	0.90	0.41	88,88,88,88	0
58	MG	14	3249	1/1	0.90	0.24	80,80,80,80	0
58	MG	1H	3088	1/1	0.90	0.34	68,68,68,68	0
58	MG	13	1629	1/1	0.90	0.39	96,96,96,96	0
58	MG	14	3165	1/1	0.90	0.51	77,77,77,77	0
58	MG	1H	3446	1/1	0.90	0.09	84,84,84,84	0
58	MG	1H	3132	1/1	0.90	0.65	85,85,85,85	0
58	MG	1H	3215	1/1	0.90	0.28	63,63,63,63	0
58	MG	1H	3318	1/1	0.90	0.42	79,79,79,79	0
58	MG	14	3115	1/1	0.90	0.40	80,80,80,80	0
58	MG	14	3049	1/1	0.90	0.21	70,70,70,70	0
58	MG	16	207	1/1	0.90	0.07	80,80,80,80	0
58	MG	14	3365	1/1	0.91	0.05	94,94,94,94	0
58	MG	14	3099	1/1	0.91	0.56	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	G8	201	1/1	0.91	0.11	149,149,149,149	0
58	MG	14	3178	1/1	0.91	0.50	84,84,84,84	0
58	MG	1H	3118	1/1	0.91	0.84	77,77,77,77	0
58	MG	14	3305	1/1	0.91	0.49	75,75,75,75	0
58	MG	1H	3270	1/1	0.91	0.86	80,80,80,80	0
58	MG	14	3215	1/1	0.91	0.22	72,72,72,72	0
58	MG	1H	3220	1/1	0.91	0.27	82,82,82,82	0
58	MG	13	1720	1/1	0.91	0.10	90,90,90,90	0
58	MG	14	3352	1/1	0.91	0.07	97,97,97,97	0
58	MG	14	3397	1/1	0.91	0.50	73,73,73,73	0
58	MG	13	1710	1/1	0.91	0.09	97,97,97,97	0
58	MG	1H	3265	1/1	0.91	0.40	78,78,78,78	0
58	MG	1H	3100	1/1	0.91	0.24	61,61,61,61	0
58	MG	1H	3204	1/1	0.91	0.42	69,69,69,69	0
58	MG	1H	3162	1/1	0.91	0.39	88,88,88,88	0
58	MG	14	3148	1/1	0.91	0.31	77,77,77,77	0
58	MG	14	3239	1/1	0.91	0.17	80,80,80,80	0
58	MG	J8	101	1/1	0.91	0.19	66,66,66,66	0
58	MG	1G	1602	1/1	0.91	0.42	79,79,79,79	0
58	MG	14	3241	1/1	0.91	0.35	56,56,56,56	0
58	MG	1G	1645	1/1	0.91	0.52	74,74,74,74	0
58	MG	13	1654	1/1	0.91	0.38	74,74,74,74	0
58	MG	1H	3367	1/1	0.91	0.09	71,71,71,71	0
58	MG	13	1657	1/1	0.91	0.28	103,103,103,103	0
58	MG	1H	3095	1/1	0.91	0.33	65,65,65,65	0
58	MG	1G	1674	1/1	0.91	0.44	102,102,102,102	0
58	MG	14	3279	1/1	0.91	0.09	104,104,104,104	0
58	MG	14	3217	1/1	0.91	0.43	83,83,83,83	0
58	MG	14	3223	1/1	0.91	0.35	86,86,86,86	0
58	MG	14	3031	1/1	0.91	0.42	68,68,68,68	0
58	MG	1H	3002	1/1	0.91	0.25	38,38,38,38	0
58	MG	14	3242	1/1	0.91	0.52	67,67,67,67	0
58	MG	14	3384	1/1	0.91	0.14	83,83,83,83	0
58	MG	1H	3104	1/1	0.91	0.58	69,69,69,69	0
58	MG	13	1731	1/1	0.91	0.14	84,84,84,84	0
58	MG	13	1627	1/1	0.91	0.55	69,69,69,69	0
58	MG	14	3122	1/1	0.91	0.28	88,88,88,88	0
58	MG	1H	3418	1/1	0.91	0.08	92,92,92,92	0
58	MG	1H	3047	1/1	0.91	0.32	47,47,47,47	0
58	MG	1G	1614	1/1	0.91	0.30	107,107,107,107	0
58	MG	1H	3004	1/1	0.91	0.32	57,57,57,57	0
58	MG	1H	3460	1/1	0.91	0.09	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3294	1/1	0.91	0.34	57,57,57,57	0
58	MG	1G	1670	1/1	0.91	0.43	86,86,86,86	0
58	MG	14	3171	1/1	0.91	0.32	99,99,99,99	0
58	MG	14	3056	1/1	0.92	0.34	55,55,55,55	0
58	MG	14	3394	1/1	0.92	0.05	109,109,109,109	0
58	MG	1H	3317	1/1	0.92	0.38	68,68,68,68	0
58	MG	14	3355	1/1	0.92	0.10	102,102,102,102	0
58	MG	1H	3078	1/1	0.92	0.51	67,67,67,67	0
58	MG	14	3340	1/1	0.92	0.09	79,79,79,79	0
58	MG	1H	3244	1/1	0.92	0.28	62,62,62,62	0
58	MG	1H	3198	1/1	0.92	0.43	69,69,69,69	0
58	MG	1H	3371	1/1	0.92	0.12	59,59,59,59	0
58	MG	1G	1632	1/1	0.92	0.43	75,75,75,75	0
58	MG	14	3240	1/1	0.92	0.21	83,83,83,83	0
58	MG	1H	3038	1/1	0.92	0.34	92,92,92,92	0
58	MG	1H	3214	1/1	0.92	0.63	76,76,76,76	0
58	MG	1H	3161	1/1	0.92	0.30	84,84,84,84	0
58	MG	14	3086	1/1	0.92	0.43	83,83,83,83	0
58	MG	1H	3177	1/1	0.92	0.23	74,74,74,74	0
58	MG	13	1623	1/1	0.92	0.23	108,108,108,108	0
58	MG	14	3374	1/1	0.92	0.07	76,76,76,76	0
58	MG	13	1636	1/1	0.92	0.28	64,64,64,64	0
58	MG	13	1729	1/1	0.92	0.07	113,113,113,113	0
58	MG	1H	3387	1/1	0.92	0.07	80,80,80,80	0
58	MG	1H	3304	1/1	0.92	0.33	86,86,86,86	0
58	MG	14	3119	1/1	0.92	0.37	62,62,62,62	0
58	MG	14	3233	1/1	0.92	0.15	86,86,86,86	0
58	MG	14	3267	1/1	0.92	0.25	92,92,92,92	0
58	MG	1G	1629	1/1	0.92	0.63	104,104,104,104	0
58	MG	14	3362	1/1	0.92	0.12	77,77,77,77	0
58	MG	1G	1673	1/1	0.92	0.33	93,93,93,93	0
58	MG	1H	3105	1/1	0.92	0.33	66,66,66,66	0
58	MG	14	3314	1/1	0.92	0.32	94,94,94,94	0
58	MG	1H	3044	1/1	0.92	0.27	82,82,82,82	0
58	MG	1G	1655	1/1	0.92	0.25	100,100,100,100	0
58	MG	1H	3166	1/1	0.92	0.27	71,71,71,71	0
58	MG	14	3175	1/1	0.92	0.16	92,92,92,92	0
58	MG	1H	3028	1/1	0.92	0.28	68,68,68,68	0
58	MG	45	202	1/1	0.92	0.41	72,72,72,72	0
58	MG	1H	3355	1/1	0.92	0.20	48,48,48,48	0
58	MG	13	1625	1/1	0.92	0.33	86,86,86,86	0
58	MG	1H	3273	1/1	0.92	0.22	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3239	1/1	0.92	0.21	75,75,75,75	0
58	MG	1H	3392	1/1	0.92	0.11	68,68,68,68	0
58	MG	1G	1656	1/1	0.92	0.41	78,78,78,78	0
58	MG	1G	1653	1/1	0.92	0.15	97,97,97,97	0
58	MG	13	1626	1/1	0.92	0.37	69,69,69,69	0
58	MG	16	201	1/1	0.92	0.11	85,85,85,85	0
58	MG	14	3047	1/1	0.92	0.18	74,74,74,74	0
58	MG	14	3343	1/1	0.92	0.08	82,82,82,82	0
58	MG	1G	1681	1/1	0.92	0.10	78,78,78,78	0
58	MG	14	3347	1/1	0.92	0.06	108,108,108,108	0
58	MG	14	3076	1/1	0.92	0.34	62,62,62,62	0
58	MG	1H	3149	1/1	0.92	0.34	60,60,60,60	0
58	MG	1H	3150	1/1	0.92	0.23	72,72,72,72	0
58	MG	14	3381	1/1	0.92	0.14	81,81,81,81	0
58	MG	14	3141	1/1	0.93	0.21	93,93,93,93	0
58	MG	1H	3456	1/1	0.93	0.07	97,97,97,97	0
58	MG	1H	3211	1/1	0.93	0.24	83,83,83,83	0
58	MG	1H	3116	1/1	0.93	0.44	55,55,55,55	0
58	MG	1H	3012	1/1	0.93	0.80	83,83,83,83	0
58	MG	1H	3225	1/1	0.93	0.35	78,78,78,78	0
58	MG	1G	1644	1/1	0.93	0.67	92,92,92,92	0
58	MG	1G	1658	1/1	0.93	0.23	92,92,92,92	0
58	MG	14	3162	1/1	0.93	0.54	70,70,70,70	0
58	MG	1H	3407	1/1	0.93	0.12	116,116,116,116	0
58	MG	14	3106	1/1	0.93	0.40	61,61,61,61	0
58	MG	1G	1676	1/1	0.93	0.11	90,90,90,90	0
58	MG	1H	3343	1/1	0.93	0.15	54,54,54,54	0
58	MG	14	3216	1/1	0.93	0.31	77,77,77,77	0
58	MG	13	1725	1/1	0.93	0.08	94,94,94,94	0
58	MG	1H	3447	1/1	0.93	0.04	86,86,86,86	0
58	MG	14	3289	1/1	0.93	0.76	83,83,83,83	0
58	MG	1H	3172	1/1	0.93	0.41	87,87,87,87	0
58	MG	14	3208	1/1	0.93	0.15	91,91,91,91	0
58	MG	13	1713	1/1	0.93	0.05	101,101,101,101	0
58	MG	1H	3410	1/1	0.93	0.10	58,58,58,58	0
58	MG	1H	3466	1/1	0.93	0.30	56,56,56,56	0
58	MG	1H	3261	1/1	0.93	0.19	69,69,69,69	0
58	MG	14	3105	1/1	0.93	0.31	67,67,67,67	0
58	MG	14	3142	1/1	0.93	0.41	76,76,76,76	0
58	MG	13	1660	1/1	0.93	0.24	103,103,103,103	0
58	MG	14	3166	1/1	0.93	0.21	60,60,60,60	0
58	MG	13	1645	1/1	0.93	0.42	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3064	1/1	0.93	0.32	65,65,65,65	0
58	MG	1H	3370	1/1	0.93	0.16	71,71,71,71	0
58	MG	13	1665	1/1	0.93	0.09	82,82,82,82	0
58	MG	13	1693	1/1	0.93	0.21	55,55,55,55	0
58	MG	1H	3243	1/1	0.93	0.50	65,65,65,65	0
58	MG	1G	1688	1/1	0.93	0.07	138,138,138,138	0
58	MG	1H	3145	1/1	0.93	0.14	73,73,73,73	0
58	MG	1H	3056	1/1	0.93	0.50	56,56,56,56	0
58	MG	1H	3127	1/1	0.93	0.14	59,59,59,59	0
58	MG	13	1607	1/1	0.93	0.19	116,116,116,116	0
58	MG	13	1724	1/1	0.93	0.09	102,102,102,102	0
58	MG	14	3077	1/1	0.93	0.45	68,68,68,68	0
58	MG	14	3383	1/1	0.93	0.12	86,86,86,86	0
58	MG	1H	3050	1/1	0.93	0.39	60,60,60,60	0
58	MG	1G	1660	1/1	0.93	0.45	85,85,85,85	0
58	MG	14	3156	1/1	0.93	0.61	63,63,63,63	0
58	MG	14	3219	1/1	0.93	0.31	48,48,48,48	0
58	MG	14	3164	1/1	0.93	0.79	74,74,74,74	0
58	MG	1H	3274	1/1	0.93	0.18	59,59,59,59	0
58	MG	14	3054	1/1	0.93	0.37	70,70,70,70	0
58	MG	1H	3107	1/1	0.93	0.28	71,71,71,71	0
58	MG	14	3326	1/1	0.93	0.09	90,90,90,90	0
58	MG	14	3387	1/1	0.93	0.10	96,96,96,96	0
58	MG	1H	3111	1/1	0.93	0.53	74,74,74,74	0
58	MG	1H	3311	1/1	0.93	0.29	75,75,75,75	0
58	MG	1H	3070	1/1	0.93	0.47	58,58,58,58	0
58	MG	1H	3395	1/1	0.93	0.07	77,77,77,77	0
58	MG	13	1726	1/1	0.93	0.05	126,126,126,126	0
58	MG	14	3276	1/1	0.93	0.37	92,92,92,92	0
58	MG	1H	3040	1/1	0.93	0.44	70,70,70,70	0
58	MG	14	3396	1/1	0.93	0.06	108,108,108,108	0
58	MG	14	3225	1/1	0.93	0.41	82,82,82,82	0
58	MG	1G	1651	1/1	0.93	0.20	104,104,104,104	0
58	MG	1H	3014	1/1	0.94	0.33	70,70,70,70	0
58	MG	13	1664	1/1	0.94	0.12	89,89,89,89	0
58	MG	14	3198	1/1	0.94	0.18	107,107,107,107	0
58	MG	14	3057	1/1	0.94	0.27	101,101,101,101	0
58	MG	1G	1652	1/1	0.94	0.54	71,71,71,71	0
58	MG	14	3053	1/1	0.94	0.23	61,61,61,61	0
58	MG	1H	3379	1/1	0.94	0.11	73,73,73,73	0
58	MG	14	3020	1/1	0.94	0.47	75,75,75,75	0
58	MG	1H	3431	1/1	0.94	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1601	1/1	0.94	0.34	68,68,68,68	0
58	MG	14	3082	1/1	0.94	0.47	61,61,61,61	0
58	MG	1G	1624	1/1	0.94	0.62	65,65,65,65	0
58	MG	1H	3451	1/1	0.94	0.13	114,114,114,114	0
58	MG	1H	3415	1/1	0.94	0.06	73,73,73,73	0
58	MG	1H	3112	1/1	0.94	0.41	56,56,56,56	0
58	MG	13	1676	1/1	0.94	0.51	76,76,76,76	0
58	MG	1H	3393	1/1	0.94	0.20	54,54,54,54	0
58	MG	1H	3421	1/1	0.94	0.06	64,64,64,64	0
58	MG	1H	3181	1/1	0.94	0.25	61,61,61,61	0
58	MG	1H	3299	1/1	0.94	0.17	74,74,74,74	0
58	MG	14	3132	1/1	0.94	0.27	68,68,68,68	0
58	MG	14	3002	1/1	0.94	0.37	57,57,57,57	0
58	MG	1H	3110	1/1	0.94	0.51	55,55,55,55	0
58	MG	1H	3055	1/1	0.94	0.34	49,49,49,49	0
58	MG	1G	1607	1/1	0.94	0.34	73,73,73,73	0
58	MG	1H	3189	1/1	0.94	0.57	67,67,67,67	0
58	MG	14	3014	1/1	0.94	0.47	57,57,57,57	0
58	MG	14	3112	1/1	0.94	0.48	65,65,65,65	0
58	MG	1H	3098	1/1	0.94	0.24	53,53,53,53	0
58	MG	14	3063	1/1	0.94	0.28	58,58,58,58	0
58	MG	1H	3117	1/1	0.94	0.23	48,48,48,48	0
58	MG	1H	3436	1/1	0.94	0.17	73,73,73,73	0
58	MG	14	3350	1/1	0.94	0.11	85,85,85,85	0
58	MG	1H	3420	1/1	0.94	0.06	92,92,92,92	0
58	MG	13	1663	1/1	0.94	0.26	82,82,82,82	0
58	MG	1H	3240	1/1	0.94	0.30	74,74,74,74	0
58	MG	14	3003	1/1	0.94	0.24	62,62,62,62	0
58	MG	1H	3266	1/1	0.94	0.25	81,81,81,81	0
58	MG	1H	3208	1/1	0.94	0.51	88,88,88,88	0
58	MG	1H	3165	1/1	0.94	0.52	78,78,78,78	0
58	MG	1H	3073	1/1	0.94	0.50	81,81,81,81	0
58	MG	14	3315	1/1	0.94	1.07	93,93,93,93	0
58	MG	1G	1626	1/1	0.94	0.29	82,82,82,82	0
58	MG	13	1719	1/1	0.94	0.13	71,71,71,71	0
58	MG	1H	3443	1/1	0.94	0.19	76,76,76,76	0
58	MG	14	3322	1/1	0.94	0.22	65,65,65,65	0
58	MG	13	1712	1/1	0.94	0.12	83,83,83,83	0
58	MG	14	3069	1/1	0.94	0.38	70,70,70,70	0
58	MG	1H	3275	1/1	0.94	0.37	75,75,75,75	0
58	MG	13	1640	1/1	0.94	0.35	74,74,74,74	0
58	MG	14	3348	1/1	0.94	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3017	1/1	0.94	0.44	71,71,71,71	0
58	MG	1H	3065	1/1	0.94	0.35	61,61,61,61	0
58	MG	13	1683	1/1	0.94	0.23	94,94,94,94	0
58	MG	14	3114	1/1	0.94	0.42	58,58,58,58	0
58	MG	1H	3037	1/1	0.94	0.46	121,121,121,121	0
58	MG	1H	3115	1/1	0.94	0.26	43,43,43,43	0
58	MG	14	3323	1/1	0.94	0.14	64,64,64,64	0
58	MG	14	3189	1/1	0.94	0.33	82,82,82,82	0
58	MG	1H	3300	1/1	0.94	0.42	87,87,87,87	0
58	MG	14	3151	1/1	0.94	0.77	79,79,79,79	0
58	MG	1H	3091	1/1	0.94	0.46	65,65,65,65	0
58	MG	1H	3458	1/1	0.94	0.07	73,73,73,73	0
58	MG	1H	3449	1/1	0.94	0.12	106,106,106,106	0
58	MG	1H	3361	1/1	0.94	0.13	63,63,63,63	0
58	MG	14	3159	1/1	0.94	0.47	63,63,63,63	0
58	MG	1H	3461	1/1	0.94	0.04	92,92,92,92	0
58	MG	1H	3106	1/1	0.94	0.41	63,63,63,63	0
58	MG	14	3136	1/1	0.94	0.17	62,62,62,62	0
58	MG	1G	1612	1/1	0.94	0.36	81,81,81,81	0
58	MG	1G	1611	1/1	0.94	0.38	104,104,104,104	0
58	MG	14	3385	1/1	0.94	0.07	116,116,116,116	0
58	MG	1H	3123	1/1	0.94	0.39	69,69,69,69	0
58	MG	1H	3381	1/1	0.94	0.14	63,63,63,63	0
58	MG	1H	3229	1/1	0.94	0.27	48,48,48,48	0
58	MG	13	1619	1/1	0.94	0.13	91,91,91,91	0
58	MG	14	3390	1/1	0.94	0.10	89,89,89,89	0
58	MG	1H	3061	1/1	0.94	0.30	48,48,48,48	0
58	MG	1H	3023	1/1	0.94	0.46	56,56,56,56	0
58	MG	1H	3146	1/1	0.94	0.39	72,72,72,72	0
58	MG	1H	3223	1/1	0.95	0.52	78,78,78,78	0
58	MG	1H	3250	1/1	0.95	0.27	74,74,74,74	0
58	MG	13	1643	1/1	0.95	0.11	99,99,99,99	0
58	MG	14	3016	1/1	0.95	0.40	61,61,61,61	0
58	MG	1H	3236	1/1	0.95	0.18	99,99,99,99	0
58	MG	14	3121	1/1	0.95	0.48	78,78,78,78	0
58	MG	14	3124	1/1	0.95	0.40	54,54,54,54	0
58	MG	1H	3005	1/1	0.95	0.34	54,54,54,54	0
58	MG	1H	3218	1/1	0.95	0.25	56,56,56,56	0
58	MG	13	1616	1/1	0.95	0.04	88,88,88,88	0
58	MG	1H	3048	1/1	0.95	0.30	56,56,56,56	0
58	MG	14	3051	1/1	0.95	0.11	81,81,81,81	0
58	MG	13	1673	1/1	0.95	0.53	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3066	1/1	0.95	0.41	62,62,62,62	0
58	MG	1H	3394	1/1	0.95	0.20	53,53,53,53	0
58	MG	14	3380	1/1	0.95	0.10	96,96,96,96	0
58	MG	1H	3058	1/1	0.95	0.43	46,46,46,46	0
58	MG	14	3371	1/1	0.95	0.12	53,53,53,53	0
58	MG	1H	3153	1/1	0.95	0.20	62,62,62,62	0
58	MG	14	3133	1/1	0.95	0.19	107,107,107,107	0
58	MG	14	3110	1/1	0.95	0.37	57,57,57,57	0
58	MG	1H	3235	1/1	0.95	0.16	53,53,53,53	0
58	MG	1H	3113	1/1	0.95	0.44	51,51,51,51	0
58	MG	14	3336	1/1	0.95	0.17	62,62,62,62	0
60	ZN	C5	201	1/1	0.95	0.07	165,165,165,165	0
58	MG	14	3351	1/1	0.95	0.12	85,85,85,85	0
58	MG	13	1671	1/1	0.95	0.31	87,87,87,87	0
58	MG	14	3094	1/1	0.95	0.64	60,60,60,60	0
58	MG	1H	3237	1/1	0.95	0.28	84,84,84,84	0
58	MG	14	3358	1/1	0.95	0.09	91,91,91,91	0
58	MG	1H	3428	1/1	0.95	0.19	51,51,51,51	0
58	MG	1H	3357	1/1	0.95	0.23	71,71,71,71	0
58	MG	14	3095	1/1	0.95	0.41	71,71,71,71	0
58	MG	1H	3377	1/1	0.95	0.13	70,70,70,70	0
58	MG	1H	3375	1/1	0.95	0.29	60,60,60,60	0
58	MG	1H	3192	1/1	0.95	0.23	80,80,80,80	0
58	MG	1H	3455	1/1	0.95	0.08	59,59,59,59	0
58	MG	14	3317	1/1	0.95	0.70	89,89,89,89	0
58	MG	1H	3084	1/1	0.95	0.20	94,94,94,94	0
58	MG	1H	3346	1/1	0.95	0.14	45,45,45,45	0
58	MG	1H	3432	1/1	0.95	0.11	50,50,50,50	0
58	MG	14	3137	1/1	0.95	0.09	57,57,57,57	0
58	MG	13	1628	1/1	0.95	0.41	65,65,65,65	0
58	MG	14	3388	1/1	0.95	0.10	68,68,68,68	0
58	MG	1H	3345	1/1	0.95	0.18	61,61,61,61	0
58	MG	14	3338	1/1	0.95	0.23	60,60,60,60	0
58	MG	1H	3049	1/1	0.95	0.50	52,52,52,52	0
58	MG	1H	3256	1/1	0.95	0.17	61,61,61,61	0
58	MG	14	3346	1/1	0.95	0.09	85,85,85,85	0
58	MG	14	3173	1/1	0.95	0.30	66,66,66,66	0
58	MG	14	3134	1/1	0.95	0.28	74,74,74,74	0
58	MG	16	208	1/1	0.95	0.16	86,86,86,86	0
58	MG	1H	3230	1/1	0.95	0.41	43,43,43,43	0
58	MG	14	3158	1/1	0.95	0.42	75,75,75,75	0
58	MG	1H	3444	1/1	0.95	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1633	1/1	0.95	0.63	62,62,62,62	0
58	MG	1G	1675	1/1	0.95	0.33	91,91,91,91	0
58	MG	14	3087	1/1	0.95	0.35	40,40,40,40	0
58	MG	14	3319	1/1	0.95	0.10	59,59,59,59	0
58	MG	14	3174	1/1	0.95	0.27	101,101,101,101	0
58	MG	1H	3310	1/1	0.95	0.17	75,75,75,75	0
58	MG	1H	3007	1/1	0.95	0.34	54,54,54,54	0
58	MG	1H	3011	1/1	0.95	0.38	51,51,51,51	0
58	MG	1H	3434	1/1	0.96	0.08	51,51,51,51	0
58	MG	14	3214	1/1	0.96	0.34	88,88,88,88	0
58	MG	1G	1610	1/1	0.96	0.31	98,98,98,98	0
58	MG	1H	3442	1/1	0.96	0.08	69,69,69,69	0
58	MG	14	3321	1/1	0.96	0.09	78,78,78,78	0
58	MG	1H	3354	1/1	0.96	0.13	49,49,49,49	0
58	MG	I8	103	1/1	0.96	0.04	73,73,73,73	0
58	MG	14	3366	1/1	0.96	0.04	86,86,86,86	0
58	MG	1H	3454	1/1	0.96	0.07	96,96,96,96	0
58	MG	14	3376	1/1	0.96	0.07	94,94,94,94	0
58	MG	14	3078	1/1	0.96	0.38	64,64,64,64	0
58	MG	14	3206	1/1	0.96	0.09	80,80,80,80	0
58	MG	14	3377	1/1	0.96	0.20	52,52,52,52	0
58	MG	1G	1605	1/1	0.96	0.38	101,101,101,101	0
58	MG	1H	3129	1/1	0.96	0.52	85,85,85,85	0
58	MG	13	1711	1/1	0.96	0.11	97,97,97,97	0
58	MG	14	3039	1/1	0.96	0.23	50,50,50,50	0
58	MG	1H	3397	1/1	0.96	0.07	71,71,71,71	0
58	MG	1H	3067	1/1	0.96	0.32	55,55,55,55	0
58	MG	1H	3121	1/1	0.96	0.38	62,62,62,62	0
58	MG	13	1618	1/1	0.96	0.36	80,80,80,80	0
58	MG	1H	3081	1/1	0.96	0.39	87,87,87,87	0
58	MG	14	3015	1/1	0.96	0.44	49,49,49,49	0
58	MG	1G	1625	1/1	0.96	0.32	93,93,93,93	0
58	MG	1H	3212	1/1	0.96	0.43	76,76,76,76	0
58	MG	13	1723	1/1	0.96	0.10	87,87,87,87	0
58	MG	1G	1627	1/1	0.96	0.22	94,94,94,94	0
58	MG	1H	3423	1/1	0.96	0.10	66,66,66,66	0
58	MG	1H	3399	1/1	0.96	0.15	62,62,62,62	0
58	MG	14	3382	1/1	0.96	0.07	87,87,87,87	0
58	MG	1H	3174	1/1	0.96	0.36	88,88,88,88	0
58	MG	14	3330	1/1	0.96	0.14	77,77,77,77	0
58	MG	1H	3430	1/1	0.96	0.17	49,49,49,49	0
58	MG	13	1727	1/1	0.96	0.08	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3360	1/1	0.96	0.06	83,83,83,83	0
58	MG	14	3235	1/1	0.96	0.66	72,72,72,72	0
58	MG	14	3167	1/1	0.96	0.29	87,87,87,87	0
58	MG	13	1722	1/1	0.96	0.08	103,103,103,103	0
58	MG	1H	3433	1/1	0.96	0.17	87,87,87,87	0
58	MG	13	1730	1/1	0.96	0.17	86,86,86,86	0
58	MG	1H	3046	1/1	0.96	0.32	47,47,47,47	0
58	MG	13	1666	1/1	0.96	0.13	78,78,78,78	0
58	MG	14	3328	1/1	0.96	0.06	74,74,74,74	0
58	MG	1H	3412	1/1	0.96	0.10	78,78,78,78	0
58	MG	13	1714	1/1	0.96	0.10	73,73,73,73	0
58	MG	13	1649	1/1	0.96	0.37	72,72,72,72	0
58	MG	1G	1617	1/1	0.96	0.14	135,135,135,135	0
58	MG	13	1690	1/1	0.96	0.13	74,74,74,74	0
58	MG	21	301	1/1	0.96	0.38	54,54,54,54	0
58	MG	1H	3389	1/1	0.96	0.10	38,38,38,38	0
58	MG	14	3369	1/1	0.96	0.12	59,59,59,59	0
58	MG	13	1658	1/1	0.96	0.24	83,83,83,83	0
58	MG	1H	3231	1/1	0.96	0.20	58,58,58,58	0
58	MG	14	3120	1/1	0.96	0.38	82,82,82,82	0
58	MG	1H	3405	1/1	0.96	0.09	63,63,63,63	0
58	MG	14	3008	1/1	0.96	0.36	65,65,65,65	0
58	MG	1H	3082	1/1	0.96	0.26	78,78,78,78	0
58	MG	1G	1683	1/1	0.96	0.13	89,89,89,89	0
58	MG	14	3083	1/1	0.96	0.63	72,72,72,72	0
58	MG	13	1610	1/1	0.96	0.25	80,80,80,80	0
58	MG	14	3213	1/1	0.96	0.36	64,64,64,64	0
58	MG	1H	3295	1/1	0.96	0.46	93,93,93,93	0
58	MG	1H	3406	1/1	0.96	0.07	76,76,76,76	0
58	MG	13	1615	1/1	0.96	0.40	77,77,77,77	0
58	MG	1H	3183	1/1	0.96	0.52	67,67,67,67	0
58	MG	1H	3382	1/1	0.96	0.06	77,77,77,77	0
58	MG	14	3101	1/1	0.96	0.43	64,64,64,64	0
58	MG	14	3093	1/1	0.96	0.42	42,42,42,42	0
58	MG	1H	3391	1/1	0.96	0.09	61,61,61,61	0
58	MG	1H	3114	1/1	0.96	0.54	74,74,74,74	0
58	MG	13	1612	1/1	0.96	0.33	63,63,63,63	0
58	MG	1H	3120	1/1	0.96	0.34	74,74,74,74	0
58	MG	2K	101	1/1	0.96	0.36	68,68,68,68	0
58	MG	14	3349	1/1	0.96	0.15	83,83,83,83	0
58	MG	1H	3090	1/1	0.96	0.36	71,71,71,71	0
58	MG	1H	3025	1/1	0.96	0.40	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3368	1/1	0.96	0.21	62,62,62,62	0
58	MG	13	1614	1/1	0.96	0.20	78,78,78,78	0
58	MG	14	3123	1/1	0.96	0.30	64,64,64,64	0
58	MG	1H	3429	1/1	0.96	0.12	71,71,71,71	0
58	MG	1H	3312	1/1	0.96	0.24	67,67,67,67	0
58	MG	1H	3260	1/1	0.96	0.37	72,72,72,72	0
58	MG	14	3209	1/1	0.96	0.24	66,66,66,66	0
58	MG	13	1613	1/1	0.97	0.22	81,81,81,81	0
58	MG	14	3270	1/1	0.97	0.30	63,63,63,63	0
58	MG	1H	3358	1/1	0.97	0.14	45,45,45,45	0
58	MG	1H	3163	1/1	0.97	0.35	50,50,50,50	0
58	MG	13	1732	1/1	0.97	0.20	65,65,65,65	0
58	MG	1H	3010	1/1	0.97	0.36	63,63,63,63	0
58	MG	13	1667	1/1	0.97	0.47	71,71,71,71	0
58	MG	13	1642	1/1	0.97	0.27	74,74,74,74	0
58	MG	1H	3356	1/1	0.97	0.17	42,42,42,42	0
58	MG	13	1622	1/1	0.97	0.37	74,74,74,74	0
58	MG	1G	1682	1/1	0.97	0.13	97,97,97,97	0
58	MG	14	3152	1/1	0.97	0.33	92,92,92,92	0
58	MG	14	3341	1/1	0.97	0.08	68,68,68,68	0
58	MG	1H	3057	1/1	0.97	0.41	66,66,66,66	0
58	MG	14	3367	1/1	0.97	0.09	65,65,65,65	0
58	MG	14	3161	1/1	0.97	0.52	70,70,70,70	0
58	MG	14	3088	1/1	0.97	0.45	52,52,52,52	0
58	MG	14	3070	1/1	0.97	0.51	60,60,60,60	0
58	MG	1G	1621	1/1	0.97	0.12	92,92,92,92	0
58	MG	1H	3404	1/1	0.97	0.13	48,48,48,48	0
58	MG	14	3103	1/1	0.97	0.28	51,51,51,51	0
58	MG	1H	3416	1/1	0.97	0.08	69,69,69,69	0
58	MG	1H	3069	1/1	0.97	0.42	90,90,90,90	0
58	MG	13	1648	1/1	0.97	0.50	95,95,95,95	0
58	MG	14	3210	1/1	0.97	0.17	80,80,80,80	0
58	MG	1G	1601	1/1	0.97	0.29	91,91,91,91	0
58	MG	14	3359	1/1	0.97	0.06	79,79,79,79	0
58	MG	14	3004	1/1	0.97	0.37	67,67,67,67	0
58	MG	1H	3359	1/1	0.97	0.12	59,59,59,59	0
58	MG	14	3098	1/1	0.97	0.17	93,93,93,93	0
58	MG	1H	3448	1/1	0.97	0.08	82,82,82,82	0
58	MG	1H	3408	1/1	0.97	0.12	82,82,82,82	0
58	MG	1H	3384	1/1	0.97	0.06	58,58,58,58	0
58	MG	1H	3133	1/1	0.97	0.34	71,71,71,71	0
58	MG	14	3036	1/1	0.97	0.74	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3075	1/1	0.97	0.29	68,68,68,68	0
58	MG	1H	3380	1/1	0.97	0.11	59,59,59,59	0
58	MG	1H	3257	1/1	0.97	0.30	70,70,70,70	0
58	MG	1H	3396	1/1	0.97	0.10	78,78,78,78	0
58	MG	1H	3026	1/1	0.97	0.47	56,56,56,56	0
58	MG	1H	3259	1/1	0.97	0.48	79,79,79,79	0
58	MG	14	3062	1/1	0.97	0.17	68,68,68,68	0
58	MG	1H	3086	1/1	0.97	0.37	70,70,70,70	0
58	MG	14	3344	1/1	0.97	0.15	81,81,81,81	0
58	MG	14	3116	1/1	0.97	0.20	64,64,64,64	0
58	MG	14	3038	1/1	0.97	0.33	71,71,71,71	0
58	MG	16	206	1/1	0.97	0.05	73,73,73,73	0
58	MG	13	1701	1/1	0.97	0.14	114,114,114,114	0
58	MG	14	3335	1/1	0.97	0.09	61,61,61,61	0
58	MG	14	3196	1/1	0.97	0.55	75,75,75,75	0
58	MG	1H	3148	1/1	0.97	0.24	50,50,50,50	0
58	MG	14	3072	1/1	0.97	0.22	45,45,45,45	0
58	MG	1H	3398	1/1	0.97	0.16	66,66,66,66	0
58	MG	1H	3403	1/1	0.97	0.14	76,76,76,76	0
58	MG	13	1635	1/1	0.97	0.52	74,74,74,74	0
58	MG	1H	3068	1/1	0.97	0.28	86,86,86,86	0
58	MG	14	3254	1/1	0.97	0.19	111,111,111,111	0
58	MG	13	1609	1/1	0.97	0.37	75,75,75,75	0
58	MG	1H	3409	1/1	0.97	0.07	85,85,85,85	0
58	MG	1H	3245	1/1	0.97	0.70	62,62,62,62	0
58	MG	1H	3062	1/1	0.97	0.20	64,64,64,64	0
58	MG	14	3065	1/1	0.97	0.32	67,67,67,67	0
58	MG	88	201	1/1	0.97	0.21	81,81,81,81	0
58	MG	14	3370	1/1	0.97	0.10	64,64,64,64	0
58	MG	1H	3462	1/1	0.97	0.04	97,97,97,97	0
58	MG	14	3192	1/1	0.97	0.51	63,63,63,63	0
58	MG	14	3334	1/1	0.97	0.05	64,64,64,64	0
58	MG	1H	3440	1/1	0.97	0.05	58,58,58,58	0
58	MG	1H	3330	1/1	0.97	0.34	102,102,102,102	0
58	MG	14	3006	1/1	0.97	0.63	56,56,56,56	0
58	MG	14	3226	1/1	0.97	0.41	73,73,73,73	0
58	MG	13	1717	1/1	0.97	0.08	92,92,92,92	0
58	MG	1H	3347	1/1	0.97	0.28	51,51,51,51	0
58	MG	13	1718	1/1	0.97	0.04	83,83,83,83	0
58	MG	1G	1685	1/1	0.97	0.09	87,87,87,87	0
58	MG	1H	3103	1/1	0.97	0.28	54,54,54,54	0
58	MG	1H	3030	1/1	0.97	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3075	1/1	0.97	0.48	43,43,43,43	0
58	MG	14	3379	1/1	0.97	0.12	60,60,60,60	0
58	MG	13	1617	1/1	0.97	0.24	83,83,83,83	0
58	MG	14	3064	1/1	0.97	0.19	78,78,78,78	0
58	MG	1G	1690	1/1	0.97	0.16	93,93,93,93	0
58	MG	1G	1642	1/1	0.97	0.48	91,91,91,91	0
58	MG	14	3005	1/1	0.97	0.45	48,48,48,48	0
58	MG	1H	3401	1/1	0.97	0.18	69,69,69,69	0
58	MG	1H	3202	1/1	0.97	0.82	70,70,70,70	0
58	MG	14	3332	1/1	0.97	0.10	53,53,53,53	0
58	MG	14	3318	1/1	0.97	0.24	64,64,64,64	0
58	MG	1H	3450	1/1	0.97	0.10	54,54,54,54	0
58	MG	14	3398	1/1	0.97	0.07	108,108,108,108	0
58	MG	1H	3210	1/1	0.97	0.47	71,71,71,71	0
58	MG	13	1684	1/1	0.97	0.14	128,128,128,128	0
58	MG	1H	3195	1/1	0.97	0.50	62,62,62,62	0
58	MG	1H	3465	1/1	0.97	0.15	71,71,71,71	0
58	MG	14	3001	1/1	0.97	0.16	46,46,46,46	0
58	MG	1H	3350	1/1	0.97	0.12	48,48,48,48	0
58	MG	14	3048	1/1	0.98	0.29	90,90,90,90	0
58	MG	1H	3074	1/1	0.98	0.29	64,64,64,64	0
58	MG	14	3356	1/1	0.98	0.17	58,58,58,58	0
58	MG	1H	3076	1/1	0.98	0.41	65,65,65,65	0
59	SF4	3E	301	8/8	0.98	0.17	86,99,103,105	0
58	MG	1H	3124	1/1	0.98	0.36	46,46,46,46	0
58	MG	1H	3191	1/1	0.98	0.50	90,90,90,90	0
58	MG	1H	3143	1/1	0.98	0.14	56,56,56,56	0
58	MG	1H	3344	1/1	0.98	0.13	58,58,58,58	0
58	MG	14	3043	1/1	0.98	0.38	57,57,57,57	0
58	MG	14	3375	1/1	0.98	0.07	97,97,97,97	0
58	MG	13	1716	1/1	0.98	0.07	76,76,76,76	0
58	MG	14	3145	1/1	0.98	0.32	65,65,65,65	0
58	MG	1H	3369	1/1	0.98	0.18	49,49,49,49	0
58	MG	1H	3052	1/1	0.98	0.33	53,53,53,53	0
58	MG	1H	3437	1/1	0.98	0.09	58,58,58,58	0
58	MG	14	3081	1/1	0.98	0.32	76,76,76,76	0
58	MG	14	3011	1/1	0.98	0.59	48,48,48,48	0
58	MG	13	1611	1/1	0.98	0.24	72,72,72,72	0
58	MG	14	3373	1/1	0.98	0.19	61,61,61,61	0
58	MG	13	1602	1/1	0.98	0.28	86,86,86,86	0
58	MG	1H	3102	1/1	0.98	0.39	35,35,35,35	0
58	MG	1H	3006	1/1	0.98	0.36	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1674	1/1	0.98	0.09	91,91,91,91	0
58	MG	1H	3169	1/1	0.98	0.21	85,85,85,85	0
58	MG	1H	3365	1/1	0.98	0.14	74,74,74,74	0
58	MG	14	3113	1/1	0.98	0.41	73,73,73,73	0
58	MG	1H	3390	1/1	0.98	0.09	50,50,50,50	0
58	MG	14	3207	1/1	0.98	0.37	80,80,80,80	0
58	MG	14	3218	1/1	0.98	0.56	62,62,62,62	0
58	MG	1H	3425	1/1	0.98	0.12	63,63,63,63	0
58	MG	14	3327	1/1	0.98	0.16	59,59,59,59	0
58	MG	1H	3109	1/1	0.98	0.30	47,47,47,47	0
58	MG	1H	3453	1/1	0.98	0.10	84,84,84,84	0
58	MG	1H	3289	1/1	0.98	0.17	49,49,49,49	0
58	MG	14	3337	1/1	0.98	0.06	66,66,66,66	0
58	MG	14	3046	1/1	0.98	0.28	66,66,66,66	0
58	MG	14	3050	1/1	0.98	0.51	59,59,59,59	0
58	MG	29	303	1/1	0.98	0.40	52,52,52,52	0
58	MG	14	3139	1/1	0.98	0.34	99,99,99,99	0
58	MG	14	3361	1/1	0.98	0.15	64,64,64,64	0
58	MG	1H	3060	1/1	0.98	0.40	61,61,61,61	0
58	MG	1H	3349	1/1	0.98	0.18	64,64,64,64	0
60	ZN	5A	101	1/1	0.98	0.08	142,142,142,142	0
58	MG	14	3102	1/1	0.98	0.26	61,61,61,61	0
58	MG	1H	3134	1/1	0.98	0.08	69,69,69,69	0
58	MG	1H	3385	1/1	0.98	0.20	47,47,47,47	0
58	MG	1G	1669	1/1	0.98	0.36	107,107,107,107	0
58	MG	14	3092	1/1	0.98	0.32	76,76,76,76	0
58	MG	1H	3402	1/1	0.98	0.15	51,51,51,51	0
58	MG	1H	3255	1/1	0.98	0.39	73,73,73,73	0
58	MG	1H	3427	1/1	0.98	0.07	72,72,72,72	0
58	MG	1H	3348	1/1	0.98	0.19	50,50,50,50	0
58	MG	14	3071	1/1	0.98	0.58	68,68,68,68	0
58	MG	1H	3400	1/1	0.98	0.11	72,72,72,72	0
58	MG	14	3202	1/1	0.98	0.31	63,63,63,63	0
58	MG	1H	3366	1/1	0.98	0.14	76,76,76,76	0
58	MG	1H	3093	1/1	0.98	0.36	72,72,72,72	0
58	MG	1H	3001	1/1	0.98	0.32	43,43,43,43	0
58	MG	1H	3360	1/1	0.98	0.10	61,61,61,61	0
58	MG	14	3127	1/1	0.98	0.27	69,69,69,69	0
58	MG	14	3342	1/1	0.98	0.07	80,80,80,80	0
58	MG	14	3040	1/1	0.98	0.35	59,59,59,59	0
58	MG	14	3372	1/1	0.98	0.09	70,70,70,70	0
58	MG	1H	3008	1/1	0.98	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3130	1/1	0.98	0.53	86,86,86,86	0
58	MG	1H	3241	1/1	0.98	0.35	66,66,66,66	0
58	MG	1H	3339	1/1	0.98	0.43	48,48,48,48	0
58	MG	1H	3424	1/1	0.98	0.10	48,48,48,48	0
58	MG	1H	3013	1/1	0.98	0.29	82,82,82,82	0
58	MG	1H	3386	1/1	0.98	0.11	57,57,57,57	0
58	MG	14	3009	1/1	0.98	0.46	52,52,52,52	0
58	MG	1H	3373	1/1	0.98	0.12	51,51,51,51	0
58	MG	14	3041	1/1	0.98	0.35	54,54,54,54	0
58	MG	1H	3374	1/1	0.98	0.16	53,53,53,53	0
58	MG	1H	3029	1/1	0.98	0.35	42,42,42,42	0
58	MG	14	3044	1/1	0.98	0.51	64,64,64,64	0
58	MG	14	3010	1/1	0.98	0.48	41,41,41,41	0
58	MG	14	3079	1/1	0.98	0.46	70,70,70,70	0
58	MG	1H	3051	1/1	0.98	0.35	45,45,45,45	0
58	MG	14	3331	1/1	0.98	0.14	63,63,63,63	0
58	MG	1H	3077	1/1	0.98	0.23	60,60,60,60	0
58	MG	13	1721	1/1	0.98	0.12	66,66,66,66	0
58	MG	1G	1623	1/1	0.99	0.50	62,62,62,62	0
58	MG	14	3339	1/1	0.99	0.11	82,82,82,82	0
58	MG	1H	3053	1/1	0.99	0.34	50,50,50,50	0
60	ZN	5I	101	1/1	0.99	0.13	102,102,102,102	0
58	MG	1H	3378	1/1	0.99	0.16	53,53,53,53	0
58	MG	2L	101	1/1	0.99	0.56	73,73,73,73	0
58	MG	14	3045	1/1	0.99	0.33	58,58,58,58	0
58	MG	1H	3372	1/1	0.99	0.11	62,62,62,62	0
58	MG	13	1709	1/1	0.99	0.07	92,92,92,92	0
58	MG	14	3354	1/1	0.99	0.10	70,70,70,70	0
58	MG	14	3357	1/1	0.99	0.22	76,76,76,76	0
58	MG	1H	3094	1/1	0.99	0.37	64,64,64,64	0
58	MG	13	1638	1/1	0.99	0.26	59,59,59,59	0
58	MG	1H	3411	1/1	0.99	0.12	69,69,69,69	0
58	MG	1H	3248	1/1	0.99	0.50	74,74,74,74	0
58	MG	14	3320	1/1	0.99	0.18	64,64,64,64	0
58	MG	1H	3059	1/1	0.99	0.24	49,49,49,49	0
58	MG	1H	3147	1/1	0.99	0.31	64,64,64,64	0
58	MG	1H	3352	1/1	0.99	0.12	61,61,61,61	0
58	MG	1H	3092	1/1	0.99	0.26	49,49,49,49	0
58	MG	1H	3363	1/1	0.99	0.06	68,68,68,68	0
58	MG	14	3091	1/1	0.99	0.43	86,86,86,86	0
58	MG	1H	3099	1/1	0.99	0.20	55,55,55,55	0
58	MG	14	3329	1/1	0.99	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1G	1608	1/1	0.99	0.18	89,89,89,89	0
58	MG	1H	3435	1/1	0.99	0.13	56,56,56,56	0
59	SF4	32	301	8/8	0.99	0.15	115,123,133,136	0
58	MG	14	3138	1/1	0.99	0.32	45,45,45,45	0
58	MG	14	3128	1/1	0.99	0.45	58,58,58,58	0
58	MG	14	3298	1/1	0.99	0.90	64,64,64,64	0
58	MG	1H	3351	1/1	0.99	0.08	46,46,46,46	0
58	MG	1H	3138	1/1	0.99	0.41	58,58,58,58	0
58	MG	1H	3383	1/1	0.99	0.17	60,60,60,60	0
58	MG	14	3097	1/1	0.99	0.22	65,65,65,65	0
58	MG	14	3042	1/1	0.99	0.54	70,70,70,70	0
58	MG	1H	3054	1/1	0.99	0.24	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.