



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:21 PM UTC

PDB ID : 4WU1 / pdb_00004wu1
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with G-U mismatch in the second position in the P-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-30
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 types of validation reports are described at

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

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

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

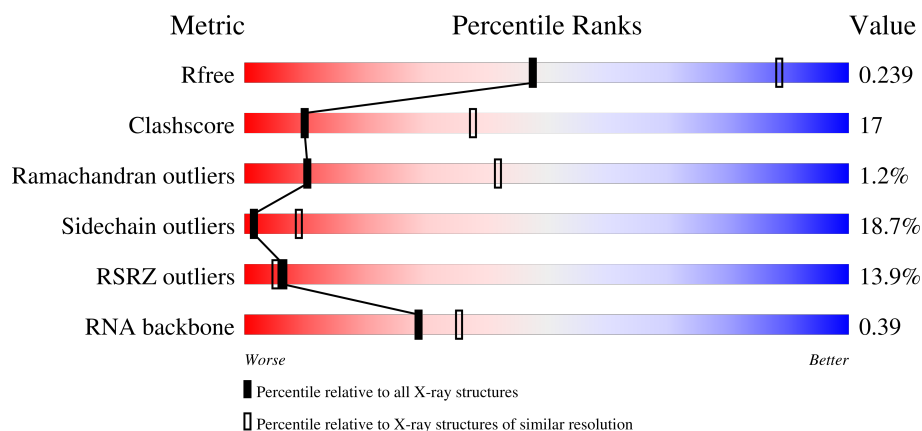
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	13% 38% 48% 13%
2	12	256	16% 41% 40% 11% 7%
2	1E	256	11% 40% 39% 13% 7%
3	22	239	19% 49% 30% 8% 14%

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Mol	Chain	Length	Quality of chain
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	
15	6I	89	

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Mol	Chain	Length	Quality of chain
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	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	27	
23	4L	27	
24	14	2917	
24	1H	2917	
25	16	122	
25	1J	122	
26	71	229	
26	79	229	
27	11	276	

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Mol	Chain	Length	Quality of chain
27	19	276	
28	21	206	
28	29	206	
29	31	210	
29	39	210	
30	41	182	
30	49	182	
31	51	180	
31	59	180	
32	61	148	
32	69	148	
33	15	140	
33	58	140	
34	25	122	
34	68	122	
35	35	150	
35	78	150	
36	45	141	
36	88	141	
37	55	118	
37	98	118	
38	65	112	
38	A8	112	
39	75	146	
39	B8	146	

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Mol	Chain	Length	Quality of chain
40	85	118	
40	C8	118	
41	95	101	
41	D8	101	
42	A5	113	
42	E8	113	
43	B5	96	
43	F8	96	
44	C5	110	
44	G8	110	
45	D5	206	
45	H8	206	
46	E5	85	
46	I8	85	
47	F5	98	
47	J8	98	
48	G5	72	
48	K8	72	
49	H5	60	
49	L8	60	
50	I5	71	
50	M8	71	
51	J5	60	
51	N8	60	
52	L5	49	

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Mol	Chain	Length	Quality of chain
52	P8	49	
53	M5	65	
53	Q8	65	
54	1G	1522	

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
22	MIA	3K	38	-	-	-	X
55	MG	13	1667	-	-	-	X
55	MG	13	1692	-	-	-	X
55	MG	14	3016	-	-	-	X
55	MG	14	3031	-	-	-	X
55	MG	14	3041	-	-	-	X
55	MG	14	3077	-	-	-	X
55	MG	14	3081	-	-	-	X
55	MG	14	3154	-	-	-	X
55	MG	14	3196	-	-	-	X
55	MG	14	3197	-	-	-	X
55	MG	14	3211	-	-	-	X
55	MG	14	3246	-	-	-	X
55	MG	14	3249	-	-	-	X
55	MG	14	3255	-	-	-	X
55	MG	14	3295	-	-	-	X
55	MG	14	3311	-	-	-	X
55	MG	14	3312	-	-	-	X
55	MG	14	3314	-	-	-	X
55	MG	14	3317	-	-	-	X
55	MG	14	3319	-	-	-	X
55	MG	14	3323	-	-	-	X
55	MG	14	3324	-	-	-	X
55	MG	14	3327	-	-	-	X
55	MG	1G	1628	-	-	-	X
55	MG	1G	1657	-	-	-	X
55	MG	1G	1666	-	-	-	X
55	MG	1G	1696	-	-	-	X
55	MG	1G	1709	-	-	-	X
55	MG	1H	3059	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3069	-	-	-	X
55	MG	1H	3078	-	-	-	X
55	MG	1H	3111	-	-	-	X
55	MG	1H	3118	-	-	-	X
55	MG	1H	3123	-	-	-	X
55	MG	1H	3131	-	-	-	X
55	MG	1H	3135	-	-	-	X
55	MG	1H	3146	-	-	-	X
55	MG	1H	3149	-	-	-	X
55	MG	1H	3154	-	-	-	X
55	MG	1H	3157	-	-	-	X
55	MG	1H	3163	-	-	-	X
55	MG	1H	3207	-	-	-	X
55	MG	1H	3220	-	-	-	X
55	MG	1H	3235	-	-	-	X
55	MG	1H	3237	-	-	-	X
55	MG	1H	3249	-	-	-	X
55	MG	1H	3262	-	-	-	X
55	MG	1H	3290	-	-	-	X
55	MG	1H	3333	-	-	-	X
55	MG	1H	3351	-	-	-	X
55	MG	1H	3353	-	-	-	X
55	MG	1H	3358	-	-	-	X
55	MG	1J	206	-	-	-	X
55	MG	3L	102	-	-	-	X
55	MG	88	202	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1501	Total	C	N	O	P	0	3	0
			32334	14391	5996	10443	1504			

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

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

- 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	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			
9	82	126	Total	C	N	O	0	0	0
			998	633	193	172			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	117	Total	C	N	O	S	0	0	0
			933	577	192	162	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	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	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	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	82	Total	C	N	O	S	0	0	0
			644	410	119	113	2			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	2K	82	Total	C	N	O	P	S	0	0	0
			1765	795	315	571	82	2			
22	3K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			
22	2L	78	Total	C	N	O	P	S	0	0	0
			1678	756	297	545	78	2			
22	3L	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	4K	11	Total	C	N	O	P	0	0	0
			239	108	50	70	11			
23	4L	6	Total	C	N	O	P	0	0	0
			129	58	25	40	6			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1H	2912	Total	C	N	O	P	0	1	0
			62729	27921	11727	20169	2912			
24	14	2909	Total	C	N	O	P	0	1	0
			62669	27894	11721	20145	2909			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	71	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			
26	79	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	59	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
34	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
36	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
37	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
38	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	75	137	Total	C	N	O		0	0	0
			1131	704	232	195				

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
40	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
41	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	F8	94	Total	C	N	O		0	0	0
			738	480	133	125				
43	B5	93	Total	C	N	O		0	0	0
			730	474	132	124				

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	I8	83	Total	C	N	O	S	0	0	0
			639	395	135	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	G5	69	Total	C	N	O	S	0	0	0
			580	358	118	103	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	P8	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
52	L5	49	Total	C	N	O	S	0	0	0
			429	263	108	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Q8	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			
53	M5	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 54 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1G	1504	Total	C	N	O	P	0	0	0
			32329	14390	5993	10443	1503			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	129	Total	Mg	0	0
			129	129		
55	5E	2	Total	Mg	0	0
			2	2		
55	3I	1	Total	Mg	0	0
			1	1		
55	2K	4	Total	Mg	0	0
			4	4		
55	1H	548	Total	Mg	0	0
			548	548		
55	16	12	Total	Mg	0	0
			12	12		
55	11	2	Total	Mg	0	0
			2	2		
55	21	1	Total	Mg	0	0
			1	1		
55	78	2	Total	Mg	0	0
			2	2		
55	88	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	I8	3	Total 3	Mg 3	0	0
55	J8	1	Total 1	Mg 1	0	0
55	Q8	1	Total 1	Mg 1	0	0
55	1G	147	Total 147	Mg 147	0	0
55	32	1	Total 1	Mg 1	0	0
55	42	1	Total 1	Mg 1	0	0
55	2L	3	Total 3	Mg 3	0	0
55	3L	2	Total 2	Mg 2	0	0
55	14	489	Total 489	Mg 489	0	0
55	1J	11	Total 11	Mg 11	0	0
55	19	1	Total 1	Mg 1	0	0
55	29	5	Total 5	Mg 5	0	0
55	39	1	Total 1	Mg 1	0	0
55	49	1	Total 1	Mg 1	0	0
55	15	1	Total 1	Mg 1	0	0
55	25	1	Total 1	Mg 1	0	0
55	45	1	Total 1	Mg 1	0	0
55	55	3	Total 3	Mg 3	0	0
55	C5	1	Total 1	Mg 1	0	0
55	E5	2	Total 2	Mg 2	0	0
55	F5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	M5	1	Total	Mg	0	0
			1	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	3E	1	Total	Zn	0	0
			1	1		
56	5I	1	Total	Zn	0	0
			1	1		
56	G8	1	Total	Zn	0	0
			1	1		
56	32	1	Total	Zn	0	0
			1	1		
56	5A	1	Total	Zn	0	0
			1	1		
56	C5	1	Total	Zn	0	0
			1	1		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	3	Total	O	0	0
			3	3		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		
57	13	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	13	6	Total O 6 6	0	0
57	2K	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	5	Total O 5 5	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
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57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	5	Total O 5 5	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
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57	1H	5	Total O 5 5	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
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57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	5	Total 5	O 5	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	4	Total 4	O 4	0	0
57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
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57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0
57	1H	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			6	6		
57	1H	6	Total	O	0	0
			6	6		
57	1H	6	Total	O	0	0
			6	6		
57	1H	6	Total	O	0	0
			6	6		
57	1H	6	Total	O	0	0
			6	6		
57	1H	6	Total	O	0	0
			6	6		
57	1H	6	Total	O	0	0
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57	1H	6	Total	O	0	0
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57	1H	6	Total	O	0	0
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57	1H	6	Total	O	0	0
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57	1H	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
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57	1H	6	Total O 6 6	0	0
57	1H	6	Total O 6 6	0	0
57	16	6	Total O 6 6	0	0
57	16	6	Total O 6 6	0	0
57	J8	6	Total O 6 6	0	0
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57	1G	6	Total O 6 6	0	0
57	1G	6	Total O 6 6	0	0
57	1G	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	6	Total 6	O 6	0	0
57	1G	6	Total 6	O 6	0	0
57	1G	6	Total 6	O 6	0	0
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57	1G	6	Total 6	O 6	0	0
57	1G	6	Total 6	O 6	0	0
57	1G	6	Total 6	O 6	0	0
57	2L	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	14	6	Total O 6 6	0	0
57	14	4	Total O 4 4	0	0
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57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
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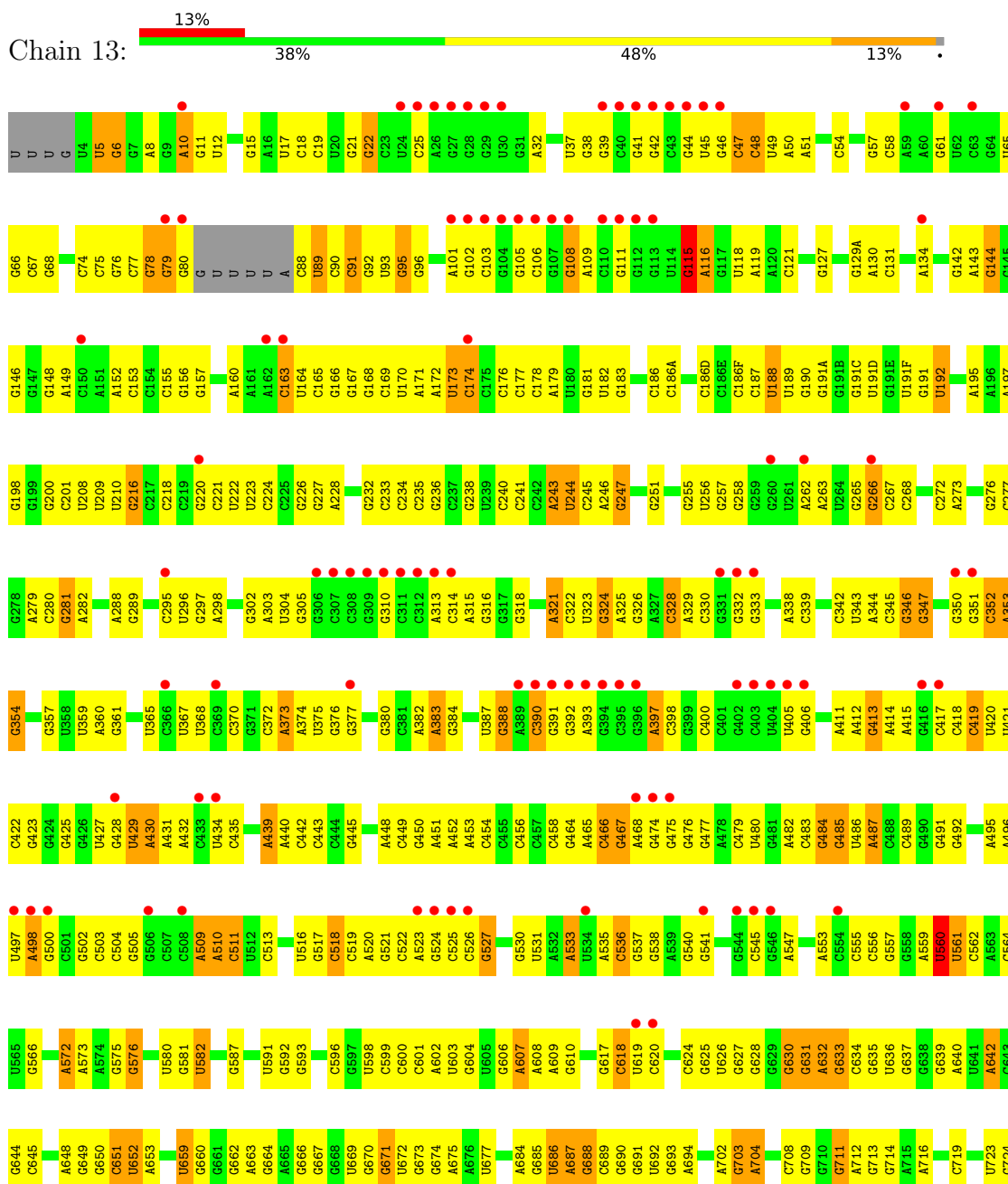
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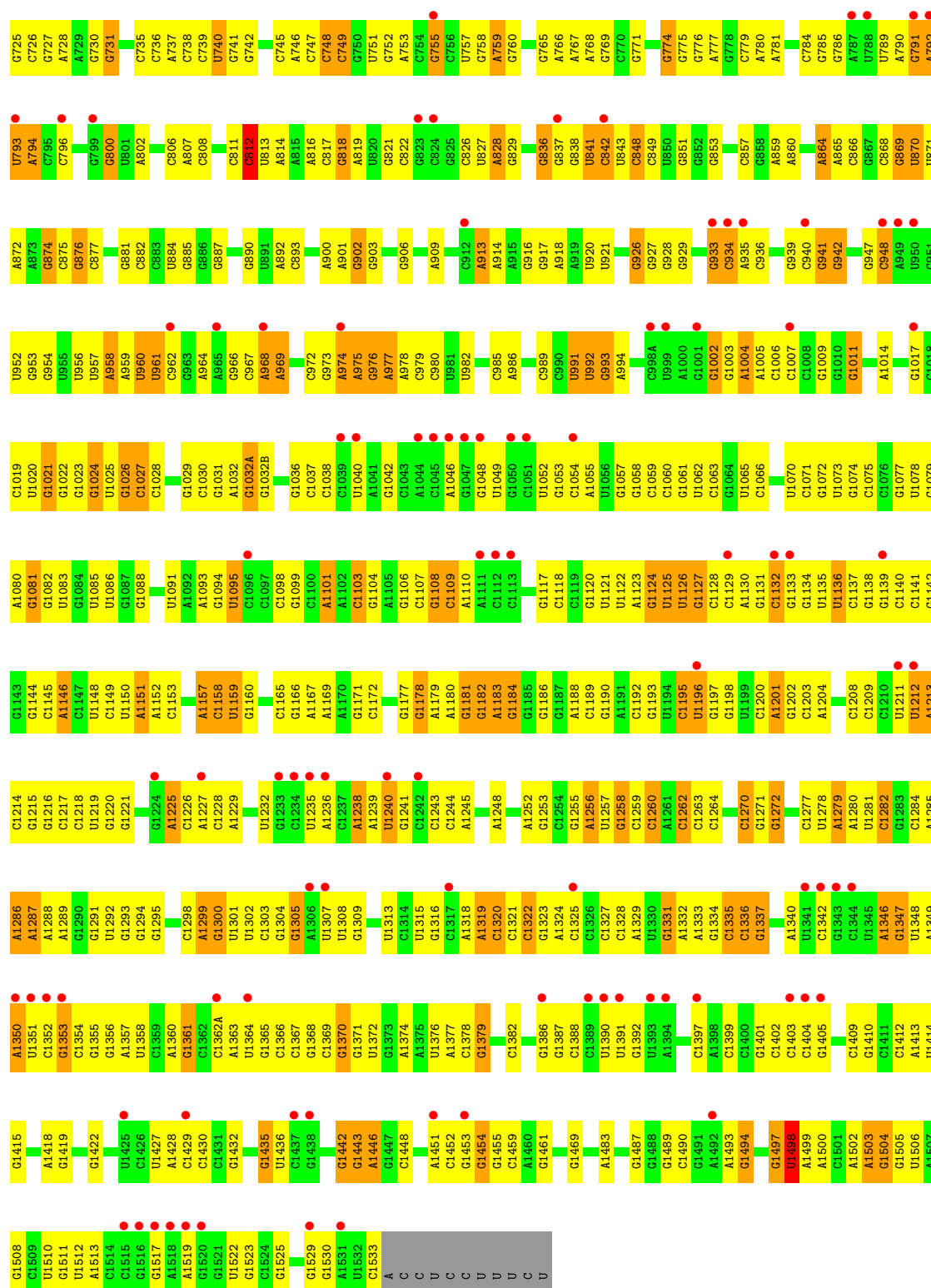
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57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	14	6	Total 6	O 6	0	0
57	1J	6	Total 6	O 6	0	0
57	1J	6	Total 6	O 6	0	0
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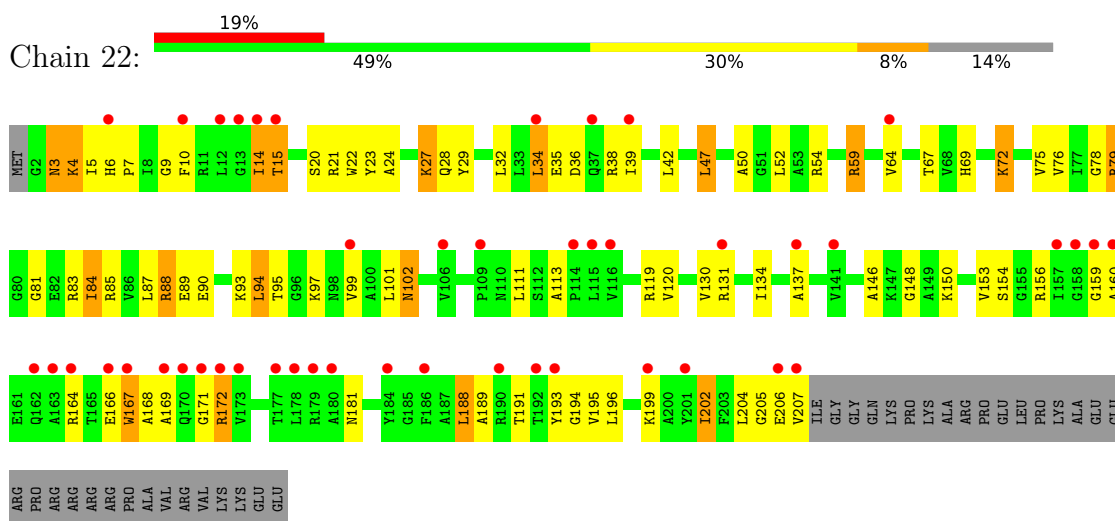
3 Residue-property plots

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

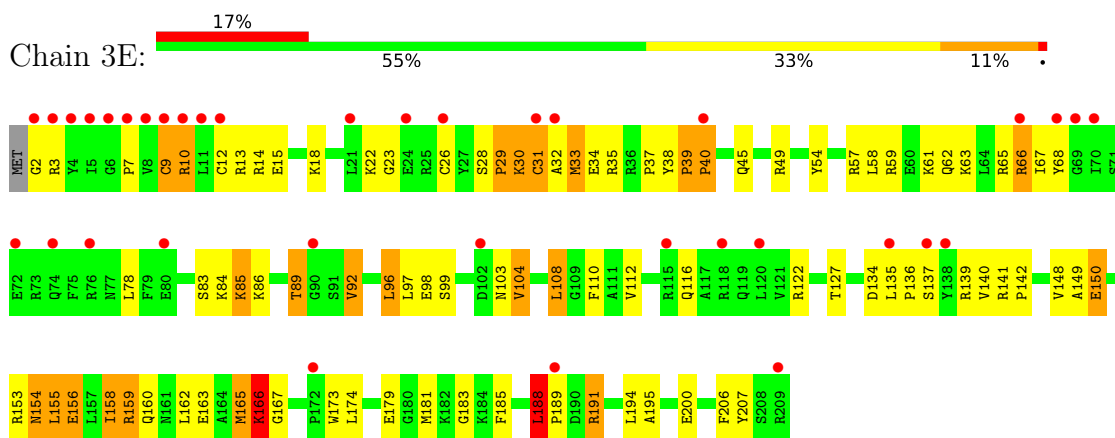
• Molecule 1: 16S ribosomal RNA



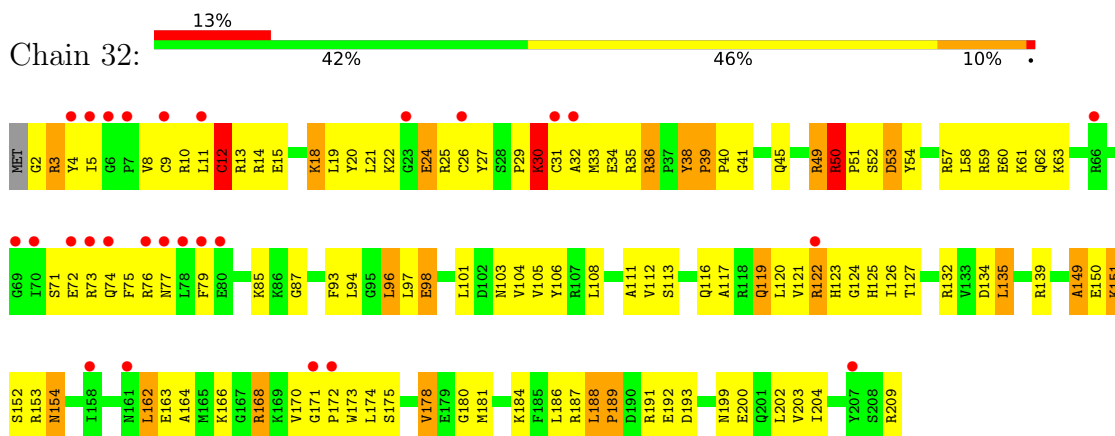




• Molecule 4: 30S ribosomal protein S4

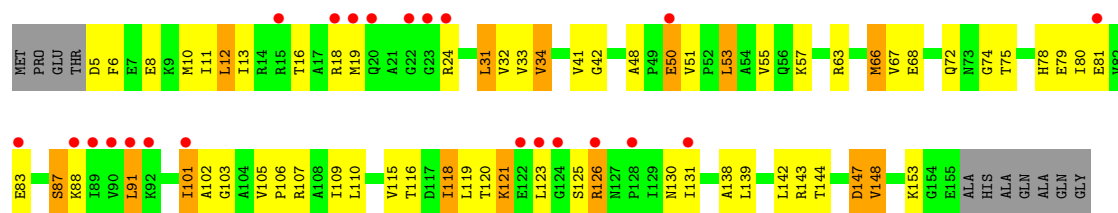


• Molecule 4: 30S ribosomal protein S4

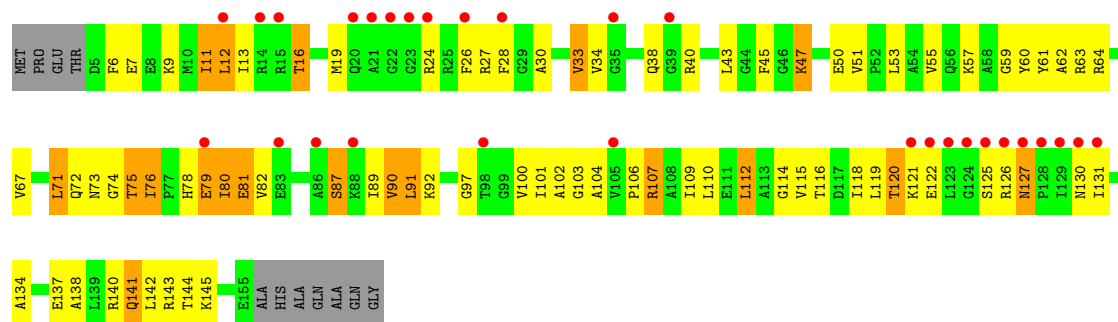
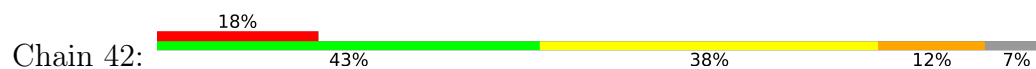


• Molecule 5: 30S ribosomal protein S5

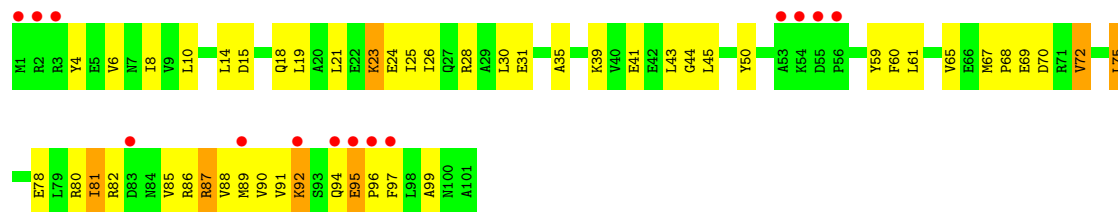




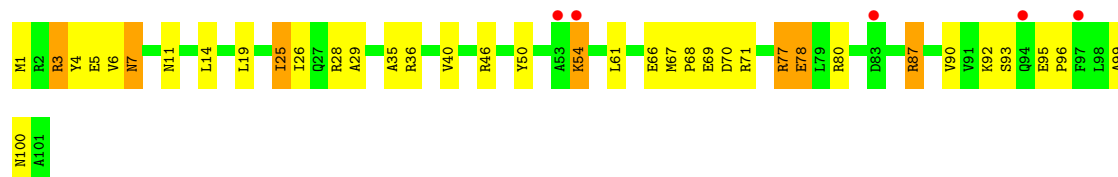
• Molecule 5: 30S ribosomal protein S5



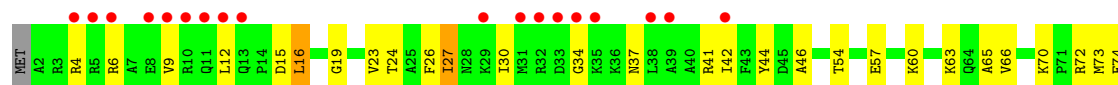
• Molecule 6: 30S ribosomal protein S6

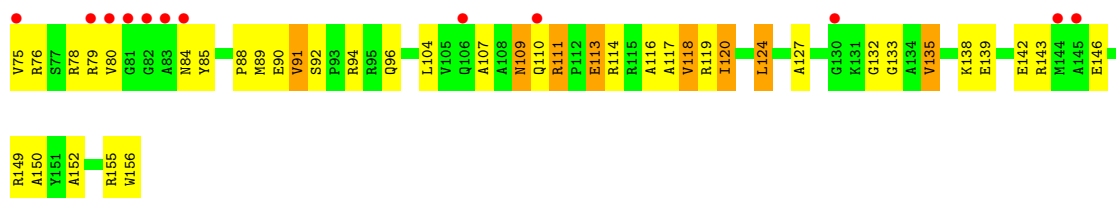


• Molecule 6: 30S ribosomal protein S6

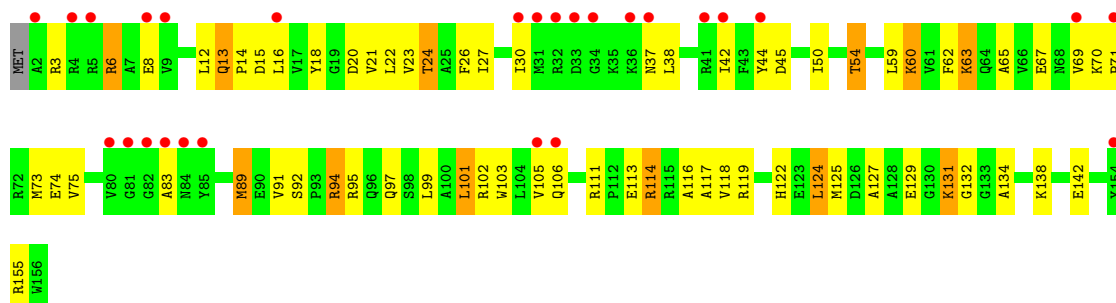


• Molecule 7: 30S ribosomal protein S7

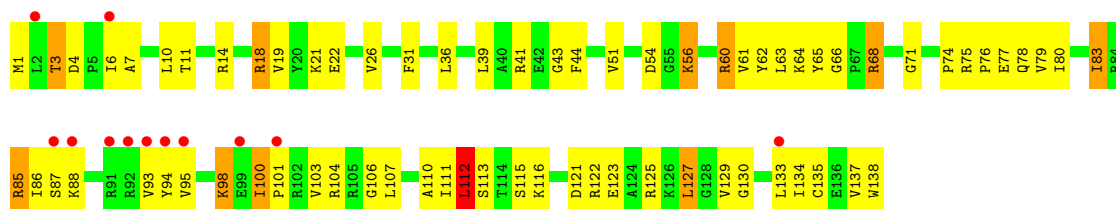




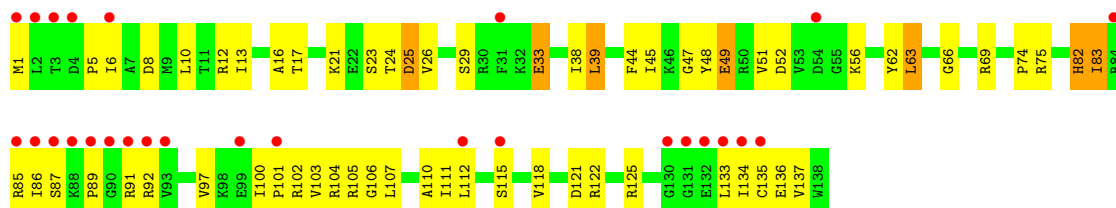
• Molecule 7: 30S ribosomal protein S7



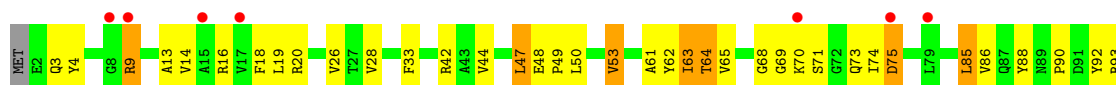
• Molecule 8: 30S ribosomal protein S8

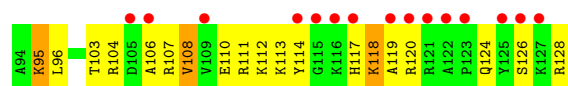


• Molecule 8: 30S ribosomal protein S8

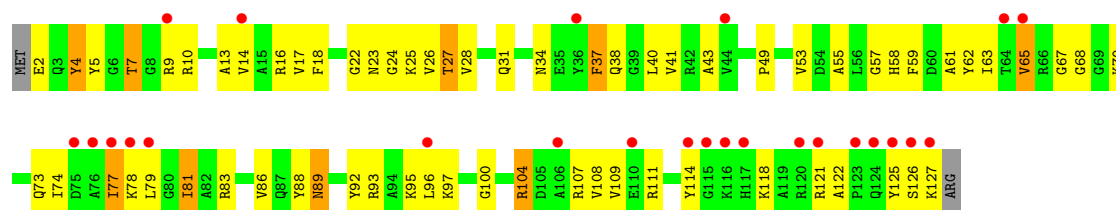


• Molecule 9: 30S ribosomal protein S9

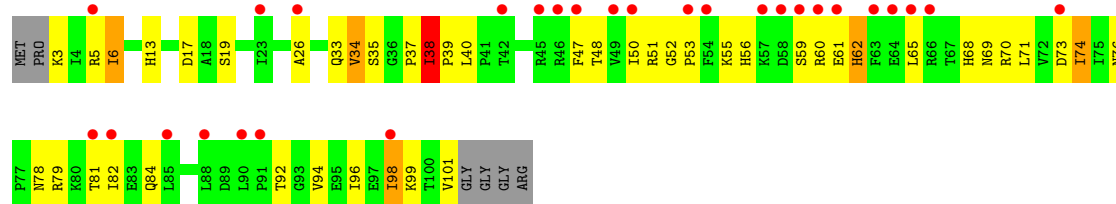




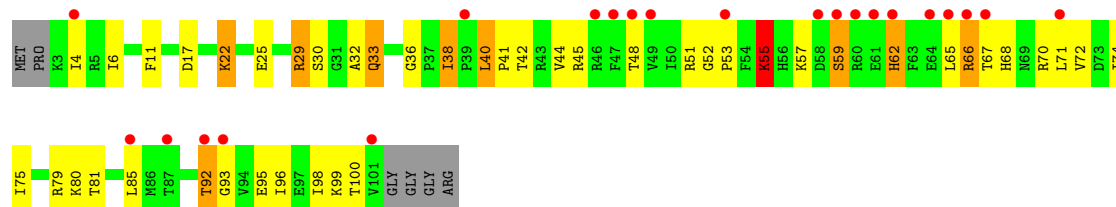
• Molecule 9: 30S ribosomal protein S9



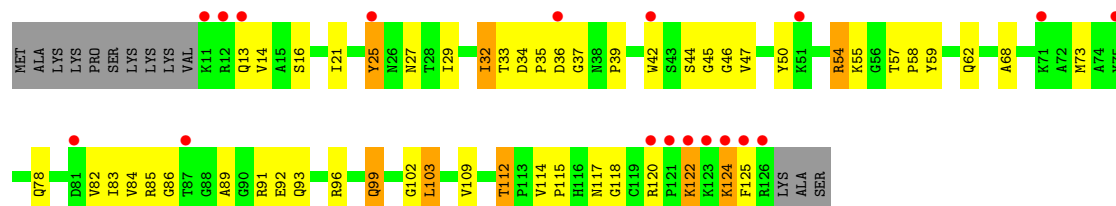
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

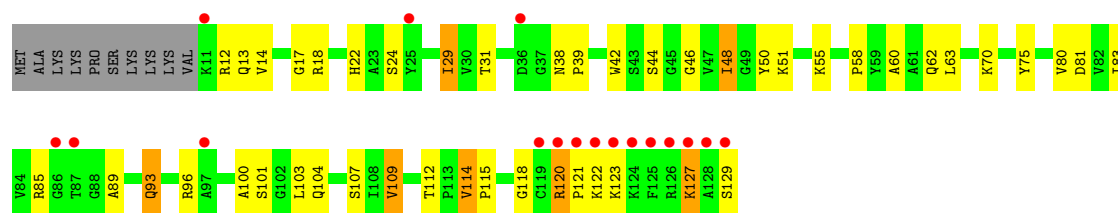


• Molecule 11: 30S ribosomal protein S11

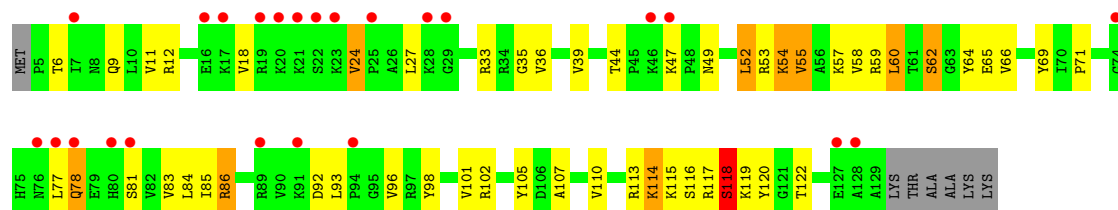


• Molecule 11: 30S ribosomal protein S11

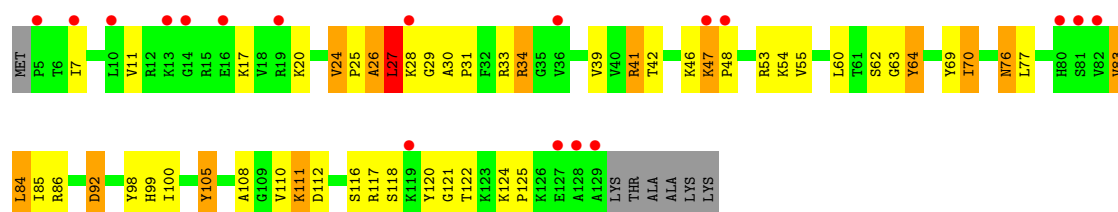




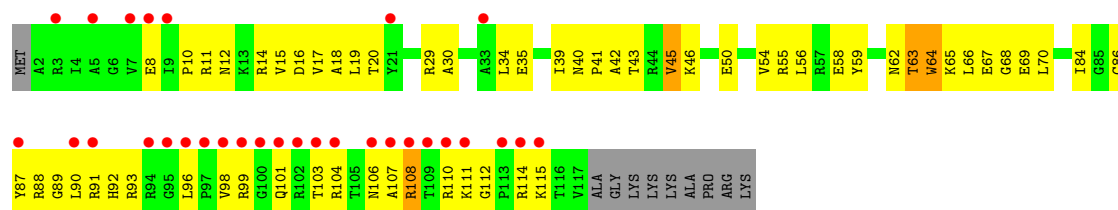
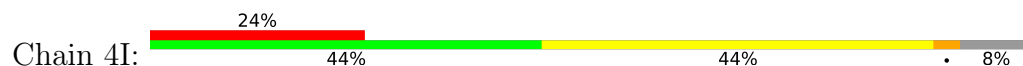
• Molecule 12: 30S ribosomal protein S12



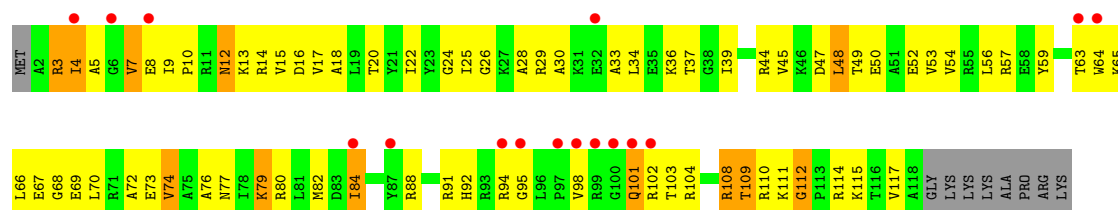
• Molecule 12: 30S ribosomal protein S12



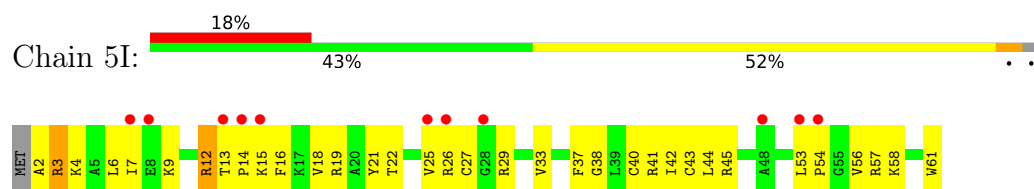
• Molecule 13: 30S ribosomal protein S13



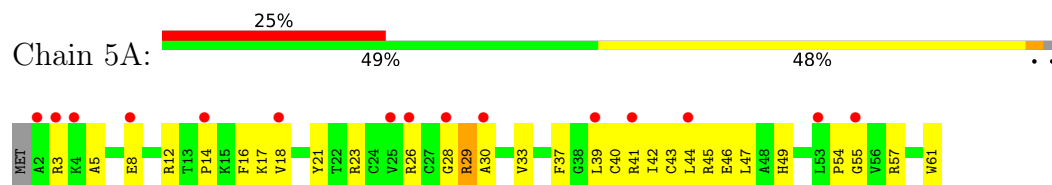
• Molecule 13: 30S ribosomal protein S13



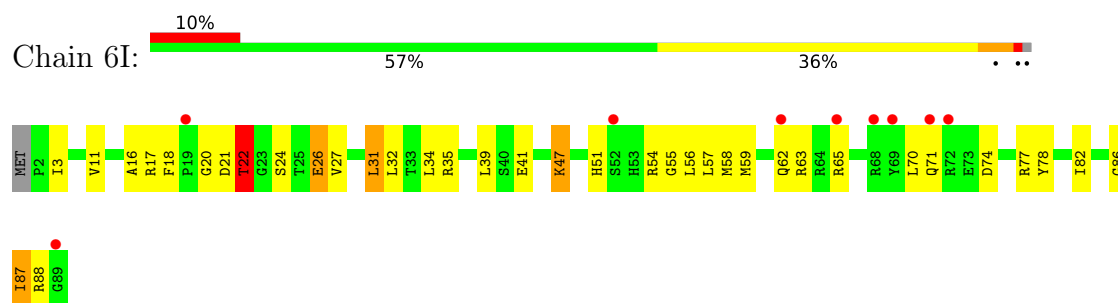
- Molecule 14: 30S ribosomal protein S14 type Z



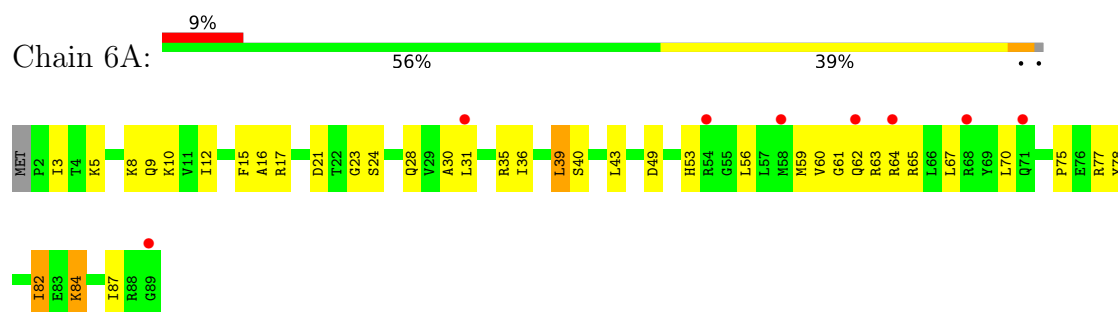
- Molecule 14: 30S ribosomal protein S14 type Z



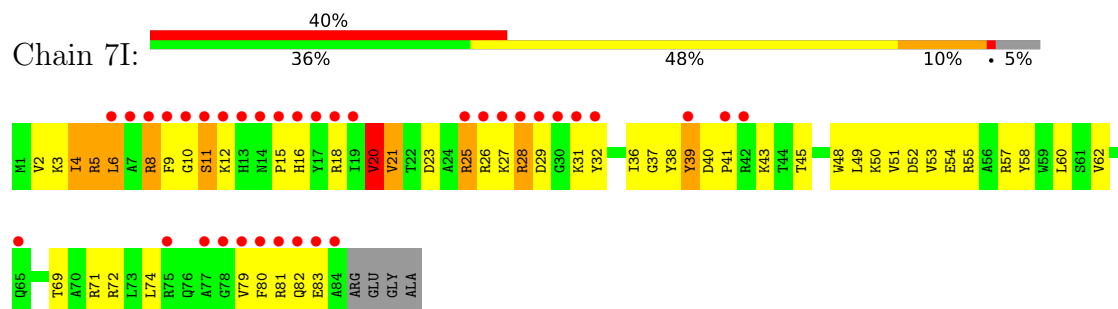
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

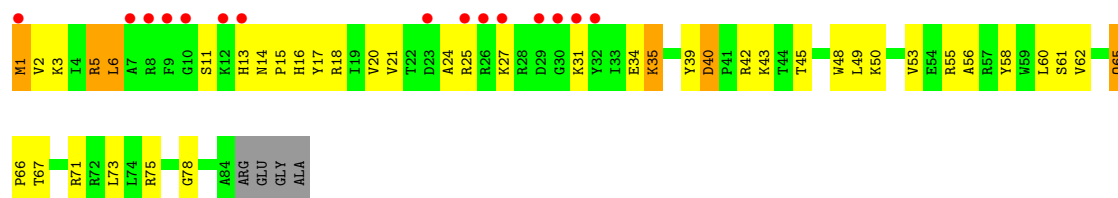


- Molecule 16: 30S ribosomal protein S16

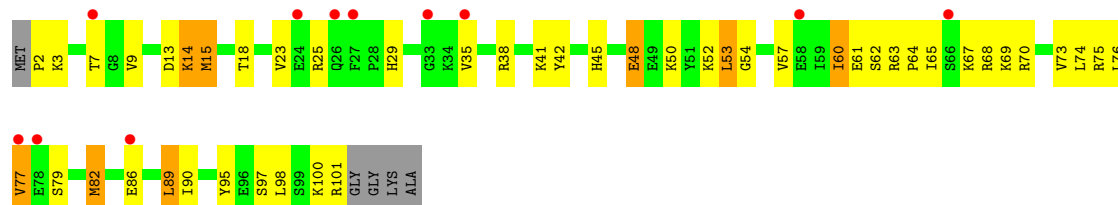


- Molecule 16: 30S ribosomal protein S16

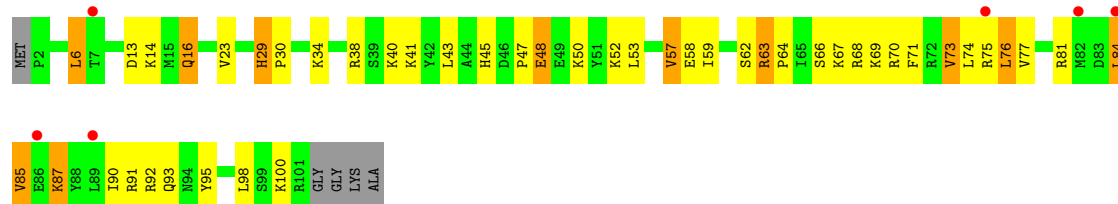




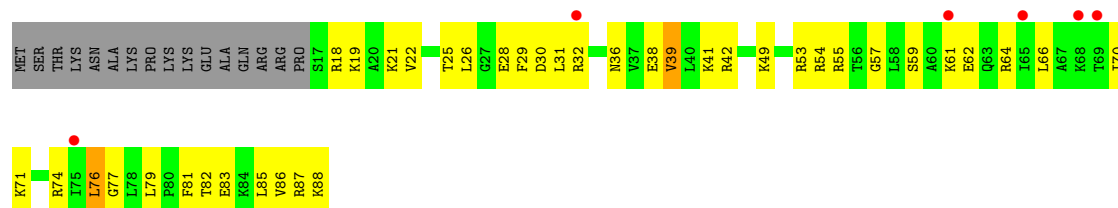
• Molecule 17: 30S ribosomal protein S17



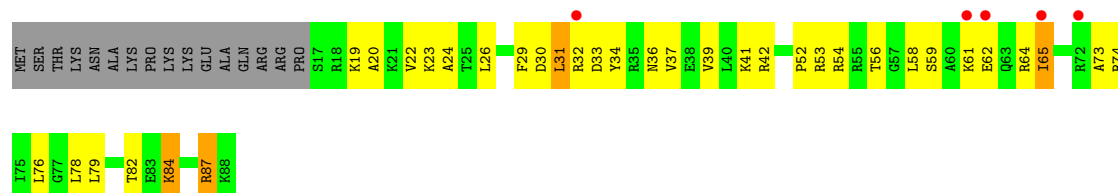
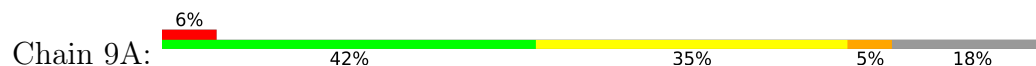
• Molecule 17: 30S ribosomal protein S17



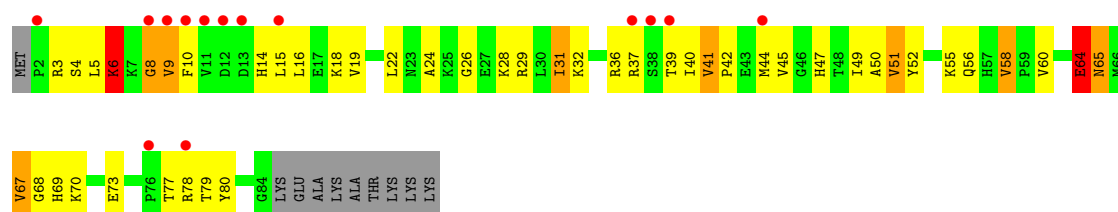
• Molecule 18: 30S ribosomal protein S18



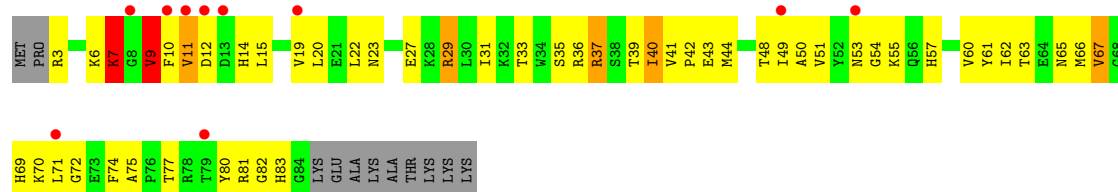
• Molecule 18: 30S ribosomal protein S18



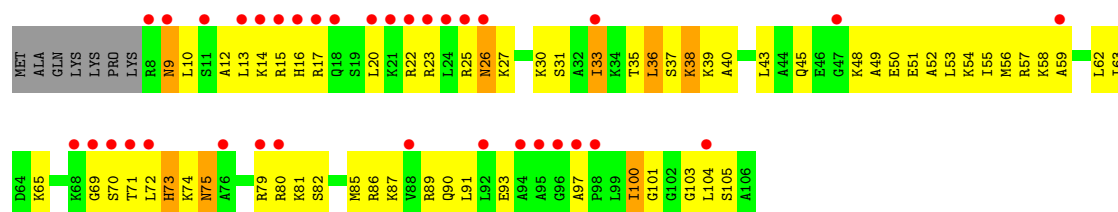
- Molecule 19: 30S ribosomal protein S19



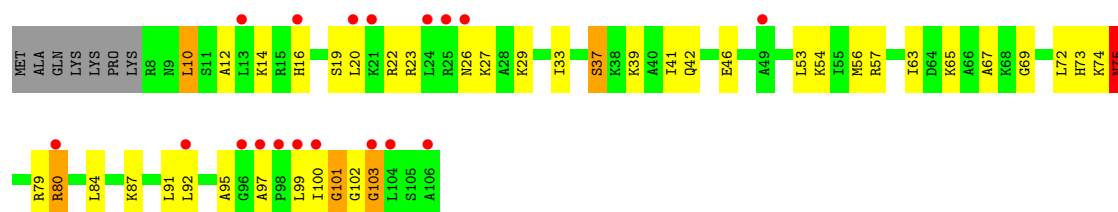
- Molecule 19: 30S ribosomal protein S19



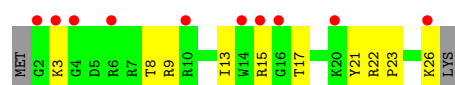
- Molecule 20: 30S ribosomal protein S20



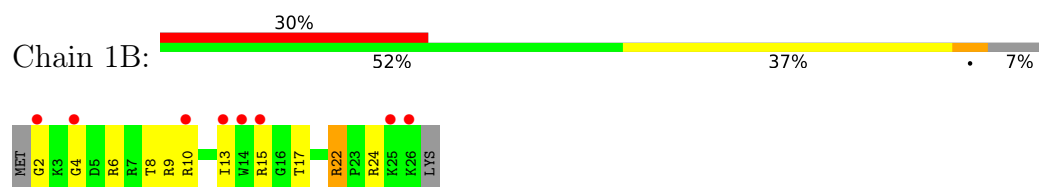
- Molecule 20: 30S ribosomal protein S20



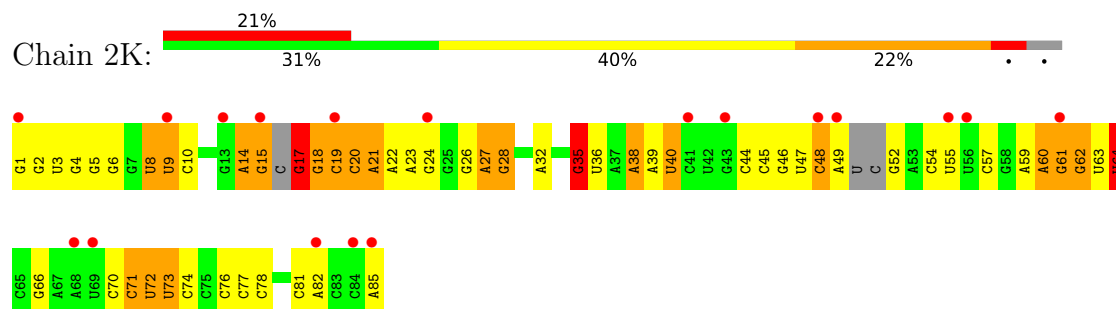
- Molecule 21: 30S ribosomal protein Thx



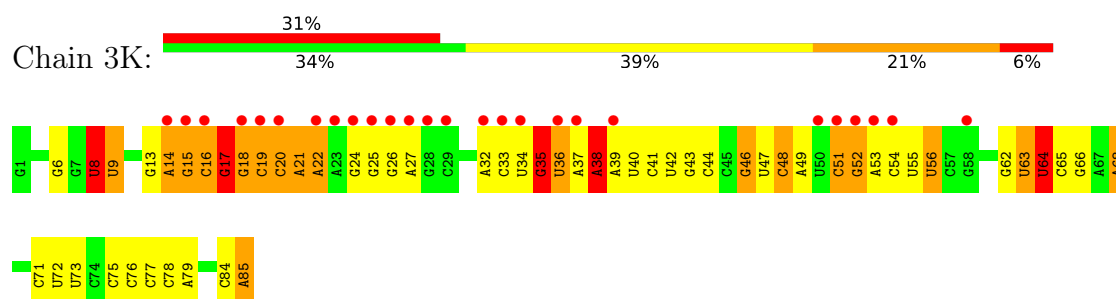
- Molecule 21: 30S ribosomal protein Thx



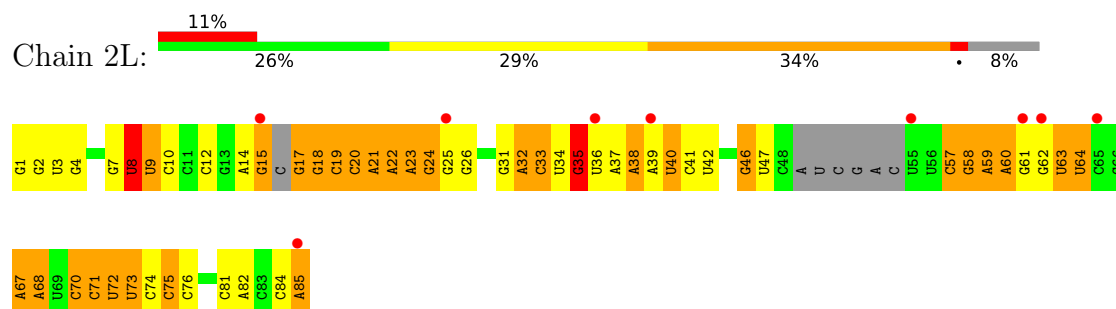
- Molecule 22: tRNA-Tyr



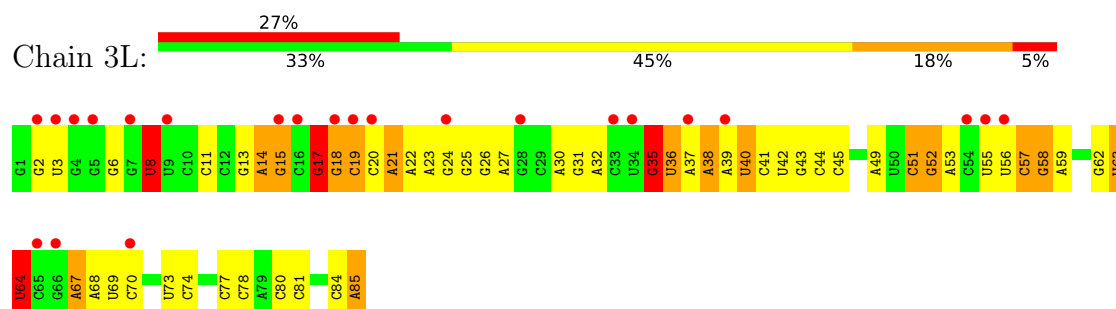
- Molecule 22: tRNA-Tyr

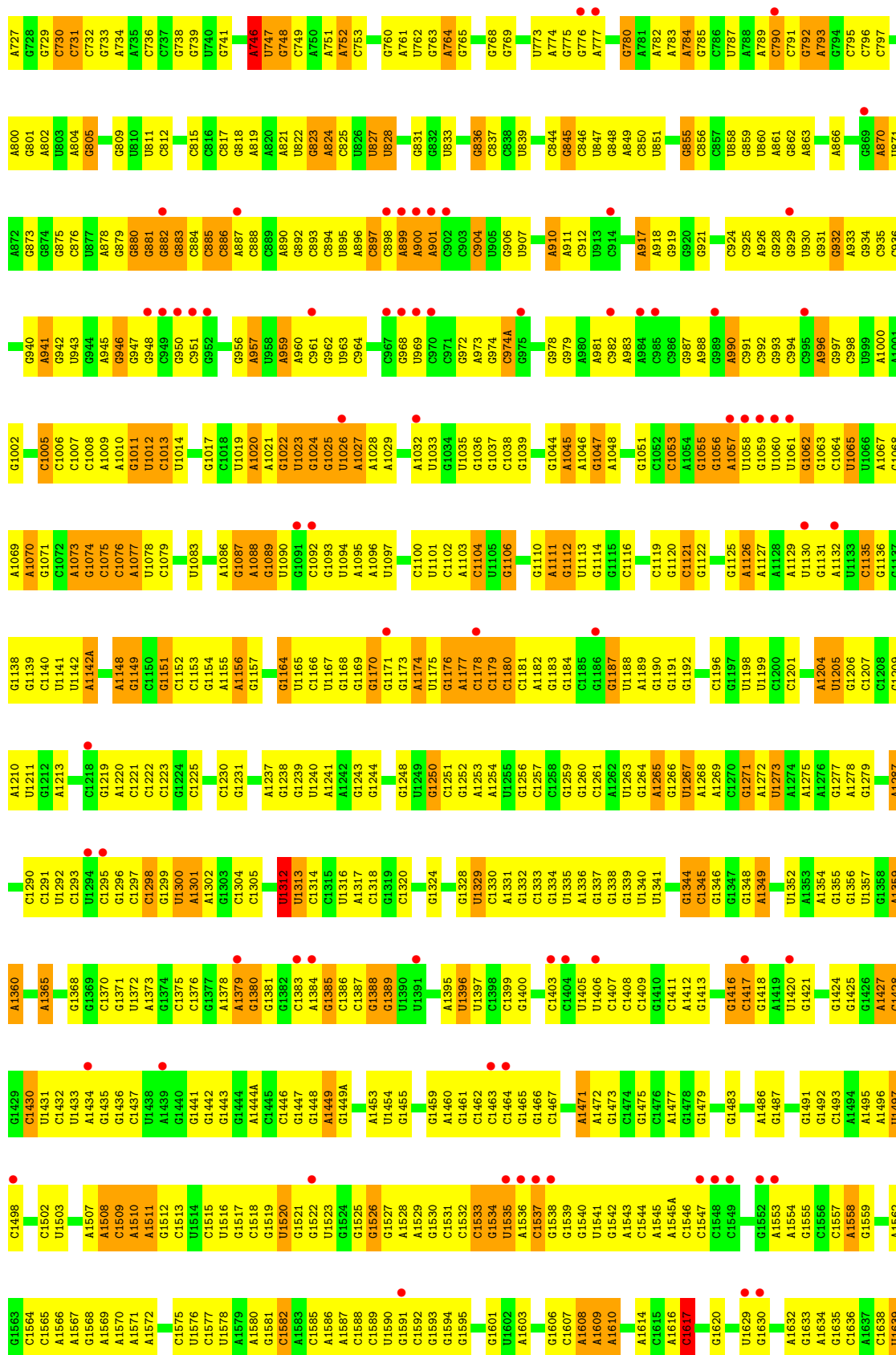


- Molecule 22: tRNA-Tyr

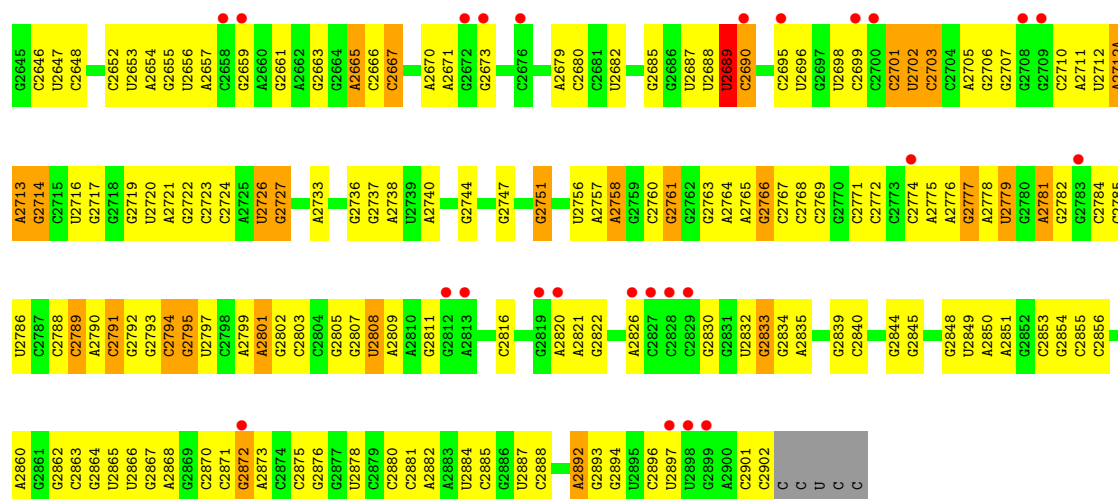


- Molecule 22: tRNA-Tyr

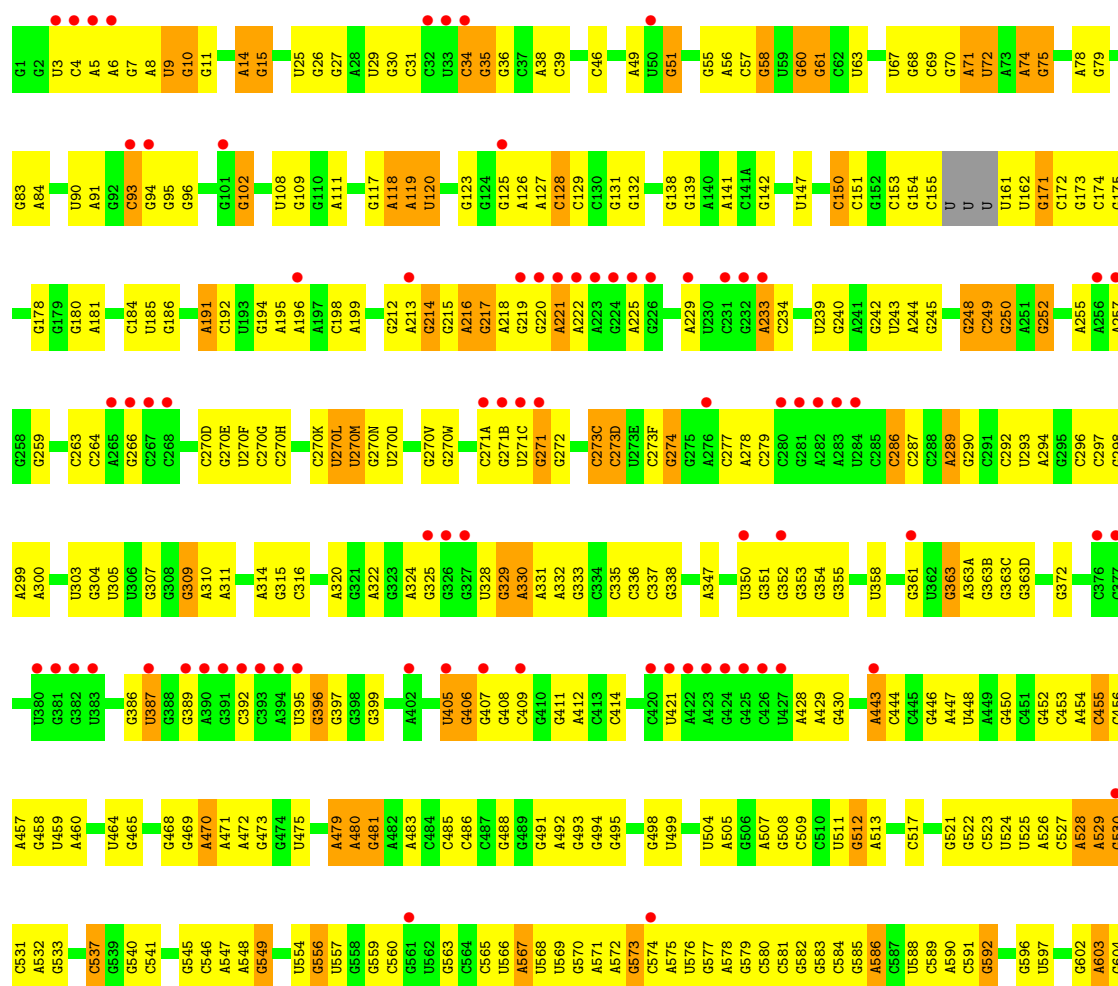
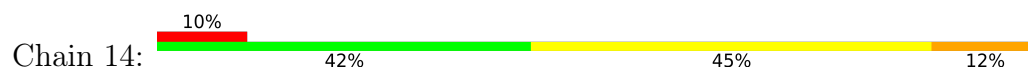


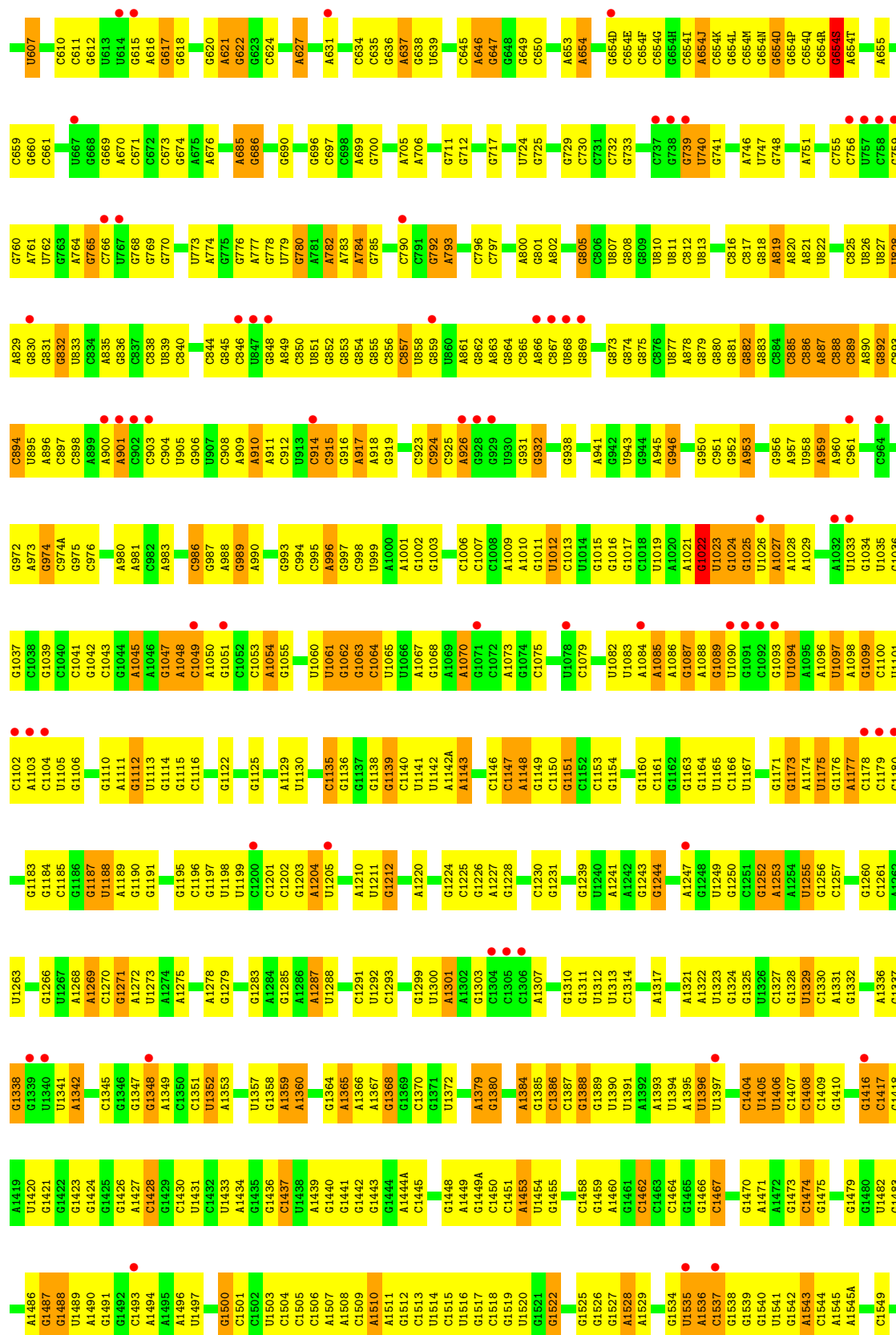


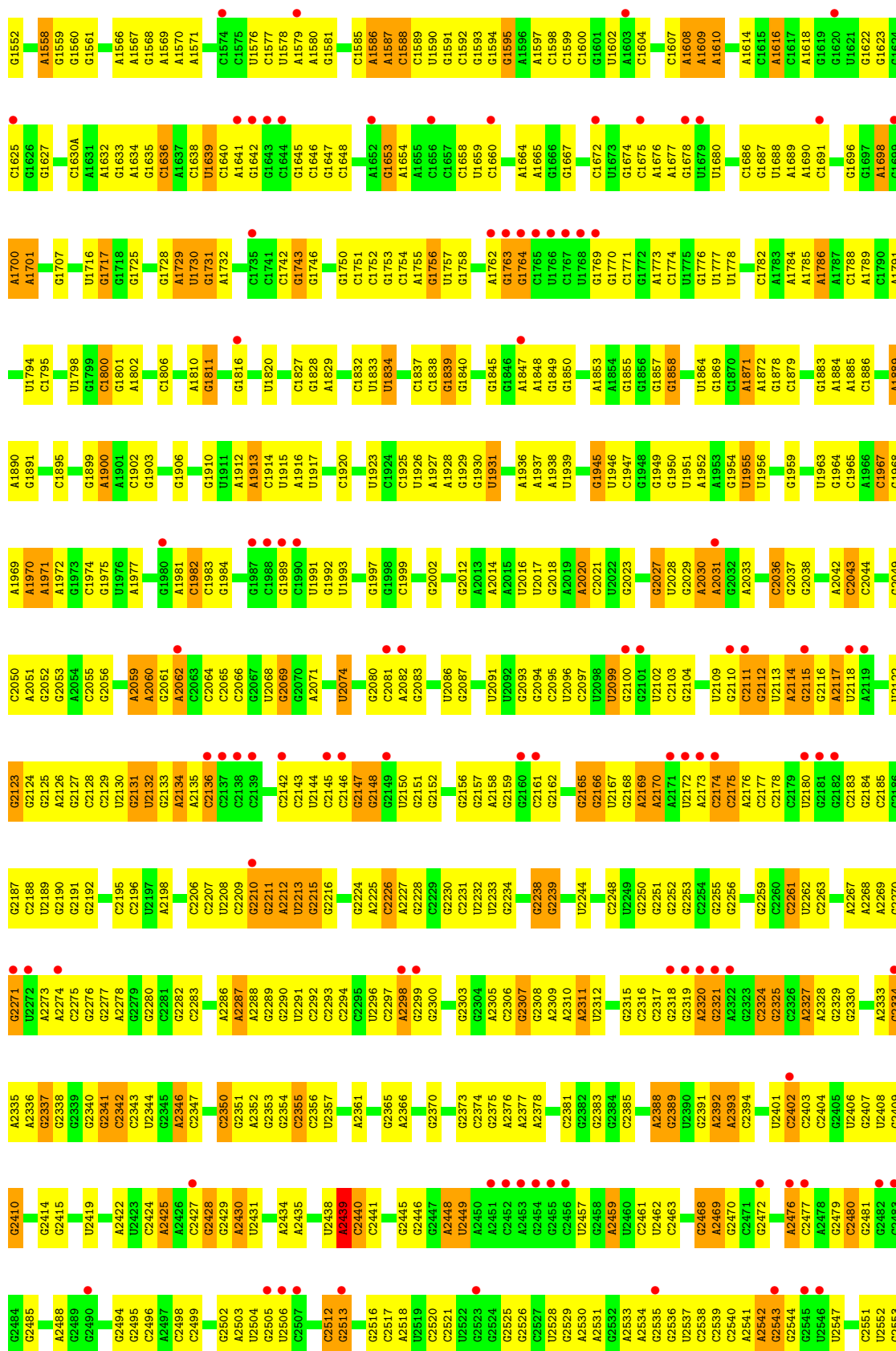


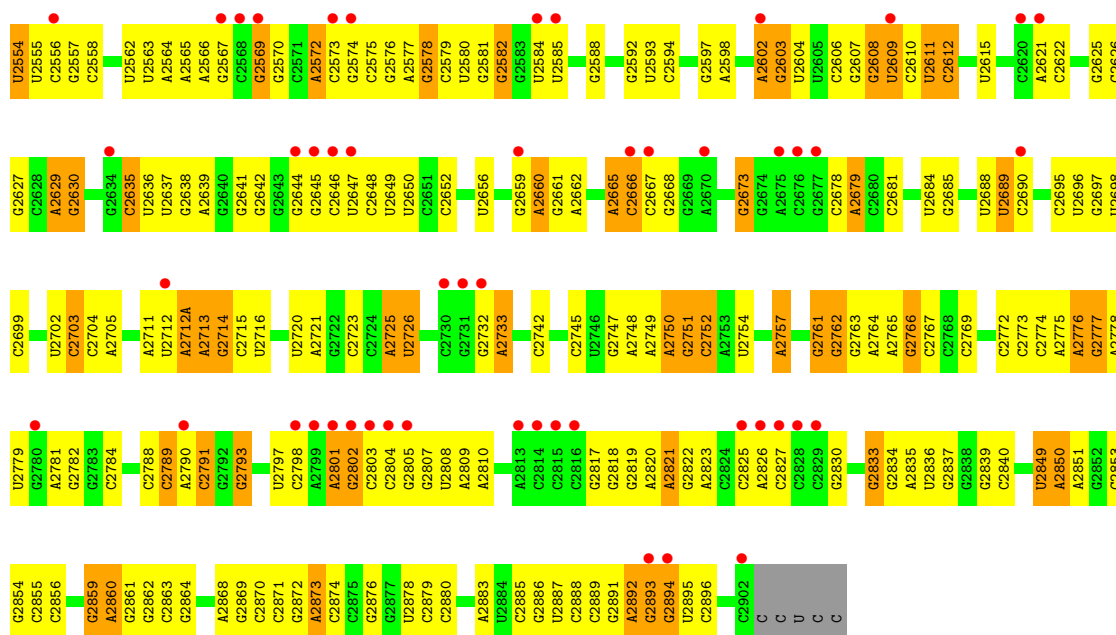


• Molecule 24: 23S ribosomal RNA

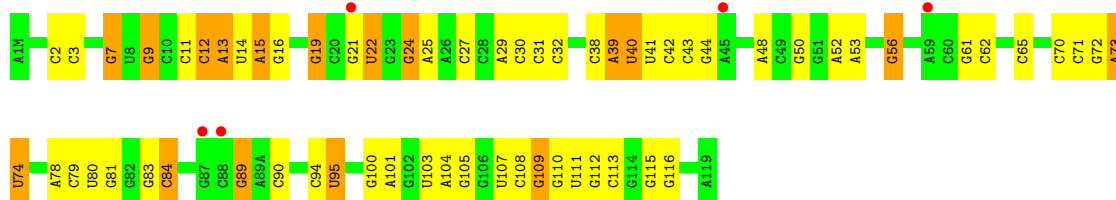




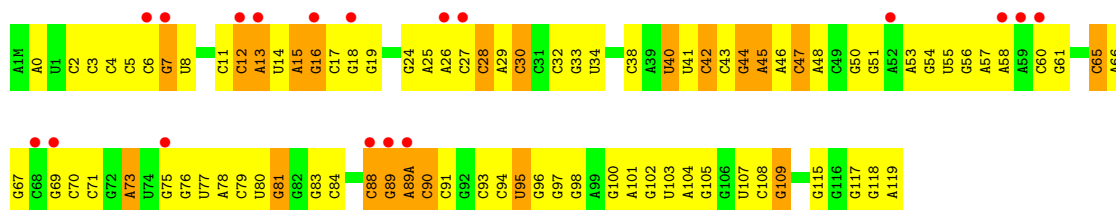




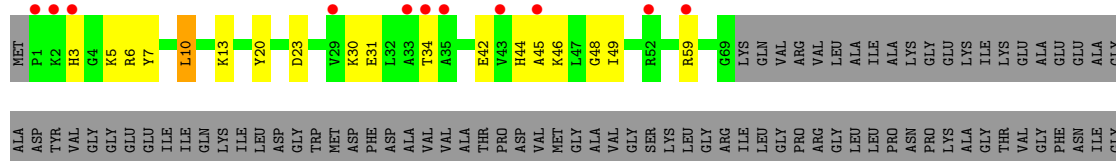
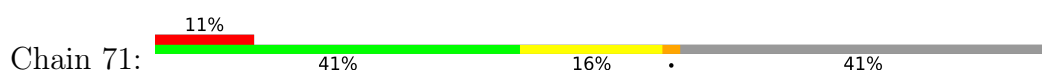
• Molecule 25: 5S ribosomal RNA

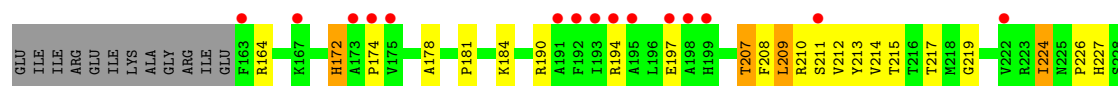


• Molecule 25: 5S ribosomal RNA

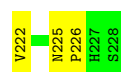
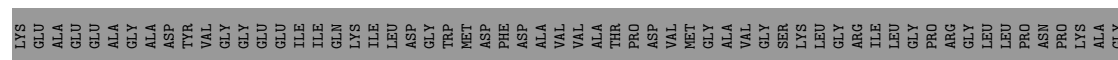


• Molecule 26: 50S ribosomal protein L1

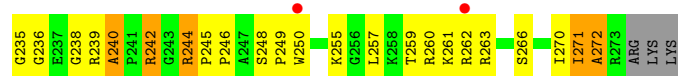
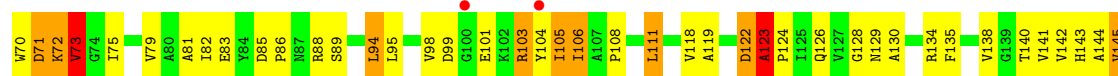
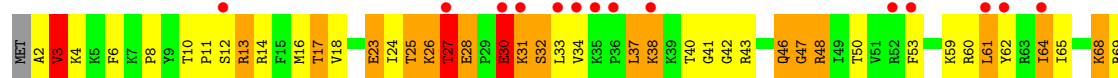




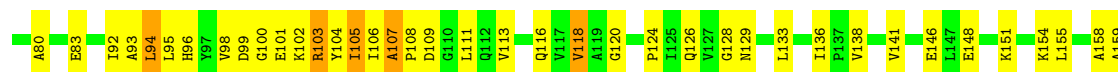
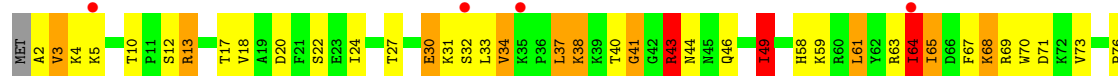
• Molecule 26: 50S ribosomal protein L1

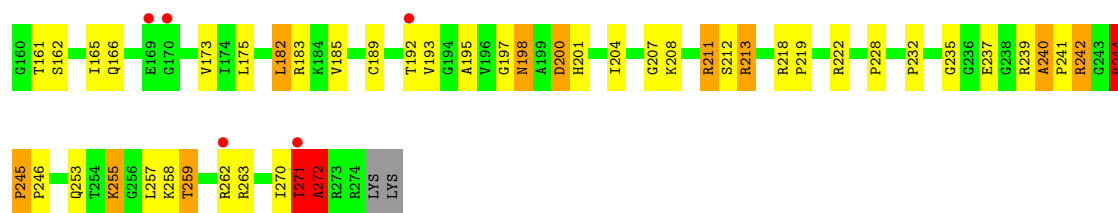


• Molecule 27: 50S ribosomal protein L2

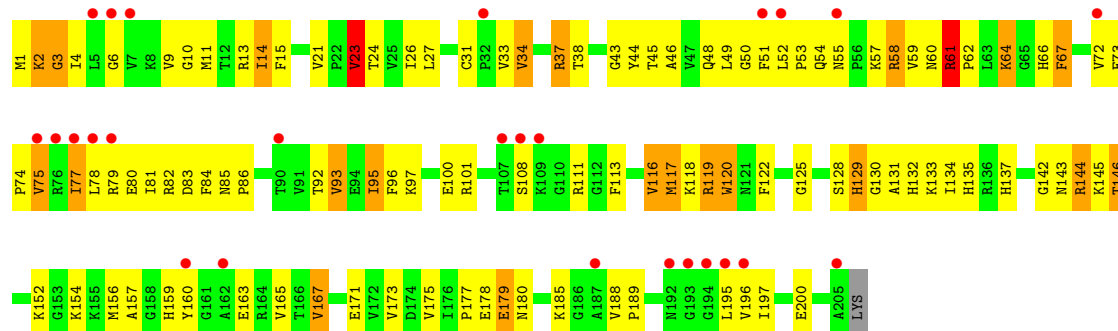


• Molecule 27: 50S ribosomal protein L2

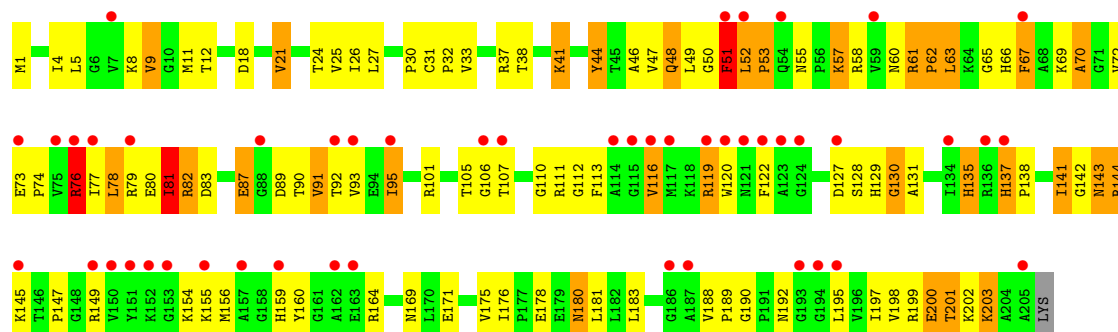




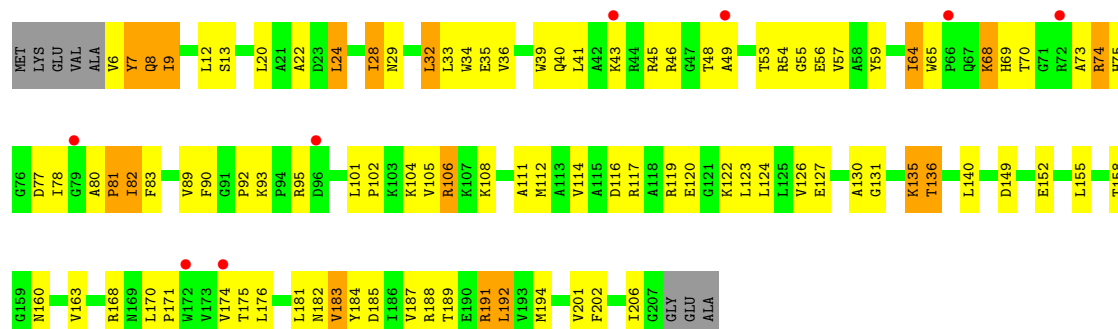
• Molecule 28: 50S ribosomal protein L3



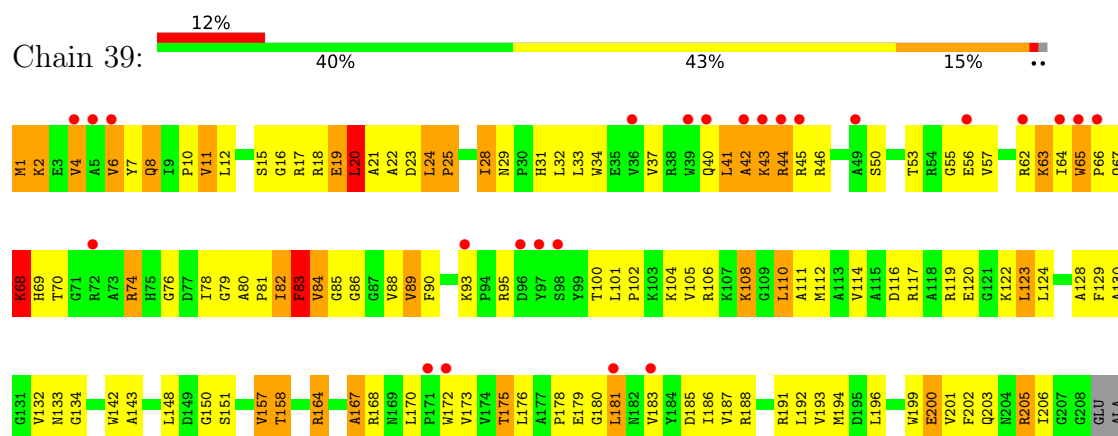
• Molecule 28: 50S ribosomal protein L3



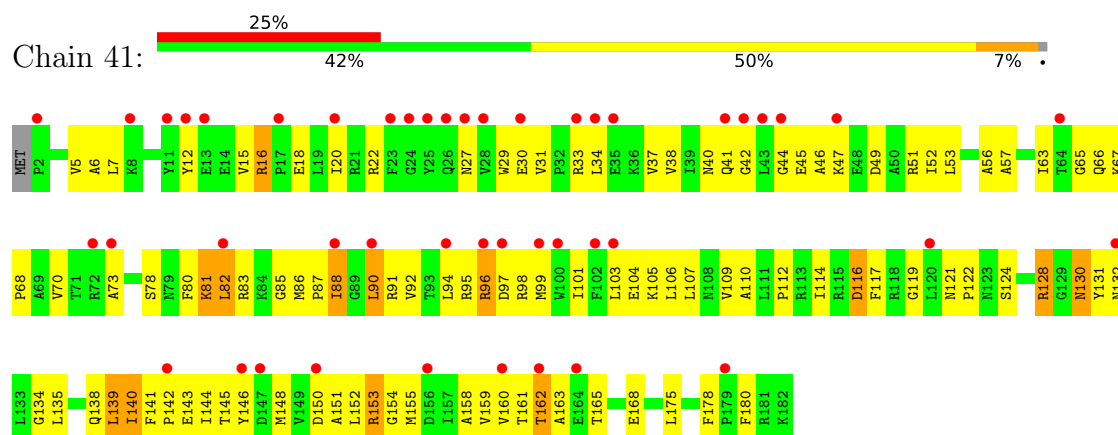
• Molecule 29: 50S ribosomal protein L4



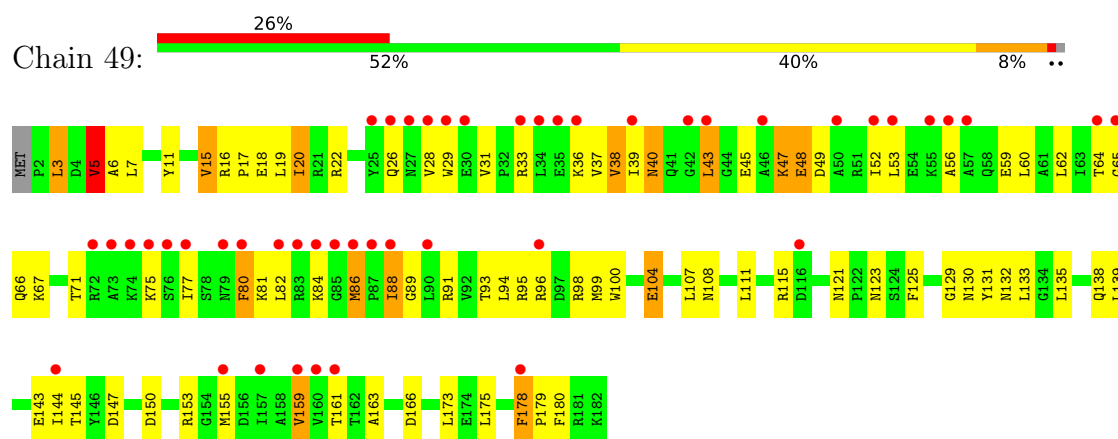
- Molecule 29: 50S ribosomal protein L4



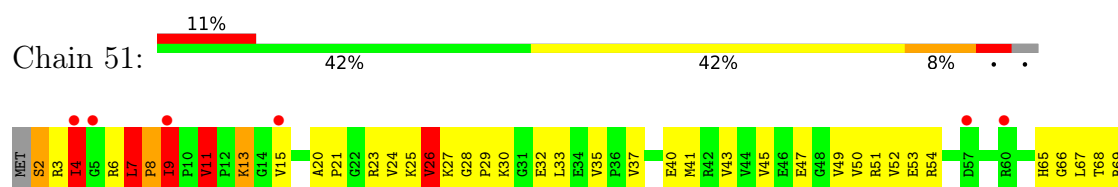
- Molecule 30: 50S ribosomal protein L5

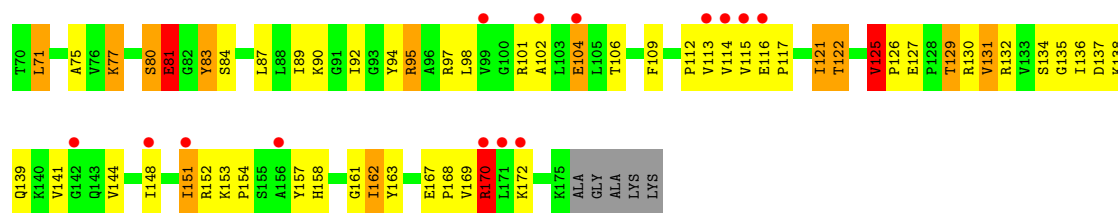


- Molecule 30: 50S ribosomal protein L5

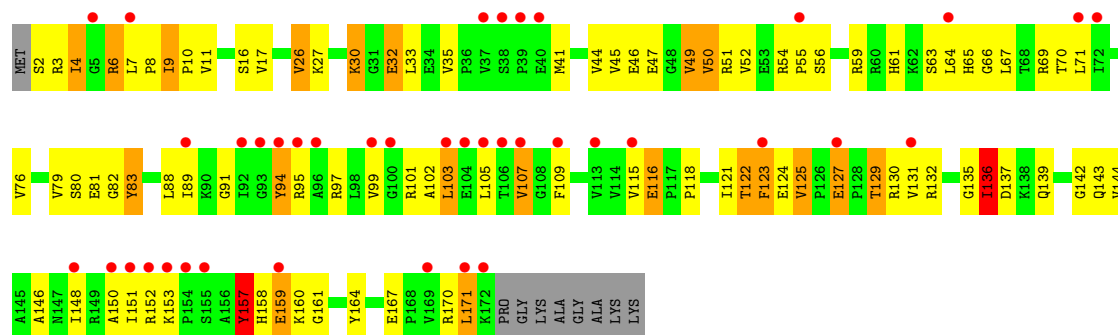
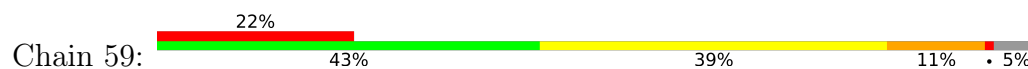


- Molecule 31: 50S ribosomal protein L6

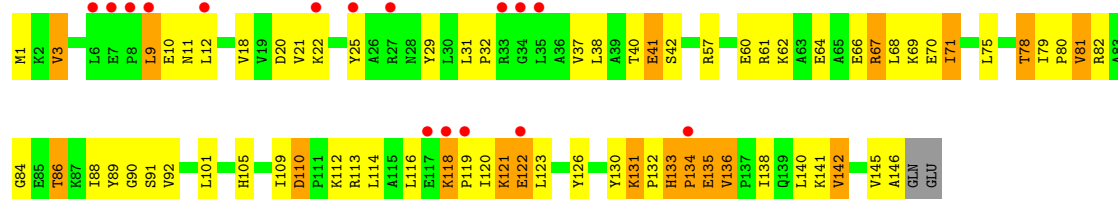




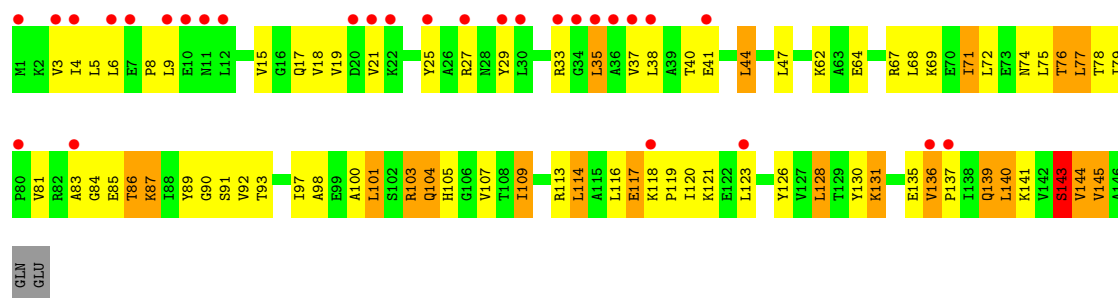
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

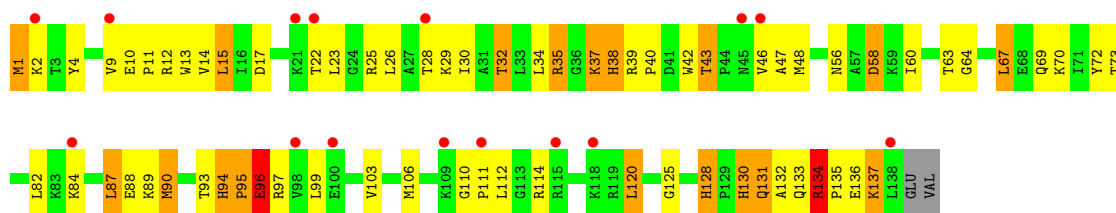


• Molecule 32: 50S ribosomal protein L9

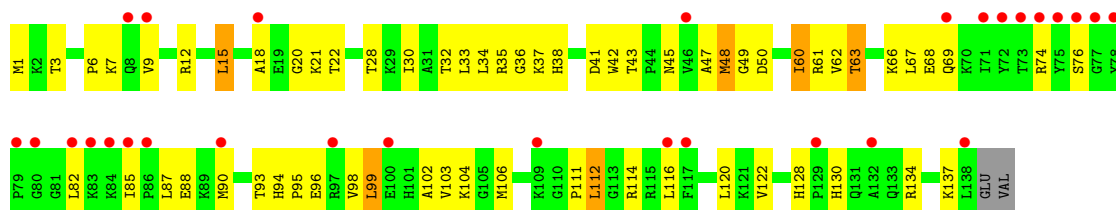


• Molecule 33: 50S ribosomal protein L13

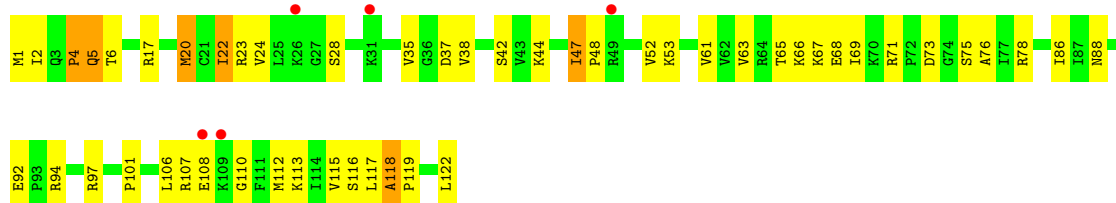




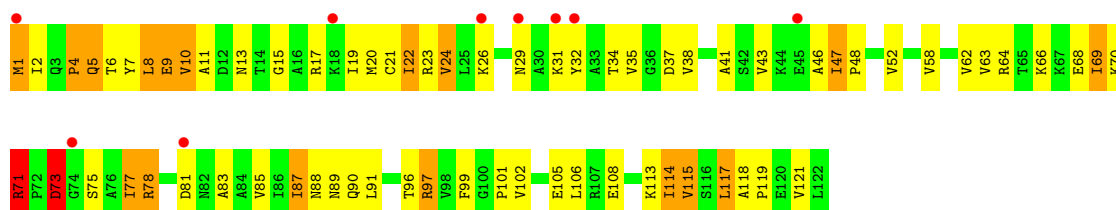
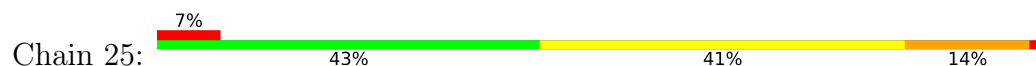
• Molecule 33: 50S ribosomal protein L13



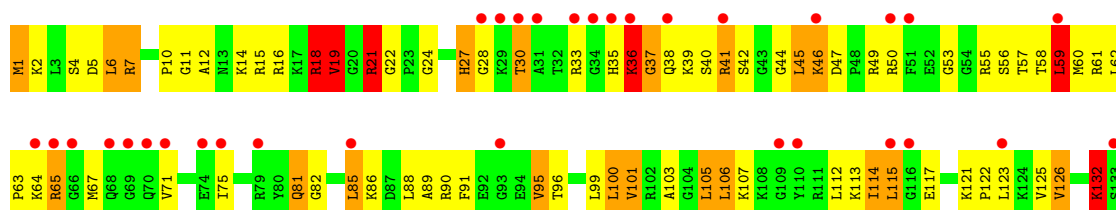
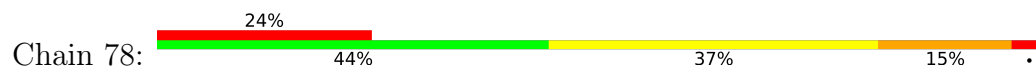
• Molecule 34: 50S ribosomal protein L14

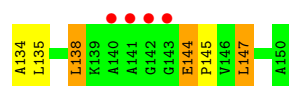


• Molecule 34: 50S ribosomal protein L14

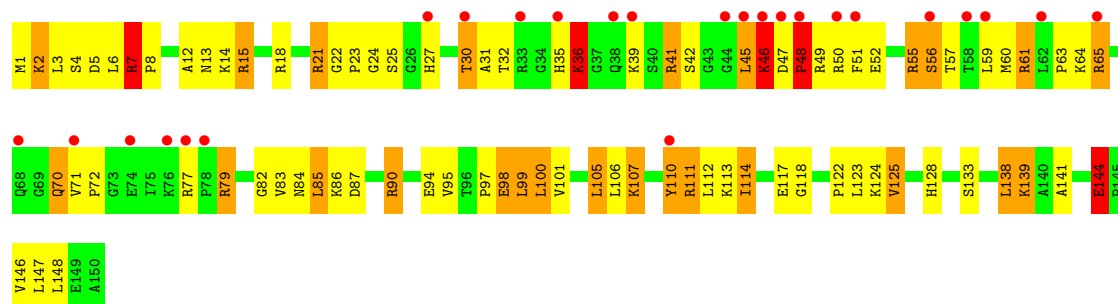
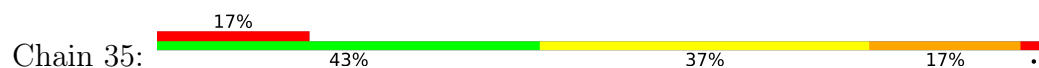


• Molecule 35: 50S ribosomal protein L15

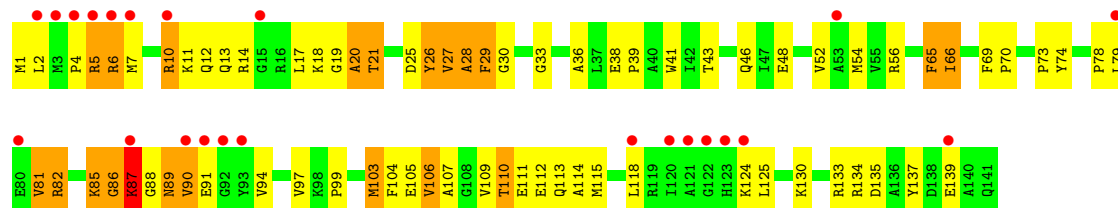




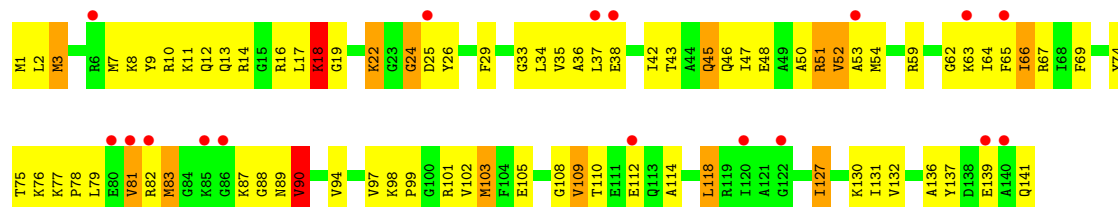
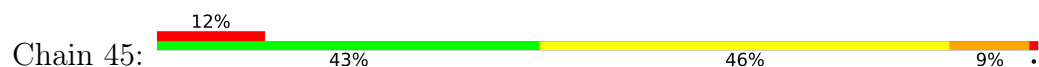
• Molecule 35: 50S ribosomal protein L15



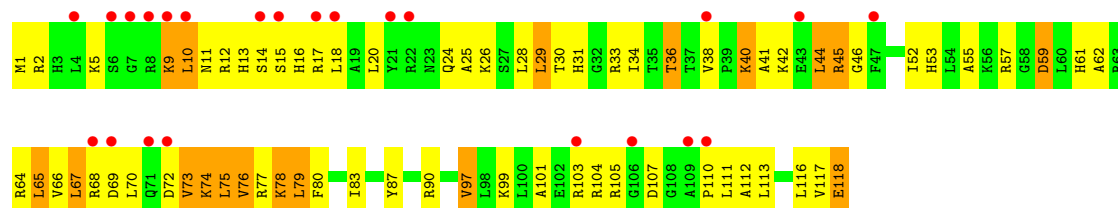
• Molecule 36: 50S ribosomal protein L16



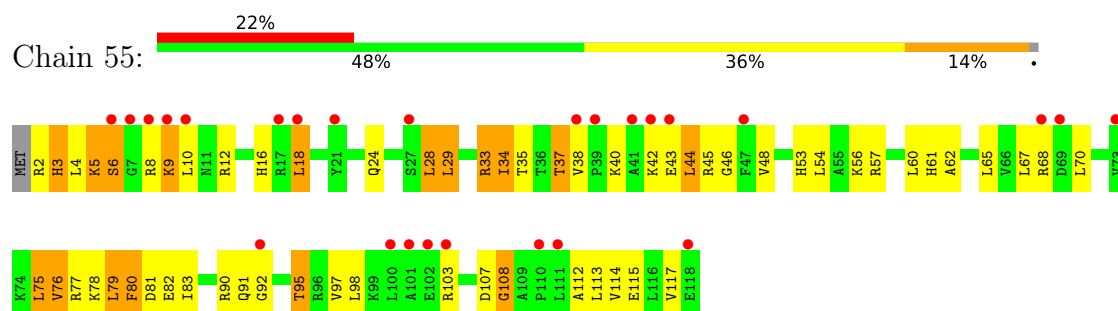
• Molecule 36: 50S ribosomal protein L16



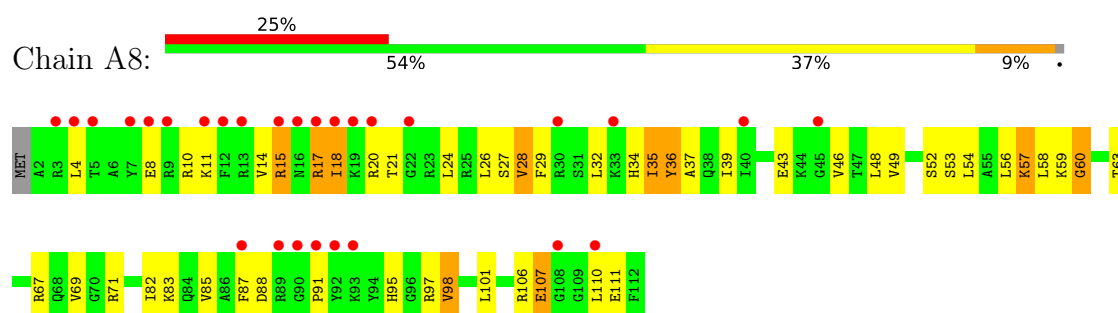
• Molecule 37: 50S ribosomal protein L17



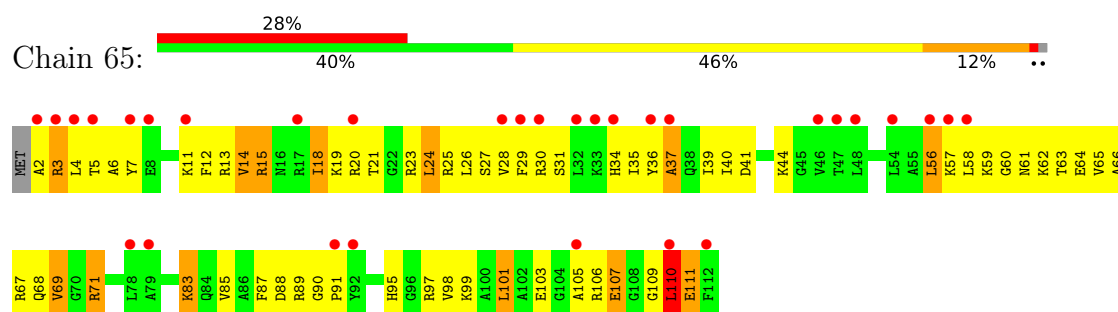
- Molecule 37: 50S ribosomal protein L17



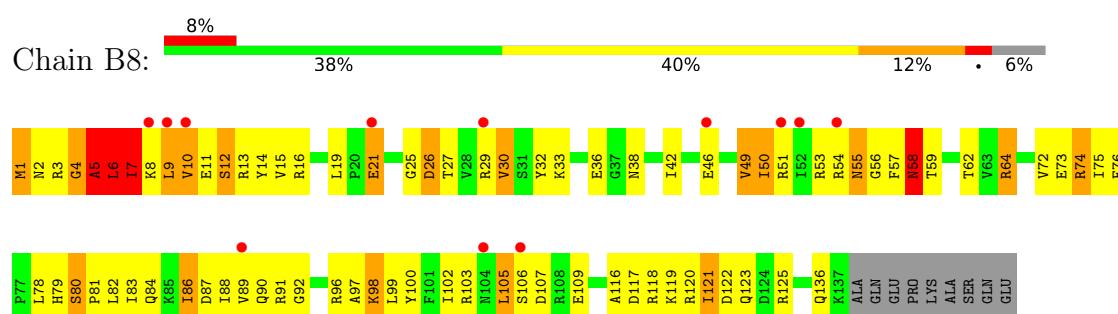
- Molecule 38: 50S ribosomal protein L18



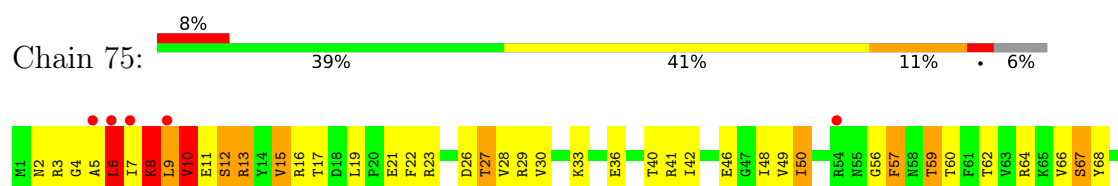
- Molecule 38: 50S ribosomal protein L18

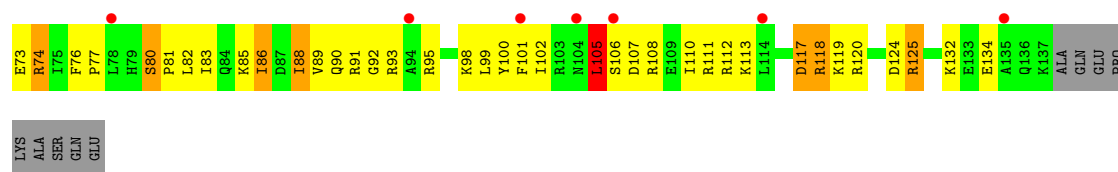


- Molecule 39: 50S ribosomal protein L19

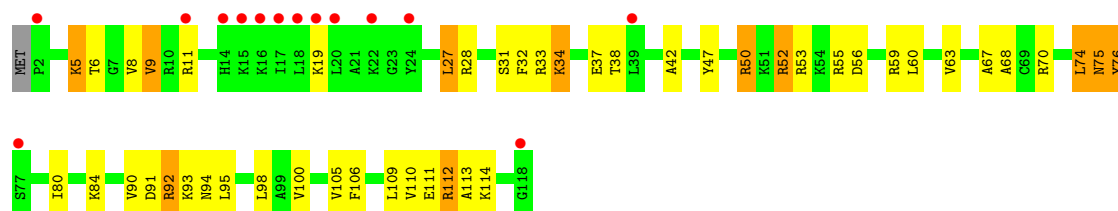


- Molecule 39: 50S ribosomal protein L19

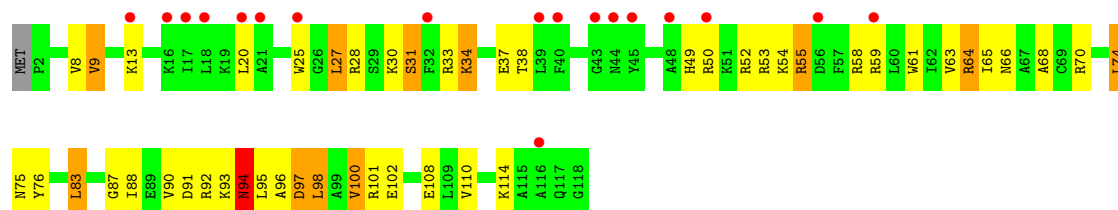




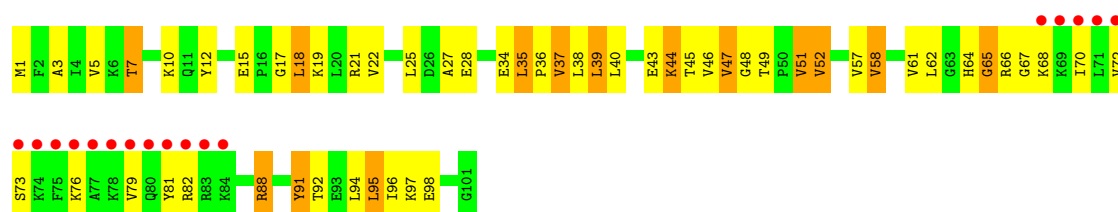
- Molecule 40: 50S ribosomal protein L20



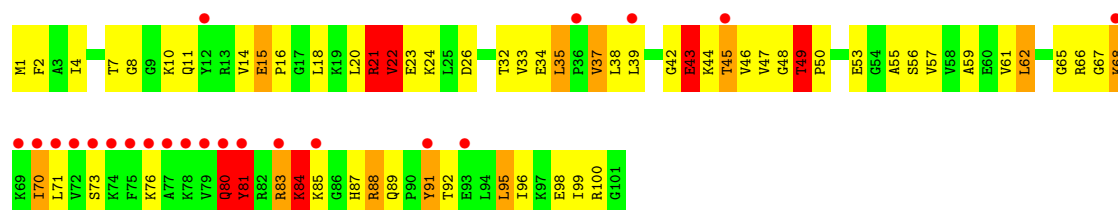
- Molecule 40: 50S ribosomal protein L20



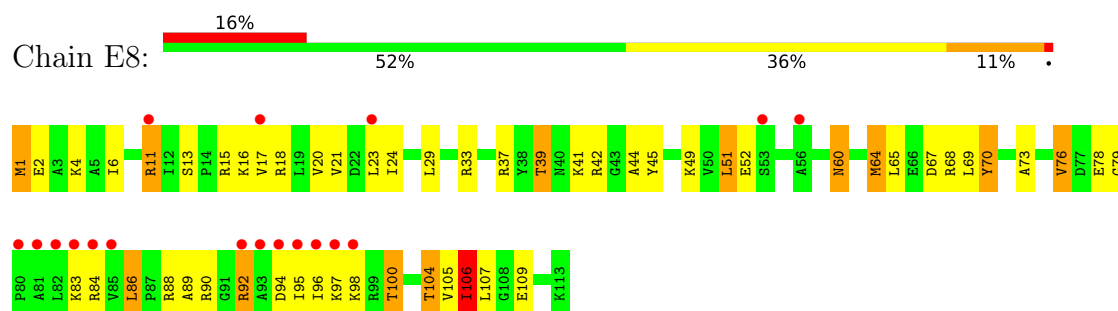
- Molecule 41: 50S ribosomal protein L21



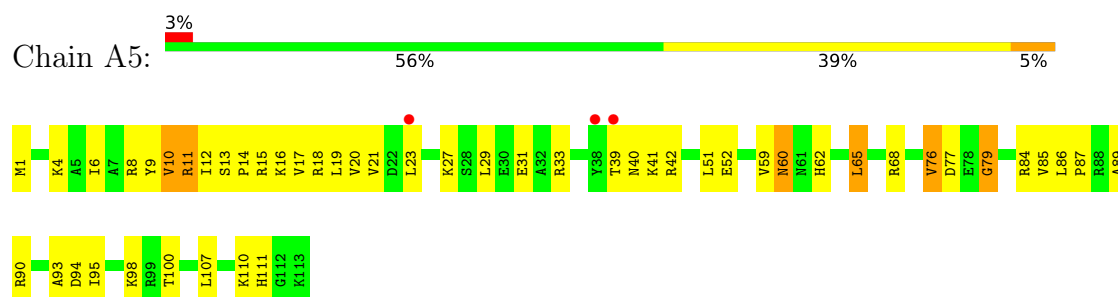
- Molecule 41: 50S ribosomal protein L21



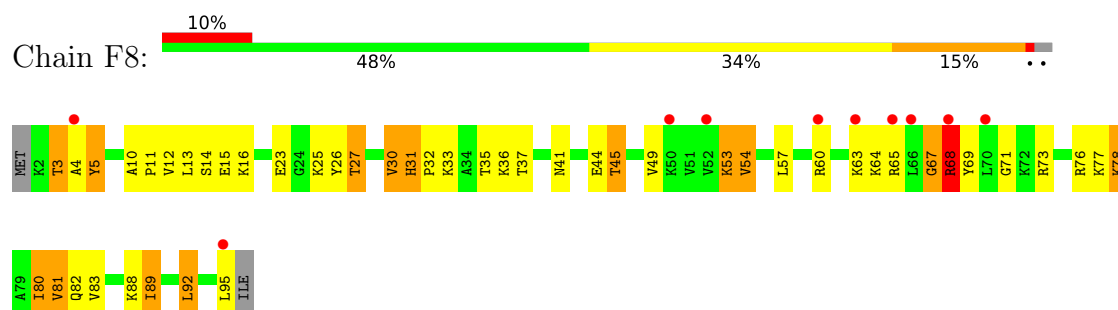
- Molecule 42: 50S ribosomal protein L22



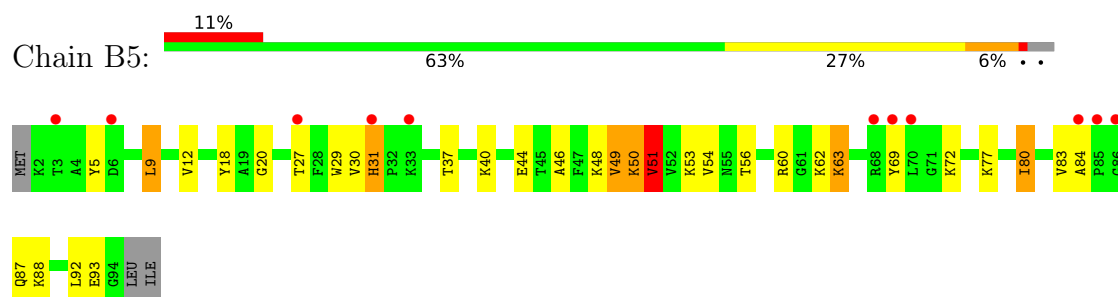
- Molecule 42: 50S ribosomal protein L22



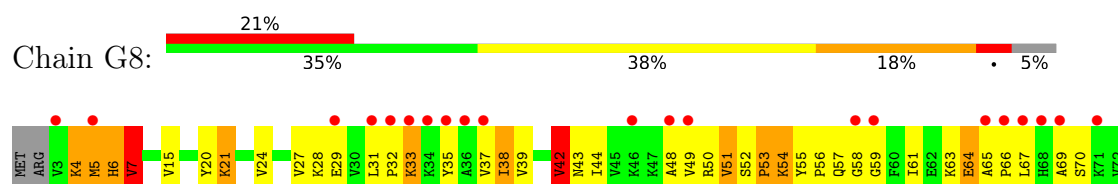
- Molecule 43: 50S ribosomal protein L23

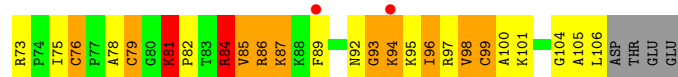


- Molecule 43: 50S ribosomal protein L23

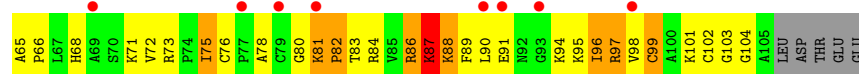
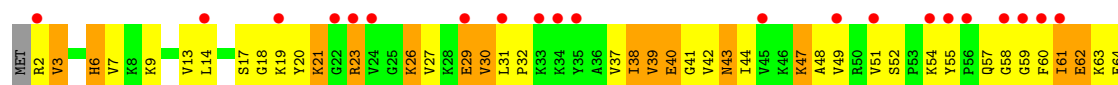


- Molecule 44: 50S ribosomal protein L24

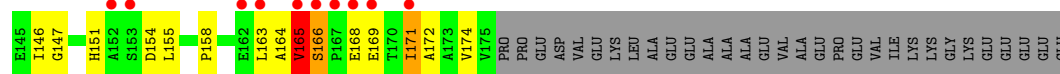
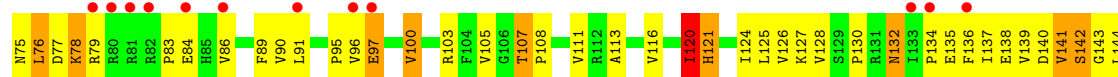




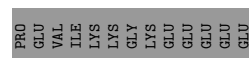
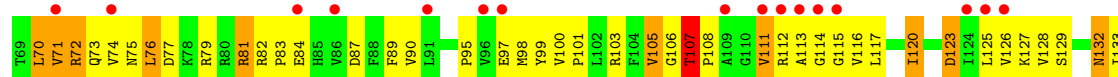
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25

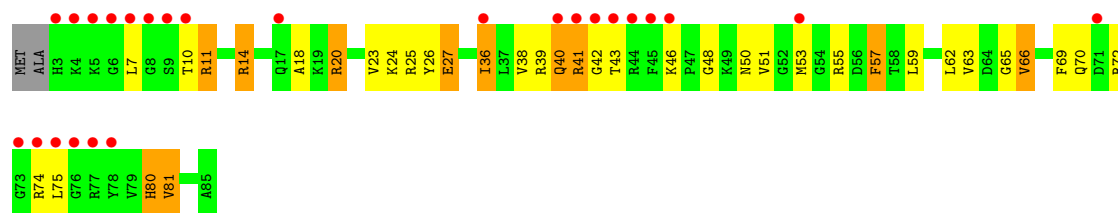


• Molecule 45: 50S ribosomal protein L25

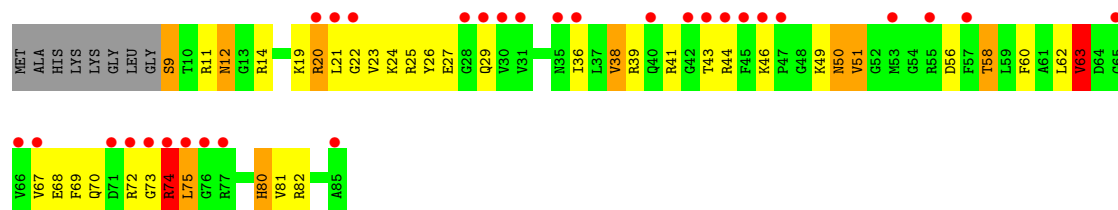
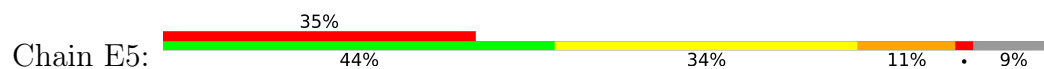


• Molecule 46: 50S ribosomal protein L27

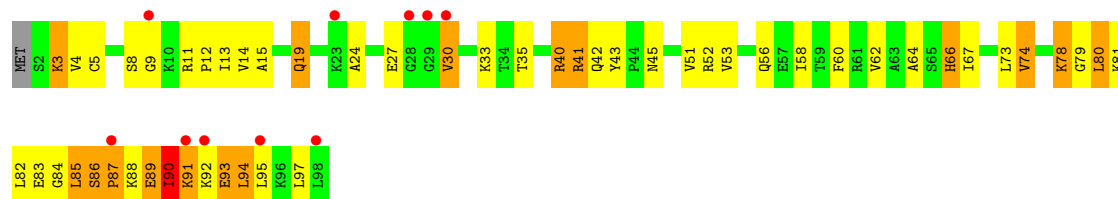




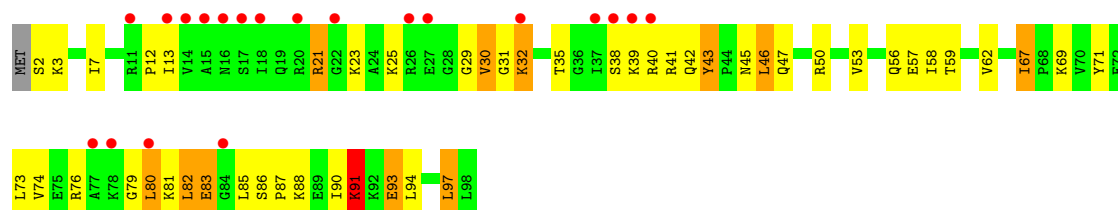
- Molecule 46: 50S ribosomal protein L27



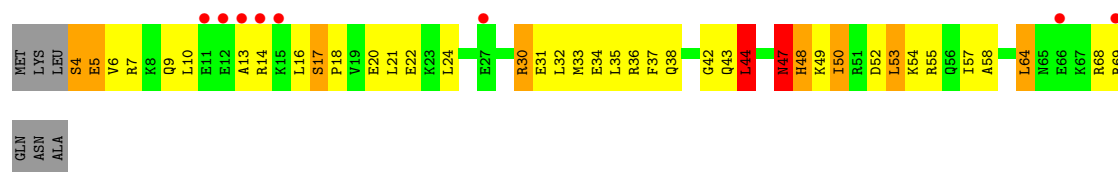
- Molecule 47: 50S ribosomal protein L28



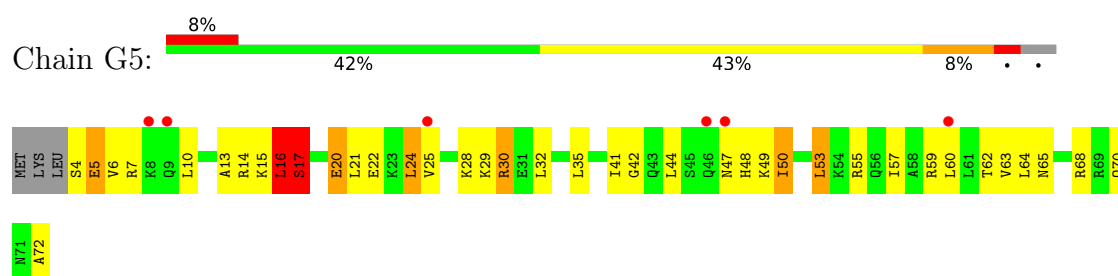
- Molecule 47: 50S ribosomal protein L28



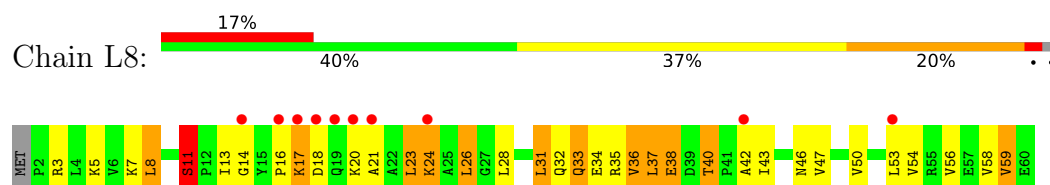
- Molecule 48: 50S ribosomal protein L29



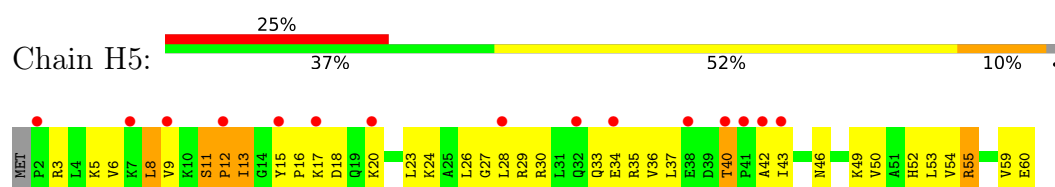
- Molecule 48: 50S ribosomal protein L29



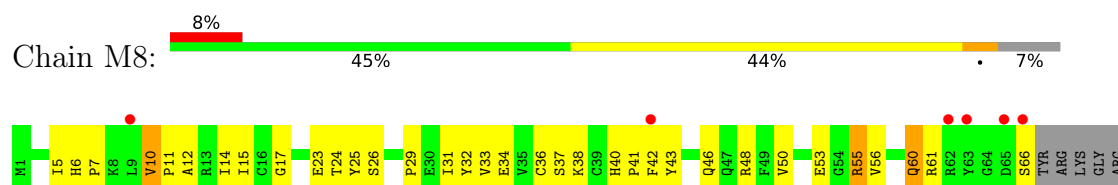
- Molecule 49: 50S ribosomal protein L30



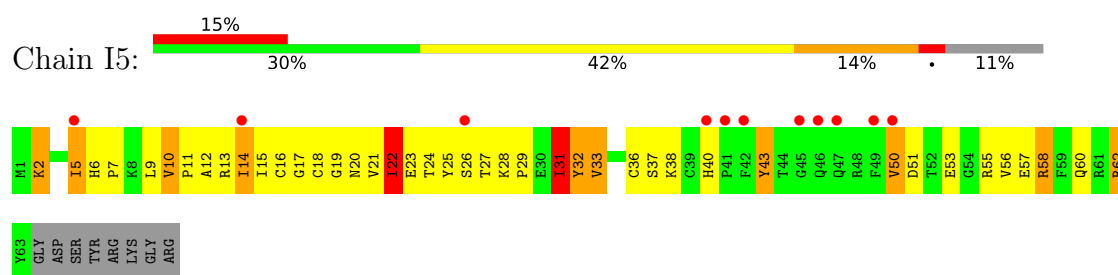
- Molecule 49: 50S ribosomal protein L30



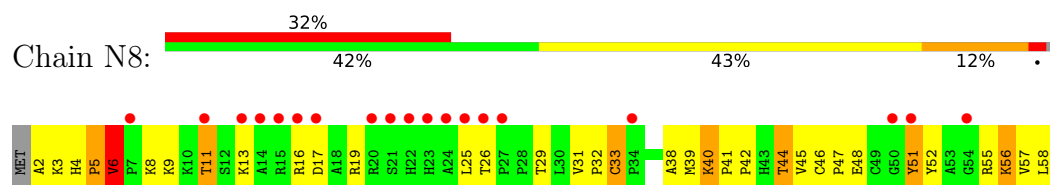
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



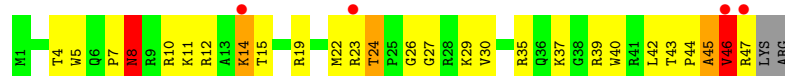
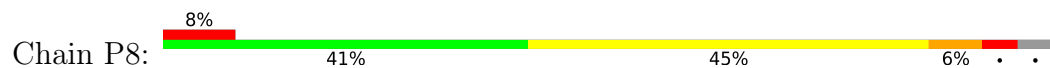
- Molecule 51: 50S ribosomal protein L32



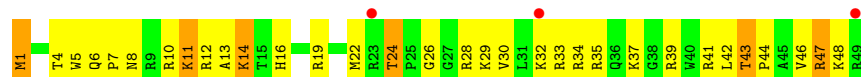
- Molecule 51: 50S ribosomal protein L32



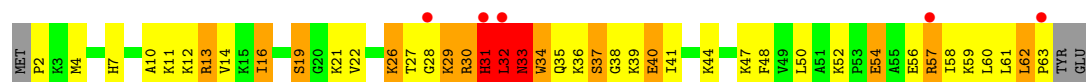
- Molecule 52: 50S ribosomal protein L34



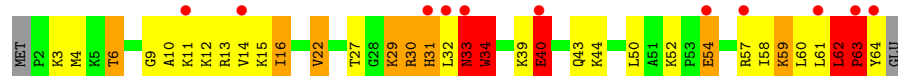
- Molecule 52: 50S ribosomal protein L34



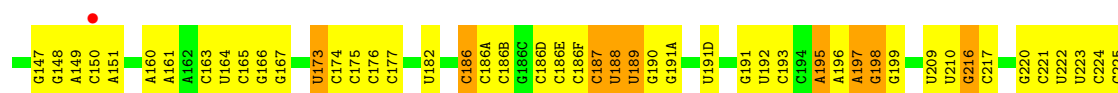
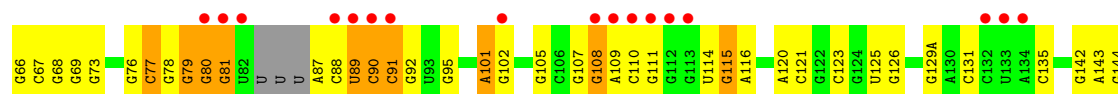
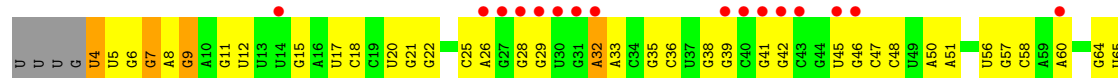
- Molecule 53: 50S ribosomal protein L35



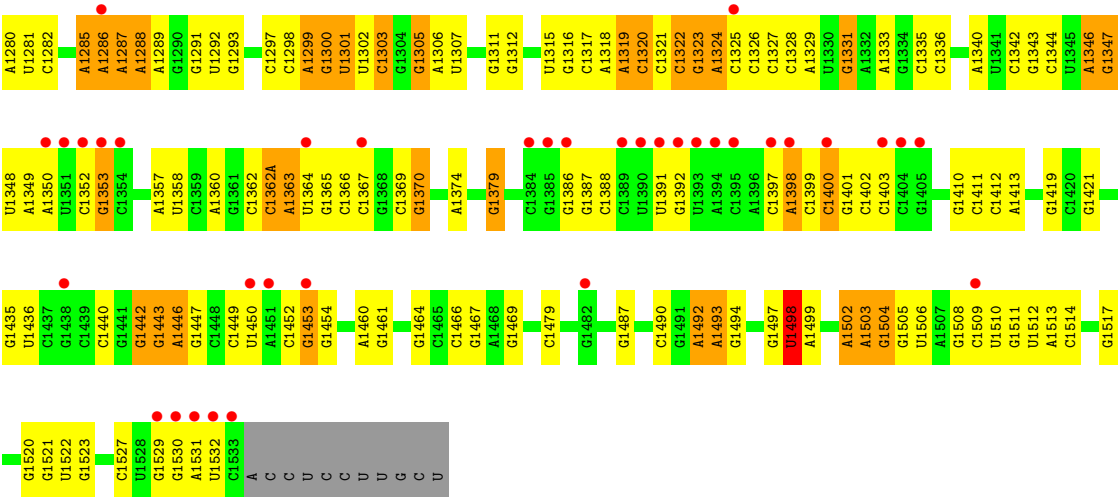
- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 16S ribosomal RNA







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 451.50Å 616.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	198.79 – 3.20 198.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (198.79-3.20) 92.9 (198.79-3.20)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.188 , 0.238 0.188 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 187.2	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	0.90	EDS
Total number of atoms	299678	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.40	0/36195	0.64	6/56491 (0.0%)
2	12	0.51	0/1959	1.01	5/2642 (0.2%)
2	1E	0.55	0/1959	1.00	8/2642 (0.3%)
3	22	0.58	0/1636	0.94	0/2205
3	2E	0.58	0/1629	0.95	2/2195 (0.1%)
4	32	0.62	0/1732	1.16	14/2318 (0.6%)
4	3E	0.69	0/1732	1.19	16/2318 (0.7%)
5	42	0.67	0/1171	1.15	5/1576 (0.3%)
5	4E	0.66	0/1171	1.05	6/1576 (0.4%)
6	52	0.67	0/855	1.04	2/1154 (0.2%)
6	5E	0.70	0/855	1.05	3/1154 (0.3%)
7	62	0.54	0/1275	0.97	3/1709 (0.2%)
7	6E	0.55	0/1275	1.01	3/1709 (0.2%)
8	72	0.61	0/1135	1.05	7/1527 (0.5%)
8	7E	0.64	0/1135	1.22	11/1527 (0.7%)
9	82	0.57	0/1017	0.96	0/1365
9	8E	0.56	0/1028	0.92	0/1379
10	1A	0.54	0/814	0.97	2/1095 (0.2%)
10	1I	0.58	0/814	1.04	8/1095 (0.7%)
11	2A	0.65	0/899	1.07	3/1213 (0.2%)
11	2I	0.69	0/879	1.07	2/1187 (0.2%)
12	3A	0.73	0/991	1.26	7/1327 (0.5%)
12	3I	0.79	1/991 (0.1%)	1.23	5/1327 (0.4%)
13	4A	0.51	0/943	0.92	3/1265 (0.2%)
13	4I	0.52	0/938	1.00	3/1258 (0.2%)
14	5A	0.58	0/500	0.95	1/664 (0.2%)
14	5I	0.63	0/500	0.96	0/664
15	6A	0.70	0/744	0.97	0/992
15	6I	0.69	0/744	1.09	1/992 (0.1%)
16	7A	0.71	0/721	1.11	6/970 (0.6%)
16	7I	0.61	0/721	1.04	4/970 (0.4%)
17	8A	0.62	0/847	1.08	4/1131 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8I	0.62	0/847	1.01	0/1131
18	9A	0.63	0/595	0.96	1/790 (0.1%)
18	9I	0.68	0/595	0.98	2/790 (0.3%)
19	AA	0.52	0/658	1.09	4/888 (0.5%)
19	AI	0.52	0/680	1.10	5/915 (0.5%)
20	BA	0.69	0/764	1.14	4/1007 (0.4%)
20	BI	0.54	0/764	1.09	4/1007 (0.4%)
21	1B	0.55	0/221	0.90	2/288 (0.7%)
21	1F	0.51	0/221	0.87	0/288
22	2K	0.42	1/1784 (0.1%)	0.66	0/2771
22	2L	0.40	0/1686	0.67	0/2618
22	3K	0.29	1/1851 (0.1%)	0.43	0/2877
22	3L	0.29	0/1851	0.46	0/2877
23	4K	0.49	0/269	0.69	0/417
23	4L	0.50	0/144	0.63	0/222
24	14	0.53	0/70192	0.75	9/109580 (0.0%)
24	1H	0.57	0/70258	0.79	21/109682 (0.0%)
25	16	0.45	0/2928	0.70	0/4568
25	1J	0.42	0/2928	0.68	0/4568
26	71	0.39	0/1072	0.80	0/1447
26	79	0.42	0/1072	0.86	6/1447 (0.4%)
27	11	1.04	3/2165 (0.1%)	1.52	35/2919 (1.2%)
27	19	0.97	4/2170 (0.2%)	1.33	17/2926 (0.6%)
28	21	0.88	0/1601	1.33	16/2160 (0.7%)
28	29	0.86	0/1601	1.38	18/2160 (0.8%)
29	31	0.92	0/1620	1.26	14/2194 (0.6%)
29	39	0.82	0/1662	1.28	17/2249 (0.8%)
30	41	0.57	0/1498	1.01	2/2016 (0.1%)
30	49	0.52	0/1498	1.01	6/2016 (0.3%)
31	51	0.81	0/1362	1.36	20/1841 (1.1%)
31	59	0.57	0/1337	1.20	18/1809 (1.0%)
32	61	0.72	0/1151	1.13	11/1558 (0.7%)
32	69	0.64	0/1151	1.06	4/1558 (0.3%)
33	15	0.70	0/1131	1.11	2/1525 (0.1%)
33	58	0.81	0/1131	1.22	7/1525 (0.5%)
34	25	0.92	0/942	1.26	9/1269 (0.7%)
34	68	0.89	0/942	1.22	4/1269 (0.3%)
35	35	0.80	0/1161	1.33	8/1544 (0.5%)
35	78	0.94	2/1161 (0.2%)	1.42	12/1544 (0.8%)
36	45	0.79	1/1142 (0.1%)	1.24	5/1527 (0.3%)
36	88	0.91	0/1142	1.35	11/1527 (0.7%)
37	55	0.90	0/973	1.27	6/1302 (0.5%)
37	98	0.82	0/981	1.13	4/1312 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	65	0.71	0/891	1.16	3/1187 (0.3%)
38	A8	0.80	0/891	1.20	2/1187 (0.2%)
39	75	0.81	0/1145	1.23	3/1531 (0.2%)
39	B8	0.83	1/1155 (0.1%)	1.26	14/1542 (0.9%)
40	85	0.80	0/981	1.12	2/1306 (0.2%)
40	C8	0.83	0/981	1.13	1/1306 (0.1%)
41	95	2.55	10/789 (1.3%)	1.54	16/1057 (1.5%)
41	D8	0.84	0/789	1.20	8/1057 (0.8%)
42	A5	0.87	0/910	1.20	5/1220 (0.4%)
42	E8	0.95	1/910 (0.1%)	1.29	3/1220 (0.2%)
43	B5	0.91	0/744	1.17	3/1000 (0.3%)
43	F8	1.03	0/752	1.36	9/1011 (0.9%)
44	C5	0.87	0/807	1.27	4/1076 (0.4%)
44	G8	0.96	0/804	1.53	21/1073 (2.0%)
45	D5	0.56	0/1460	1.07	10/1982 (0.5%)
45	H8	0.62	0/1427	1.09	12/1935 (0.6%)
46	E5	0.85	0/620	1.28	5/827 (0.6%)
46	I8	0.95	0/647	1.19	2/864 (0.2%)
47	F5	0.87	0/769	1.25	9/1022 (0.9%)
47	J8	0.89	0/769	1.25	3/1022 (0.3%)
48	G5	0.67	0/582	1.14	2/771 (0.3%)
48	K8	0.90	0/560	1.34	4/741 (0.5%)
49	H5	0.68	0/473	1.07	1/635 (0.2%)
49	L8	0.79	0/473	1.21	3/635 (0.5%)
50	I5	0.63	0/527	0.98	0/709
50	M8	0.54	0/545	0.90	0/733
51	J5	0.84	0/472	1.29	5/639 (0.8%)
51	N8	0.91	1/472 (0.2%)	1.32	5/639 (0.8%)
52	L5	0.99	1/437 (0.2%)	1.21	2/575 (0.3%)
52	P8	1.03	0/417	1.34	1/550 (0.2%)
53	M5	1.14	2/515 (0.4%)	1.30	3/679 (0.4%)
53	Q8	1.12	0/502	1.56	10/661 (1.5%)
54	1G	0.40	0/36189	0.63	4/56482 (0.0%)
All	All	0.59	29/321112 (0.0%)	0.86	619/480439 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	3E	0	1
10	1A	0	1
12	3A	0	2
14	5I	0	1
19	AI	0	2
20	BA	0	1
27	11	0	4
27	19	0	4
28	29	0	9
31	59	0	1
32	61	0	1
35	35	0	6
35	78	0	3
36	45	0	2
36	88	0	2
38	65	0	1
39	75	0	3
39	B8	0	4
40	85	0	1
41	95	0	2
44	C5	0	1
45	D5	0	1
47	F5	0	1
48	G5	0	2
48	K8	0	1
49	H5	0	1
51	J5	0	1
52	P8	0	1
53	M5	0	5
53	Q8	0	1
All	All	0	68

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	95	91	TYR	CD1-CE1	30.54	2.30	1.38
41	95	91	TYR	CD2-CE2	30.00	2.28	1.38
41	95	21	ARG	CD-NE	28.42	1.86	1.46
41	95	91	TYR	CE1-CZ	21.55	1.90	1.38
41	95	91	TYR	CE2-CZ	20.92	1.88	1.38

The worst 5 of 619 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	95	21	ARG	CD-NE-CZ	21.92	155.09	124.40
27	11	272	ALA	N-CA-C	12.50	124.32	108.19
27	19	244	ARG	CA-C-N	-12.36	107.65	120.38
27	19	244	ARG	C-N-CA	-12.36	107.65	120.38
53	Q8	34	TRP	N-CA-C	12.22	126.65	112.72

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	71	VAL	Peptide
4	3E	166	LYS	Peptide
14	5I	13	THR	Peptide
19	AI	6	LYS	Peptide
19	AI	64	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32334	0	16320	774	0
2	12	1924	0	1975	90	0
2	1E	1924	0	1975	110	0
3	22	1612	0	1677	66	0
3	2E	1605	0	1668	64	0
4	32	1702	0	1763	104	1
4	3E	1702	0	1762	63	0
5	42	1155	0	1213	60	0
5	4E	1155	0	1213	41	0
6	52	842	0	857	27	0
6	5E	842	0	857	48	1
7	62	1256	0	1296	43	0
7	6E	1256	0	1296	46	0
8	72	1115	0	1177	32	0
8	7E	1115	0	1177	46	0
9	82	998	0	1024	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	8E	1009	0	1037	51	0
10	1A	801	0	849	36	0
10	1I	801	0	849	30	0
11	2A	884	0	904	29	0
11	2I	864	0	881	35	0
12	3A	975	0	1062	37	0
12	3I	975	0	1062	40	0
13	4A	933	0	992	58	0
13	4I	928	0	987	44	0
14	5A	491	0	529	30	0
14	5I	491	0	529	33	0
15	6A	733	0	771	27	0
15	6I	733	0	771	30	0
16	7A	705	0	725	29	0
16	7I	705	0	725	48	0
17	8A	834	0	904	34	0
17	8I	834	0	904	37	0
18	9A	590	0	662	24	0
18	9I	590	0	662	28	0
19	AA	644	0	644	49	0
19	AI	665	0	686	35	0
20	BA	762	0	861	35	0
20	BI	762	0	861	50	0
21	1B	217	0	234	13	0
21	1F	217	0	234	10	0
22	2K	1765	0	916	58	0
22	2L	1678	0	872	70	0
22	3K	1825	0	946	59	0
22	3L	1825	0	946	49	0
23	4K	239	0	121	12	0
23	4L	129	0	66	3	0
24	14	62669	0	31591	1360	0
24	1H	62729	0	31622	1445	1
25	16	2617	0	1328	60	0
25	1J	2617	0	1328	89	0
26	71	1049	0	1071	32	0
26	79	1049	0	1071	33	0
27	11	2115	0	2195	105	0
27	19	2120	0	2197	104	0
28	21	1568	0	1634	92	0
28	29	1568	0	1634	91	0
29	31	1585	0	1632	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	39	1627	0	1680	94	0
30	41	1473	0	1535	79	0
30	49	1473	0	1535	74	0
31	51	1336	0	1418	73	0
31	59	1312	0	1384	58	0
32	61	1136	0	1223	45	0
32	69	1136	0	1223	68	0
33	15	1104	0	1180	37	0
33	58	1104	0	1180	54	0
34	25	932	0	996	50	0
34	68	932	0	996	34	0
35	35	1144	0	1228	79	0
35	78	1144	0	1228	89	0
36	45	1121	0	1179	63	0
36	88	1121	0	1179	63	0
37	55	959	0	1021	46	0
37	98	967	0	1033	61	0
38	65	881	0	943	62	0
38	A8	881	0	943	35	0
39	75	1131	0	1180	72	0
39	B8	1141	0	1202	77	0
40	85	963	0	1022	50	0
40	C8	963	0	1022	36	0
41	95	778	0	852	86	0
41	D8	778	0	852	30	0
42	A5	899	0	964	34	0
42	E8	899	0	964	31	0
43	B5	730	0	780	24	0
43	F8	738	0	791	41	0
44	C5	794	0	884	72	0
44	G8	791	0	881	46	0
45	D5	1428	0	1454	99	0
45	H8	1397	0	1430	59	0
46	E5	612	0	633	38	0
46	I8	639	0	644	43	0
47	F5	762	0	848	27	0
47	J8	762	0	848	44	0
48	G5	580	0	629	30	1
48	K8	558	0	610	31	0
49	H5	468	0	518	27	0
49	L8	468	0	518	20	0
50	I5	515	0	514	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	M8	533	0	526	29	0
51	J5	458	0	480	23	0
51	N8	458	0	480	33	0
52	L5	429	0	480	32	0
52	P8	409	0	454	21	0
53	M5	507	0	576	37	0
53	Q8	495	0	567	50	0
54	1G	32329	0	16319	734	0
55	11	2	0	0	0	0
55	13	129	0	0	0	0
55	14	489	0	0	0	0
55	15	1	0	0	0	0
55	16	12	0	0	0	0
55	19	1	0	0	0	0
55	1G	147	0	0	0	0
55	1H	548	0	0	0	0
55	1J	11	0	0	0	0
55	21	1	0	0	0	0
55	25	1	0	0	0	0
55	29	5	0	0	0	0
55	2K	4	0	0	0	0
55	2L	3	0	0	0	0
55	32	1	0	0	0	0
55	39	1	0	0	0	0
55	3I	1	0	0	0	0
55	3L	2	0	0	0	0
55	42	1	0	0	0	0
55	45	1	0	0	0	0
55	49	1	0	0	0	0
55	55	3	0	0	0	0
55	5E	2	0	0	0	0
55	78	2	0	0	0	0
55	88	2	0	0	0	0
55	C5	1	0	0	0	0
55	E5	2	0	0	0	0
55	F5	1	0	0	0	0
55	I8	3	0	0	0	0
55	J8	1	0	0	0	0
55	M5	1	0	0	0	0
55	Q8	1	0	0	0	0
56	32	1	0	0	0	0
56	3E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	5A	1	0	0	0	0
56	5I	1	0	0	0	0
56	C5	1	0	0	0	0
56	G8	1	0	0	0	0
57	13	188	0	0	32	0
57	14	821	0	0	195	0
57	16	12	0	0	2	0
57	1G	156	0	0	26	0
57	1H	1038	0	0	253	0
57	1J	24	0	0	3	0
57	25	6	0	0	0	0
57	2K	6	0	0	0	0
57	2L	6	0	0	0	0
57	E5	6	0	0	0	0
57	J8	6	0	0	0	0
All	All	299678	0	200771	8367	2

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 8367 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)
41:95:91:TYR:CD2	41:95:91:TYR:CG	1.79	1.66
41:95:91:TYR:CG	41:95:91:TYR:CD1	1.80	1.63
41:95:91:TYR:CE1	41:95:91:TYR:CZ	1.90	1.59
41:95:91:TYR:CZ	41:95:91:TYR:CE2	1.88	1.58
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.71	1.53

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD1	4:32:27:TYR:OH[4_555]	2.13	0.07
24:1H:277:C:O2'	48:G5:49:LYS:NZ[2_564]	2.14	0.06

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	235/256 (92%)	201 (86%)	32 (14%)	2 (1%)	14	47
2	1E	235/256 (92%)	198 (84%)	32 (14%)	5 (2%)	5	31
3	22	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	24	59
4	3E	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12	45
5	42	149/162 (92%)	144 (97%)	5 (3%)	0	100	100
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	18	52
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	72	136/138 (99%)	129 (95%)	5 (4%)	2 (2%)	8	37
8	7E	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	82	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
9	8E	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	1A	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	1I	97/105 (92%)	83 (86%)	14 (14%)	0	100	100
11	2A	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	2I	114/129 (88%)	104 (91%)	9 (8%)	1 (1%)	14	47
12	3A	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	7	36
12	3I	123/132 (93%)	114 (93%)	9 (7%)	0	100	100
13	4A	115/126 (91%)	100 (87%)	11 (10%)	4 (4%)	3	20
13	4I	114/126 (90%)	100 (88%)	14 (12%)	0	100	100
14	5A	58/61 (95%)	50 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	6A	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	8A	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	70/88 (80%)	66 (94%)	4 (6%)	0	100	100
18	9I	70/88 (80%)	66 (94%)	3 (4%)	1 (1%)	9	39
19	AA	80/93 (86%)	59 (74%)	18 (22%)	3 (4%)	2	18
19	AI	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	10	42
20	BA	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	BI	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	1B	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	7I	131/229 (57%)	130 (99%)	1 (1%)	0	100	100
26	79	131/229 (57%)	129 (98%)	2 (2%)	0	100	100
27	11	270/276 (98%)	246 (91%)	19 (7%)	5 (2%)	6	33
27	19	271/276 (98%)	252 (93%)	16 (6%)	3 (1%)	11	43
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	24	59
28	29	203/206 (98%)	158 (78%)	38 (19%)	7 (3%)	3	20
29	31	200/210 (95%)	187 (94%)	13 (6%)	0	100	100
29	39	206/210 (98%)	176 (85%)	25 (12%)	5 (2%)	4	28
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	21	56
30	49	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	21	56
31	51	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	35
31	59	169/180 (94%)	133 (79%)	34 (20%)	2 (1%)	10	42
32	61	144/148 (97%)	123 (85%)	18 (12%)	3 (2%)	5	31
32	69	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9	39
33	15	136/140 (97%)	126 (93%)	9 (7%)	1 (1%)	18	52
33	58	136/140 (97%)	115 (85%)	15 (11%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	35	148/150 (99%)	119 (80%)	24 (16%)	5 (3%)	3	20
35	78	148/150 (99%)	114 (77%)	30 (20%)	4 (3%)	4	25
36	45	139/141 (99%)	113 (81%)	23 (16%)	3 (2%)	5	29
36	88	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	3	24
37	55	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	14	47
37	98	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
38	65	109/112 (97%)	95 (87%)	12 (11%)	2 (2%)	6	34
38	A8	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	14	47
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	5	29
39	B8	135/146 (92%)	115 (85%)	20 (15%)	0	100	100
40	85	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
40	C8	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
41	95	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	3	23
41	D8	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
42	A5	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	E8	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
43	B5	91/96 (95%)	86 (94%)	4 (4%)	1 (1%)	11	43
43	F8	92/96 (96%)	85 (92%)	6 (6%)	1 (1%)	11	43
44	C5	102/110 (93%)	70 (69%)	29 (28%)	3 (3%)	3	24
44	G8	102/110 (93%)	80 (78%)	19 (19%)	3 (3%)	3	24
45	D5	177/206 (86%)	141 (80%)	31 (18%)	5 (3%)	4	25
45	H8	173/206 (84%)	141 (82%)	25 (14%)	7 (4%)	2	17
46	E5	75/85 (88%)	69 (92%)	5 (7%)	1 (1%)	9	40
46	I8	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	10	42
47	F5	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	11	43
47	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	5	31
48	G5	67/72 (93%)	57 (85%)	10 (15%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	1 (2%)	2 (3%)	3	22
49	H5	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	I5	61/71 (86%)	35 (57%)	22 (36%)	4 (7%)	1	7
50	M8	64/71 (90%)	44 (69%)	19 (30%)	1 (2%)	7	36
51	J5	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	3	20
51	N8	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	6	34
52	L5	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
52	P8	45/49 (92%)	41 (91%)	2 (4%)	2 (4%)	2	15
53	M5	61/65 (94%)	54 (88%)	4 (7%)	3 (5%)	1	13
53	Q8	60/65 (92%)	49 (82%)	7 (12%)	4 (7%)	1	7
All	All	11538/12404 (93%)	10164 (88%)	1238 (11%)	136 (1%)	10	42

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
27	11	122	ASP
33	58	22	THR
33	58	95	PRO
33	58	96	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	205/220 (93%)	166 (81%)	39 (19%)	1	9
2	1E	205/220 (93%)	163 (80%)	42 (20%)	1	7
3	22	160/188 (85%)	131 (82%)	29 (18%)	2	9
3	2E	159/188 (85%)	134 (84%)	25 (16%)	2	13
4	32	180/181 (99%)	148 (82%)	32 (18%)	2	10
4	3E	180/181 (99%)	152 (84%)	28 (16%)	2	13
5	42	116/123 (94%)	93 (80%)	23 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4E	116/123 (94%)	88 (76%)	28 (24%)	1	4
6	52	90/90 (100%)	78 (87%)	12 (13%)	4	19
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6	25
7	62	126/127 (99%)	107 (85%)	19 (15%)	3	14
7	6E	126/127 (99%)	104 (82%)	22 (18%)	2	10
8	72	119/119 (100%)	103 (87%)	16 (13%)	4	19
8	7E	119/119 (100%)	107 (90%)	12 (10%)	7	30
9	82	97/99 (98%)	82 (84%)	15 (16%)	2	14
9	8E	98/99 (99%)	84 (86%)	14 (14%)	3	16
10	1A	89/92 (97%)	74 (83%)	15 (17%)	2	11
10	1I	89/92 (97%)	77 (86%)	12 (14%)	4	19
11	2A	90/99 (91%)	77 (86%)	13 (14%)	3	16
11	2I	88/99 (89%)	74 (84%)	14 (16%)	2	13
12	3A	104/109 (95%)	88 (85%)	16 (15%)	2	14
12	3I	104/109 (95%)	91 (88%)	13 (12%)	4	21
13	4A	94/101 (93%)	80 (85%)	14 (15%)	3	15
13	4I	94/101 (93%)	84 (89%)	10 (11%)	6	27
14	5A	49/50 (98%)	44 (90%)	5 (10%)	7	29
14	5I	49/50 (98%)	42 (86%)	7 (14%)	3	16
15	6A	79/80 (99%)	72 (91%)	7 (9%)	9	34
15	6I	79/80 (99%)	72 (91%)	7 (9%)	9	34
16	7A	72/74 (97%)	61 (85%)	11 (15%)	3	14
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	8
17	8A	95/97 (98%)	80 (84%)	15 (16%)	2	13
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	9
18	9A	63/77 (82%)	55 (87%)	8 (13%)	4	20
18	9I	63/77 (82%)	55 (87%)	8 (13%)	4	20
19	AA	67/80 (84%)	61 (91%)	6 (9%)	9	34
19	AI	72/80 (90%)	61 (85%)	11 (15%)	3	14
20	BA	76/82 (93%)	68 (90%)	8 (10%)	6	28
20	BI	76/82 (93%)	62 (82%)	14 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1B	20/22 (91%)	19 (95%)	1 (5%)	22	55
21	1F	20/22 (91%)	19 (95%)	1 (5%)	22	55
26	71	111/181 (61%)	104 (94%)	7 (6%)	16	48
26	79	111/181 (61%)	108 (97%)	3 (3%)	39	68
27	11	214/218 (98%)	169 (79%)	45 (21%)	1	6
27	19	214/218 (98%)	172 (80%)	42 (20%)	1	8
28	21	165/166 (99%)	136 (82%)	29 (18%)	2	10
28	29	165/166 (99%)	137 (83%)	28 (17%)	2	11
29	31	161/166 (97%)	129 (80%)	32 (20%)	1	7
29	39	165/166 (99%)	125 (76%)	40 (24%)	1	4
30	41	155/156 (99%)	134 (86%)	21 (14%)	4	19
30	49	155/156 (99%)	135 (87%)	20 (13%)	4	20
31	51	145/148 (98%)	111 (77%)	34 (23%)	1	4
31	59	142/148 (96%)	112 (79%)	30 (21%)	1	6
32	61	122/124 (98%)	99 (81%)	23 (19%)	1	9
32	69	122/124 (98%)	91 (75%)	31 (25%)	0	3
33	15	117/119 (98%)	93 (80%)	24 (20%)	1	7
33	58	117/119 (98%)	95 (81%)	22 (19%)	1	9
34	25	100/100 (100%)	72 (72%)	28 (28%)	0	2
34	68	100/100 (100%)	87 (87%)	13 (13%)	4	20
35	35	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	78	116/116 (100%)	79 (68%)	37 (32%)	0	1
36	45	111/111 (100%)	89 (80%)	22 (20%)	1	8
36	88	111/111 (100%)	94 (85%)	17 (15%)	3	14
37	55	100/101 (99%)	79 (79%)	21 (21%)	1	6
37	98	101/101 (100%)	81 (80%)	20 (20%)	1	8
38	65	87/88 (99%)	66 (76%)	21 (24%)	1	4
38	A8	87/88 (99%)	63 (72%)	24 (28%)	0	2
39	75	117/127 (92%)	87 (74%)	30 (26%)	0	3
39	B8	120/127 (94%)	92 (77%)	28 (23%)	1	5
40	85	93/94 (99%)	77 (83%)	16 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	C8	93/94 (99%)	76 (82%)	17 (18%)	2	9
41	95	82/82 (100%)	59 (72%)	23 (28%)	0	2
41	D8	82/82 (100%)	56 (68%)	26 (32%)	0	1
42	A5	92/92 (100%)	76 (83%)	16 (17%)	2	10
42	E8	92/92 (100%)	70 (76%)	22 (24%)	1	4
43	B5	74/78 (95%)	62 (84%)	12 (16%)	2	12
43	F8	75/78 (96%)	56 (75%)	19 (25%)	0	3
44	C5	85/91 (93%)	59 (69%)	26 (31%)	0	1
44	G8	85/91 (93%)	58 (68%)	27 (32%)	0	1
45	D5	158/179 (88%)	128 (81%)	30 (19%)	1	9
45	H8	154/179 (86%)	118 (77%)	36 (23%)	1	4
46	E5	62/67 (92%)	48 (77%)	14 (23%)	1	5
46	I8	61/67 (91%)	50 (82%)	11 (18%)	2	9
47	F5	82/83 (99%)	62 (76%)	20 (24%)	1	4
47	J8	82/83 (99%)	62 (76%)	20 (24%)	1	4
48	G5	64/67 (96%)	51 (80%)	13 (20%)	1	7
48	K8	62/67 (92%)	47 (76%)	15 (24%)	1	4
49	H5	51/52 (98%)	39 (76%)	12 (24%)	1	4
49	L8	51/52 (98%)	33 (65%)	18 (35%)	0	0
50	I5	57/63 (90%)	44 (77%)	13 (23%)	1	5
50	M8	59/63 (94%)	52 (88%)	7 (12%)	5	23
51	J5	51/52 (98%)	41 (80%)	10 (20%)	1	8
51	N8	51/52 (98%)	40 (78%)	11 (22%)	1	6
52	L5	42/42 (100%)	32 (76%)	10 (24%)	1	4
52	P8	40/42 (95%)	34 (85%)	6 (15%)	3	15
53	M5	53/55 (96%)	41 (77%)	12 (23%)	1	5
53	Q8	52/55 (94%)	36 (69%)	16 (31%)	0	1
All	All	9717/10256 (95%)	7901 (81%)	1816 (19%)	1	9

5 of 1816 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	12	90	MET

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Mol	Chain	Res	Type
50	I5	10	VAL
13	4A	47	ASP
48	G5	35	LEU
40	85	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
26	79	57	ASN
37	55	61	HIS
26	79	165	ASN
28	29	135	HIS
48	G5	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	329 (21%)	24 (1%)
22	2K	80/85 (94%)	29 (36%)	5 (6%)
22	2L	75/85 (88%)	25 (33%)	7 (9%)
22	3K	84/85 (98%)	24 (28%)	3 (3%)
22	3L	84/85 (98%)	23 (27%)	3 (3%)
23	4K	11/27 (40%)	3 (27%)	1 (9%)
23	4L	5/27 (18%)	2 (40%)	0
24	14	2907/2917 (99%)	659 (22%)	38 (1%)
24	1H	2910/2917 (99%)	680 (23%)	45 (1%)
25	16	121/122 (99%)	26 (21%)	0
25	1J	121/122 (99%)	29 (23%)	1 (0%)
54	1G	1503/1522 (98%)	323 (21%)	33 (2%)
All	All	9397/9516 (98%)	2152 (22%)	160 (1%)

5 of 2152 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	6	G
1	13	10	A
1	13	22	G
1	13	25	C
1	13	32	A

5 of 160 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	2L	60	A
24	14	1558	A
22	3L	18	G
24	14	669	G
24	14	2406	U

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

28 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
22	MIA	3K	38	22	28,31,32	2.59	3 (10%)	38,44,47	3.11	15 (39%)
22	QUO	2L	35	22,23	32,35,36	4.79	12 (37%)	36,52,55	4.76	13 (36%)
22	QUO	2K	35	22,23	32,35,36	4.82	11 (34%)	36,52,55	4.55	11 (30%)
22	5MU	2L	63	22	19,22,23	3.98	5 (26%)	27,32,35	3.48	9 (33%)
22	MIA	3L	38	22	28,31,32	2.43	4 (14%)	38,44,47	3.58	14 (36%)
22	MIA	2L	38	22	28,31,32	2.43	4 (14%)	38,44,47	3.42	14 (36%)
22	4SU	3L	8	22,55	18,21,22	2.02	5 (27%)	25,30,33	2.10	5 (20%)
22	MIA	2K	38	22	28,31,32	2.48	4 (14%)	38,44,47	4.01	14 (36%)
22	4SU	2L	8	22	18,21,22	1.94	4 (22%)	25,30,33	2.28	5 (20%)
22	OMG	3L	17	22	23,26,27	5.20	11 (47%)	32,38,41	4.74	19 (59%)
22	5MU	2K	63	22	19,22,23	3.91	5 (26%)	27,32,35	3.51	9 (33%)
22	5MU	3L	63	22	19,22,23	3.95	5 (26%)	27,32,35	3.06	8 (29%)
22	OMG	2K	17	22	23,26,27	5.12	11 (47%)	32,38,41	4.72	19 (59%)
22	QUO	3K	35	22	32,35,36	4.78	12 (37%)	36,52,55	4.59	12 (33%)
22	PSU	2K	40	22	18,21,22	2.28	5 (27%)	21,30,33	1.66	4 (19%)
22	PSU	3L	40	22	18,21,22	2.52	5 (27%)	21,30,33	1.95	4 (19%)
22	4SU	3K	8	22	18,21,22	1.87	3 (16%)	25,30,33	2.90	6 (24%)
22	OMG	3K	17	22	23,26,27	5.02	11 (47%)	32,38,41	4.61	17 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	2L	40	22	18,21,22	2.42	5 (27%)	21,30,33	1.71	3 (14%)
22	5MU	3K	63	22	19,22,23	3.90	5 (26%)	27,32,35	3.08	8 (29%)
22	PSU	2K	64	22	18,21,22	2.65	5 (27%)	21,30,33	1.85	5 (23%)
22	PSU	3K	40	22	18,21,22	2.45	5 (27%)	21,30,33	1.56	2 (9%)
22	PSU	2L	64	22	18,21,22	2.71	6 (33%)	21,30,33	1.79	5 (23%)
22	4SU	2K	8	22	18,21,22	1.96	3 (16%)	25,30,33	2.61	6 (24%)
22	PSU	3L	64	22	18,21,22	2.66	6 (33%)	21,30,33	1.78	4 (19%)
22	OMG	2L	17	22	23,26,27	5.06	11 (47%)	32,38,41	4.72	18 (56%)
22	PSU	3K	64	22	18,21,22	2.54	5 (27%)	21,30,33	1.86	3 (14%)
22	QUO	3L	35	22	32,35,36	4.87	13 (40%)	36,52,55	4.62	11 (30%)

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
22	MIA	3K	38	22	-	8/15/33/34	0/3/3/3
22	QUO	2L	35	22,23	-	0/12/43/44	0/4/4/4
22	QUO	2K	35	22,23	-	4/12/43/44	0/4/4/4
22	5MU	2L	63	22	-	0/7/25/26	0/2/2/2
22	MIA	3L	38	22	-	1/15/33/34	0/3/3/3
22	MIA	2L	38	22	-	7/15/33/34	0/3/3/3
22	4SU	3L	8	22,55	-	0/7/25/26	0/2/2/2
22	MIA	2K	38	22	-	7/15/33/34	0/3/3/3
22	4SU	2L	8	22	-	2/7/25/26	0/2/2/2
22	OMG	3L	17	22	-	0/9/27/28	0/3/3/3
22	5MU	2K	63	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/7/25/26	0/2/2/2
22	OMG	2K	17	22	-	3/9/27/28	0/3/3/3
22	QUO	3K	35	22	-	1/12/43/44	0/4/4/4
22	PSU	2K	40	22	-	0/7/25/26	0/2/2/2
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	3/7/25/26	0/2/2/2
22	OMG	3K	17	22	-	4/9/27/28	0/3/3/3
22	PSU	2L	40	22	-	1/7/25/26	0/2/2/2
22	5MU	3K	63	22	-	0/7/25/26	0/2/2/2
22	PSU	2K	64	22	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	PSU	2L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	2K	8	22	-	0/7/25/26	0/2/2/2
22	PSU	3L	64	22	-	3/7/25/26	0/2/2/2
22	OMG	2L	17	22	-	4/9/27/28	0/3/3/3
22	PSU	3K	64	22	-	4/7/25/26	0/2/2/2
22	QUO	3L	35	22	-	5/12/43/44	0/4/4/4

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2L	35	QUO	C4-N3	16.68	1.72	1.34
22	3L	35	QUO	C4-N3	16.42	1.71	1.34
22	3K	35	QUO	C4-N3	16.35	1.71	1.34
22	2K	35	QUO	C4-N3	15.83	1.70	1.34
22	2L	63	5MU	C2-N1	13.36	1.59	1.38

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3K	35	QUO	C5-C4-N3	-18.19	106.65	127.53
22	3L	35	QUO	C5-C4-N3	-18.13	106.71	127.53
22	2L	35	QUO	C5-C4-N3	-17.88	107.00	127.53
22	2K	38	MIA	C11-S10-C2	17.57	115.43	102.25
22	2K	35	QUO	C5-C4-N3	-17.40	107.55	127.53

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2K	35	QUO	O4'-C4'-C5'-O5'
22	2K	35	QUO	N11-C10-C7-C5
22	2K	38	MIA	N1-C2-S10-C11
22	2K	38	MIA	N3-C2-S10-C11
22	2K	38	MIA	N6-C12-C13-C14

There are no ring outliers.

25 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3K	38	MIA	3	0
22	2L	35	QUO	6	0
22	2K	35	QUO	4	0
22	2L	63	5MU	3	0
22	3L	38	MIA	1	0
22	2L	38	MIA	2	0
22	3L	8	4SU	2	0
22	2K	38	MIA	4	0
22	2L	8	4SU	2	0
22	3L	17	OMG	1	0
22	3L	63	5MU	1	0
22	2K	17	OMG	3	0
22	3K	35	QUO	5	0
22	2K	40	PSU	1	0
22	3L	40	PSU	1	0
22	3K	8	4SU	2	0
22	3K	17	OMG	2	0
22	2L	40	PSU	2	0
22	3K	63	5MU	2	0
22	2K	64	PSU	2	0
22	2L	64	PSU	2	0
22	3L	64	PSU	1	0
22	2L	17	OMG	3	0
22	3K	64	PSU	3	0
22	3L	35	QUO	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1387 ligands modelled in this entry, 1387 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1501/1522 (98%)	0.68	195 (12%) 7 6	63, 129, 208, 407	3 (0%)
2	12	237/256 (92%)	1.11	40 (16%) 4 3	137, 175, 213, 240	0
2	1E	237/256 (92%)	0.79	28 (11%) 9 6	131, 168, 201, 234	0
3	22	206/239 (86%)	1.36	46 (22%) 2 2	135, 156, 189, 209	0
3	2E	205/239 (85%)	0.77	26 (12%) 8 6	122, 142, 197, 207	0
4	32	208/209 (99%)	0.82	27 (12%) 7 6	108, 130, 156, 169	0
4	3E	208/209 (99%)	0.92	36 (17%) 4 3	104, 129, 155, 182	0
5	42	151/162 (93%)	1.21	29 (19%) 3 2	107, 128, 153, 194	0
5	4E	151/162 (93%)	0.84	22 (14%) 6 4	102, 125, 153, 204	0
6	52	101/101 (100%)	0.09	5 (4%) 34 22	101, 120, 138, 153	0
6	5E	101/101 (100%)	0.82	14 (13%) 6 5	105, 129, 146, 163	0
7	62	155/156 (99%)	1.08	27 (17%) 4 3	128, 144, 162, 171	0
7	6E	155/156 (99%)	1.20	30 (19%) 3 2	123, 149, 172, 184	0
8	72	138/138 (100%)	0.86	27 (19%) 3 2	111, 132, 143, 170	0
8	7E	138/138 (100%)	0.38	12 (8%) 16 11	115, 134, 145, 157	0
9	82	126/128 (98%)	1.24	25 (19%) 3 2	124, 170, 197, 213	0
9	8E	127/128 (99%)	0.90	22 (17%) 4 3	119, 163, 179, 191	0
10	1A	99/105 (94%)	1.21	22 (22%) 2 2	135, 170, 191, 206	0
10	1I	99/105 (94%)	1.49	28 (28%) 1 1	121, 166, 195, 209	0
11	2A	119/129 (92%)	1.26	17 (14%) 6 5	105, 125, 157, 256	0
11	2I	116/129 (89%)	1.06	18 (15%) 5 4	93, 126, 153, 203	0
12	3A	125/132 (94%)	0.98	18 (14%) 6 5	96, 114, 144, 188	0
12	3I	125/132 (94%)	1.09	24 (19%) 3 2	91, 104, 136, 239	0
13	4A	117/126 (92%)	0.75	16 (13%) 6 5	138, 174, 197, 229	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4I	116/126 (92%)	1.41	30 (25%) 1 2	127, 173, 195, 208	0
14	5A	60/61 (98%)	1.49	15 (25%) 2 2	145, 163, 185, 186	0
14	5I	60/61 (98%)	1.13	11 (18%) 3 3	127, 137, 167, 186	0
15	6A	88/89 (98%)	0.43	8 (9%) 15 9	100, 128, 146, 152	0
15	6I	88/89 (98%)	0.61	9 (10%) 12 8	103, 127, 147, 154	0
16	7A	84/88 (95%)	0.99	15 (17%) 3 3	108, 121, 141, 189	0
16	7I	84/88 (95%)	2.28	35 (41%) 0 1	119, 136, 162, 196	0
17	8A	100/105 (95%)	0.39	6 (6%) 27 17	104, 121, 140, 197	0
17	8I	100/105 (95%)	0.77	11 (11%) 10 7	112, 132, 146, 150	0
18	9A	72/88 (81%)	0.27	5 (6%) 23 14	107, 127, 185, 223	0
18	9I	72/88 (81%)	0.54	6 (8%) 17 11	111, 130, 164, 208	0
19	AA	82/93 (88%)	0.98	10 (12%) 8 6	152, 196, 219, 232	0
19	AI	83/93 (89%)	0.87	14 (16%) 4 3	150, 176, 207, 222	0
20	BA	99/106 (93%)	0.97	18 (18%) 3 3	96, 125, 161, 175	0
20	BI	99/106 (93%)	1.78	35 (35%) 1 1	127, 147, 191, 205	0
21	1B	25/27 (92%)	1.56	8 (32%) 1 1	135, 158, 186, 196	0
21	1F	25/27 (92%)	1.71	10 (40%) 1 1	139, 156, 182, 190	0
22	2K	75/85 (88%)	1.27	18 (24%) 2 2	95, 145, 276, 308	0
22	2L	71/85 (83%)	0.76	9 (12%) 8 6	95, 146, 228, 250	0
22	3K	78/85 (91%)	1.72	26 (33%) 1 1	95, 199, 288, 312	0
22	3L	78/85 (91%)	1.64	23 (29%) 1 1	93, 213, 284, 309	0
23	4K	11/27 (40%)	0.40	0 100 100	105, 139, 160, 164	0
23	4L	6/27 (22%)	0.26	0 100 100	116, 126, 146, 163	0
24	14	2909/2917 (99%)	0.35	291 (10%) 12 8	48, 99, 266, 424	1 (0%)
24	1H	2912/2917 (99%)	0.23	214 (7%) 21 13	49, 92, 251, 431	1 (0%)
25	16	122/122 (100%)	0.19	5 (4%) 41 25	96, 125, 153, 258	0
25	1J	122/122 (100%)	0.86	18 (14%) 5 4	102, 138, 160, 226	0
26	71	135/229 (58%)	1.29	26 (19%) 3 2	152, 213, 248, 256	0
26	79	135/229 (58%)	1.24	20 (14%) 5 4	159, 237, 261, 265	0
27	11	272/276 (98%)	0.40	24 (8%) 15 10	60, 82, 103, 122	0
27	19	273/276 (98%)	0.19	9 (3%) 49 30	64, 87, 104, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	21	205/206 (99%)	0.80	26 (12%) 8 6	68, 105, 159, 229	0
28	29	205/206 (99%)	1.31	48 (23%) 2 2	71, 102, 169, 251	0
29	31	202/210 (96%)	0.26	8 (3%) 42 26	61, 94, 137, 152	0
29	39	208/210 (99%)	0.61	25 (12%) 9 6	71, 113, 184, 198	0
30	41	181/182 (99%)	1.27	46 (25%) 1 2	127, 159, 197, 218	0
30	49	181/182 (99%)	1.46	47 (25%) 1 2	142, 165, 197, 213	0
31	51	174/180 (96%)	0.83	20 (11%) 9 7	98, 122, 145, 174	0
31	59	171/180 (95%)	1.37	40 (23%) 2 2	148, 205, 246, 335	0
32	61	146/148 (98%)	0.62	16 (10%) 10 7	99, 136, 162, 176	0
32	69	146/148 (98%)	1.08	29 (19%) 3 2	100, 143, 171, 191	0
33	15	138/140 (98%)	1.24	29 (21%) 2 2	86, 115, 153, 196	0
33	58	138/140 (98%)	0.87	15 (10%) 10 7	86, 108, 153, 174	0
34	25	122/122 (100%)	0.29	9 (7%) 20 13	77, 98, 113, 122	0
34	68	122/122 (100%)	0.25	5 (4%) 41 25	73, 96, 115, 134	0
35	35	150/150 (100%)	0.86	25 (16%) 4 3	74, 119, 159, 213	0
35	78	150/150 (100%)	1.18	36 (24%) 2 2	65, 101, 126, 244	0
36	45	141/141 (100%)	0.85	17 (12%) 8 6	88, 117, 144, 179	0
36	88	141/141 (100%)	0.90	23 (16%) 4 3	78, 107, 139, 170	0
37	55	117/118 (99%)	1.30	26 (22%) 2 2	74, 94, 109, 130	0
37	98	118/118 (100%)	1.03	23 (19%) 3 2	79, 100, 119, 136	0
38	65	111/112 (99%)	1.49	31 (27%) 1 1	109, 130, 159, 180	0
38	A8	111/112 (99%)	1.66	28 (25%) 1 2	102, 123, 157, 203	0
39	75	137/146 (93%)	0.59	12 (8%) 15 10	88, 105, 157, 218	0
39	B8	137/146 (93%)	0.54	12 (8%) 15 10	92, 113, 171, 204	0
40	85	117/118 (99%)	0.97	18 (15%) 5 4	77, 109, 146, 183	0
40	C8	117/118 (99%)	0.61	14 (11%) 9 6	66, 97, 138, 182	0
41	95	101/101 (100%)	1.33	22 (21%) 2 2	80, 136, 158, 200	0
41	D8	101/101 (100%)	1.03	17 (16%) 4 3	71, 118, 159, 234	0
42	A5	113/113 (100%)	0.16	3 (2%) 56 36	74, 89, 125, 209	0
42	E8	113/113 (100%)	0.90	18 (15%) 5 3	74, 89, 121, 226	0
43	B5	93/96 (96%)	0.74	11 (11%) 9 6	86, 97, 119, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	F8	94/96 (97%)	0.51	10 (10%) 11 8	68, 87, 111, 124	0
44	C5	104/110 (94%)	1.32	29 (27%) 1 1	102, 136, 209, 232	0
44	G8	104/110 (94%)	1.03	23 (22%) 2 2	85, 108, 158, 205	0
45	D5	179/206 (86%)	1.44	47 (26%) 1 2	121, 163, 275, 332	0
45	H8	175/206 (84%)	1.04	30 (17%) 4 3	111, 157, 273, 304	0
46	E5	77/85 (90%)	1.84	30 (38%) 1 1	86, 102, 123, 174	0
46	I8	83/85 (97%)	1.44	25 (30%) 1 1	83, 99, 122, 165	0
47	F5	97/98 (98%)	0.98	20 (20%) 2 2	76, 96, 155, 197	0
47	J8	97/98 (98%)	0.71	10 (10%) 12 8	70, 93, 171, 227	0
48	G5	69/72 (95%)	0.55	6 (8%) 16 11	99, 124, 152, 184	0
48	K8	66/72 (91%)	0.81	8 (12%) 8 6	74, 95, 120, 165	0
49	H5	59/60 (98%)	1.07	15 (25%) 1 2	90, 112, 169, 182	0
49	L8	59/60 (98%)	0.84	10 (16%) 4 3	87, 103, 149, 177	0
50	I5	63/71 (88%)	1.15	11 (17%) 4 3	165, 225, 254, 292	0
50	M8	66/71 (92%)	0.68	6 (9%) 15 9	156, 231, 273, 282	0
51	J5	59/60 (98%)	0.54	6 (10%) 12 8	71, 96, 206, 229	0
51	N8	59/60 (98%)	1.88	19 (32%) 1 1	64, 101, 224, 243	0
52	L5	49/49 (100%)	0.34	3 (6%) 27 17	69, 74, 108, 147	0
52	P8	47/49 (95%)	0.18	4 (8%) 16 11	60, 66, 88, 140	0
53	M5	63/65 (96%)	0.74	11 (17%) 4 3	82, 96, 122, 134	0
53	Q8	62/65 (95%)	0.46	5 (8%) 18 11	77, 92, 120, 133	0
54	1G	1504/1522 (98%)	0.74	227 (15%) 5 4	83, 130, 201, 419	0
All	All	21123/21920 (96%)	0.73	2937 (13%) 6 5	48, 120, 217, 431	5 (0%)

The worst 5 of 2937 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2A	128	ALA	32.6
30	49	75	LYS	17.5
11	2A	127	LYS	15.1
7	62	81	GLY	14.9
11	2A	125	PHE	14.1

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
22	OMG	2K	17	24/25	0.52	0.18	150,155,165,169	0
22	5MU	3K	63	21/22	0.65	0.13	168,182,188,191	0
22	4SU	3L	8	20/21	0.66	0.19	193,208,220,222	0
22	PSU	2K	64	20/21	0.69	0.13	139,143,148,152	0
22	OMG	3K	17	24/25	0.69	0.20	201,213,227,235	0
22	PSU	3K	64	20/21	0.70	0.12	175,186,200,205	0
22	4SU	3K	8	20/21	0.71	0.15	182,197,218,229	0
22	PSU	2L	64	20/21	0.72	0.15	147,156,162,165	0
22	OMG	2L	17	24/25	0.72	0.15	161,167,175,176	0
22	5MU	2L	63	21/22	0.77	0.18	144,157,165,169	0
22	5MU	3L	63	21/22	0.78	0.17	164,182,191,194	0
22	4SU	2L	8	20/21	0.79	0.14	142,153,161,169	0
22	4SU	2K	8	20/21	0.79	0.16	139,144,148,151	0
22	PSU	3L	64	20/21	0.79	0.18	167,198,215,220	0
22	MIA	3K	38	29/30	0.80	0.41	128,138,144,146	0
22	MIA	3L	38	29/30	0.83	0.35	131,140,149,159	0
22	OMG	3L	17	24/25	0.84	0.31	201,218,239,245	0
22	5MU	2K	63	21/22	0.85	0.10	136,142,148,150	0
22	PSU	3L	40	20/21	0.85	0.18	132,140,144,144	0
22	QUO	2L	35	32/33	0.86	0.38	111,120,135,136	8
22	QUO	3L	35	32/33	0.87	0.32	131,137,152,158	0
22	QUO	3K	35	32/33	0.89	0.41	131,138,151,152	0
22	PSU	3K	40	20/21	0.89	0.15	132,136,141,143	0
22	PSU	2L	40	20/21	0.91	0.18	108,120,128,130	0
22	MIA	2K	38	29/30	0.91	0.17	101,114,121,126	0
22	QUO	2K	35	32/33	0.93	0.13	103,113,118,124	9
22	PSU	2K	40	20/21	0.94	0.15	96,112,117,120	0
22	MIA	2L	38	29/30	0.94	0.15	112,124,132,146	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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(Å ²)	Q<0.9
55	MG	13	1680	1/1	-0.02	0.33	160,160,160,160	0
55	MG	14	3346	1/1	0.01	0.26	194,194,194,194	0
55	MG	1J	206	1/1	0.02	0.42	129,129,129,129	0
55	MG	13	1670	1/1	0.05	0.39	150,150,150,150	0
55	MG	3L	101	1/1	0.26	0.37	189,189,189,189	0
55	MG	14	3324	1/1	0.27	0.47	119,119,119,119	0
55	MG	14	3299	1/1	0.29	0.29	138,138,138,138	0
55	MG	1G	1696	1/1	0.30	0.49	112,112,112,112	0
55	MG	1H	3163	1/1	0.30	0.46	111,111,111,111	0
55	MG	1G	1682	1/1	0.30	0.32	145,145,145,145	0
55	MG	1G	1670	1/1	0.33	0.28	115,115,115,115	0
55	MG	14	3214	1/1	0.33	0.38	122,122,122,122	0
55	MG	14	3154	1/1	0.37	0.42	102,102,102,102	0
55	MG	1H	3339	1/1	0.39	0.33	122,122,122,122	0
55	MG	14	3222	1/1	0.40	0.35	112,112,112,112	0
55	MG	1G	1692	1/1	0.42	0.34	141,141,141,141	0
55	MG	1G	1676	1/1	0.42	0.32	129,129,129,129	0
55	MG	14	3189	1/1	0.42	0.33	98,98,98,98	0
55	MG	14	3238	1/1	0.43	0.29	153,153,153,153	0
55	MG	14	3249	1/1	0.43	0.47	106,106,106,106	0
55	MG	13	1675	1/1	0.44	0.34	127,127,127,127	0
55	MG	1G	1702	1/1	0.45	0.25	173,173,173,173	0
55	MG	13	1616	1/1	0.45	0.33	133,133,133,133	0
55	MG	1G	1691	1/1	0.45	0.40	122,122,122,122	0
55	MG	1H	3225	1/1	0.46	0.35	113,113,113,113	0
55	MG	1H	3249	1/1	0.47	0.46	102,102,102,102	0
55	MG	14	3137	1/1	0.47	0.34	107,107,107,107	0
55	MG	1G	1715	1/1	0.49	0.35	116,116,116,116	0
55	MG	14	3196	1/1	0.49	0.41	107,107,107,107	0
55	MG	1H	3273	1/1	0.49	0.34	98,98,98,98	0
55	MG	1G	1669	1/1	0.49	0.19	119,119,119,119	0
55	MG	1H	3297	1/1	0.49	0.26	104,104,104,104	0
55	MG	13	1690	1/1	0.50	0.26	136,136,136,136	0
55	MG	14	3311	1/1	0.51	0.42	106,106,106,106	0
55	MG	1G	1709	1/1	0.51	0.57	111,111,111,111	0
55	MG	14	3295	1/1	0.51	0.48	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1J	202	1/1	0.51	0.35	107,107,107,107	0
55	MG	1H	3268	1/1	0.51	0.31	85,85,85,85	0
55	MG	14	3135	1/1	0.52	0.38	101,101,101,101	0
55	MG	14	3236	1/1	0.53	0.33	113,113,113,113	0
55	MG	13	1610	1/1	0.53	0.22	104,104,104,104	0
55	MG	1G	1642	1/1	0.53	0.38	117,117,117,117	0
55	MG	1G	1712	1/1	0.53	0.34	122,122,122,122	0
55	MG	1H	3235	1/1	0.53	0.40	107,107,107,107	0
55	MG	2K	103	1/1	0.54	0.34	140,140,140,140	0
55	MG	16	210	1/1	0.54	0.37	117,117,117,117	0
55	MG	1H	3119	1/1	0.55	0.40	92,92,92,92	0
55	MG	1H	3135	1/1	0.55	0.51	102,102,102,102	0
55	MG	1H	3259	1/1	0.55	0.32	165,165,165,165	0
55	MG	1H	3228	1/1	0.55	0.27	90,90,90,90	0
55	MG	88	202	1/1	0.55	0.41	98,98,98,98	0
55	MG	1G	1628	1/1	0.55	0.46	95,95,95,95	0
55	MG	1H	3027	1/1	0.56	0.37	88,88,88,88	0
55	MG	1H	3233	1/1	0.56	0.35	117,117,117,117	0
55	MG	14	3325	1/1	0.57	0.39	107,107,107,107	0
55	MG	14	3231	1/1	0.57	0.26	112,112,112,112	0
55	MG	1H	3305	1/1	0.58	0.20	107,107,107,107	0
55	MG	1H	3146	1/1	0.58	0.46	98,98,98,98	0
55	MG	1H	3254	1/1	0.58	0.32	104,104,104,104	0
55	MG	1H	3207	1/1	0.58	0.46	101,101,101,101	0
55	MG	14	3314	1/1	0.58	0.43	111,111,111,111	0
55	MG	1H	3059	1/1	0.59	0.43	90,90,90,90	0
55	MG	14	3319	1/1	0.59	0.47	110,110,110,110	0
55	MG	1H	3306	1/1	0.59	0.25	109,109,109,109	0
55	MG	13	1650	1/1	0.59	0.33	116,116,116,116	0
55	MG	1H	3342	1/1	0.59	0.28	87,87,87,87	0
55	MG	1H	3298	1/1	0.59	0.31	114,114,114,114	0
55	MG	1G	1673	1/1	0.59	0.31	101,101,101,101	0
55	MG	14	3312	1/1	0.60	0.40	98,98,98,98	0
55	MG	13	1674	1/1	0.60	0.30	142,142,142,142	0
55	MG	1H	3020	1/1	0.60	0.35	103,103,103,103	0
55	MG	1J	204	1/1	0.60	0.27	128,128,128,128	0
55	MG	14	3257	1/1	0.60	0.39	109,109,109,109	0
55	MG	13	1685	1/1	0.61	0.32	119,119,119,119	0
55	MG	1G	1637	1/1	0.61	0.28	127,127,127,127	0
55	MG	1H	3358	1/1	0.61	0.64	115,115,115,115	0
55	MG	1H	3320	1/1	0.61	0.24	106,106,106,106	0
55	MG	13	1686	1/1	0.61	0.26	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3364	1/1	0.62	0.37	101,101,101,101	0
55	MG	14	3147	1/1	0.62	0.28	115,115,115,115	0
55	MG	1H	3123	1/1	0.62	0.41	93,93,93,93	0
55	MG	13	1638	1/1	0.63	0.37	103,103,103,103	0
55	MG	1H	3546	1/1	0.63	0.35	89,89,89,89	0
55	MG	16	203	1/1	0.63	0.29	105,105,105,105	0
55	MG	13	1641	1/1	0.63	0.34	117,117,117,117	0
55	MG	1H	3111	1/1	0.63	0.43	111,111,111,111	0
55	MG	I8	101	1/1	0.63	0.37	93,93,93,93	0
55	MG	1G	1613	1/1	0.63	0.34	104,104,104,104	0
55	MG	1J	205	1/1	0.63	0.32	112,112,112,112	0
55	MG	1H	3291	1/1	0.63	0.20	120,120,120,120	0
55	MG	14	3074	1/1	0.64	0.19	97,97,97,97	0
55	MG	13	1652	1/1	0.64	0.33	98,98,98,98	0
55	MG	1H	3505	1/1	0.64	0.27	122,122,122,122	0
55	MG	29	304	1/1	0.64	0.35	115,115,115,115	0
55	MG	16	209	1/1	0.65	0.22	101,101,101,101	0
55	MG	13	1691	1/1	0.65	0.39	98,98,98,98	0
55	MG	13	1669	1/1	0.65	0.26	115,115,115,115	0
55	MG	1H	3142	1/1	0.65	0.36	81,81,81,81	0
55	MG	1G	1606	1/1	0.65	0.29	108,108,108,108	0
55	MG	1H	3028	1/1	0.65	0.31	93,93,93,93	0
55	MG	16	204	1/1	0.65	0.26	121,121,121,121	0
55	MG	14	3320	1/1	0.65	0.23	114,114,114,114	0
55	MG	14	3126	1/1	0.66	0.27	110,110,110,110	0
55	MG	1H	3260	1/1	0.66	0.29	114,114,114,114	0
55	MG	14	3136	1/1	0.66	0.32	109,109,109,109	0
55	MG	1H	3199	1/1	0.66	0.36	106,106,106,106	0
55	MG	1H	3149	1/1	0.66	0.42	98,98,98,98	0
55	MG	1G	1653	1/1	0.66	0.31	90,90,90,90	0
55	MG	1G	1718	1/1	0.66	0.28	94,94,94,94	0
55	MG	1H	3029	1/1	0.66	0.36	84,84,84,84	0
55	MG	1H	3319	1/1	0.66	0.31	91,91,91,91	0
55	MG	14	3110	1/1	0.66	0.34	95,95,95,95	0
55	MG	14	3323	1/1	0.67	0.46	113,113,113,113	0
55	MG	1G	1675	1/1	0.67	0.30	111,111,111,111	0
55	MG	14	3092	1/1	0.67	0.30	84,84,84,84	0
55	MG	14	3327	1/1	0.67	0.53	101,101,101,101	0
55	MG	1H	3242	1/1	0.67	0.36	107,107,107,107	0
55	MG	1G	1643	1/1	0.67	0.25	128,128,128,128	0
55	MG	14	3240	1/1	0.67	0.22	100,100,100,100	0
55	MG	1G	1638	1/1	0.67	0.27	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3033	1/1	0.67	0.39	83,83,83,83	0
55	MG	14	3321	1/1	0.67	0.29	93,93,93,93	0
55	MG	13	1664	1/1	0.68	0.31	142,142,142,142	0
55	MG	14	3081	1/1	0.68	0.44	80,80,80,80	0
55	MG	14	3241	1/1	0.68	0.20	117,117,117,117	0
55	MG	14	3181	1/1	0.68	0.34	97,97,97,97	0
55	MG	1G	1714	1/1	0.68	0.21	115,115,115,115	0
55	MG	14	3259	1/1	0.68	0.36	86,86,86,86	0
55	MG	16	205	1/1	0.68	0.18	109,109,109,109	0
55	MG	1H	3545	1/1	0.68	0.29	71,71,71,71	0
55	MG	14	3220	1/1	0.68	0.30	89,89,89,89	0
55	MG	13	1613	1/1	0.68	0.30	123,123,123,123	0
55	MG	14	3016	1/1	0.68	0.43	86,86,86,86	0
55	MG	1H	3365	1/1	0.68	0.31	96,96,96,96	0
55	MG	14	3211	1/1	0.69	0.43	101,101,101,101	0
55	MG	14	3014	1/1	0.69	0.37	88,88,88,88	0
55	MG	1G	1706	1/1	0.69	0.24	116,116,116,116	0
55	MG	14	3264	1/1	0.69	0.22	100,100,100,100	0
55	MG	13	1676	1/1	0.69	0.31	120,120,120,120	0
55	MG	14	3337	1/1	0.69	0.28	111,111,111,111	0
55	MG	1H	3279	1/1	0.69	0.29	101,101,101,101	0
55	MG	14	3235	1/1	0.69	0.34	109,109,109,109	0
55	MG	13	1663	1/1	0.69	0.20	108,108,108,108	0
55	MG	1H	3237	1/1	0.69	0.44	99,99,99,99	0
55	MG	5E	201	1/1	0.69	0.37	121,121,121,121	0
55	MG	1H	3243	1/1	0.69	0.22	119,119,119,119	0
55	MG	1H	3131	1/1	0.70	0.41	96,96,96,96	0
55	MG	1H	3333	1/1	0.70	0.54	97,97,97,97	0
55	MG	14	3205	1/1	0.70	0.26	82,82,82,82	0
55	MG	1G	1608	1/1	0.70	0.35	110,110,110,110	0
55	MG	1G	1674	1/1	0.70	0.33	106,106,106,106	0
55	MG	1H	3277	1/1	0.70	0.23	88,88,88,88	0
55	MG	1H	3069	1/1	0.70	0.63	86,86,86,86	0
55	MG	14	3100	1/1	0.70	0.38	81,81,81,81	0
55	MG	14	3103	1/1	0.70	0.38	74,74,74,74	0
55	MG	13	1684	1/1	0.71	0.29	99,99,99,99	0
55	MG	14	3097	1/1	0.71	0.38	94,94,94,94	0
55	MG	1H	3261	1/1	0.71	0.28	109,109,109,109	0
55	MG	1H	3353	1/1	0.71	0.88	100,100,100,100	0
55	MG	1H	3024	1/1	0.71	0.35	98,98,98,98	0
55	MG	1H	3280	1/1	0.71	0.27	97,97,97,97	0
55	MG	1G	1620	1/1	0.71	0.35	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3292	1/1	0.71	0.23	104,104,104,104	0
55	MG	1G	1622	1/1	0.71	0.24	124,124,124,124	0
55	MG	14	3041	1/1	0.71	0.43	76,76,76,76	0
55	MG	14	3303	1/1	0.71	0.31	122,122,122,122	0
55	MG	14	3234	1/1	0.71	0.37	96,96,96,96	0
55	MG	1H	3334	1/1	0.71	0.23	88,88,88,88	0
55	MG	1H	3336	1/1	0.71	0.38	103,103,103,103	0
55	MG	14	3015	1/1	0.72	0.32	78,78,78,78	0
55	MG	1H	3351	1/1	0.72	0.47	114,114,114,114	0
55	MG	14	3031	1/1	0.72	0.49	95,95,95,95	0
55	MG	14	3293	1/1	0.72	0.37	105,105,105,105	0
55	MG	1G	1705	1/1	0.72	0.26	110,110,110,110	0
55	MG	1H	3307	1/1	0.72	0.40	105,105,105,105	0
55	MG	1H	3208	1/1	0.72	0.35	110,110,110,110	0
55	MG	1G	1700	1/1	0.72	0.37	99,99,99,99	0
55	MG	1H	3355	1/1	0.73	0.32	92,92,92,92	0
55	MG	13	1615	1/1	0.73	0.36	146,146,146,146	0
55	MG	14	3071	1/1	0.73	0.28	95,95,95,95	0
55	MG	2L	102	1/1	0.73	0.16	113,113,113,113	0
55	MG	14	3077	1/1	0.73	0.44	80,80,80,80	0
55	MG	1H	3255	1/1	0.73	0.21	107,107,107,107	0
55	MG	3L	102	1/1	0.73	0.40	95,95,95,95	0
55	MG	14	3183	1/1	0.73	0.32	98,98,98,98	0
55	MG	13	1633	1/1	0.73	0.25	107,107,107,107	0
55	MG	13	1646	1/1	0.73	0.31	100,100,100,100	0
55	MG	1G	1713	1/1	0.73	0.26	106,106,106,106	0
55	MG	13	1649	1/1	0.73	0.20	121,121,121,121	0
55	MG	1H	3130	1/1	0.74	0.37	91,91,91,91	0
55	MG	1G	1719	1/1	0.74	0.27	118,118,118,118	0
55	MG	1H	3167	1/1	0.74	0.23	119,119,119,119	0
55	MG	1H	3348	1/1	0.74	0.20	126,126,126,126	0
55	MG	1G	1657	1/1	0.74	0.46	93,93,93,93	0
55	MG	1G	1612	1/1	0.74	0.32	108,108,108,108	0
55	MG	1H	3178	1/1	0.74	0.38	92,92,92,92	0
55	MG	1H	3191	1/1	0.74	0.31	90,90,90,90	0
55	MG	14	3132	1/1	0.74	0.22	90,90,90,90	0
55	MG	13	1631	1/1	0.74	0.30	101,101,101,101	0
55	MG	1H	3294	1/1	0.74	0.31	91,91,91,91	0
55	MG	1H	3114	1/1	0.74	0.40	94,94,94,94	0
55	MG	1H	3154	1/1	0.74	0.47	88,88,88,88	0
55	MG	1G	1684	1/1	0.74	0.27	108,108,108,108	0
55	MG	1H	3073	1/1	0.75	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3143	1/1	0.75	0.24	90,90,90,90	0
55	MG	1H	3097	1/1	0.75	0.39	75,75,75,75	0
55	MG	13	1606	1/1	0.75	0.23	100,100,100,100	0
55	MG	1G	1664	1/1	0.75	0.32	112,112,112,112	0
55	MG	14	3331	1/1	0.75	0.23	79,79,79,79	0
55	MG	1H	3033	1/1	0.75	0.26	113,113,113,113	0
55	MG	1H	3133	1/1	0.75	0.26	92,92,92,92	0
55	MG	1H	3118	1/1	0.75	0.41	56,56,56,56	0
55	MG	14	3082	1/1	0.75	0.33	100,100,100,100	0
55	MG	14	3317	1/1	0.75	0.42	92,92,92,92	0
55	MG	14	3217	1/1	0.75	0.25	88,88,88,88	0
55	MG	14	3087	1/1	0.75	0.30	101,101,101,101	0
55	MG	1H	3322	1/1	0.76	0.25	103,103,103,103	0
55	MG	1H	3274	1/1	0.76	0.16	97,97,97,97	0
55	MG	1G	1644	1/1	0.76	0.15	104,104,104,104	0
55	MG	1G	1649	1/1	0.76	0.34	125,125,125,125	0
55	MG	5E	202	1/1	0.76	0.22	109,109,109,109	0
55	MG	14	3266	1/1	0.76	0.20	101,101,101,101	0
55	MG	1G	1656	1/1	0.76	0.20	104,104,104,104	0
55	MG	13	1619	1/1	0.76	0.36	81,81,81,81	0
55	MG	1G	1658	1/1	0.76	0.24	106,106,106,106	0
55	MG	13	1679	1/1	0.76	0.28	101,101,101,101	0
55	MG	1H	3252	1/1	0.76	0.22	76,76,76,76	0
55	MG	14	3160	1/1	0.76	0.24	82,82,82,82	0
55	MG	14	3167	1/1	0.76	0.25	107,107,107,107	0
55	MG	1H	3220	1/1	0.76	0.58	92,92,92,92	0
55	MG	1H	3224	1/1	0.76	0.25	87,87,87,87	0
55	MG	13	1671	1/1	0.76	0.26	155,155,155,155	0
55	MG	14	3194	1/1	0.76	0.29	92,92,92,92	0
55	MG	1H	3139	1/1	0.76	0.34	101,101,101,101	0
55	MG	1G	1611	1/1	0.76	0.22	92,92,92,92	0
55	MG	1H	3176	1/1	0.76	0.33	93,93,93,93	0
55	MG	1H	3360	1/1	0.76	0.33	96,96,96,96	0
55	MG	14	3044	1/1	0.76	0.28	78,78,78,78	0
55	MG	14	3330	1/1	0.76	0.19	85,85,85,85	0
55	MG	1H	3363	1/1	0.76	0.33	93,93,93,93	0
55	MG	1H	3262	1/1	0.76	0.42	101,101,101,101	0
55	MG	1G	1694	1/1	0.76	0.29	103,103,103,103	0
55	MG	1J	201	1/1	0.76	0.22	125,125,125,125	0
55	MG	1G	1695	1/1	0.76	0.22	108,108,108,108	0
55	MG	1H	3315	1/1	0.76	0.25	107,107,107,107	0
55	MG	1G	1636	1/1	0.76	0.32	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3109	1/1	0.76	0.26	57,57,57,57	0
55	MG	1H	3126	1/1	0.76	0.16	87,87,87,87	0
55	MG	1H	3362	1/1	0.77	0.28	112,112,112,112	0
55	MG	1H	3045	1/1	0.77	0.33	104,104,104,104	0
55	MG	14	3255	1/1	0.77	0.52	107,107,107,107	0
55	MG	1H	3226	1/1	0.77	0.26	89,89,89,89	0
55	MG	13	1692	1/1	0.77	0.59	101,101,101,101	0
55	MG	1G	1665	1/1	0.77	0.27	107,107,107,107	0
55	MG	14	3216	1/1	0.77	0.13	104,104,104,104	0
55	MG	14	3268	1/1	0.77	0.33	87,87,87,87	0
55	MG	1H	3352	1/1	0.77	0.21	84,84,84,84	0
55	MG	1G	1740	1/1	0.77	0.23	135,135,135,135	0
55	MG	14	3340	1/1	0.77	0.21	103,103,103,103	0
55	MG	13	1682	1/1	0.77	0.20	98,98,98,98	0
55	MG	1H	3312	1/1	0.77	0.21	106,106,106,106	0
55	MG	14	3083	1/1	0.77	0.16	64,64,64,64	0
55	MG	1H	3034	1/1	0.77	0.14	93,93,93,93	0
55	MG	1H	3318	1/1	0.77	0.30	86,86,86,86	0
55	MG	1H	3361	1/1	0.77	0.30	103,103,103,103	0
55	MG	1G	1678	1/1	0.77	0.15	107,107,107,107	0
55	MG	13	1609	1/1	0.78	0.21	130,130,130,130	0
55	MG	14	3157	1/1	0.78	0.30	95,95,95,95	0
55	MG	1G	1693	1/1	0.78	0.16	106,106,106,106	0
55	MG	14	3163	1/1	0.78	0.21	86,86,86,86	0
55	MG	14	3271	1/1	0.78	0.26	99,99,99,99	0
55	MG	1H	3187	1/1	0.78	0.32	103,103,103,103	0
55	MG	1H	3158	1/1	0.78	0.32	93,93,93,93	0
55	MG	14	3332	1/1	0.78	0.31	89,89,89,89	0
55	MG	1H	3193	1/1	0.78	0.18	79,79,79,79	0
55	MG	14	3339	1/1	0.78	0.13	107,107,107,107	0
55	MG	13	1644	1/1	0.78	0.36	91,91,91,91	0
55	MG	1H	3078	1/1	0.78	0.40	81,81,81,81	0
55	MG	14	3195	1/1	0.78	0.18	103,103,103,103	0
55	MG	13	1667	1/1	0.78	0.49	99,99,99,99	0
55	MG	14	3246	1/1	0.78	0.42	101,101,101,101	0
55	MG	14	3138	1/1	0.78	0.33	90,90,90,90	0
55	MG	1H	3236	1/1	0.78	0.40	77,77,77,77	0
55	MG	14	3152	1/1	0.78	0.31	80,80,80,80	0
55	MG	1H	3157	1/1	0.79	0.48	98,98,98,98	0
55	MG	1G	1666	1/1	0.79	0.43	99,99,99,99	0
55	MG	1H	3210	1/1	0.79	0.32	97,97,97,97	0
55	MG	1H	3216	1/1	0.79	0.25	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1671	1/1	0.79	0.26	102,102,102,102	0
55	MG	1H	3049	1/1	0.79	0.31	78,78,78,78	0
55	MG	1H	3053	1/1	0.79	0.28	74,74,74,74	0
55	MG	13	1642	1/1	0.79	0.26	99,99,99,99	0
55	MG	1H	3141	1/1	0.79	0.27	90,90,90,90	0
55	MG	13	1630	1/1	0.79	0.28	92,92,92,92	0
55	MG	1G	1679	1/1	0.79	0.13	106,106,106,106	0
55	MG	13	1665	1/1	0.79	0.32	106,106,106,106	0
55	MG	14	3186	1/1	0.79	0.17	90,90,90,90	0
55	MG	13	1635	1/1	0.79	0.27	106,106,106,106	0
55	MG	1G	1687	1/1	0.79	0.23	120,120,120,120	0
55	MG	14	3102	1/1	0.79	0.20	86,86,86,86	0
55	MG	13	1658	1/1	0.79	0.18	84,84,84,84	0
55	MG	14	3197	1/1	0.79	0.41	105,105,105,105	0
55	MG	1H	3151	1/1	0.79	0.26	80,80,80,80	0
55	MG	1H	3205	1/1	0.79	0.14	101,101,101,101	0
55	MG	13	1659	1/1	0.79	0.28	108,108,108,108	0
55	MG	14	3134	1/1	0.79	0.24	77,77,77,77	0
55	MG	1H	3290	1/1	0.79	0.49	88,88,88,88	0
55	MG	14	3309	1/1	0.79	0.16	85,85,85,85	0
55	MG	1H	3217	1/1	0.80	0.38	85,85,85,85	0
55	MG	14	3207	1/1	0.80	0.26	96,96,96,96	0
55	MG	1H	3281	1/1	0.80	0.34	103,103,103,103	0
55	MG	13	1660	1/1	0.80	0.20	108,108,108,108	0
55	MG	1H	3116	1/1	0.80	0.28	92,92,92,92	0
55	MG	1H	3189	1/1	0.80	0.24	83,83,83,83	0
55	MG	13	1639	1/1	0.80	0.30	89,89,89,89	0
55	MG	14	3275	1/1	0.80	0.23	84,84,84,84	0
55	MG	14	3283	1/1	0.80	0.28	81,81,81,81	0
55	MG	14	3285	1/1	0.80	0.31	107,107,107,107	0
55	MG	14	3179	1/1	0.80	0.34	107,107,107,107	0
55	MG	13	1604	1/1	0.80	0.23	96,96,96,96	0
55	MG	1H	3058	1/1	0.80	0.18	88,88,88,88	0
55	MG	1H	3043	1/1	0.80	0.33	89,89,89,89	0
55	MG	1H	3129	1/1	0.80	0.19	80,80,80,80	0
55	MG	1H	3170	1/1	0.80	0.30	69,69,69,69	0
55	MG	1H	3239	1/1	0.80	0.29	71,71,71,71	0
55	MG	1H	3174	1/1	0.80	0.30	80,80,80,80	0
55	MG	1H	3061	1/1	0.80	0.26	90,90,90,90	0
55	MG	14	3201	1/1	0.80	0.17	84,84,84,84	0
55	MG	55	201	1/1	0.80	0.13	92,92,92,92	0
55	MG	1G	1654	1/1	0.81	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1601	1/1	0.81	0.25	89,89,89,89	0
55	MG	1H	3162	1/1	0.81	0.33	87,87,87,87	0
55	MG	1G	1698	1/1	0.81	0.19	86,86,86,86	0
55	MG	1G	1699	1/1	0.81	0.20	157,157,157,157	0
55	MG	1G	1607	1/1	0.81	0.23	94,94,94,94	0
55	MG	14	3153	1/1	0.81	0.23	91,91,91,91	0
55	MG	14	3213	1/1	0.81	0.23	108,108,108,108	0
55	MG	14	3089	1/1	0.81	0.41	78,78,78,78	0
55	MG	14	3005	1/1	0.81	0.33	72,72,72,72	0
55	MG	14	3328	1/1	0.81	0.20	103,103,103,103	0
55	MG	14	3329	1/1	0.81	0.29	85,85,85,85	0
55	MG	14	3274	1/1	0.81	0.17	88,88,88,88	0
55	MG	1H	3311	1/1	0.81	0.26	85,85,85,85	0
55	MG	14	3276	1/1	0.81	0.12	75,75,75,75	0
55	MG	14	3219	1/1	0.81	0.22	105,105,105,105	0
55	MG	1G	1680	1/1	0.81	0.15	101,101,101,101	0
55	MG	14	3287	1/1	0.81	0.36	111,111,111,111	0
55	MG	1H	3099	1/1	0.81	0.23	90,90,90,90	0
55	MG	13	1607	1/1	0.81	0.16	97,97,97,97	0
55	MG	1H	3303	1/1	0.81	0.23	88,88,88,88	0
55	MG	14	3115	1/1	0.81	0.22	94,94,94,94	0
55	MG	1H	3214	1/1	0.81	0.32	94,94,94,94	0
55	MG	14	3307	1/1	0.81	0.14	90,90,90,90	0
55	MG	1J	207	1/1	0.81	0.46	97,97,97,97	0
55	MG	1G	1652	1/1	0.81	0.24	100,100,100,100	0
55	MG	1H	3190	1/1	0.81	0.15	98,98,98,98	0
55	MG	13	1648	1/1	0.82	0.28	94,94,94,94	0
55	MG	13	1645	1/1	0.82	0.30	84,84,84,84	0
55	MG	1G	1625	1/1	0.82	0.44	97,97,97,97	0
55	MG	1G	1626	1/1	0.82	0.24	108,108,108,108	0
55	MG	1H	3206	1/1	0.82	0.32	89,89,89,89	0
55	MG	13	1694	1/1	0.82	0.14	108,108,108,108	0
55	MG	13	1687	1/1	0.82	0.18	111,111,111,111	0
55	MG	1H	3266	1/1	0.82	0.26	106,106,106,106	0
55	MG	1H	3209	1/1	0.82	0.29	85,85,85,85	0
55	MG	14	3193	1/1	0.82	0.19	90,90,90,90	0
55	MG	13	1689	1/1	0.82	0.11	102,102,102,102	0
55	MG	42	201	1/1	0.82	0.26	103,103,103,103	0
55	MG	1H	3031	1/1	0.82	0.20	73,73,73,73	0
55	MG	13	1603	1/1	0.82	0.18	107,107,107,107	0
55	MG	Q8	101	1/1	0.82	0.34	95,95,95,95	0
55	MG	1H	3016	1/1	0.82	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3248	1/1	0.82	0.22	89,89,89,89	0
55	MG	14	3279	1/1	0.82	0.31	103,103,103,103	0
55	MG	1H	3018	1/1	0.82	0.35	76,76,76,76	0
55	MG	1H	3223	1/1	0.82	0.41	77,77,77,77	0
55	MG	1H	3323	1/1	0.82	0.26	84,84,84,84	0
55	MG	1H	3164	1/1	0.82	0.40	95,95,95,95	0
55	MG	1J	203	1/1	0.82	0.10	121,121,121,121	0
55	MG	1H	3368	1/1	0.82	0.21	64,64,64,64	0
55	MG	14	3141	1/1	0.82	0.26	64,64,64,64	0
55	MG	1G	1616	1/1	0.82	0.21	85,85,85,85	0
55	MG	14	3056	1/1	0.82	0.20	74,74,74,74	0
55	MG	14	3070	1/1	0.82	0.33	72,72,72,72	0
55	MG	15	201	1/1	0.82	0.31	110,110,110,110	0
55	MG	1G	1618	1/1	0.82	0.15	110,110,110,110	0
55	MG	14	3243	1/1	0.83	0.21	89,89,89,89	0
55	MG	14	3184	1/1	0.83	0.32	92,92,92,92	0
55	MG	14	3101	1/1	0.83	0.31	100,100,100,100	0
55	MG	1H	3289	1/1	0.83	0.52	104,104,104,104	0
55	MG	1H	3321	1/1	0.83	0.17	88,88,88,88	0
55	MG	1G	1703	1/1	0.83	0.29	113,113,113,113	0
55	MG	1H	3175	1/1	0.83	0.43	96,96,96,96	0
55	MG	14	3122	1/1	0.83	0.20	81,81,81,81	0
55	MG	1H	3124	1/1	0.83	0.38	85,85,85,85	0
55	MG	1G	1645	1/1	0.83	0.33	104,104,104,104	0
55	MG	14	3046	1/1	0.83	0.35	88,88,88,88	0
55	MG	1H	3035	1/1	0.83	0.31	98,98,98,98	0
55	MG	14	3062	1/1	0.83	0.34	79,79,79,79	0
55	MG	14	3064	1/1	0.83	0.21	84,84,84,84	0
55	MG	14	3066	1/1	0.83	0.47	82,82,82,82	0
55	MG	1H	3160	1/1	0.83	0.35	91,91,91,91	0
55	MG	1H	3188	1/1	0.83	0.48	88,88,88,88	0
55	MG	1H	3263	1/1	0.83	0.32	78,78,78,78	0
55	MG	1H	3238	1/1	0.83	0.26	97,97,97,97	0
55	MG	2K	102	1/1	0.83	0.22	106,106,106,106	0
55	MG	1H	3117	1/1	0.83	0.30	83,83,83,83	0
55	MG	13	1612	1/1	0.83	0.19	117,117,117,117	0
55	MG	16	206	1/1	0.83	0.20	76,76,76,76	0
55	MG	1H	3166	1/1	0.83	0.22	86,86,86,86	0
55	MG	13	1688	1/1	0.83	0.28	107,107,107,107	0
55	MG	49	201	1/1	0.83	0.18	134,134,134,134	0
55	MG	13	1678	1/1	0.83	0.18	124,124,124,124	0
55	MG	1H	3136	1/1	0.83	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1651	1/1	0.84	0.27	91,91,91,91	0
55	MG	1H	3329	1/1	0.84	0.27	96,96,96,96	0
55	MG	1G	1723	1/1	0.84	0.23	131,131,131,131	0
55	MG	1H	3039	1/1	0.84	0.29	55,55,55,55	0
55	MG	1H	3068	1/1	0.84	0.37	72,72,72,72	0
55	MG	14	3098	1/1	0.84	0.38	86,86,86,86	0
55	MG	1H	3335	1/1	0.84	0.35	90,90,90,90	0
55	MG	14	3199	1/1	0.84	0.59	94,94,94,94	0
55	MG	14	3200	1/1	0.84	0.30	89,89,89,89	0
55	MG	13	1668	1/1	0.84	0.35	94,94,94,94	0
55	MG	1H	3295	1/1	0.84	0.24	87,87,87,87	0
55	MG	1H	3023	1/1	0.84	0.46	101,101,101,101	0
55	MG	1H	3346	1/1	0.84	0.13	80,80,80,80	0
55	MG	14	3313	1/1	0.84	0.16	91,91,91,91	0
55	MG	14	3114	1/1	0.84	0.31	83,83,83,83	0
55	MG	1H	3347	1/1	0.84	0.12	117,117,117,117	0
55	MG	14	3116	1/1	0.84	0.28	89,89,89,89	0
55	MG	1H	3032	1/1	0.84	0.23	76,76,76,76	0
55	MG	14	3017	1/1	0.84	0.30	79,79,79,79	0
55	MG	14	3023	1/1	0.84	0.20	89,89,89,89	0
55	MG	14	3030	1/1	0.84	0.23	92,92,92,92	0
55	MG	14	3223	1/1	0.84	0.20	97,97,97,97	0
55	MG	1H	3081	1/1	0.84	0.31	66,66,66,66	0
55	MG	1H	3084	1/1	0.84	0.25	83,83,83,83	0
55	MG	1G	1602	1/1	0.84	0.24	84,84,84,84	0
55	MG	1H	3265	1/1	0.84	0.13	85,85,85,85	0
55	MG	14	3139	1/1	0.84	0.28	102,102,102,102	0
55	MG	1H	3009	1/1	0.84	0.30	67,67,67,67	0
55	MG	14	3142	1/1	0.84	0.35	67,67,67,67	0
55	MG	14	3050	1/1	0.84	0.23	75,75,75,75	0
55	MG	1H	3267	1/1	0.84	0.40	95,95,95,95	0
55	MG	1H	3057	1/1	0.84	0.34	76,76,76,76	0
55	MG	14	3347	1/1	0.84	0.15	72,72,72,72	0
55	MG	1H	3211	1/1	0.84	0.36	94,94,94,94	0
55	MG	1H	3102	1/1	0.84	0.27	82,82,82,82	0
55	MG	14	3067	1/1	0.84	0.25	66,66,66,66	0
55	MG	1G	1707	1/1	0.84	0.26	91,91,91,91	0
55	MG	1H	3215	1/1	0.84	0.37	84,84,84,84	0
55	MG	14	3170	1/1	0.84	0.43	77,77,77,77	0
55	MG	14	3269	1/1	0.84	0.20	93,93,93,93	0
55	MG	1H	3106	1/1	0.84	0.45	81,81,81,81	0
55	MG	13	1666	1/1	0.84	0.13	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3219	1/1	0.84	0.23	90,90,90,90	0
55	MG	1H	3451	1/1	0.84	0.14	123,123,123,123	0
55	MG	M5	101	1/1	0.84	0.18	97,97,97,97	0
55	MG	13	1628	1/1	0.85	0.31	89,89,89,89	0
55	MG	1H	3366	1/1	0.85	0.16	113,113,113,113	0
55	MG	14	3305	1/1	0.85	0.26	94,94,94,94	0
55	MG	1H	3184	1/1	0.85	0.31	66,66,66,66	0
55	MG	1H	3309	1/1	0.85	0.25	96,96,96,96	0
55	MG	1H	3014	1/1	0.85	0.20	69,69,69,69	0
55	MG	1H	3343	1/1	0.85	0.09	75,75,75,75	0
55	MG	1H	3345	1/1	0.85	0.15	104,104,104,104	0
55	MG	1G	1624	1/1	0.85	0.18	101,101,101,101	0
55	MG	14	3156	1/1	0.85	0.29	84,84,84,84	0
55	MG	13	1643	1/1	0.85	0.17	111,111,111,111	0
55	MG	1H	3120	1/1	0.85	0.39	69,69,69,69	0
55	MG	1H	3317	1/1	0.85	0.35	87,87,87,87	0
55	MG	14	3322	1/1	0.85	0.12	91,91,91,91	0
55	MG	1G	1747	1/1	0.85	0.12	123,123,123,123	0
55	MG	1H	3349	1/1	0.85	0.13	95,95,95,95	0
55	MG	14	3244	1/1	0.85	0.19	90,90,90,90	0
55	MG	14	3177	1/1	0.85	0.27	91,91,91,91	0
55	MG	1H	3246	1/1	0.85	0.29	86,86,86,86	0
55	MG	1H	3292	1/1	0.85	0.21	100,100,100,100	0
55	MG	1H	3110	1/1	0.85	0.21	65,65,65,65	0
55	MG	1H	3155	1/1	0.85	0.36	92,92,92,92	0
55	MG	1G	1688	1/1	0.85	0.33	115,115,115,115	0
55	MG	14	3333	1/1	0.85	0.15	96,96,96,96	0
55	MG	14	3334	1/1	0.85	0.30	93,93,93,93	0
55	MG	I8	102	1/1	0.85	0.27	73,73,73,73	0
55	MG	I8	103	1/1	0.85	0.08	94,94,94,94	0
55	MG	13	1657	1/1	0.85	0.16	109,109,109,109	0
55	MG	14	3343	1/1	0.85	0.11	83,83,83,83	0
55	MG	14	3270	1/1	0.85	0.15	88,88,88,88	0
55	MG	14	3018	1/1	0.85	0.26	81,81,81,81	0
55	MG	1G	1651	1/1	0.85	0.39	92,92,92,92	0
55	MG	1H	3005	1/1	0.85	0.27	64,64,64,64	0
55	MG	1H	3328	1/1	0.85	0.34	94,94,94,94	0
55	MG	14	3125	1/1	0.85	0.23	93,93,93,93	0
55	MG	1H	3299	1/1	0.85	0.42	80,80,80,80	0
55	MG	1H	3056	1/1	0.85	0.18	67,67,67,67	0
55	MG	1H	3257	1/1	0.85	0.12	102,102,102,102	0
55	MG	14	3289	1/1	0.85	0.10	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3290	1/1	0.85	0.07	102,102,102,102	0
55	MG	1G	1610	1/1	0.85	0.18	156,156,156,156	0
55	MG	1G	1660	1/1	0.85	0.22	112,112,112,112	0
55	MG	F5	101	1/1	0.85	0.23	90,90,90,90	0
55	MG	1G	1663	1/1	0.85	0.22	110,110,110,110	0
55	MG	14	3111	1/1	0.86	0.20	85,85,85,85	0
55	MG	14	3316	1/1	0.86	0.20	97,97,97,97	0
55	MG	14	3040	1/1	0.86	0.27	67,67,67,67	0
55	MG	1H	3025	1/1	0.86	0.15	95,95,95,95	0
55	MG	14	3251	1/1	0.86	0.31	90,90,90,90	0
55	MG	1H	3218	1/1	0.86	0.30	87,87,87,87	0
55	MG	1G	1681	1/1	0.86	0.31	105,105,105,105	0
55	MG	1H	3002	1/1	0.86	0.31	61,61,61,61	0
55	MG	1H	3022	1/1	0.86	0.34	83,83,83,83	0
55	MG	1G	1717	1/1	0.86	0.35	111,111,111,111	0
55	MG	14	3267	1/1	0.86	0.26	99,99,99,99	0
55	MG	1G	1619	1/1	0.86	0.37	92,92,92,92	0
55	MG	13	1632	1/1	0.86	0.28	87,87,87,87	0
55	MG	1G	1690	1/1	0.86	0.22	122,122,122,122	0
55	MG	1H	3127	1/1	0.86	0.29	93,93,93,93	0
55	MG	1H	3325	1/1	0.86	0.14	78,78,78,78	0
55	MG	1H	3367	1/1	0.86	0.14	97,97,97,97	0
55	MG	1H	3140	1/1	0.86	0.15	87,87,87,87	0
55	MG	1H	3370	1/1	0.86	0.49	87,87,87,87	0
55	MG	14	3280	1/1	0.86	0.14	79,79,79,79	0
55	MG	14	3144	1/1	0.86	0.31	78,78,78,78	0
55	MG	1G	1632	1/1	0.86	0.29	88,88,88,88	0
55	MG	14	3149	1/1	0.86	0.34	81,81,81,81	0
55	MG	14	3001	1/1	0.86	0.27	84,84,84,84	0
55	MG	14	3086	1/1	0.86	0.25	68,68,68,68	0
55	MG	1H	3395	1/1	0.86	0.13	107,107,107,107	0
55	MG	13	1656	1/1	0.86	0.22	89,89,89,89	0
55	MG	14	3227	1/1	0.86	0.10	112,112,112,112	0
55	MG	1H	3172	1/1	0.86	0.29	94,94,94,94	0
55	MG	1G	1701	1/1	0.86	0.19	106,106,106,106	0
55	MG	1H	3087	1/1	0.86	0.26	81,81,81,81	0
55	MG	1H	3159	1/1	0.86	0.36	90,90,90,90	0
55	MG	1G	1704	1/1	0.86	0.16	98,98,98,98	0
55	MG	14	3310	1/1	0.86	0.13	107,107,107,107	0
55	MG	1G	1609	1/1	0.86	0.22	106,106,106,106	0
55	MG	55	202	1/1	0.86	0.20	108,108,108,108	0
55	MG	16	201	1/1	0.86	0.20	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3269	1/1	0.86	0.17	107,107,107,107	0
55	MG	1H	3231	1/1	0.87	0.31	81,81,81,81	0
55	MG	14	3253	1/1	0.87	0.52	94,94,94,94	0
55	MG	1H	3341	1/1	0.87	0.41	94,94,94,94	0
55	MG	1H	3132	1/1	0.87	0.21	77,77,77,77	0
55	MG	1G	1623	1/1	0.87	0.29	99,99,99,99	0
55	MG	14	3263	1/1	0.87	0.24	101,101,101,101	0
55	MG	14	3069	1/1	0.87	0.36	86,86,86,86	0
55	MG	14	3265	1/1	0.87	0.12	85,85,85,85	0
55	MG	1H	3064	1/1	0.87	0.38	82,82,82,82	0
55	MG	14	3326	1/1	0.87	0.18	103,103,103,103	0
55	MG	1H	3134	1/1	0.87	0.35	78,78,78,78	0
55	MG	1H	3066	1/1	0.87	0.31	81,81,81,81	0
55	MG	14	3203	1/1	0.87	0.42	98,98,98,98	0
55	MG	1H	3195	1/1	0.87	0.21	78,78,78,78	0
55	MG	14	3078	1/1	0.87	0.26	70,70,70,70	0
55	MG	14	3209	1/1	0.87	0.23	89,89,89,89	0
55	MG	1G	1631	1/1	0.87	0.20	81,81,81,81	0
55	MG	1H	3198	1/1	0.87	0.18	58,58,58,58	0
55	MG	14	3013	1/1	0.87	0.25	75,75,75,75	0
55	MG	13	1683	1/1	0.87	0.12	111,111,111,111	0
55	MG	1H	3091	1/1	0.87	0.14	81,81,81,81	0
55	MG	14	3341	1/1	0.87	0.31	102,102,102,102	0
55	MG	1H	3543	1/1	0.87	0.16	121,121,121,121	0
55	MG	1G	1639	1/1	0.87	0.26	102,102,102,102	0
55	MG	14	3093	1/1	0.87	0.19	66,66,66,66	0
55	MG	14	3348	1/1	0.87	0.22	96,96,96,96	0
55	MG	14	3481	1/1	0.87	0.33	112,112,112,112	0
55	MG	1H	3113	1/1	0.87	0.14	98,98,98,98	0
55	MG	1H	3094	1/1	0.87	0.25	72,72,72,72	0
55	MG	1H	3548	1/1	0.87	0.20	76,76,76,76	0
55	MG	13	1654	1/1	0.87	0.11	104,104,104,104	0
55	MG	1H	3042	1/1	0.87	0.30	69,69,69,69	0
55	MG	14	3171	1/1	0.87	0.16	82,82,82,82	0
55	MG	1H	3253	1/1	0.87	0.39	92,92,92,92	0
55	MG	1G	1615	1/1	0.87	0.38	83,83,83,83	0
55	MG	1G	1686	1/1	0.87	0.14	121,121,121,121	0
55	MG	14	3242	1/1	0.87	0.16	100,100,100,100	0
55	MG	1G	1716	1/1	0.87	0.15	98,98,98,98	0
55	MG	14	3047	1/1	0.87	0.20	78,78,78,78	0
55	MG	C5	201	1/1	0.87	0.24	95,95,95,95	0
55	MG	E5	101	1/1	0.87	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1605	1/1	0.87	0.22	103,103,103,103	0
55	MG	1H	3230	1/1	0.87	0.44	91,91,91,91	0
56	ZN	G8	201	1/1	0.87	0.12	201,201,201,201	0
55	MG	14	3294	1/1	0.88	0.36	82,82,82,82	0
55	MG	1H	3112	1/1	0.88	0.36	64,64,64,64	0
55	MG	14	3117	1/1	0.88	0.14	87,87,87,87	0
55	MG	14	3210	1/1	0.88	0.19	89,89,89,89	0
55	MG	1H	3088	1/1	0.88	0.27	55,55,55,55	0
55	MG	1H	3156	1/1	0.88	0.20	76,76,76,76	0
55	MG	14	3039	1/1	0.88	0.36	90,90,90,90	0
55	MG	14	3130	1/1	0.88	0.29	85,85,85,85	0
55	MG	1H	3179	1/1	0.88	0.26	69,69,69,69	0
55	MG	1H	3180	1/1	0.88	0.21	53,53,53,53	0
55	MG	1G	1621	1/1	0.88	0.10	90,90,90,90	0
55	MG	1H	3181	1/1	0.88	0.51	69,69,69,69	0
55	MG	1H	3310	1/1	0.88	0.27	84,84,84,84	0
55	MG	14	3226	1/1	0.88	0.10	85,85,85,85	0
55	MG	13	1695	1/1	0.88	0.17	108,108,108,108	0
55	MG	14	3229	1/1	0.88	0.12	71,71,71,71	0
55	MG	14	3055	1/1	0.88	0.23	72,72,72,72	0
55	MG	14	3233	1/1	0.88	0.18	84,84,84,84	0
55	MG	13	1629	1/1	0.88	0.24	88,88,88,88	0
55	MG	1H	3314	1/1	0.88	0.12	80,80,80,80	0
55	MG	1G	1627	1/1	0.88	0.25	89,89,89,89	0
55	MG	14	3145	1/1	0.88	0.16	75,75,75,75	0
55	MG	1H	3096	1/1	0.88	0.19	74,74,74,74	0
55	MG	1H	3276	1/1	0.88	0.19	89,89,89,89	0
55	MG	11	301	1/1	0.88	0.30	93,93,93,93	0
55	MG	1G	1634	1/1	0.88	0.27	107,107,107,107	0
55	MG	1G	1635	1/1	0.88	0.46	98,98,98,98	0
55	MG	14	3155	1/1	0.88	0.19	99,99,99,99	0
55	MG	1H	3071	1/1	0.88	0.21	80,80,80,80	0
55	MG	1H	3357	1/1	0.88	0.16	87,87,87,87	0
55	MG	32	301	1/1	0.88	0.12	109,109,109,109	0
55	MG	14	3254	1/1	0.88	0.31	95,95,95,95	0
55	MG	14	3162	1/1	0.88	0.20	92,92,92,92	0
55	MG	1H	3278	1/1	0.88	0.42	79,79,79,79	0
55	MG	14	3166	1/1	0.88	0.15	86,86,86,86	0
55	MG	1H	3098	1/1	0.88	0.29	73,73,73,73	0
55	MG	13	1622	1/1	0.88	0.18	96,96,96,96	0
55	MG	1H	3250	1/1	0.88	0.49	80,80,80,80	0
55	MG	14	3446	1/1	0.88	0.30	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3474	1/1	0.88	0.08	142,142,142,142	0
55	MG	14	3172	1/1	0.88	0.12	74,74,74,74	0
55	MG	14	3487	1/1	0.88	0.18	73,73,73,73	0
55	MG	1H	3222	1/1	0.88	0.19	83,83,83,83	0
55	MG	14	3003	1/1	0.88	0.17	67,67,67,67	0
55	MG	1H	3076	1/1	0.88	0.21	74,74,74,74	0
55	MG	1H	3103	1/1	0.88	0.24	74,74,74,74	0
55	MG	14	3095	1/1	0.88	0.33	87,87,87,87	0
55	MG	14	3096	1/1	0.88	0.23	78,78,78,78	0
55	MG	13	1693	1/1	0.88	0.12	103,103,103,103	0
55	MG	1H	3332	1/1	0.88	0.33	101,101,101,101	0
55	MG	1H	3063	1/1	0.88	0.38	76,76,76,76	0
55	MG	1H	3227	1/1	0.88	0.28	83,83,83,83	0
55	MG	13	1672	1/1	0.88	0.09	105,105,105,105	0
55	MG	14	3021	1/1	0.88	0.11	87,87,87,87	0
55	MG	14	3106	1/1	0.88	0.28	75,75,75,75	0
55	MG	1H	3040	1/1	0.88	0.20	80,80,80,80	0
55	MG	14	3024	1/1	0.88	0.23	81,81,81,81	0
55	MG	14	3025	1/1	0.88	0.20	85,85,85,85	0
55	MG	14	3026	1/1	0.88	0.31	76,76,76,76	0
55	MG	1G	1641	1/1	0.89	0.27	102,102,102,102	0
55	MG	1H	3173	1/1	0.89	0.19	88,88,88,88	0
55	MG	14	3260	1/1	0.89	0.26	88,88,88,88	0
55	MG	1H	3065	1/1	0.89	0.25	74,74,74,74	0
55	MG	1H	3080	1/1	0.89	0.31	67,67,67,67	0
55	MG	1G	1708	1/1	0.89	0.22	96,96,96,96	0
55	MG	14	3084	1/1	0.89	0.10	78,78,78,78	0
55	MG	13	1655	1/1	0.89	0.16	107,107,107,107	0
55	MG	1G	1647	1/1	0.89	0.23	102,102,102,102	0
55	MG	14	3088	1/1	0.89	0.15	99,99,99,99	0
55	MG	1H	3196	1/1	0.89	0.18	106,106,106,106	0
55	MG	1G	1650	1/1	0.89	0.13	99,99,99,99	0
55	MG	14	3028	1/1	0.89	0.26	76,76,76,76	0
55	MG	13	1617	1/1	0.89	0.17	99,99,99,99	0
55	MG	14	3335	1/1	0.89	0.39	93,93,93,93	0
55	MG	1H	3085	1/1	0.89	0.23	78,78,78,78	0
55	MG	14	3032	1/1	0.89	0.11	79,79,79,79	0
55	MG	1H	3030	1/1	0.89	0.21	66,66,66,66	0
55	MG	14	3281	1/1	0.89	0.06	98,98,98,98	0
55	MG	14	3342	1/1	0.89	0.17	93,93,93,93	0
55	MG	1H	3258	1/1	0.89	0.59	94,94,94,94	0
55	MG	14	3158	1/1	0.89	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1689	1/1	0.89	0.17	126,126,126,126	0
55	MG	1H	3037	1/1	0.89	0.38	78,78,78,78	0
55	MG	14	3435	1/1	0.89	0.09	123,123,123,123	0
55	MG	1G	1725	1/1	0.89	0.11	124,124,124,124	0
55	MG	13	1653	1/1	0.89	0.13	97,97,97,97	0
55	MG	14	3107	1/1	0.89	0.23	78,78,78,78	0
55	MG	14	3108	1/1	0.89	0.16	87,87,87,87	0
55	MG	1H	3092	1/1	0.89	0.18	79,79,79,79	0
55	MG	14	3297	1/1	0.89	0.22	81,81,81,81	0
55	MG	1G	1659	1/1	0.89	0.12	97,97,97,97	0
55	MG	14	3173	1/1	0.89	0.18	103,103,103,103	0
55	MG	14	3176	1/1	0.89	0.17	75,75,75,75	0
55	MG	1G	1629	1/1	0.89	0.20	91,91,91,91	0
55	MG	14	3308	1/1	0.89	0.19	74,74,74,74	0
55	MG	1H	3330	1/1	0.89	0.31	91,91,91,91	0
55	MG	1H	3331	1/1	0.89	0.28	62,62,62,62	0
55	MG	1H	3356	1/1	0.89	0.27	98,98,98,98	0
55	MG	13	1621	1/1	0.89	0.17	116,116,116,116	0
55	MG	16	202	1/1	0.89	0.12	88,88,88,88	0
55	MG	14	3187	1/1	0.89	0.08	103,103,103,103	0
55	MG	1H	3283	1/1	0.89	0.29	104,104,104,104	0
55	MG	14	3009	1/1	0.89	0.26	67,67,67,67	0
55	MG	1H	3284	1/1	0.89	0.15	83,83,83,83	0
55	MG	1H	3137	1/1	0.89	0.18	93,93,93,93	0
55	MG	1H	3302	1/1	0.90	0.26	90,90,90,90	0
55	MG	16	208	1/1	0.90	0.27	76,76,76,76	0
55	MG	1H	3203	1/1	0.90	0.40	83,83,83,83	0
55	MG	1H	3304	1/1	0.90	0.32	84,84,84,84	0
55	MG	1H	3104	1/1	0.90	0.44	84,84,84,84	0
55	MG	1H	3251	1/1	0.90	0.31	76,76,76,76	0
55	MG	14	3051	1/1	0.90	0.22	78,78,78,78	0
55	MG	14	3215	1/1	0.90	0.14	182,182,182,182	0
55	MG	13	1636	1/1	0.90	0.14	100,100,100,100	0
55	MG	1H	3185	1/1	0.90	0.23	73,73,73,73	0
55	MG	1H	3337	1/1	0.90	0.17	87,87,87,87	0
55	MG	1H	3168	1/1	0.90	0.17	75,75,75,75	0
55	MG	14	3065	1/1	0.90	0.30	86,86,86,86	0
55	MG	1G	1633	1/1	0.90	0.23	91,91,91,91	0
55	MG	1G	1668	1/1	0.90	0.10	99,99,99,99	0
55	MG	13	1727	1/1	0.90	0.09	130,130,130,130	0
55	MG	13	1729	1/1	0.90	0.13	115,115,115,115	0
55	MG	14	3230	1/1	0.90	0.42	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3046	1/1	0.90	0.23	86,86,86,86	0
55	MG	14	3291	1/1	0.90	0.41	88,88,88,88	0
55	MG	14	3073	1/1	0.90	0.25	82,82,82,82	0
55	MG	1H	3431	1/1	0.90	0.19	127,127,127,127	0
55	MG	14	3129	1/1	0.90	0.33	77,77,77,77	0
55	MG	14	3396	1/1	0.90	0.11	94,94,94,94	0
55	MG	1H	3234	1/1	0.90	0.30	89,89,89,89	0
55	MG	14	3296	1/1	0.90	0.18	87,87,87,87	0
55	MG	1H	3062	1/1	0.90	0.21	70,70,70,70	0
55	MG	14	3133	1/1	0.90	0.39	85,85,85,85	0
55	MG	14	3301	1/1	0.90	0.15	91,91,91,91	0
55	MG	1H	3508	1/1	0.90	0.12	122,122,122,122	0
55	MG	14	3304	1/1	0.90	0.22	85,85,85,85	0
55	MG	1H	3047	1/1	0.90	0.24	84,84,84,84	0
55	MG	14	3306	1/1	0.90	0.16	92,92,92,92	0
55	MG	13	1637	1/1	0.90	0.14	113,113,113,113	0
55	MG	14	3191	1/1	0.90	0.29	97,97,97,97	0
55	MG	14	3192	1/1	0.90	0.47	74,74,74,74	0
55	MG	29	303	1/1	0.90	0.14	77,77,77,77	0
55	MG	14	3248	1/1	0.90	0.17	110,110,110,110	0
55	MG	29	305	1/1	0.90	0.13	86,86,86,86	0
55	MG	1H	3052	1/1	0.90	0.23	72,72,72,72	0
55	MG	1H	3197	1/1	0.90	0.18	93,93,93,93	0
55	MG	13	1623	1/1	0.90	0.27	104,104,104,104	0
55	MG	13	1620	1/1	0.90	0.36	67,67,67,67	0
55	MG	1G	1685	1/1	0.90	0.42	83,83,83,83	0
55	MG	14	3143	1/1	0.90	0.11	58,58,58,58	0
55	MG	1H	3200	1/1	0.90	0.28	109,109,109,109	0
55	MG	1H	3202	1/1	0.90	0.19	75,75,75,75	0
55	MG	1H	3301	1/1	0.90	0.13	93,93,93,93	0
56	ZN	C5	202	1/1	0.90	0.08	206,206,206,206	0
55	MG	14	3178	1/1	0.91	0.14	87,87,87,87	0
55	MG	14	3121	1/1	0.91	0.11	88,88,88,88	0
55	MG	14	3180	1/1	0.91	0.16	94,94,94,94	0
55	MG	14	3315	1/1	0.91	0.12	121,121,121,121	0
55	MG	14	3247	1/1	0.91	0.26	89,89,89,89	0
55	MG	14	3068	1/1	0.91	0.26	71,71,71,71	0
55	MG	14	3124	1/1	0.91	0.18	92,92,92,92	0
55	MG	13	1634	1/1	0.91	0.14	79,79,79,79	0
55	MG	1H	3122	1/1	0.91	0.24	77,77,77,77	0
55	MG	14	3127	1/1	0.91	0.23	87,87,87,87	0
55	MG	14	3019	1/1	0.91	0.21	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3256	1/1	0.91	0.38	96,96,96,96	0
55	MG	14	3190	1/1	0.91	0.20	85,85,85,85	0
55	MG	14	3072	1/1	0.91	0.27	85,85,85,85	0
55	MG	14	3131	1/1	0.91	0.10	81,81,81,81	0
55	MG	14	3020	1/1	0.91	0.25	71,71,71,71	0
55	MG	1H	3293	1/1	0.91	0.21	89,89,89,89	0
55	MG	1H	3192	1/1	0.91	0.29	97,97,97,97	0
55	MG	1H	3275	1/1	0.91	0.11	85,85,85,85	0
55	MG	14	3079	1/1	0.91	0.30	75,75,75,75	0
55	MG	1H	3316	1/1	0.91	0.14	78,78,78,78	0
55	MG	1H	3021	1/1	0.91	0.27	61,61,61,61	0
55	MG	1H	3338	1/1	0.91	0.23	88,88,88,88	0
55	MG	14	3202	1/1	0.91	0.10	90,90,90,90	0
55	MG	14	3272	1/1	0.91	0.32	94,94,94,94	0
55	MG	14	3273	1/1	0.91	0.32	92,92,92,92	0
55	MG	14	3029	1/1	0.91	0.21	85,85,85,85	0
55	MG	1H	3026	1/1	0.91	0.25	68,68,68,68	0
55	MG	1G	1728	1/1	0.91	0.07	133,133,133,133	0
55	MG	14	3278	1/1	0.91	0.12	82,82,82,82	0
55	MG	14	3208	1/1	0.91	0.12	83,83,83,83	0
55	MG	1H	3153	1/1	0.91	0.07	79,79,79,79	0
55	MG	14	3393	1/1	0.91	0.10	103,103,103,103	0
55	MG	1G	1746	1/1	0.91	0.14	162,162,162,162	0
55	MG	14	3034	1/1	0.91	0.17	67,67,67,67	0
55	MG	1H	3125	1/1	0.91	0.12	93,93,93,93	0
55	MG	14	3286	1/1	0.91	0.14	78,78,78,78	0
55	MG	14	3151	1/1	0.91	0.32	79,79,79,79	0
55	MG	1G	1672	1/1	0.91	0.21	111,111,111,111	0
55	MG	1H	3095	1/1	0.91	0.29	72,72,72,72	0
55	MG	1H	3007	1/1	0.91	0.22	53,53,53,53	0
55	MG	78	201	1/1	0.91	0.30	94,94,94,94	0
55	MG	1H	3282	1/1	0.91	0.32	87,87,87,87	0
55	MG	14	3048	1/1	0.91	0.17	69,69,69,69	0
55	MG	1H	3108	1/1	0.91	0.42	79,79,79,79	0
55	MG	14	3159	1/1	0.91	0.28	66,66,66,66	0
55	MG	19	301	1/1	0.91	0.27	76,76,76,76	0
55	MG	1H	3326	1/1	0.91	0.26	85,85,85,85	0
55	MG	14	3298	1/1	0.91	0.14	88,88,88,88	0
55	MG	14	3004	1/1	0.91	0.21	62,62,62,62	0
55	MG	1H	3327	1/1	0.91	0.12	88,88,88,88	0
55	MG	14	3059	1/1	0.91	0.18	64,64,64,64	0
55	MG	13	1618	1/1	0.91	0.17	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3063	1/1	0.91	0.25	85,85,85,85	0
55	MG	1H	3089	1/1	0.91	0.12	62,62,62,62	0
55	MG	1G	1683	1/1	0.91	0.13	102,102,102,102	0
55	MG	1H	3522	1/1	0.91	0.08	112,112,112,112	0
55	MG	14	3174	1/1	0.91	0.37	85,85,85,85	0
55	MG	1H	3204	1/1	0.91	0.39	84,84,84,84	0
55	MG	14	3118	1/1	0.91	0.23	96,96,96,96	0
55	MG	1H	3462	1/1	0.92	0.13	104,104,104,104	0
55	MG	14	3250	1/1	0.92	0.30	80,80,80,80	0
55	MG	1H	3012	1/1	0.92	0.18	67,67,67,67	0
55	MG	14	3185	1/1	0.92	0.21	92,92,92,92	0
55	MG	1H	3067	1/1	0.92	0.30	79,79,79,79	0
55	MG	13	1662	1/1	0.92	0.35	85,85,85,85	0
55	MG	1H	3525	1/1	0.92	0.07	127,127,127,127	0
55	MG	1G	1646	1/1	0.92	0.34	81,81,81,81	0
55	MG	14	3258	1/1	0.92	0.13	78,78,78,78	0
55	MG	14	3075	1/1	0.92	0.29	65,65,65,65	0
55	MG	1H	3186	1/1	0.92	0.12	74,74,74,74	0
55	MG	13	1601	1/1	0.92	0.12	110,110,110,110	0
55	MG	13	1681	1/1	0.92	0.14	117,117,117,117	0
55	MG	14	3080	1/1	0.92	0.16	66,66,66,66	0
55	MG	14	3027	1/1	0.92	0.24	80,80,80,80	0
55	MG	1H	3138	1/1	0.92	0.13	82,82,82,82	0
55	MG	14	3198	1/1	0.92	0.26	88,88,88,88	0
55	MG	13	1640	1/1	0.92	0.24	99,99,99,99	0
55	MG	13	1614	1/1	0.92	0.16	96,96,96,96	0
55	MG	1H	3300	1/1	0.92	0.19	54,54,54,54	0
55	MG	1G	1736	1/1	0.92	0.20	151,151,151,151	0
55	MG	14	3336	1/1	0.92	0.16	102,102,102,102	0
55	MG	1H	3241	1/1	0.92	0.11	99,99,99,99	0
55	MG	14	3338	1/1	0.92	0.09	80,80,80,80	0
55	MG	1G	1744	1/1	0.92	0.11	126,126,126,126	0
55	MG	14	3146	1/1	0.92	0.06	81,81,81,81	0
55	MG	14	3091	1/1	0.92	0.16	73,73,73,73	0
55	MG	14	3277	1/1	0.92	0.19	68,68,68,68	0
55	MG	14	3035	1/1	0.92	0.38	74,74,74,74	0
55	MG	14	3345	1/1	0.92	0.12	116,116,116,116	0
55	MG	14	3036	1/1	0.92	0.45	84,84,84,84	0
55	MG	14	3038	1/1	0.92	0.22	58,58,58,58	0
55	MG	1H	3077	1/1	0.92	0.22	59,59,59,59	0
55	MG	1H	3001	1/1	0.92	0.24	47,47,47,47	0
55	MG	1H	3194	1/1	0.92	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1696	1/1	0.92	0.13	89,89,89,89	0
55	MG	2L	101	1/1	0.92	0.20	92,92,92,92	0
55	MG	14	3449	1/1	0.92	0.07	135,135,135,135	0
55	MG	1H	3038	1/1	0.92	0.19	56,56,56,56	0
55	MG	1H	3148	1/1	0.92	0.30	74,74,74,74	0
55	MG	14	3104	1/1	0.92	0.40	96,96,96,96	0
55	MG	14	3105	1/1	0.92	0.30	82,82,82,82	0
55	MG	1H	3308	1/1	0.92	0.07	90,90,90,90	0
55	MG	14	3164	1/1	0.92	0.18	89,89,89,89	0
55	MG	14	3165	1/1	0.92	0.15	90,90,90,90	0
55	MG	1H	3004	1/1	0.92	0.29	74,74,74,74	0
55	MG	14	3054	1/1	0.92	0.26	65,65,65,65	0
55	MG	14	3232	1/1	0.92	0.08	86,86,86,86	0
55	MG	14	3002	1/1	0.92	0.23	64,64,64,64	0
55	MG	14	3300	1/1	0.92	0.14	85,85,85,85	0
55	MG	13	1699	1/1	0.92	0.12	137,137,137,137	0
55	MG	13	1706	1/1	0.92	0.08	117,117,117,117	0
55	MG	1H	3369	1/1	0.92	0.14	77,77,77,77	0
55	MG	14	3008	1/1	0.92	0.17	52,52,52,52	0
55	MG	14	3175	1/1	0.92	0.19	95,95,95,95	0
55	MG	1H	3008	1/1	0.92	0.29	74,74,74,74	0
55	MG	1H	3373	1/1	0.92	0.11	87,87,87,87	0
55	MG	14	3120	1/1	0.92	0.19	69,69,69,69	0
55	MG	13	1661	1/1	0.92	0.07	127,127,127,127	0
55	MG	1H	3090	1/1	0.92	0.13	80,80,80,80	0
55	MG	1H	3229	1/1	0.92	0.10	86,86,86,86	0
55	MG	14	3182	1/1	0.92	0.24	79,79,79,79	0
55	MG	1H	3086	1/1	0.93	0.31	60,60,60,60	0
55	MG	1G	1710	1/1	0.93	0.12	107,107,107,107	0
55	MG	1G	1711	1/1	0.93	0.13	107,107,107,107	0
55	MG	1H	3072	1/1	0.93	0.15	65,65,65,65	0
55	MG	1H	3152	1/1	0.93	0.50	82,82,82,82	0
55	MG	13	1677	1/1	0.93	0.08	96,96,96,96	0
55	MG	1H	3340	1/1	0.93	0.29	81,81,81,81	0
55	MG	16	207	1/1	0.93	0.08	95,95,95,95	0
55	MG	1H	3271	1/1	0.93	0.06	89,89,89,89	0
55	MG	1G	1630	1/1	0.93	0.41	75,75,75,75	0
55	MG	1H	3075	1/1	0.93	0.37	80,80,80,80	0
55	MG	1G	1677	1/1	0.93	0.09	97,97,97,97	0
55	MG	1H	3015	1/1	0.93	0.21	56,56,56,56	0
55	MG	1H	3344	1/1	0.93	0.61	95,95,95,95	0
55	MG	11	302	1/1	0.93	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3107	1/1	0.93	0.26	84,84,84,84	0
55	MG	1G	1742	1/1	0.93	0.19	116,116,116,116	0
55	MG	14	3042	1/1	0.93	0.21	71,71,71,71	0
55	MG	14	3218	1/1	0.93	0.23	77,77,77,77	0
55	MG	78	202	1/1	0.93	0.14	91,91,91,91	0
55	MG	14	3282	1/1	0.93	0.12	77,77,77,77	0
55	MG	88	201	1/1	0.93	0.16	93,93,93,93	0
55	MG	14	3221	1/1	0.93	0.31	82,82,82,82	0
55	MG	13	1624	1/1	0.93	0.31	77,77,77,77	0
55	MG	1H	3408	1/1	0.93	0.12	102,102,102,102	0
55	MG	1H	3409	1/1	0.93	0.12	84,84,84,84	0
55	MG	1H	3213	1/1	0.93	0.24	80,80,80,80	0
55	MG	14	3355	1/1	0.93	0.13	97,97,97,97	0
55	MG	14	3168	1/1	0.93	0.26	86,86,86,86	0
55	MG	14	3052	1/1	0.93	0.26	74,74,74,74	0
55	MG	13	1708	1/1	0.93	0.12	103,103,103,103	0
55	MG	14	3437	1/1	0.93	0.09	98,98,98,98	0
55	MG	1H	3454	1/1	0.93	0.10	89,89,89,89	0
55	MG	14	3448	1/1	0.93	0.09	123,123,123,123	0
55	MG	13	1709	1/1	0.93	0.06	126,126,126,126	0
55	MG	14	3454	1/1	0.93	0.09	96,96,96,96	0
55	MG	14	3457	1/1	0.93	0.10	101,101,101,101	0
55	MG	14	3464	1/1	0.93	0.09	122,122,122,122	0
55	MG	1G	1605	1/1	0.93	0.14	81,81,81,81	0
55	MG	14	3475	1/1	0.93	0.20	99,99,99,99	0
55	MG	1H	3488	1/1	0.93	0.07	117,117,117,117	0
55	MG	14	3484	1/1	0.93	0.09	146,146,146,146	0
55	MG	1H	3493	1/1	0.93	0.07	133,133,133,133	0
55	MG	3I	201	1/1	0.93	0.14	89,89,89,89	0
55	MG	1H	3083	1/1	0.93	0.12	85,85,85,85	0
55	MG	14	3123	1/1	0.93	0.41	95,95,95,95	0
55	MG	14	3007	1/1	0.93	0.25	75,75,75,75	0
55	MG	1H	3513	1/1	0.93	0.12	103,103,103,103	0
55	MG	1H	3182	1/1	0.93	0.32	68,68,68,68	0
55	MG	14	3245	1/1	0.93	0.09	109,109,109,109	0
55	MG	1J	211	1/1	0.93	0.08	133,133,133,133	0
55	MG	14	3012	1/1	0.93	0.28	62,62,62,62	0
55	MG	29	302	1/1	0.93	0.17	81,81,81,81	0
55	MG	1H	3050	1/1	0.93	0.33	73,73,73,73	0
55	MG	1H	3529	1/1	0.93	0.07	106,106,106,106	0
55	MG	1H	3530	1/1	0.93	0.11	97,97,97,97	0
55	MG	1H	3537	1/1	0.93	0.06	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1617	1/1	0.93	0.16	74,74,74,74	0
55	MG	1H	3051	1/1	0.93	0.16	76,76,76,76	0
55	MG	1H	3285	1/1	0.93	0.34	91,91,91,91	0
55	MG	1H	3288	1/1	0.93	0.21	86,86,86,86	0
55	MG	1H	3221	1/1	0.93	0.19	67,67,67,67	0
55	MG	14	3022	1/1	0.93	0.20	60,60,60,60	0
55	MG	14	3318	1/1	0.93	0.19	102,102,102,102	0
55	MG	1H	3115	1/1	0.93	0.27	89,89,89,89	0
55	MG	14	3140	1/1	0.93	0.18	97,97,97,97	0
55	MG	1H	3201	1/1	0.94	0.08	98,98,98,98	0
55	MG	1H	3465	1/1	0.94	0.10	73,73,73,73	0
55	MG	1H	3468	1/1	0.94	0.14	120,120,120,120	0
55	MG	1H	3476	1/1	0.94	0.10	106,106,106,106	0
55	MG	13	1602	1/1	0.94	0.17	88,88,88,88	0
55	MG	14	3206	1/1	0.94	0.31	93,93,93,93	0
55	MG	1H	3492	1/1	0.94	0.06	117,117,117,117	0
55	MG	1H	3079	1/1	0.94	0.18	50,50,50,50	0
55	MG	1H	3497	1/1	0.94	0.12	152,152,152,152	0
55	MG	1H	3504	1/1	0.94	0.10	131,131,131,131	0
55	MG	1H	3044	1/1	0.94	0.43	74,74,74,74	0
55	MG	14	3212	1/1	0.94	0.14	94,94,94,94	0
55	MG	13	1720	1/1	0.94	0.06	136,136,136,136	0
55	MG	1H	3512	1/1	0.94	0.22	103,103,103,103	0
55	MG	13	1726	1/1	0.94	0.11	134,134,134,134	0
55	MG	13	1702	1/1	0.94	0.07	140,140,140,140	0
55	MG	1H	3523	1/1	0.94	0.06	135,135,135,135	0
55	MG	1H	3524	1/1	0.94	0.08	123,123,123,123	0
55	MG	1G	1721	1/1	0.94	0.08	121,121,121,121	0
55	MG	14	3161	1/1	0.94	0.26	72,72,72,72	0
55	MG	1H	3121	1/1	0.94	0.15	82,82,82,82	0
55	MG	1H	3010	1/1	0.94	0.21	57,57,57,57	0
55	MG	1H	3324	1/1	0.94	0.08	96,96,96,96	0
55	MG	14	3224	1/1	0.94	0.46	87,87,87,87	0
55	MG	14	3225	1/1	0.94	0.30	94,94,94,94	0
55	MG	1H	3534	1/1	0.94	0.07	115,115,115,115	0
55	MG	14	3440	1/1	0.94	0.06	131,131,131,131	0
55	MG	1H	3011	1/1	0.94	0.22	65,65,65,65	0
55	MG	1H	3296	1/1	0.94	0.21	92,92,92,92	0
55	MG	14	3045	1/1	0.94	0.18	66,66,66,66	0
55	MG	14	3450	1/1	0.94	0.08	113,113,113,113	0
55	MG	1G	1743	1/1	0.94	0.07	128,128,128,128	0
55	MG	1H	3359	1/1	0.94	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3113	1/1	0.94	0.20	85,85,85,85	0
55	MG	14	3473	1/1	0.94	0.09	108,108,108,108	0
55	MG	1H	3036	1/1	0.94	0.11	72,72,72,72	0
55	MG	1H	3212	1/1	0.94	0.10	97,97,97,97	0
55	MG	14	3477	1/1	0.94	0.14	117,117,117,117	0
55	MG	14	3479	1/1	0.94	0.17	108,108,108,108	0
55	MG	1H	3165	1/1	0.94	0.09	81,81,81,81	0
55	MG	14	3302	1/1	0.94	0.11	82,82,82,82	0
55	MG	2K	104	1/1	0.94	0.07	153,153,153,153	0
55	MG	14	3239	1/1	0.94	0.08	101,101,101,101	0
55	MG	1H	3270	1/1	0.94	0.38	92,92,92,92	0
55	MG	13	1728	1/1	0.94	0.09	119,119,119,119	0
55	MG	1H	3147	1/1	0.94	0.39	76,76,76,76	0
55	MG	1H	3169	1/1	0.94	0.20	68,68,68,68	0
55	MG	1H	3245	1/1	0.94	0.20	74,74,74,74	0
55	MG	13	1626	1/1	0.94	0.14	69,69,69,69	0
55	MG	1H	3247	1/1	0.94	0.28	89,89,89,89	0
55	MG	1H	3371	1/1	0.94	0.10	72,72,72,72	0
55	MG	16	212	1/1	0.94	0.10	126,126,126,126	0
55	MG	13	1611	1/1	0.94	0.09	103,103,103,103	0
55	MG	1H	3150	1/1	0.94	0.24	81,81,81,81	0
55	MG	1H	3406	1/1	0.94	0.10	103,103,103,103	0
55	MG	14	3010	1/1	0.94	0.17	57,57,57,57	0
55	MG	14	3011	1/1	0.94	0.22	54,54,54,54	0
55	MG	1H	3041	1/1	0.94	0.17	68,68,68,68	0
55	MG	1H	3017	1/1	0.94	0.12	66,66,66,66	0
55	MG	1H	3419	1/1	0.94	0.07	90,90,90,90	0
55	MG	1H	3060	1/1	0.94	0.12	79,79,79,79	0
55	MG	1G	1648	1/1	0.94	0.09	109,109,109,109	0
55	MG	1H	3433	1/1	0.94	0.08	92,92,92,92	0
55	MG	1H	3313	1/1	0.94	0.21	100,100,100,100	0
55	MG	1H	3177	1/1	0.94	0.11	69,69,69,69	0
55	MG	13	1647	1/1	0.95	0.12	87,87,87,87	0
55	MG	1H	3430	1/1	0.95	0.11	99,99,99,99	0
55	MG	1H	3527	1/1	0.95	0.08	118,118,118,118	0
55	MG	13	1721	1/1	0.95	0.10	100,100,100,100	0
55	MG	1G	1667	1/1	0.95	0.10	92,92,92,92	0
55	MG	14	3150	1/1	0.95	0.19	64,64,64,64	0
55	MG	14	3357	1/1	0.95	0.10	83,83,83,83	0
55	MG	14	3358	1/1	0.95	0.07	102,102,102,102	0
55	MG	14	3380	1/1	0.95	0.14	92,92,92,92	0
55	MG	1H	3272	1/1	0.95	0.11	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3049	1/1	0.95	0.16	65,65,65,65	0
55	MG	14	3419	1/1	0.95	0.07	104,104,104,104	0
55	MG	1H	3441	1/1	0.95	0.14	97,97,97,97	0
55	MG	1H	3536	1/1	0.95	0.07	130,130,130,130	0
55	MG	1G	1603	1/1	0.95	0.14	99,99,99,99	0
55	MG	1G	1604	1/1	0.95	0.21	106,106,106,106	0
55	MG	14	3447	1/1	0.95	0.14	90,90,90,90	0
55	MG	1H	3448	1/1	0.95	0.12	79,79,79,79	0
55	MG	1H	3100	1/1	0.95	0.24	76,76,76,76	0
55	MG	14	3057	1/1	0.95	0.14	63,63,63,63	0
55	MG	1H	3240	1/1	0.95	0.28	91,91,91,91	0
55	MG	14	3455	1/1	0.95	0.10	131,131,131,131	0
55	MG	14	3456	1/1	0.95	0.11	125,125,125,125	0
55	MG	14	3060	1/1	0.95	0.32	56,56,56,56	0
55	MG	14	3459	1/1	0.95	0.06	114,114,114,114	0
55	MG	2K	101	1/1	0.95	0.20	84,84,84,84	0
55	MG	14	3468	1/1	0.95	0.06	134,134,134,134	0
55	MG	14	3261	1/1	0.95	0.22	68,68,68,68	0
55	MG	1H	3547	1/1	0.95	0.10	85,85,85,85	0
55	MG	13	1722	1/1	0.95	0.08	103,103,103,103	0
55	MG	13	1608	1/1	0.95	0.18	91,91,91,91	0
55	MG	1H	3470	1/1	0.95	0.08	98,98,98,98	0
55	MG	1H	3105	1/1	0.95	0.09	62,62,62,62	0
55	MG	14	3483	1/1	0.95	0.09	113,113,113,113	0
55	MG	1H	3483	1/1	0.95	0.07	117,117,117,117	0
55	MG	13	1625	1/1	0.95	0.17	63,63,63,63	0
55	MG	1H	3144	1/1	0.95	0.32	86,86,86,86	0
55	MG	1H	3264	1/1	0.95	0.44	85,85,85,85	0
55	MG	13	1710	1/1	0.95	0.07	119,119,119,119	0
55	MG	1G	1726	1/1	0.95	0.04	137,137,137,137	0
55	MG	1H	3354	1/1	0.95	0.16	82,82,82,82	0
55	MG	1G	1729	1/1	0.95	0.11	112,112,112,112	0
55	MG	13	1712	1/1	0.95	0.06	119,119,119,119	0
55	MG	1G	1737	1/1	0.95	0.26	147,147,147,147	0
55	MG	1G	1738	1/1	0.95	0.12	108,108,108,108	0
55	MG	14	3228	1/1	0.95	0.17	93,93,93,93	0
55	MG	1G	1739	1/1	0.95	0.11	112,112,112,112	0
55	MG	1H	3398	1/1	0.95	0.08	110,110,110,110	0
55	MG	1G	1655	1/1	0.95	0.19	88,88,88,88	0
55	MG	1H	3402	1/1	0.95	0.11	110,110,110,110	0
55	MG	1H	3161	1/1	0.95	0.20	73,73,73,73	0
55	MG	45	201	1/1	0.95	0.20	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3085	1/1	0.95	0.19	67,67,67,67	0
55	MG	1H	3521	1/1	0.95	0.07	125,125,125,125	0
55	MG	14	3288	1/1	0.95	0.07	88,88,88,88	0
55	MG	1H	3074	1/1	0.95	0.33	63,63,63,63	0
55	MG	E5	102	1/1	0.95	0.10	116,116,116,116	0
55	MG	13	1714	1/1	0.95	0.07	120,120,120,120	0
55	MG	1G	1661	1/1	0.95	0.09	82,82,82,82	0
55	MG	1G	1697	1/1	0.95	0.22	83,83,83,83	0
55	MG	1G	1662	1/1	0.95	0.09	96,96,96,96	0
55	MG	14	3367	1/1	0.96	0.07	87,87,87,87	0
55	MG	14	3379	1/1	0.96	0.05	99,99,99,99	0
55	MG	1H	3128	1/1	0.96	0.32	77,77,77,77	0
55	MG	14	3391	1/1	0.96	0.07	80,80,80,80	0
55	MG	14	3392	1/1	0.96	0.10	65,65,65,65	0
55	MG	1H	3500	1/1	0.96	0.10	87,87,87,87	0
55	MG	16	211	1/1	0.96	0.05	114,114,114,114	0
55	MG	14	3401	1/1	0.96	0.07	69,69,69,69	0
55	MG	14	3408	1/1	0.96	0.07	103,103,103,103	0
55	MG	1H	3055	1/1	0.96	0.08	55,55,55,55	0
55	MG	14	3430	1/1	0.96	0.07	114,114,114,114	0
55	MG	14	3252	1/1	0.96	0.52	79,79,79,79	0
55	MG	13	1725	1/1	0.96	0.13	157,157,157,157	0
55	MG	14	3006	1/1	0.96	0.17	53,53,53,53	0
55	MG	14	3445	1/1	0.96	0.07	104,104,104,104	0
55	MG	14	3204	1/1	0.96	0.09	104,104,104,104	0
55	MG	1H	3232	1/1	0.96	0.07	82,82,82,82	0
55	MG	1H	3411	1/1	0.96	0.08	110,110,110,110	0
55	MG	1H	3416	1/1	0.96	0.12	77,77,77,77	0
55	MG	1H	3515	1/1	0.96	0.07	125,125,125,125	0
55	MG	1H	3518	1/1	0.96	0.12	99,99,99,99	0
55	MG	1H	3519	1/1	0.96	0.07	132,132,132,132	0
55	MG	14	3262	1/1	0.96	0.16	84,84,84,84	0
55	MG	14	3061	1/1	0.96	0.14	79,79,79,79	0
55	MG	14	3112	1/1	0.96	0.27	81,81,81,81	0
55	MG	14	3460	1/1	0.96	0.06	94,94,94,94	0
55	MG	14	3461	1/1	0.96	0.16	88,88,88,88	0
55	MG	14	3462	1/1	0.96	0.12	100,100,100,100	0
55	MG	1H	3013	1/1	0.96	0.12	57,57,57,57	0
55	MG	1H	3426	1/1	0.96	0.09	68,68,68,68	0
55	MG	14	3472	1/1	0.96	0.05	121,121,121,121	0
55	MG	13	1719	1/1	0.96	0.04	140,140,140,140	0
55	MG	13	1697	1/1	0.96	0.09	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1640	1/1	0.96	0.11	95,95,95,95	0
55	MG	1H	3286	1/1	0.96	0.17	69,69,69,69	0
55	MG	1H	3287	1/1	0.96	0.11	67,67,67,67	0
55	MG	14	3480	1/1	0.96	0.07	90,90,90,90	0
55	MG	1H	3442	1/1	0.96	0.06	97,97,97,97	0
55	MG	14	3482	1/1	0.96	0.08	118,118,118,118	0
55	MG	1H	3444	1/1	0.96	0.09	111,111,111,111	0
55	MG	1H	3093	1/1	0.96	0.12	67,67,67,67	0
55	MG	14	3485	1/1	0.96	0.07	73,73,73,73	0
55	MG	1H	3535	1/1	0.96	0.14	115,115,115,115	0
55	MG	1H	3070	1/1	0.96	0.20	72,72,72,72	0
55	MG	1G	1732	1/1	0.96	0.10	113,113,113,113	0
55	MG	1G	1733	1/1	0.96	0.06	105,105,105,105	0
55	MG	14	3076	1/1	0.96	0.19	68,68,68,68	0
55	MG	1G	1735	1/1	0.96	0.06	128,128,128,128	0
55	MG	1H	3082	1/1	0.96	0.14	66,66,66,66	0
55	MG	1H	3542	1/1	0.96	0.06	123,123,123,123	0
55	MG	1H	3459	1/1	0.96	0.07	86,86,86,86	0
55	MG	13	1711	1/1	0.96	0.10	86,86,86,86	0
55	MG	1H	3256	1/1	0.96	0.06	82,82,82,82	0
55	MG	1G	1614	1/1	0.96	0.08	89,89,89,89	0
55	MG	1H	3467	1/1	0.96	0.06	101,101,101,101	0
55	MG	13	1718	1/1	0.96	0.10	125,125,125,125	0
55	MG	14	3188	1/1	0.96	0.18	71,71,71,71	0
55	MG	13	1723	1/1	0.96	0.06	107,107,107,107	0
55	MG	25	201	1/1	0.96	0.04	129,129,129,129	0
55	MG	1H	3474	1/1	0.96	0.18	88,88,88,88	0
55	MG	14	3344	1/1	0.96	0.40	89,89,89,89	0
55	MG	13	1724	1/1	0.96	0.17	113,113,113,113	0
55	MG	55	203	1/1	0.96	0.20	88,88,88,88	0
55	MG	1H	3374	1/1	0.96	0.07	64,64,64,64	0
55	MG	1H	3484	1/1	0.96	0.09	98,98,98,98	0
55	MG	1H	3394	1/1	0.96	0.15	119,119,119,119	0
55	MG	14	3354	1/1	0.96	0.08	92,92,92,92	0
55	MG	2L	103	1/1	0.96	0.10	109,109,109,109	0
55	MG	1H	3054	1/1	0.96	0.23	66,66,66,66	0
55	MG	1H	3244	1/1	0.96	0.31	75,75,75,75	0
55	MG	1G	1731	1/1	0.97	0.07	117,117,117,117	0
55	MG	1H	3392	1/1	0.97	0.06	70,70,70,70	0
55	MG	14	3436	1/1	0.97	0.05	99,99,99,99	0
55	MG	21	301	1/1	0.97	0.07	69,69,69,69	0
55	MG	13	1703	1/1	0.97	0.04	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3441	1/1	0.97	0.04	113,113,113,113	0
55	MG	14	3442	1/1	0.97	0.16	84,84,84,84	0
55	MG	1H	3478	1/1	0.97	0.05	99,99,99,99	0
55	MG	1H	3480	1/1	0.97	0.05	100,100,100,100	0
55	MG	13	1627	1/1	0.97	0.14	79,79,79,79	0
55	MG	14	3237	1/1	0.97	0.06	79,79,79,79	0
55	MG	1H	3528	1/1	0.97	0.10	115,115,115,115	0
55	MG	1H	3183	1/1	0.97	0.06	55,55,55,55	0
55	MG	1G	1741	1/1	0.97	0.03	140,140,140,140	0
55	MG	1H	3487	1/1	0.97	0.18	123,123,123,123	0
55	MG	J8	101	1/1	0.97	0.18	83,83,83,83	0
55	MG	1H	3531	1/1	0.97	0.07	116,116,116,116	0
55	MG	1G	1745	1/1	0.97	0.08	143,143,143,143	0
55	MG	1H	3399	1/1	0.97	0.11	109,109,109,109	0
55	MG	1H	3145	1/1	0.97	0.08	84,84,84,84	0
55	MG	1H	3447	1/1	0.97	0.06	78,78,78,78	0
55	MG	1H	3495	1/1	0.97	0.05	122,122,122,122	0
55	MG	14	3466	1/1	0.97	0.07	104,104,104,104	0
55	MG	14	3467	1/1	0.97	0.15	95,95,95,95	0
55	MG	14	3119	1/1	0.97	0.41	82,82,82,82	0
55	MG	14	3470	1/1	0.97	0.05	136,136,136,136	0
55	MG	14	3471	1/1	0.97	0.05	109,109,109,109	0
55	MG	1H	3404	1/1	0.97	0.07	71,71,71,71	0
55	MG	1H	3499	1/1	0.97	0.06	116,116,116,116	0
55	MG	1H	3006	1/1	0.97	0.10	58,58,58,58	0
55	MG	1H	3501	1/1	0.97	0.09	93,93,93,93	0
55	MG	14	3476	1/1	0.97	0.15	110,110,110,110	0
55	MG	1H	3502	1/1	0.97	0.10	125,125,125,125	0
55	MG	1H	3453	1/1	0.97	0.06	89,89,89,89	0
55	MG	14	3169	1/1	0.97	0.11	69,69,69,69	0
55	MG	1H	3407	1/1	0.97	0.07	83,83,83,83	0
55	MG	1H	3506	1/1	0.97	0.05	102,102,102,102	0
55	MG	14	3128	1/1	0.97	0.49	85,85,85,85	0
55	MG	14	3043	1/1	0.97	0.10	84,84,84,84	0
55	MG	1H	3171	1/1	0.97	0.22	70,70,70,70	0
55	MG	1H	3509	1/1	0.97	0.07	126,126,126,126	0
55	MG	14	3488	1/1	0.97	0.13	81,81,81,81	0
55	MG	1H	3510	1/1	0.97	0.05	125,125,125,125	0
55	MG	14	3361	1/1	0.97	0.21	75,75,75,75	0
55	MG	14	3362	1/1	0.97	0.07	79,79,79,79	0
55	MG	1H	3101	1/1	0.97	0.10	64,64,64,64	0
55	MG	14	3370	1/1	0.97	0.06	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3373	1/1	0.97	0.07	101,101,101,101	0
55	MG	1H	3464	1/1	0.97	0.06	86,86,86,86	0
55	MG	1J	210	1/1	0.97	0.05	105,105,105,105	0
55	MG	1G	1720	1/1	0.97	0.05	97,97,97,97	0
55	MG	14	3381	1/1	0.97	0.10	69,69,69,69	0
55	MG	14	3389	1/1	0.97	0.06	102,102,102,102	0
55	MG	13	1715	1/1	0.97	0.06	108,108,108,108	0
55	MG	1H	3516	1/1	0.97	0.05	126,126,126,126	0
55	MG	1H	3517	1/1	0.97	0.05	121,121,121,121	0
55	MG	39	301	1/1	0.97	0.07	108,108,108,108	0
55	MG	1H	3377	1/1	0.97	0.06	66,66,66,66	0
55	MG	14	3400	1/1	0.97	0.10	61,61,61,61	0
55	MG	1H	3379	1/1	0.97	0.06	71,71,71,71	0
55	MG	14	3403	1/1	0.97	0.07	88,88,88,88	0
55	MG	14	3407	1/1	0.97	0.06	109,109,109,109	0
55	MG	1H	3390	1/1	0.97	0.09	67,67,67,67	0
55	MG	14	3410	1/1	0.97	0.06	109,109,109,109	0
55	MG	14	3415	1/1	0.97	0.05	96,96,96,96	0
55	MG	14	3416	1/1	0.97	0.06	87,87,87,87	0
55	MG	14	3417	1/1	0.97	0.07	119,119,119,119	0
55	MG	14	3099	1/1	0.97	0.06	75,75,75,75	0
55	MG	14	3420	1/1	0.97	0.04	125,125,125,125	0
55	MG	14	3423	1/1	0.97	0.07	101,101,101,101	0
56	ZN	5A	101	1/1	0.97	0.05	155,155,155,155	0
55	MG	14	3424	1/1	0.97	0.10	113,113,113,113	0
55	MG	14	3425	1/1	0.98	0.09	89,89,89,89	0
55	MG	14	3426	1/1	0.98	0.08	96,96,96,96	0
55	MG	14	3037	1/1	0.98	0.14	48,48,48,48	0
55	MG	14	3432	1/1	0.98	0.04	107,107,107,107	0
55	MG	14	3434	1/1	0.98	0.03	102,102,102,102	0
55	MG	13	1707	1/1	0.98	0.05	101,101,101,101	0
55	MG	14	3094	1/1	0.98	0.04	68,68,68,68	0
55	MG	1H	3403	1/1	0.98	0.06	78,78,78,78	0
55	MG	14	3438	1/1	0.98	0.06	104,104,104,104	0
55	MG	14	3439	1/1	0.98	0.05	109,109,109,109	0
55	MG	13	1713	1/1	0.98	0.07	94,94,94,94	0
55	MG	1H	3375	1/1	0.98	0.07	65,65,65,65	0
55	MG	1H	3466	1/1	0.98	0.15	78,78,78,78	0
55	MG	14	3444	1/1	0.98	0.05	113,113,113,113	0
55	MG	1H	3520	1/1	0.98	0.04	104,104,104,104	0
55	MG	1H	3376	1/1	0.98	0.06	78,78,78,78	0
55	MG	1H	3019	1/1	0.98	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1673	1/1	0.98	0.11	86,86,86,86	0
55	MG	1H	3471	1/1	0.98	0.07	89,89,89,89	0
55	MG	1H	3472	1/1	0.98	0.09	94,94,94,94	0
55	MG	14	3452	1/1	0.98	0.03	96,96,96,96	0
55	MG	1H	3526	1/1	0.98	0.04	106,106,106,106	0
55	MG	1H	3381	1/1	0.98	0.08	78,78,78,78	0
55	MG	1H	3475	1/1	0.98	0.05	69,69,69,69	0
55	MG	1H	3415	1/1	0.98	0.06	91,91,91,91	0
55	MG	14	3109	1/1	0.98	0.14	77,77,77,77	0
55	MG	14	3053	1/1	0.98	0.15	49,49,49,49	0
55	MG	1H	3382	1/1	0.98	0.06	61,61,61,61	0
55	MG	1H	3479	1/1	0.98	0.04	97,97,97,97	0
55	MG	14	3463	1/1	0.98	0.13	98,98,98,98	0
55	MG	14	3284	1/1	0.98	0.36	83,83,83,83	0
55	MG	14	3465	1/1	0.98	0.05	92,92,92,92	0
55	MG	1H	3383	1/1	0.98	0.05	74,74,74,74	0
55	MG	1H	3423	1/1	0.98	0.06	64,64,64,64	0
55	MG	14	3058	1/1	0.98	0.09	64,64,64,64	0
55	MG	14	3469	1/1	0.98	0.04	115,115,115,115	0
55	MG	1H	3384	1/1	0.98	0.05	72,72,72,72	0
55	MG	1H	3486	1/1	0.98	0.05	104,104,104,104	0
55	MG	1H	3538	1/1	0.98	0.04	67,67,67,67	0
55	MG	1H	3539	1/1	0.98	0.09	123,123,123,123	0
55	MG	1H	3541	1/1	0.98	0.07	89,89,89,89	0
55	MG	14	3356	1/1	0.98	0.05	64,64,64,64	0
55	MG	1H	3427	1/1	0.98	0.07	71,71,71,71	0
55	MG	1H	3387	1/1	0.98	0.04	83,83,83,83	0
55	MG	14	3478	1/1	0.98	0.11	102,102,102,102	0
55	MG	1H	3489	1/1	0.98	0.04	108,108,108,108	0
55	MG	1H	3490	1/1	0.98	0.07	88,88,88,88	0
55	MG	14	3366	1/1	0.98	0.05	71,71,71,71	0
55	MG	1H	3491	1/1	0.98	0.08	97,97,97,97	0
55	MG	1H	3388	1/1	0.98	0.04	77,77,77,77	0
55	MG	14	3371	1/1	0.98	0.05	66,66,66,66	0
55	MG	1H	3389	1/1	0.98	0.05	72,72,72,72	0
55	MG	14	3486	1/1	0.98	0.04	64,64,64,64	0
55	MG	14	3377	1/1	0.98	0.05	91,91,91,91	0
55	MG	1H	3434	1/1	0.98	0.04	109,109,109,109	0
55	MG	14	3489	1/1	0.98	0.08	91,91,91,91	0
55	MG	1H	3438	1/1	0.98	0.06	69,69,69,69	0
55	MG	13	1704	1/1	0.98	0.05	89,89,89,89	0
55	MG	14	3383	1/1	0.98	0.04	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1716	1/1	0.98	0.06	97,97,97,97	0
55	MG	14	3390	1/1	0.98	0.05	70,70,70,70	0
55	MG	1G	1724	1/1	0.98	0.05	95,95,95,95	0
55	MG	1H	3443	1/1	0.98	0.07	97,97,97,97	0
55	MG	13	1717	1/1	0.98	0.16	91,91,91,91	0
55	MG	14	3394	1/1	0.98	0.09	100,100,100,100	0
55	MG	1G	1727	1/1	0.98	0.11	126,126,126,126	0
55	MG	29	301	1/1	0.98	0.13	67,67,67,67	0
55	MG	14	3398	1/1	0.98	0.18	109,109,109,109	0
55	MG	13	1705	1/1	0.98	0.12	85,85,85,85	0
55	MG	1H	3397	1/1	0.98	0.06	90,90,90,90	0
55	MG	1G	1730	1/1	0.98	0.05	100,100,100,100	0
55	MG	1H	3449	1/1	0.98	0.07	90,90,90,90	0
55	MG	1H	3350	1/1	0.98	0.09	72,72,72,72	0
55	MG	14	3409	1/1	0.98	0.10	99,99,99,99	0
55	MG	1H	3452	1/1	0.98	0.05	86,86,86,86	0
55	MG	14	3412	1/1	0.98	0.07	91,91,91,91	0
55	MG	14	3414	1/1	0.98	0.07	99,99,99,99	0
55	MG	1G	1734	1/1	0.98	0.07	114,114,114,114	0
55	MG	13	1698	1/1	0.98	0.07	77,77,77,77	0
55	MG	1H	3511	1/1	0.98	0.07	127,127,127,127	0
55	MG	14	3418	1/1	0.98	0.10	70,70,70,70	0
55	MG	1H	3401	1/1	0.98	0.12	82,82,82,82	0
55	MG	1H	3455	1/1	0.98	0.04	97,97,97,97	0
55	MG	14	3421	1/1	0.98	0.04	73,73,73,73	0
56	ZN	3E	301	1/1	0.98	0.21	109,109,109,109	0
55	MG	14	3422	1/1	0.98	0.04	110,110,110,110	0
55	MG	1H	3514	1/1	0.98	0.12	129,129,129,129	0
55	MG	14	3148	1/1	0.98	0.10	79,79,79,79	0
55	MG	14	3352	1/1	0.99	0.02	65,65,65,65	0
55	MG	14	3353	1/1	0.99	0.03	74,74,74,74	0
55	MG	1H	3544	1/1	0.99	0.03	59,59,59,59	0
55	MG	1H	3393	1/1	0.99	0.06	99,99,99,99	0
55	MG	1H	3498	1/1	0.99	0.03	71,71,71,71	0
55	MG	1H	3424	1/1	0.99	0.05	57,57,57,57	0
55	MG	14	3443	1/1	0.99	0.07	106,106,106,106	0
55	MG	1H	3456	1/1	0.99	0.05	86,86,86,86	0
55	MG	14	3359	1/1	0.99	0.04	87,87,87,87	0
55	MG	14	3360	1/1	0.99	0.05	64,64,64,64	0
55	MG	1H	3458	1/1	0.99	0.05	67,67,67,67	0
55	MG	1H	3425	1/1	0.99	0.03	63,63,63,63	0
55	MG	14	3363	1/1	0.99	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3364	1/1	0.99	0.03	91,91,91,91	0
55	MG	14	3451	1/1	0.99	0.08	92,92,92,92	0
55	MG	14	3365	1/1	0.99	0.05	72,72,72,72	0
55	MG	1H	3503	1/1	0.99	0.07	75,75,75,75	0
55	MG	1H	3460	1/1	0.99	0.03	94,94,94,94	0
55	MG	14	3368	1/1	0.99	0.05	75,75,75,75	0
55	MG	14	3369	1/1	0.99	0.06	63,63,63,63	0
55	MG	14	3458	1/1	0.99	0.07	94,94,94,94	0
55	MG	1G	1722	1/1	0.99	0.04	83,83,83,83	0
55	MG	1H	3372	1/1	0.99	0.04	68,68,68,68	0
55	MG	14	3372	1/1	0.99	0.05	65,65,65,65	0
55	MG	1H	3463	1/1	0.99	0.03	64,64,64,64	0
55	MG	14	3374	1/1	0.99	0.06	80,80,80,80	0
55	MG	14	3375	1/1	0.99	0.06	75,75,75,75	0
55	MG	14	3376	1/1	0.99	0.05	84,84,84,84	0
55	MG	1H	3405	1/1	0.99	0.07	94,94,94,94	0
55	MG	14	3378	1/1	0.99	0.08	99,99,99,99	0
55	MG	1H	3428	1/1	0.99	0.06	60,60,60,60	0
55	MG	1H	3429	1/1	0.99	0.06	65,65,65,65	0
55	MG	1H	3378	1/1	0.99	0.04	59,59,59,59	0
55	MG	14	3382	1/1	0.99	0.04	93,93,93,93	0
55	MG	1H	3396	1/1	0.99	0.03	84,84,84,84	0
55	MG	14	3384	1/1	0.99	0.03	75,75,75,75	0
55	MG	14	3385	1/1	0.99	0.05	96,96,96,96	0
55	MG	14	3387	1/1	0.99	0.04	77,77,77,77	0
55	MG	14	3388	1/1	0.99	0.04	80,80,80,80	0
55	MG	1H	3469	1/1	0.99	0.12	109,109,109,109	0
55	MG	1H	3432	1/1	0.99	0.09	85,85,85,85	0
55	MG	1H	3048	1/1	0.99	0.05	67,67,67,67	0
55	MG	1H	3003	1/1	0.99	0.11	51,51,51,51	0
55	MG	1H	3473	1/1	0.99	0.03	95,95,95,95	0
55	MG	1H	3435	1/1	0.99	0.07	60,60,60,60	0
55	MG	14	3395	1/1	0.99	0.06	73,73,73,73	0
55	MG	1H	3436	1/1	0.99	0.05	55,55,55,55	0
55	MG	14	3397	1/1	0.99	0.08	79,79,79,79	0
55	MG	1H	3437	1/1	0.99	0.09	94,94,94,94	0
55	MG	14	3399	1/1	0.99	0.11	63,63,63,63	0
55	MG	1H	3477	1/1	0.99	0.05	80,80,80,80	0
55	MG	1H	3410	1/1	0.99	0.04	82,82,82,82	0
55	MG	14	3402	1/1	0.99	0.06	76,76,76,76	0
55	MG	13	1701	1/1	0.99	0.02	89,89,89,89	0
55	MG	14	3404	1/1	0.99	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3405	1/1	0.99	0.06	65,65,65,65	0
55	MG	1H	3412	1/1	0.99	0.04	103,103,103,103	0
55	MG	1H	3481	1/1	0.99	0.03	77,77,77,77	0
55	MG	1H	3482	1/1	0.99	0.07	99,99,99,99	0
55	MG	1J	208	1/1	0.99	0.06	104,104,104,104	0
55	MG	1J	209	1/1	0.99	0.07	110,110,110,110	0
55	MG	1H	3413	1/1	0.99	0.07	83,83,83,83	0
55	MG	14	3411	1/1	0.99	0.05	60,60,60,60	0
55	MG	1H	3400	1/1	0.99	0.08	87,87,87,87	0
55	MG	14	3413	1/1	0.99	0.07	74,74,74,74	0
55	MG	1H	3485	1/1	0.99	0.07	97,97,97,97	0
55	MG	1H	3445	1/1	0.99	0.05	76,76,76,76	0
55	MG	14	3090	1/1	0.99	0.21	53,53,53,53	0
55	MG	1H	3446	1/1	0.99	0.05	112,112,112,112	0
55	MG	1H	3532	1/1	0.99	0.17	91,91,91,91	0
55	MG	1H	3533	1/1	0.99	0.11	88,88,88,88	0
55	MG	1H	3391	1/1	0.99	0.05	84,84,84,84	0
55	MG	1H	3417	1/1	0.99	0.04	70,70,70,70	0
55	MG	1H	3418	1/1	0.99	0.06	60,60,60,60	0
55	MG	1H	3450	1/1	0.99	0.07	100,100,100,100	0
55	MG	13	1700	1/1	0.99	0.04	97,97,97,97	0
55	MG	1H	3420	1/1	0.99	0.04	71,71,71,71	0
55	MG	1H	3540	1/1	0.99	0.04	54,54,54,54	0
55	MG	14	3428	1/1	0.99	0.05	92,92,92,92	0
55	MG	1H	3494	1/1	0.99	0.03	88,88,88,88	0
55	MG	14	3431	1/1	0.99	0.07	106,106,106,106	0
55	MG	1H	3421	1/1	0.99	0.07	63,63,63,63	0
55	MG	14	3433	1/1	0.99	0.04	105,105,105,105	0
56	ZN	5I	101	1/1	0.99	0.03	138,138,138,138	0
55	MG	1H	3496	1/1	0.99	0.03	91,91,91,91	0
56	ZN	32	302	1/1	0.99	0.22	114,114,114,114	0
55	MG	14	3350	1/1	0.99	0.06	73,73,73,73	0
55	MG	14	3351	1/1	0.99	0.06	82,82,82,82	0
55	MG	1H	3457	1/1	1.00	0.03	79,79,79,79	0
55	MG	1H	3386	1/1	1.00	0.05	72,72,72,72	0
55	MG	1H	3422	1/1	1.00	0.06	70,70,70,70	0
55	MG	14	3406	1/1	1.00	0.15	76,76,76,76	0
55	MG	14	3349	1/1	1.00	0.09	66,66,66,66	0
55	MG	1H	3414	1/1	1.00	0.04	51,51,51,51	0
55	MG	1H	3461	1/1	1.00	0.10	77,77,77,77	0
55	MG	14	3453	1/1	1.00	0.04	73,73,73,73	0
55	MG	1H	3507	1/1	1.00	0.06	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3386	1/1	1.00	0.03	67,67,67,67	0
55	MG	1H	3439	1/1	1.00	0.04	63,63,63,63	0
55	MG	1H	3440	1/1	1.00	0.02	59,59,59,59	0
55	MG	14	3427	1/1	1.00	0.02	72,72,72,72	0
55	MG	1H	3380	1/1	1.00	0.02	63,63,63,63	0
55	MG	14	3429	1/1	1.00	0.04	79,79,79,79	0
55	MG	1H	3385	1/1	1.00	0.03	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.