



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 12:01 pm BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

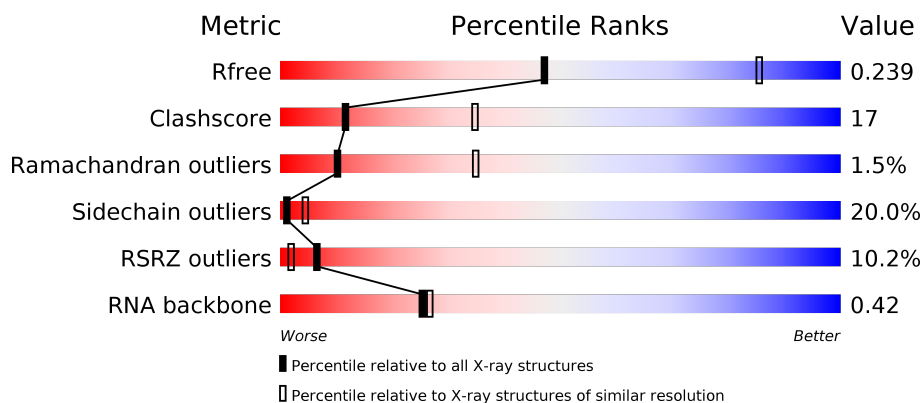
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>33%</div> <div>43%</div> <div>19%</div> <div>••</div> </div> </div>
1	1G	1522	<div> <div>5%</div> <div> <div></div> <div>33%</div> <div>46%</div> <div>17%</div> <div>••</div> </div> </div>
2	12	256	<div> <div>7%</div> <div> <div></div> <div>45%</div> <div>38%</div> <div>10%</div> <div>7%</div> </div> </div>
2	1E	256	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>39%</div> <div>12%</div> <div>7%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	1L	76	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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Mol	Chain	Length	Quality of chain
28	11	276	
28	19	276	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	

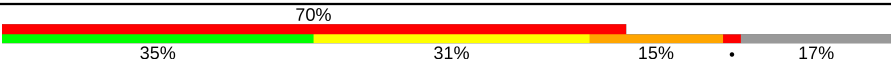

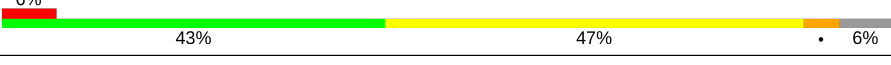
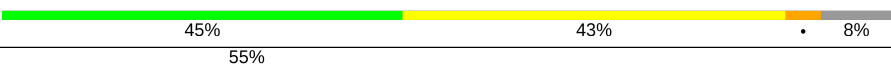

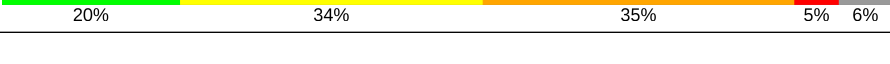
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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	

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Mol	Chain	Length	Quality of chain
53	K5	54	
53	O8	54	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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

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

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



## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 299951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- 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			
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	127	Total	C	N	O		0	0	0
			1009	639	197	173				

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			
13	4A	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	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	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 25 is a RNA chain called mRNA.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	45	2	Total	Mg	0	0
			2	2		
56	P8	1	Total	Mg	0	0
			1	1		
56	85	1	Total	Mg	0	0
			1	1		
56	32	1	Total	Mg	0	0
			1	1		
56	C5	1	Total	Mg	0	0
			1	1		
56	13	152	Total	Mg	0	0
			152	152		
56	1J	10	Total	Mg	0	0
			10	10		
56	35	1	Total	Mg	0	0
			1	1		
56	16	15	Total	Mg	0	0
			15	15		
56	25	2	Total	Mg	0	0
			2	2		
56	M5	1	Total	Mg	0	0
			1	1		
56	21	2	Total	Mg	0	0
			2	2		
56	31	1	Total	Mg	0	0
			1	1		
56	L8	1	Total	Mg	0	0
			1	1		
56	15	1	Total	Mg	0	0
			1	1		
56	3I	2	Total	Mg	0	0
			2	2		
56	I8	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	52	1	Total 1	Mg 1	0	0
56	5E	1	Total 1	Mg 1	0	0
56	29	2	Total 2	Mg 2	0	0
56	41	2	Total 2	Mg 2	0	0
56	2K	7	Total 7	Mg 7	0	0
56	J8	1	Total 1	Mg 1	0	0
56	39	3	Total 3	Mg 3	0	0
56	1G	88	Total 88	Mg 88	0	0
56	11	2	Total 2	Mg 2	0	0
56	1H	506	Total 506	Mg 506	0	0
56	E5	1	Total 1	Mg 1	0	0
56	88	2	Total 2	Mg 2	0	0
56	49	1	Total 1	Mg 1	0	0
56	14	426	Total 426	Mg 426	0	0
56	78	2	Total 2	Mg 2	0	0
56	6A	1	Total 1	Mg 1	0	0
56	4K	1	Total 1	Mg 1	0	0
56	G8	1	Total 1	Mg 1	0	0
56	2L	3	Total 3	Mg 3	0	0

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

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

- Molecule 58 is water.

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

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

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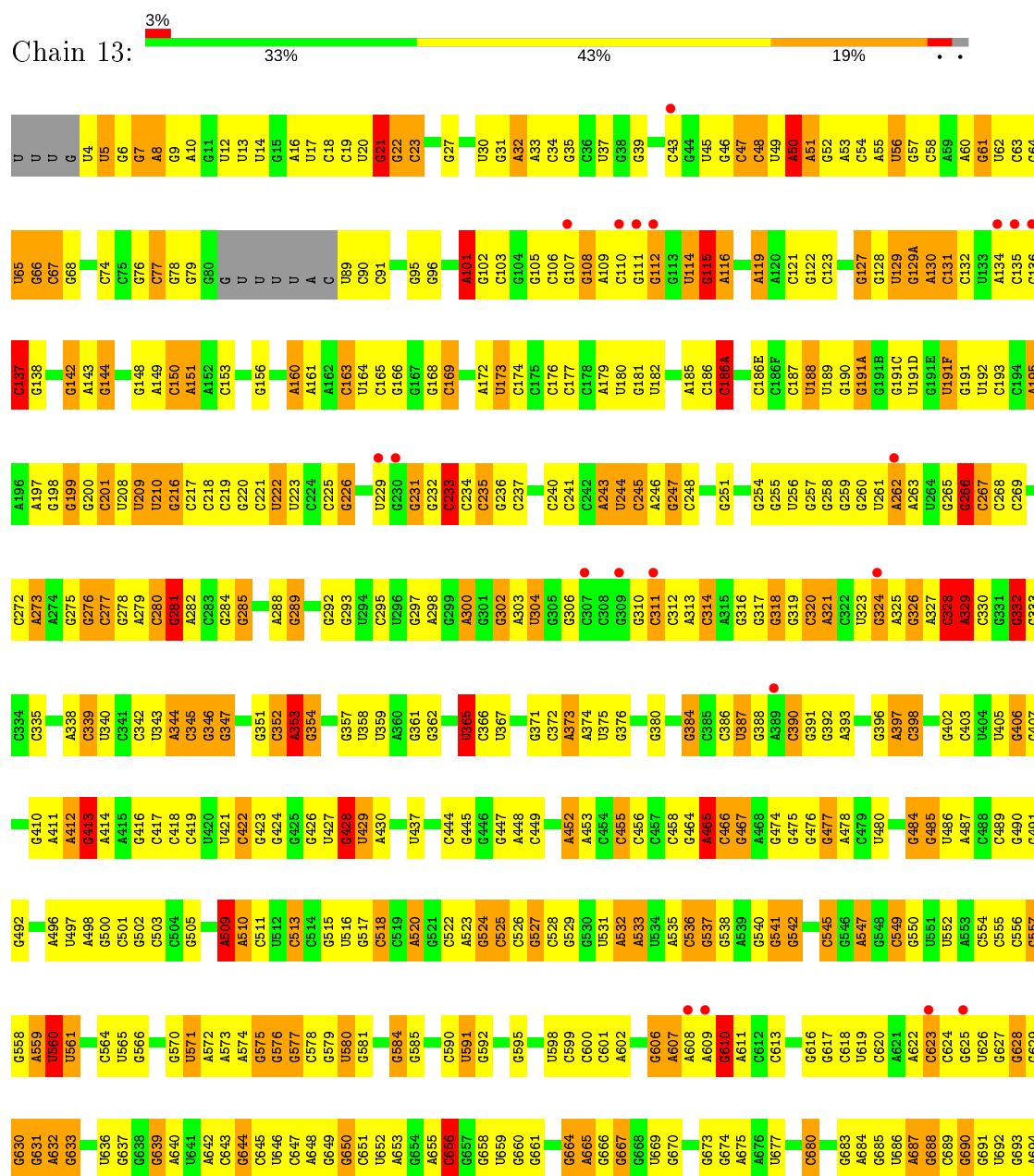
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	L5	2	Total	O	0	0
			2	2		



### 3 Residue-property plots

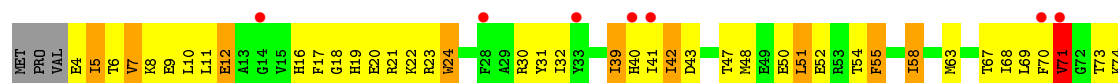
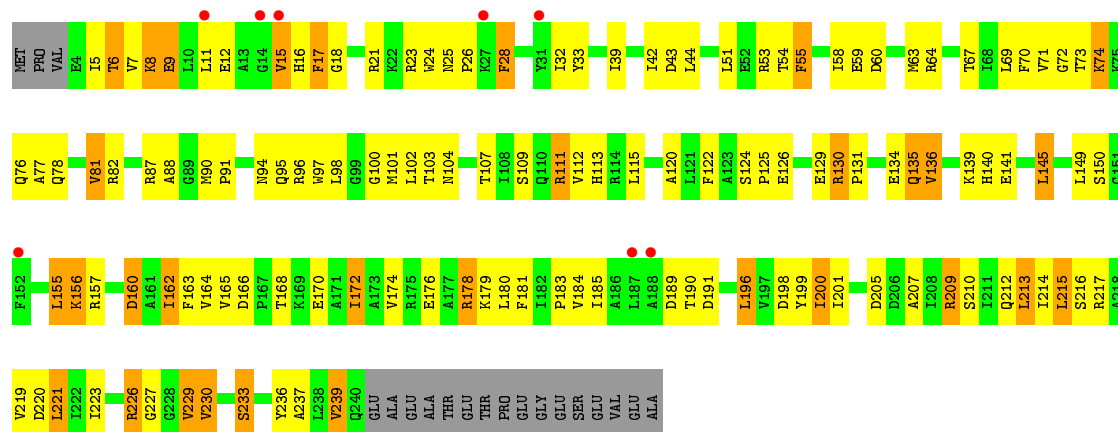
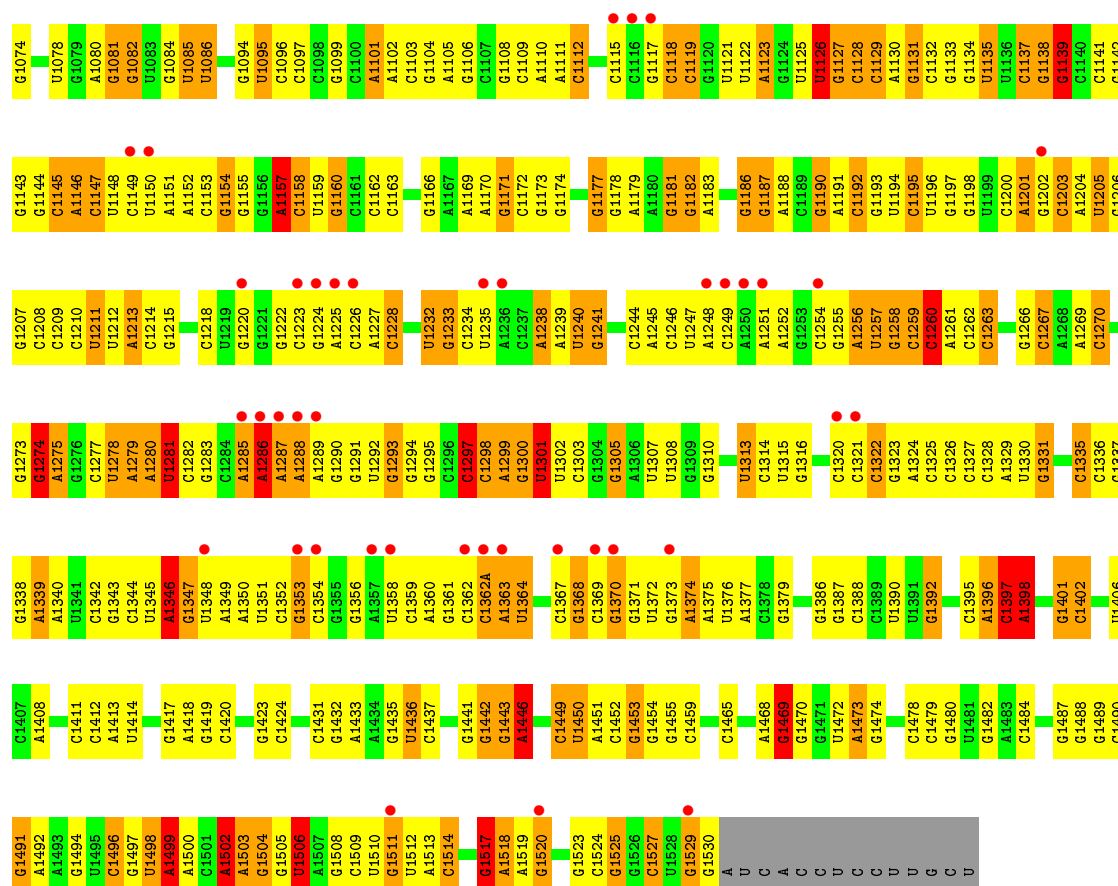
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

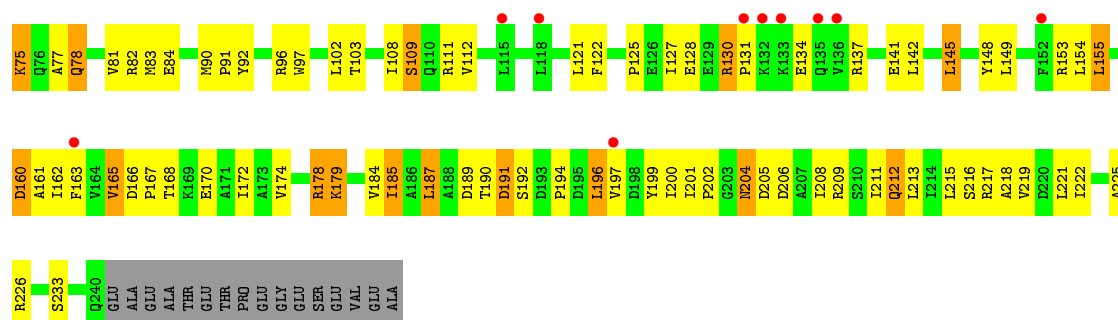
- Molecule 1: 16S ribosomal RNA





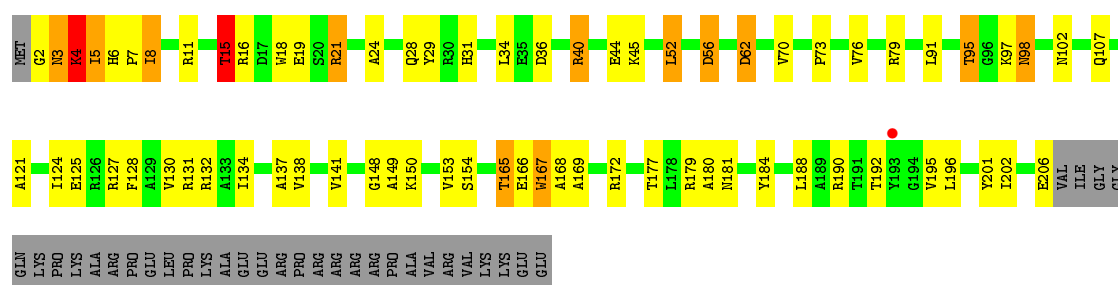
A1015	U950	G880	G731	G660	G584	G521	C443	U967	G297	G216	G146	G64
A1016	G951	G881	G735	G661	G585	C522	C443	G371	A296	C217	G147	U65
G1017	U952	C882	C736	G662	C586	A523		G372	G299	C218	G148	G66
U1018	G953	C883	C737	A663	C587	A524		C371	G300		G149	C67
C1019	G954	U884	C738	A664	C588	C525	C447	A373	G301	U222	C150	G68
U1020	U955	G885	A737	A665	C589	C526	A448	A374	G302	U223		G69
	U956	G886	C739	G666	C590	G527	C449	U975	A303		C154	G73
G1024	U957	G887		G667	U591	C528	C450	G376	U304	G230	G155	C74
U1025	A958	G888	G742	G668	C596	G529	A451	G377			G156	C75
G1026	A959	A819	U743			A530	A452		C308	G236	G157	C76
U1027	U960	U820	C744	U672		U531	A453	G380	G309	G237		C77
G1028	U961	G821	C745	G673	C600	A532	A454	C381		G238	A160	G78
C1028A	C962	G822	A746	G674	C601	A533	C455	A382	C312		A161	G79
G963	G963	G823	C747	A675	A602	U534	C456	A383	A313		A162	G80
U1029	A964	C824	C748	A676	U603	A535	C457		C314		C163	G
G1030	A965	G825	C749	U677	G604	C536	C458	C386	A315	C242	C164	U
U1031	G966	C826	G750	U678	U605	G537	G464	U387	G316	U244	U164	U
A1032	C967	U827	G751	G679	G606	A538	A465	U388	G317	C245	C165	U
G1032A	A968	A828	C754	C580	A607	A539	C466	A389		A246	G166	U
G1032B	A969	G829	G755		A608	G540	G467	C390	C320	G247	G167	A
U1033	C970	G830	G760	G683	A611	G541	A468	G391	A321		U170	C
A1035	C971	U831	G761	G684	G612	G542	G474	G392	C322	A250	A171	U89
G1036	C972		G762	G685	C613		G475	A397	U323	G251	A172	C90
C1037	G973	G836	C763	U686	C614	C545	G476	C398	G326	G254	U173	C91
U1038	A974	G837	G764	G687	C615	A546	G477	G399	A327	G255	C174	G92
U1039	A975	G838		G688		A547	A478	G400	C328		C175	U97
U1040	G976	U841		G689	G616		C479		A329	G257	C176	C99
	A977	C842		G690	G617	G550	U480	C403	G330		C177	A101
C1043	A978	U843	U772	U551	U552	U551	G481	G406	G331	U261	A179	G105
A1044	C979	C848	G773	U553	C618	A553		G407		A262	U180	G106
G1045	U981	C849	G774	G693	C620	C554	G484	A408			G181	G107
A1046	U982	U850	G775	A694		C555	G485	G409	C337	G265	U182	G108
U1047	A983	G852	G776	G703	G623	C556	G487	G410	A338	G266	G183	G109
G1048	C984	G853	G777	A704	G624			A411	C339	C267	G184	
U1049	C985	G854	G778	U705	U626	A559	G490	G412	U340	C268	A135	
G1050	A986	G855		U706	G627	U560		G413	C341	C269	G110	G111
C1051	G987	G856	A781	A706	G628	U561	A495	A414	C342		C186E	
U1052		C857	A782	C707	G629	C562	A496		U343	C272	C186F	U114
U1053	U991	G858	C783	C708	G630	A563	U497	U420	A344	A273	C187	G115
C1054	U992	A859	C784	G709	G631	C564	A498	U421	A274	A274	U188	A116
A1055	G993	G860	G785	G710	G632	U565	G500	C422	G275	G275	U189	G117
U1056	A994	G861		G711	G633	U566	C501	G423			G190	
G1057	C995	C862	U789	A712		C567	G502	G424	A349	G276	G191A	G121
G1058		U863	A790	G713	G637	G568	C503	G426	G350	G277	G191B	G122
C1059	G998	A864	G791	G714	G638	C569	C504	G426	G351	G278	G191C	G123
G1060	C998A	A865	A792	A715	G639	U570	G505	U427	C352	A279	U191D	
U1061	U999	C866	U793	G716	A640	U571	G506	G428	A383	G281	G191E	U129
U1062	A1000	G867	A794	C717		A572		U429	G354	A282	U191F	G129A
C1063	G1001	C868	C795	G718	G644	A573	A509	A430	C355	C283	G191	A130
G1064	G1002	G869		C719	G645	A574	A510	A431	A356	G284	G192	C131
U1065	G1003	C940	G800	C720	U646	G575	C511	A432	A357	G285	U192	G132
G1066	A1004	G941	U801	G721	C647	G576	C512	C433	G358	G286	C193	C137
A1067	A1005	A872	A802	A722	A648	G577	C513	U434	U359		C194	
G1068	C1006	G874	G803	U723	G649	U578	C435	A360	A360	G289	A195	
C1069		G875	U804	G724	G650	G579	U516	C436	G361	C290	A196	A141
U1070	G1009	G876	C805	G724	C651	U580	G517	U437	G362	C290	A197	G142
G1071		C877	C806	A728	U652	G582	C518	G438	A363	G293	G198	G143
C1072	G1013	G878	A807	A729	A653	U582	C519	A439			U209	A144
U1073	A1014	C879	C808	G730		A583	A520	A440	C366	U296	U210	G145





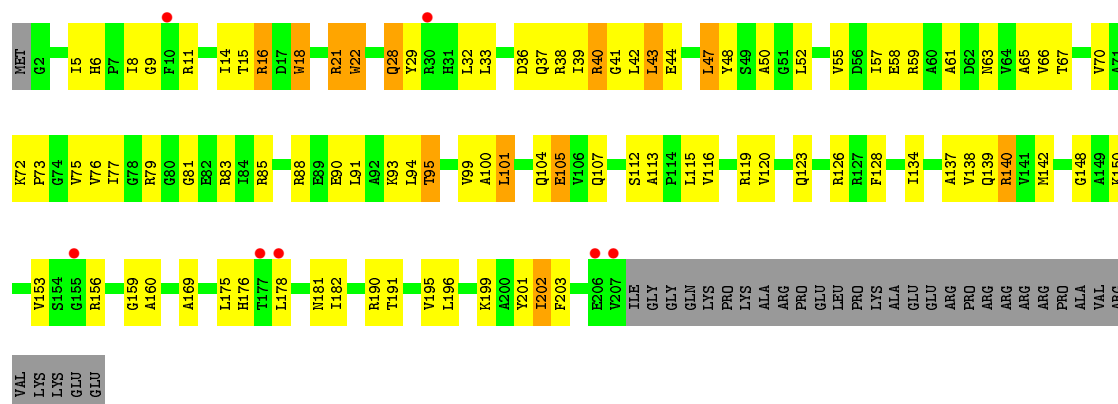
• Molecule 3: 30S ribosomal protein S3

Chain 2E: 56% 24% 5% 14%



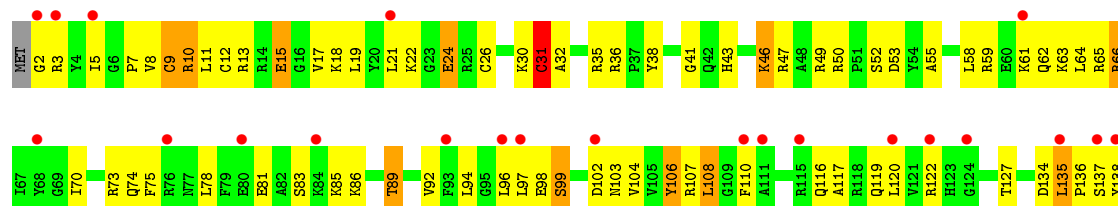
• Molecule 3: 30S ribosomal protein S3

Chain 22: 3% 47% 34% 5% 14%



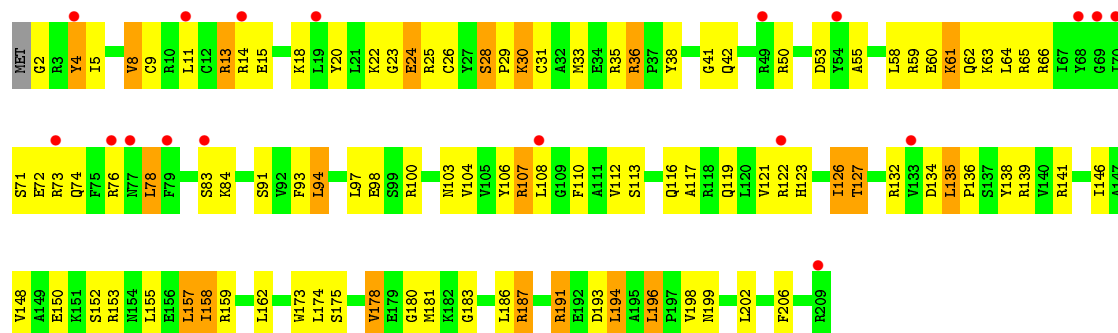
• Molecule 4: 30S ribosomal protein S4

Chain 3E: 14% 45% 46% 8%

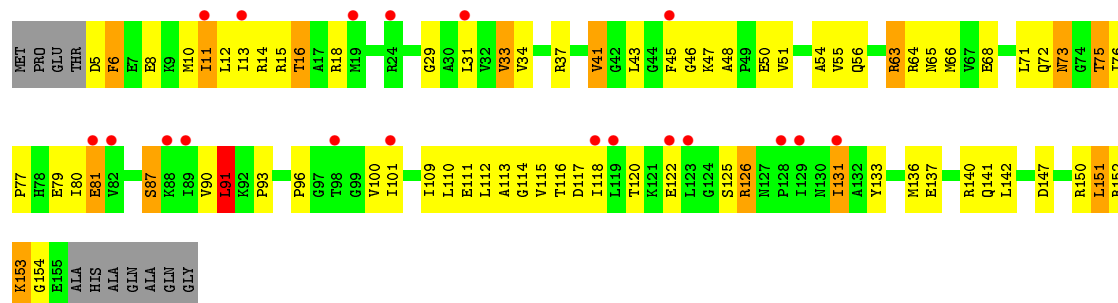




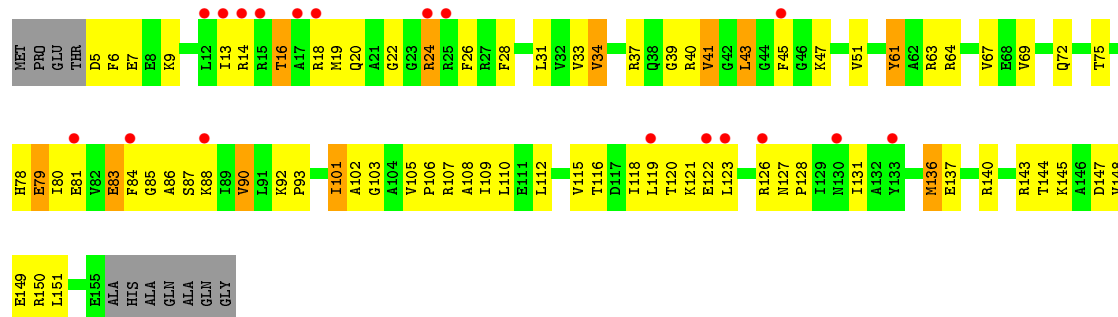
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

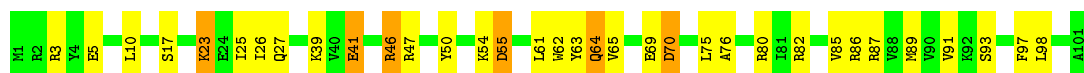


• Molecule 5: 30S ribosomal protein S5

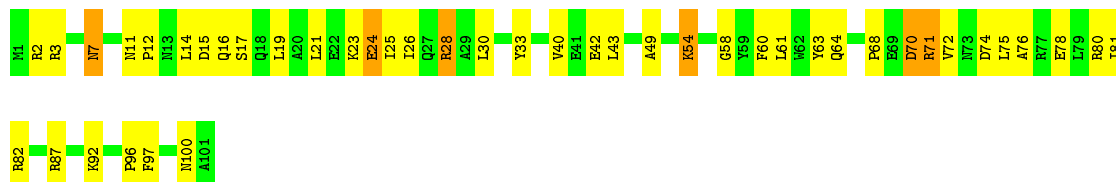


• Molecule 6: 30S ribosomal protein S6

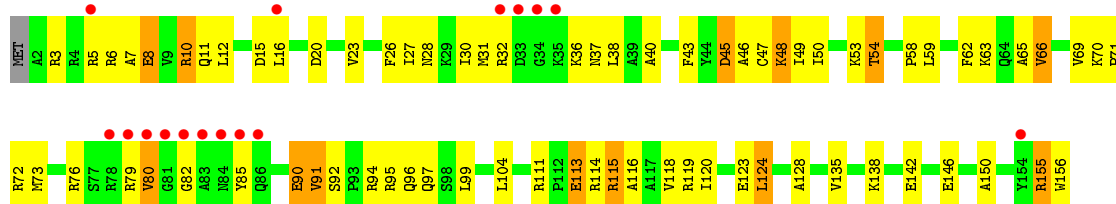




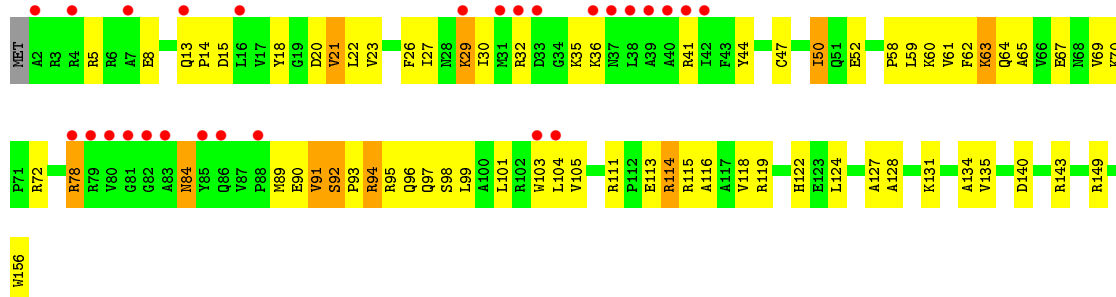
- Molecule 6: 30S ribosomal protein S6



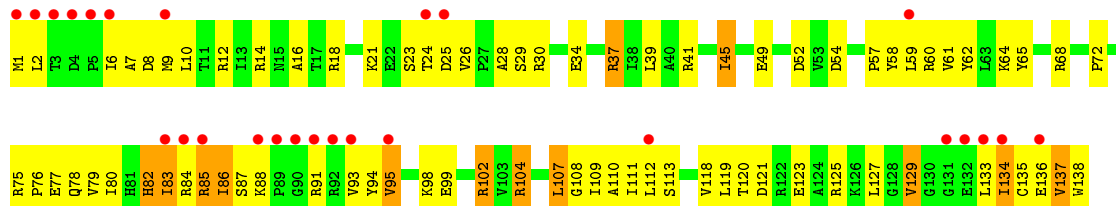
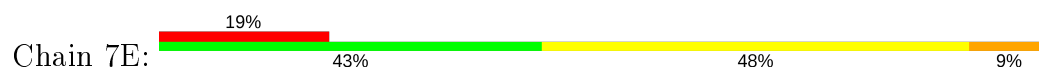
- Molecule 7: 30S ribosomal protein S7



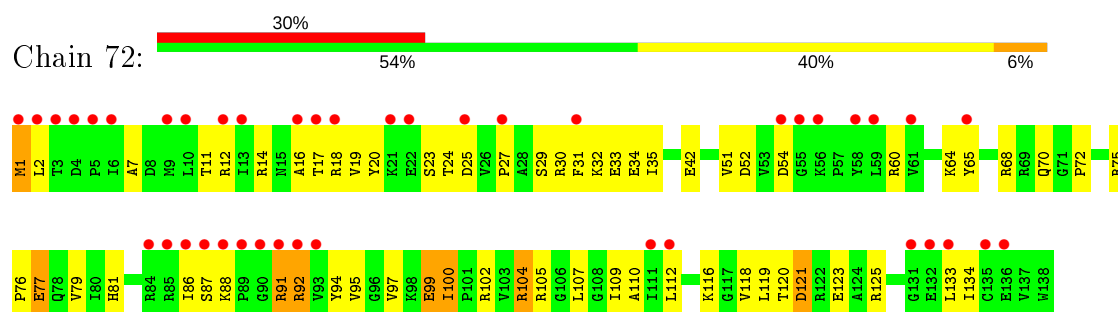
- Molecule 7: 30S ribosomal protein S7



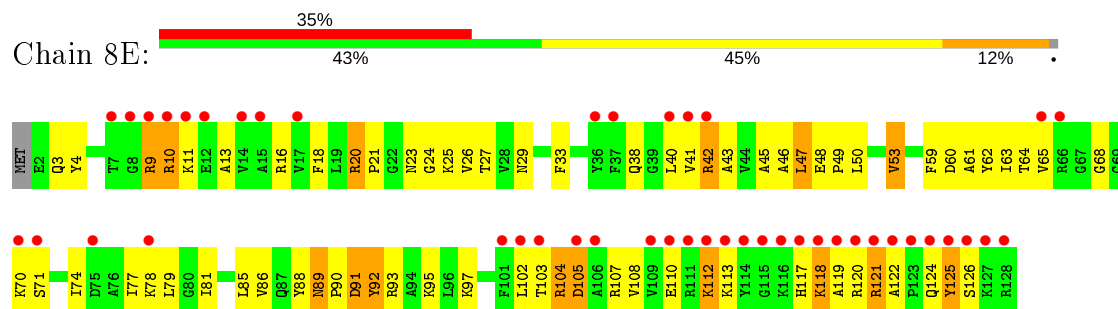
- Molecule 8: 30S ribosomal protein S8



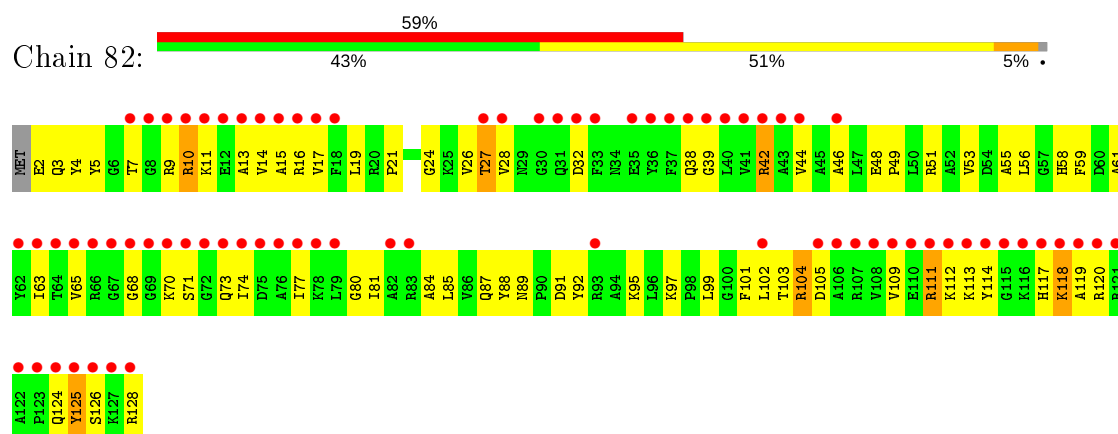
- Molecule 8: 30S ribosomal protein S8



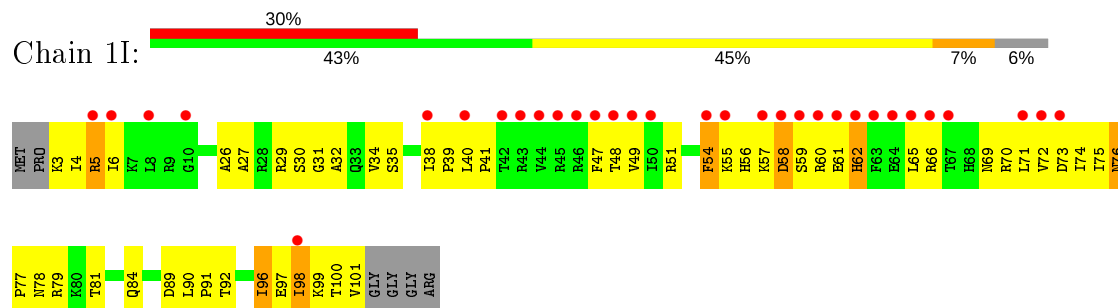
- Molecule 9: 30S ribosomal protein S9



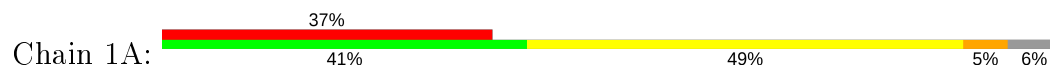
- Molecule 9: 30S ribosomal protein S9



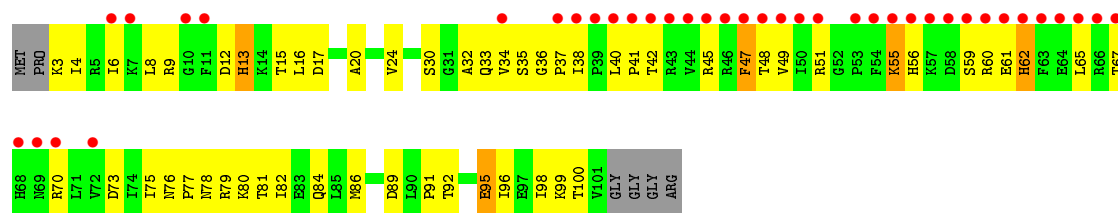
- Molecule 10: 30S ribosomal protein S10



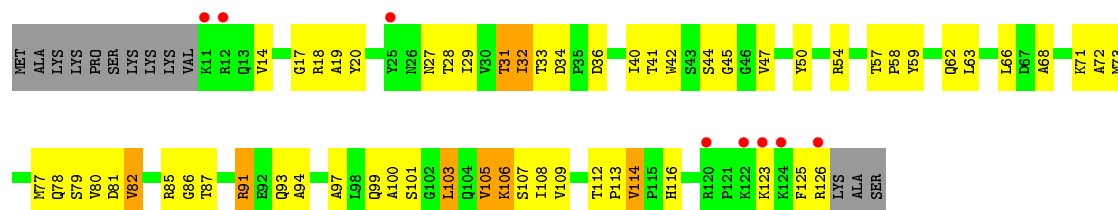
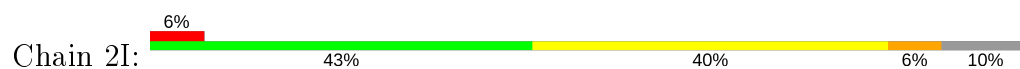
- Molecule 10: 30S ribosomal protein S10



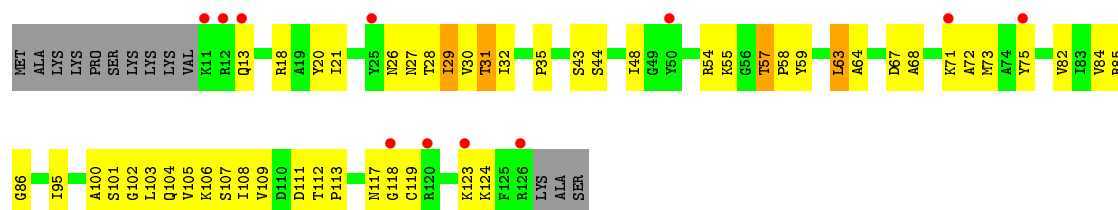




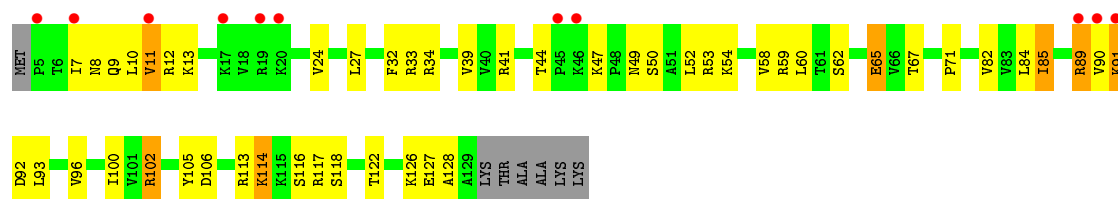
• Molecule 11: 30S ribosomal protein S11



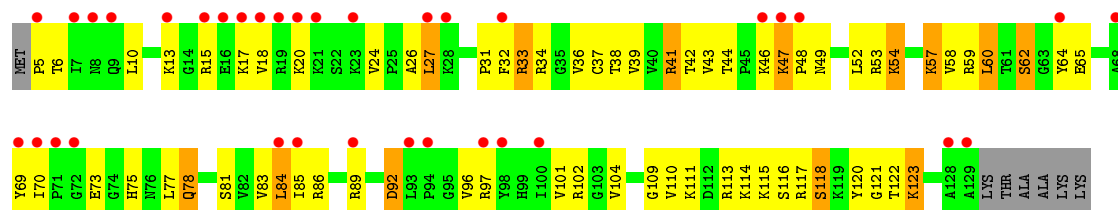
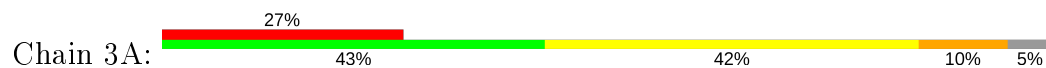
• Molecule 11: 30S ribosomal protein S11



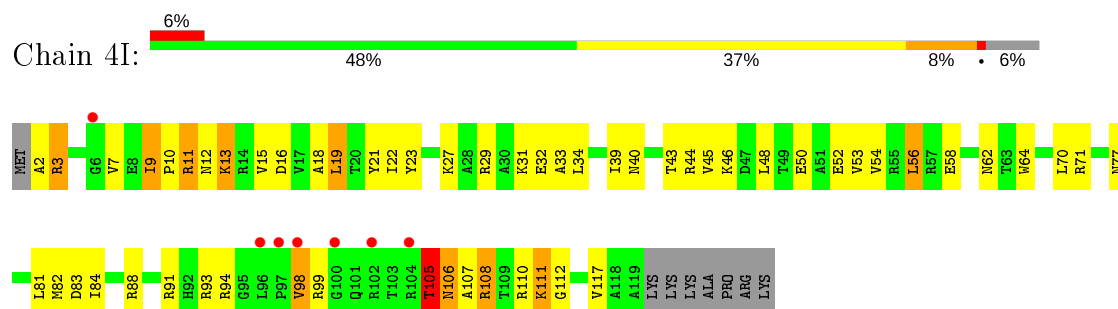
• Molecule 12: 30S ribosomal protein S12



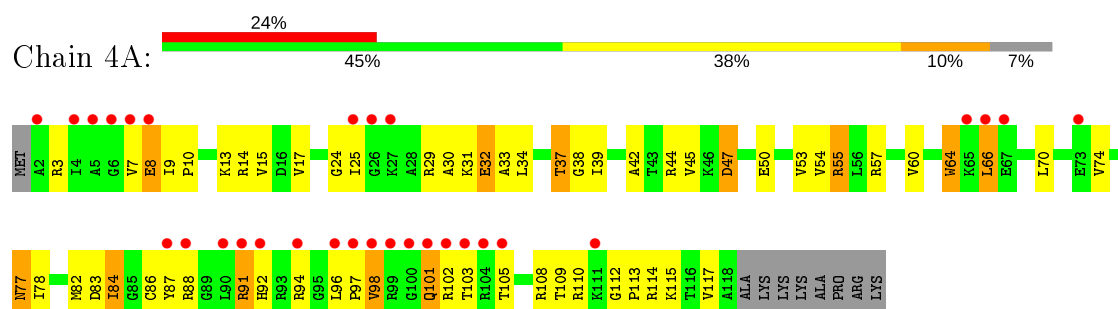
• Molecule 12: 30S ribosomal protein S12



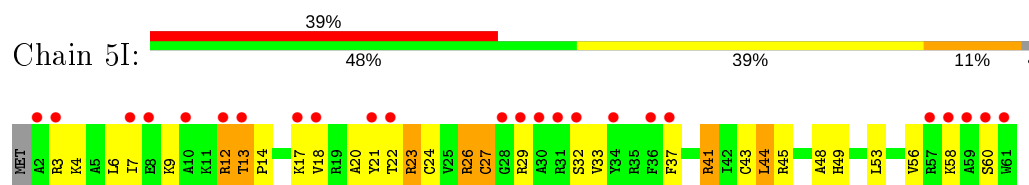
- Molecule 13: 30S ribosomal protein S13



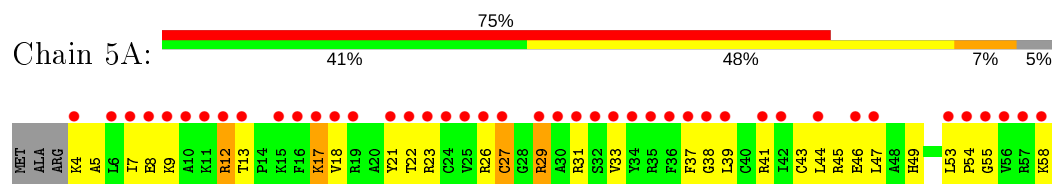
- Molecule 13: 30S ribosomal protein S13



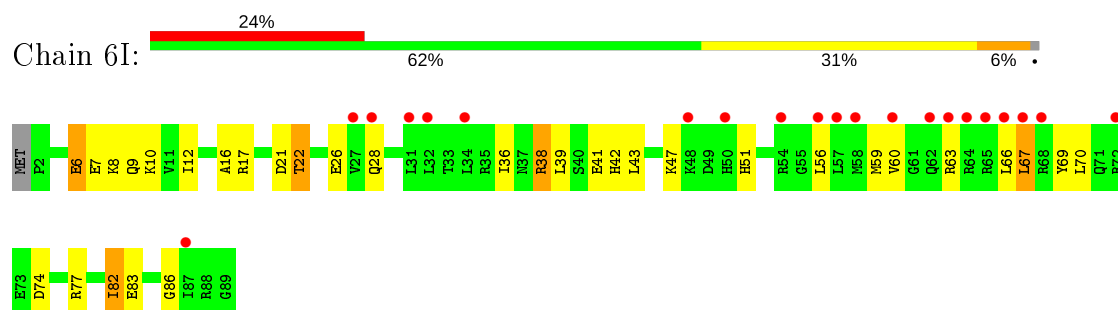
- Molecule 14: 30S ribosomal protein S14 type Z



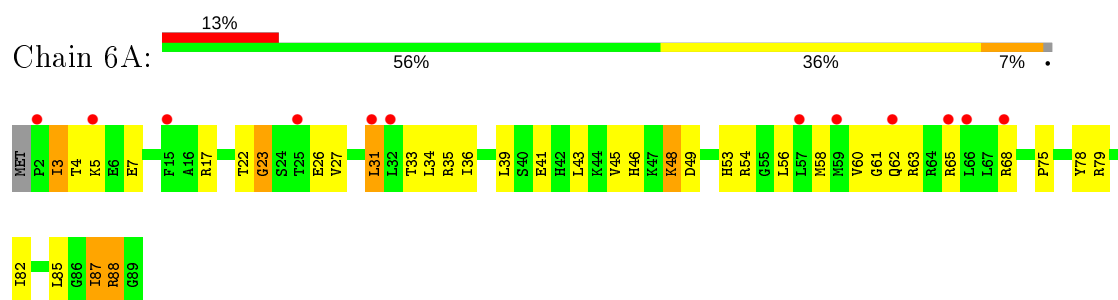
- Molecule 14: 30S ribosomal protein S14 type Z



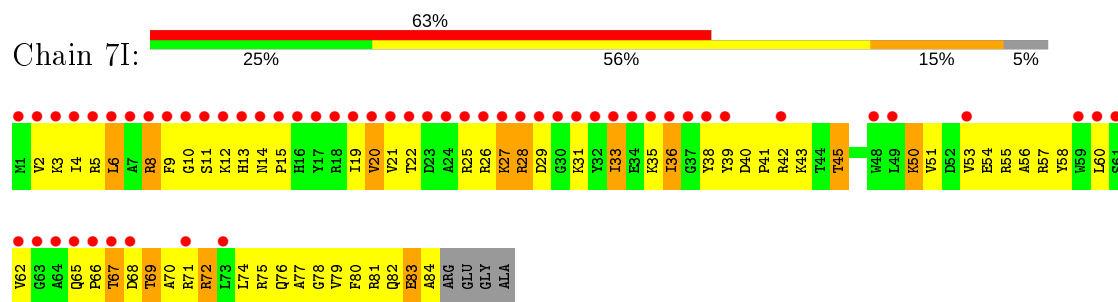
- Molecule 15: 30S ribosomal protein S15



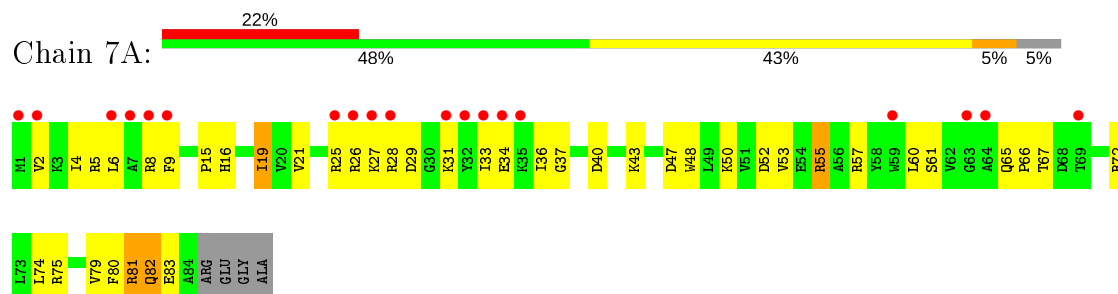
- Molecule 15: 30S ribosomal protein S15



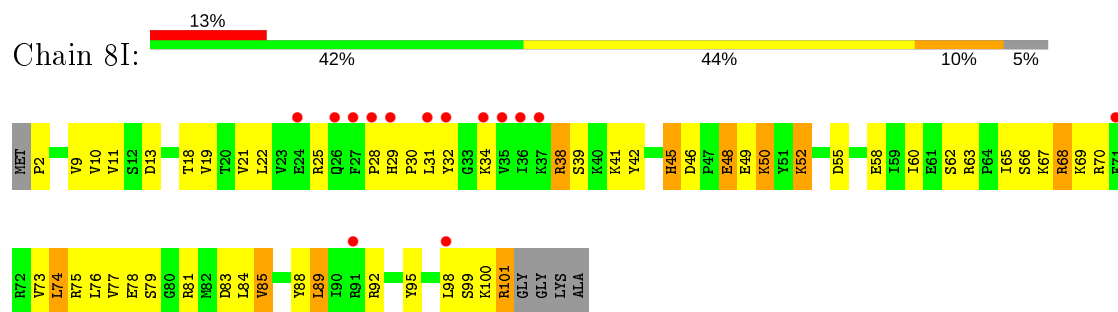
• Molecule 16: 30S ribosomal protein S16



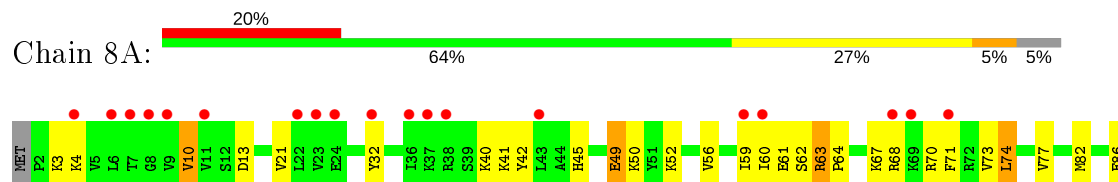
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17



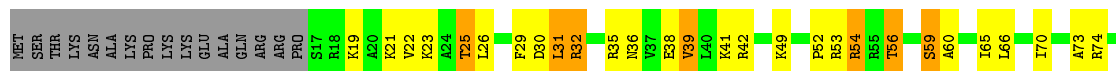
• Molecule 17: 30S ribosomal protein S17





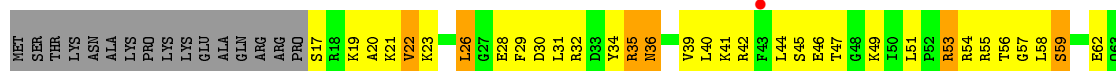
• Molecule 18: 30S ribosomal protein S18

Chain 9I: 48% 26% 8% 18%



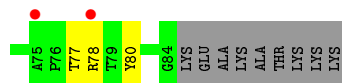
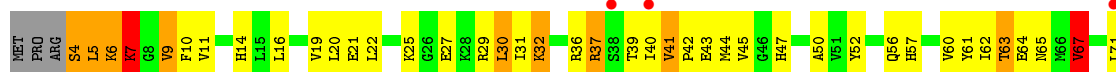
• Molecule 18: 30S ribosomal protein S18

Chain 9A: 2% 33% 41% 8% 18%



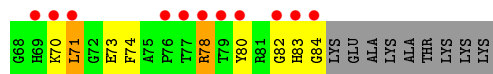
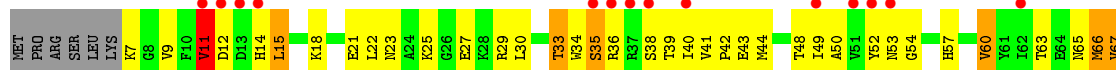
• Molecule 19: 30S ribosomal protein S19

Chain AI: 5% 40% 35% 10% 13%



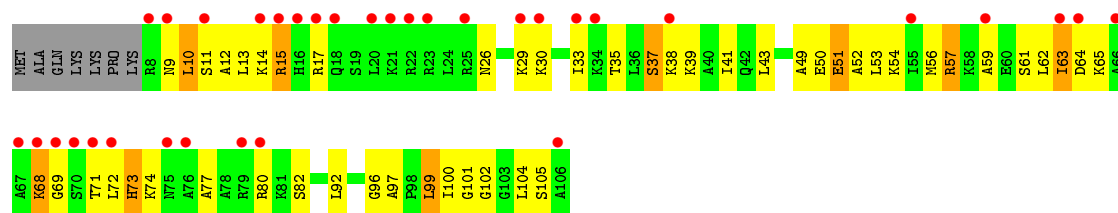
• Molecule 19: 30S ribosomal protein S19

Chain AA: 27% 34% 40% 9% 16%

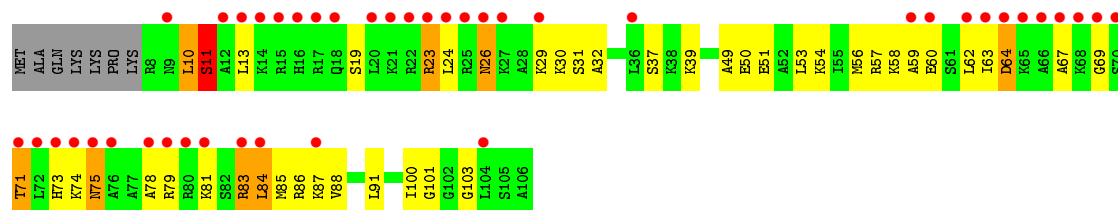
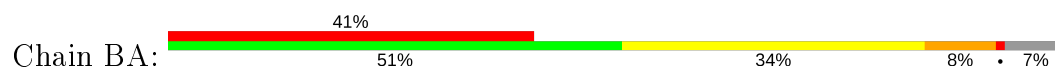


• Molecule 20: 30S ribosomal protein S20

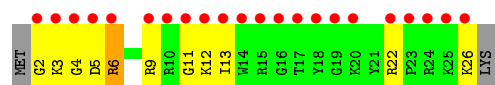
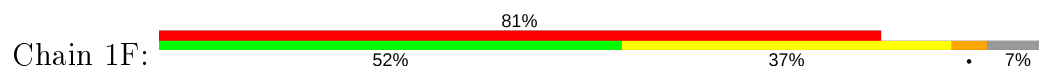
Chain BI: 32% 46% 39% 8% 7%



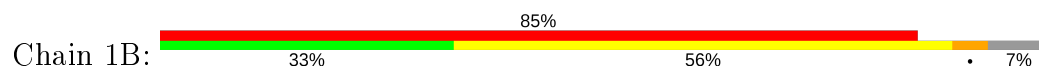
• Molecule 20: 30S ribosomal protein S20



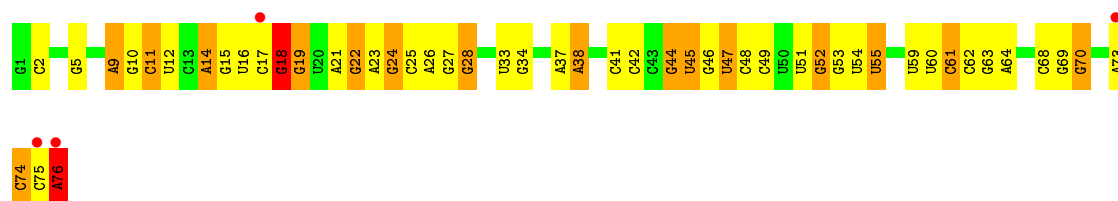
• Molecule 21: 30S ribosomal protein Thx



• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: tRNA-Phe



• Molecule 23: tRNA-fMet

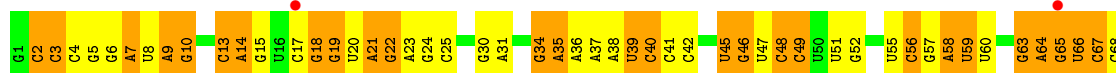
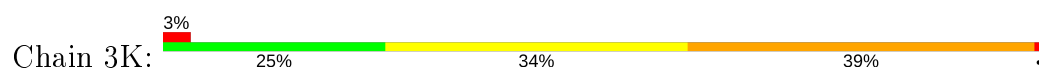




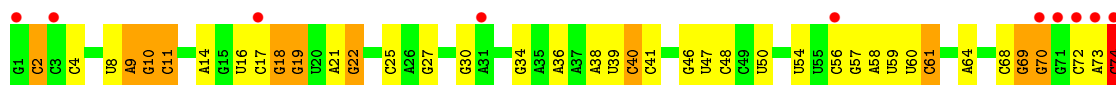
• Molecule 23: tRNA-fMet



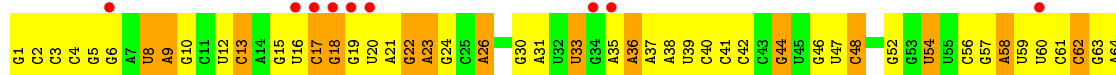
• Molecule 24: tRNA-Phe



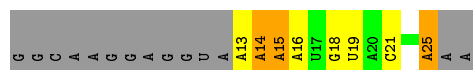
• Molecule 24: tRNA-Phe



• Molecule 24: tRNA-Phe



• Molecule 25: mRNA



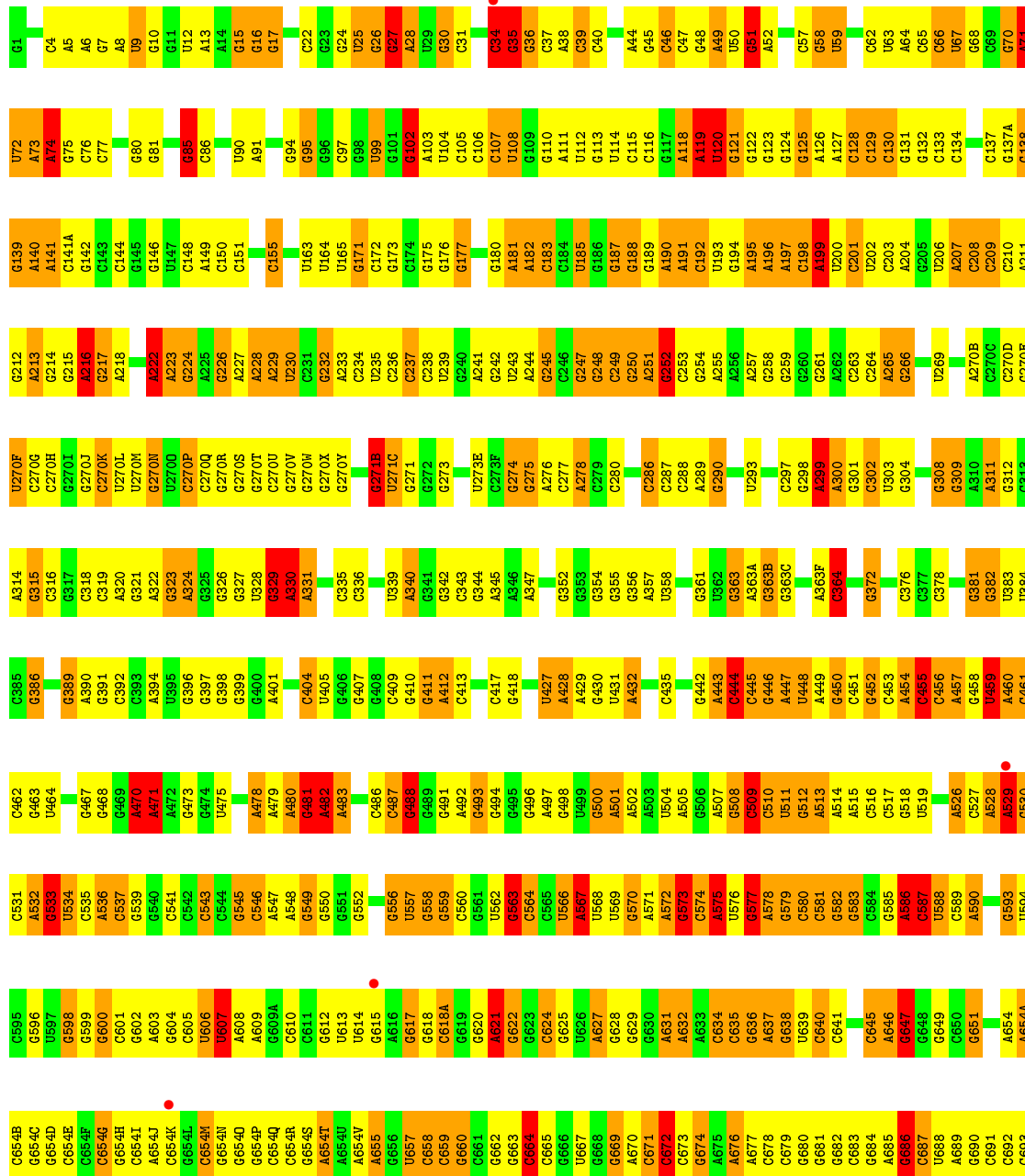
- Molecule 25: mRNA

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



- Molecule 26: 23S ribosomal RNA

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



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G1591	A1528	C1463	G1401	U1341	G1279	G1212	A1142A	A1077	G1011	G950	C885	A820	A761	G695
C1592	A1529	C1464	C1402	A1342	G1280	A1213	G1143	U1078	U1012	C951	C886	U821	A762	G696
G1593	C1403	C1465	C1403	G1343	A1214	A1214	G1144	U1079	C1013	G952	C887	U822	G952	C697
G1594	C1531	G1466	U1405	G1344	G1215	G1215	G1147	A1081	U1014	A953	C888	G823	G763	C698
G1595	C1532	C1467	U1406	G1345	G1216	G1216	G1147	U1082	G1015	G954	C889	A824	A764	A699
A1596	C1533	C1468	U1407	G1346	C1217	C1217	G1153	U1083	G1016	C955	A890	C825	G765	G700
A1597	G1534	A1469	C1408	G1347	A1287	A1287	G1154	U1084	G1017	G956	C892	U826	G766	G701
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C1600	C1537	A1472	G1410	C1350	C1290	C1222	A1156	A1086	A1020	A959	U895	A829	G769	G704
G1601	G1538	G1473	G1411	G1351	C1291	C1223	G1157	G1087	G1021	A960	A896	G830	G770	A705
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C1604	U1541	U1416	U1415	G1354	U1294	G1226	G1160	U1090	G1024	U963	A899	U833	G773	U709
C1605	G1542	A1477	G1416	G1355	C1295	A1227	G1161	G1091	G1025	C964	A900	C834	A774	
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C1615	C1551	U1489	G1425	A1365	C1304	A1242	G1170	C1100	U1035	G973	A910	C844	A783	G721
A1616	A1554	A1490	A1427	A1366	C1305	A1243	G1171	U1101	G1036	G974		G845	A784	A722
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U1629	G1563	C1501	U1438	G1377	A1317	A1254	G1183	U1113	G1051	C986	A926	U860	C737	C736
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G1633	G1568	A1507	G1440	G1380	G1319	G1256	U1188	C1119	G1055	A988	G928	U862	G799	G738
A1634	A1569	A1508	G1441	G1381	C1320	C1257	A1189	G1120	G1056	G989	U930	A863	A800	G739
G1635	C1570	C1509	G1443	G1382	A1321	G1258	G1190	C1121	A1057	C991	G931	U864	G801	U740
C1636	A1571	A1510	G1444	G1383	U1323	G1259	G1191	G1122	U1058	C992	G932	C865	A802	G741
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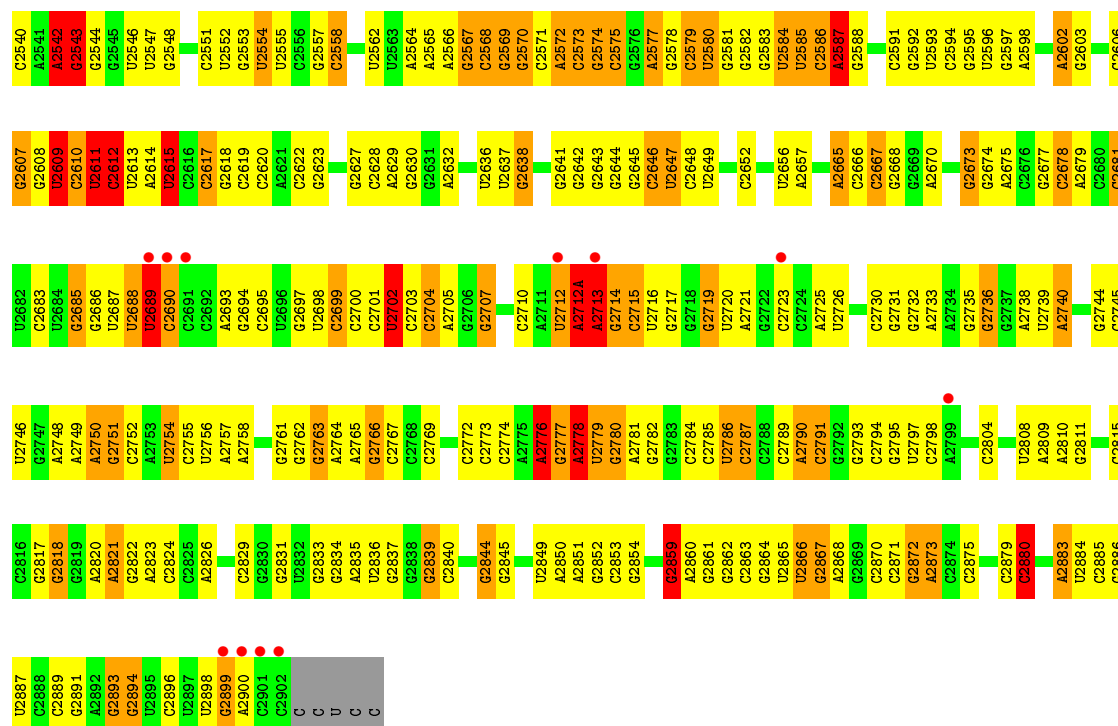




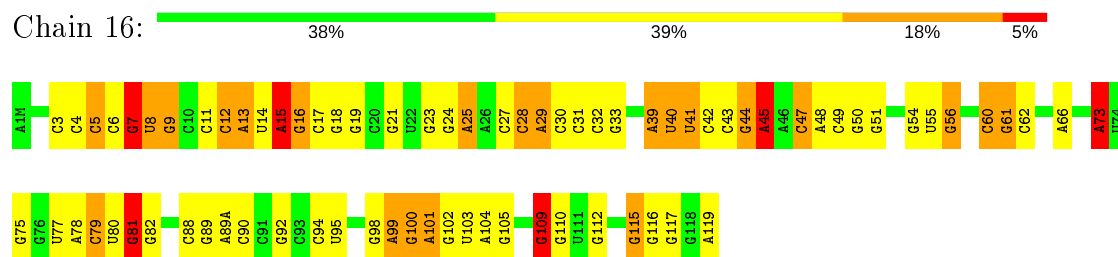


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G1436	G1371	A1307	G1244	U1166	U1097	U1032	U969	G908	G846	A777	G701	A654
U1438	A1372	A1308	G1244	U1167	U1098	U1033	G971	A909	C847	G778	G700	A654A
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A1444	A1378	C1314	C1251	U1175	A1103	C1038	G975	C914	U851	A783	G710	C654F
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C1446	G1381	A1317	A1264	C1178	G1106	C1041	G978	A917	G854	C786		C654I
G1447	C1382	C1318	U1255	G1183	G1110	G1042	G979	A918	G855	U787	A722	A654J
G1448	C1383	G1319	G1256	A1184	A1111	C1043	A980	G919	C856	A788	G723	C654K
A1449	A1384	C1320	C1257	G1185	G1112	G1044	A981	G920	C857	A789	U724	G654L
G1449A	G1385	A1321	C1258	C1185	A1045	A1045	C982	G921	U858	C790	G725	
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C1451	C1387	U1323	G1260	G1187	G1114	G1047	A984	C923	U860	G792	G729	C654Q
A1453	G1388	G1324	A1262	U1188	G1115	A1048	C985	C924	A861	A793	G730	C654R
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G1455	U1326	U1326	U1263	G1190	G1116	A1050	G987	A926	A863			
	C1327	G1264	A1265	G1191	G1122	C1051	A988	G928	G864	C797		
G1459	A1392	G1328	A1265	G1195	A1126	C1052	G989	G929	C865		G732	G656
A1460	U1393	U1329	G1266	G1196	G1126	C1053	A990	U930	A866	A800	G733	U657
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C1462	U1396	A1331	G1270	G1198	U1130	G1055	C992	G932	U868	A802	C736	C659
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C1467	C1402	A1336	U1274	A1204	G997	U1060	G997	U937	U873	C807	G741	
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A1469	C1404	C1338	G1277	G1206	G1137	U1062	U999	G939	A878	U810	U747	U667
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A1471	U1406	U1340	A1278	G1209	G1139	U1066	A1001	A941	A879	U811	G748	
	C1407	U1341	G1279	G1209	C1140	U1066	G1002	G942	G880	C812	C749	
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G1475	C1409	G1343	G1281	U1211	U1142	C1068	C1003	G944	G882	C817	A751	C673
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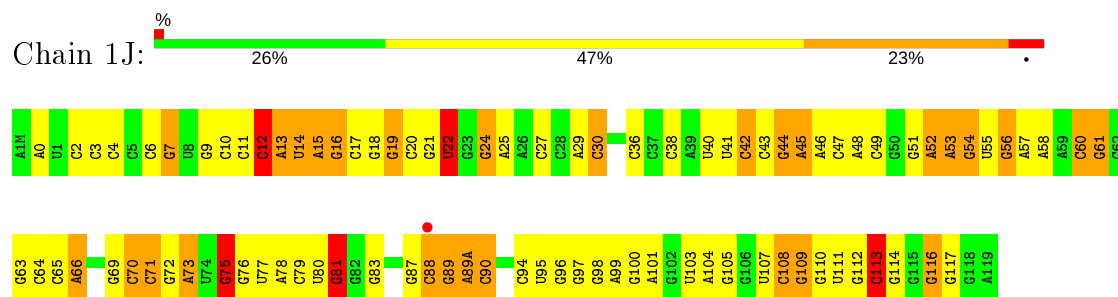
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U2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												



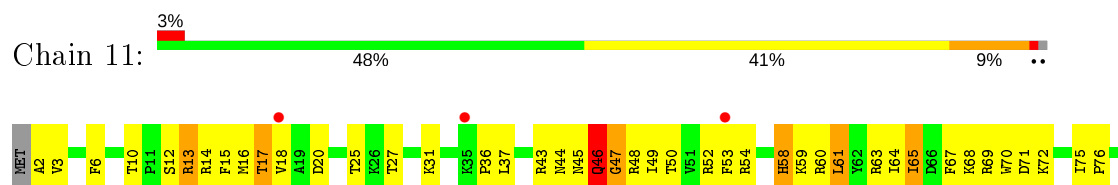
• Molecule 27: 5S ribosomal RNA

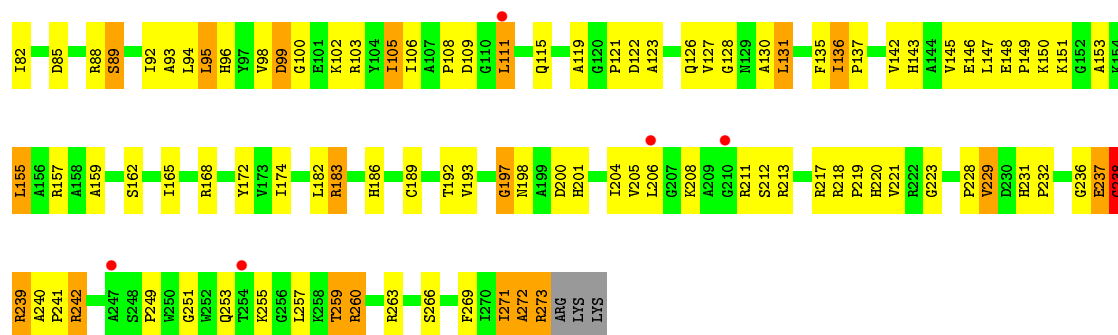


• Molecule 27: 5S ribosomal RNA

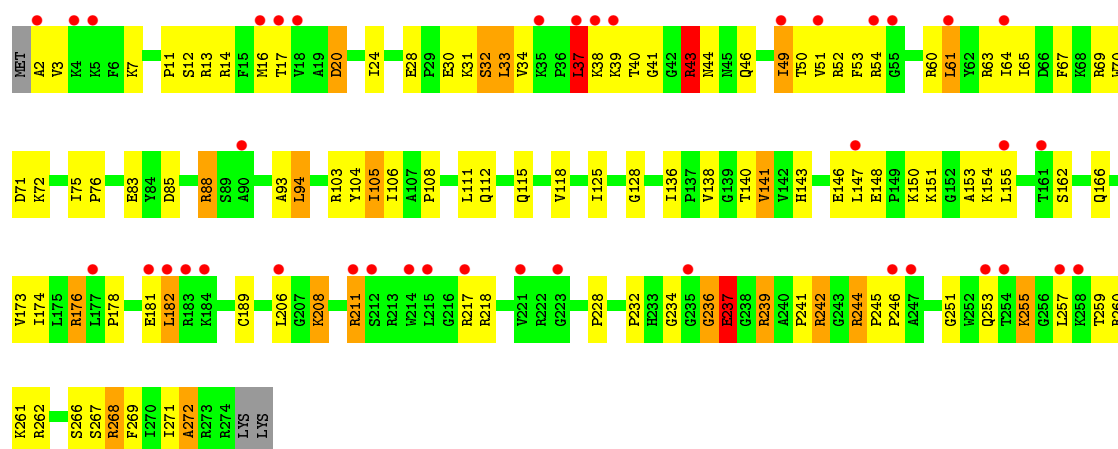


• Molecule 28: 50S ribosomal protein L2

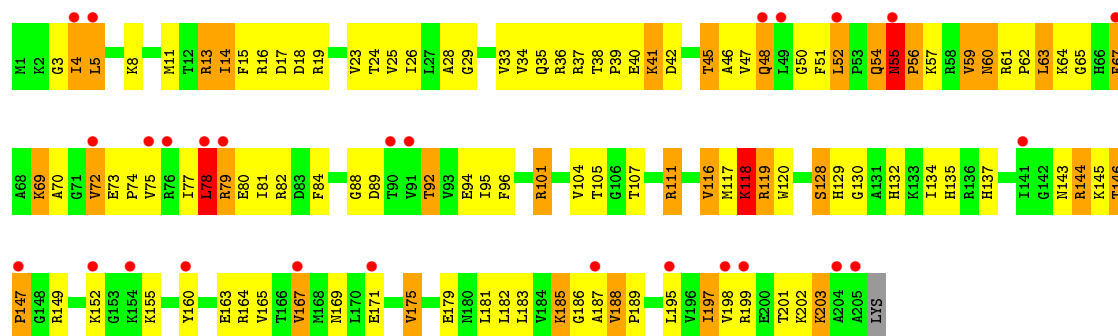
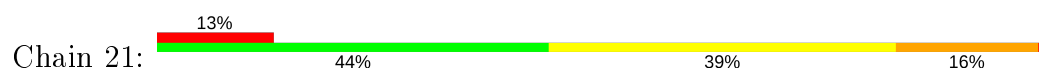




• Molecule 28: 50S ribosomal protein L2

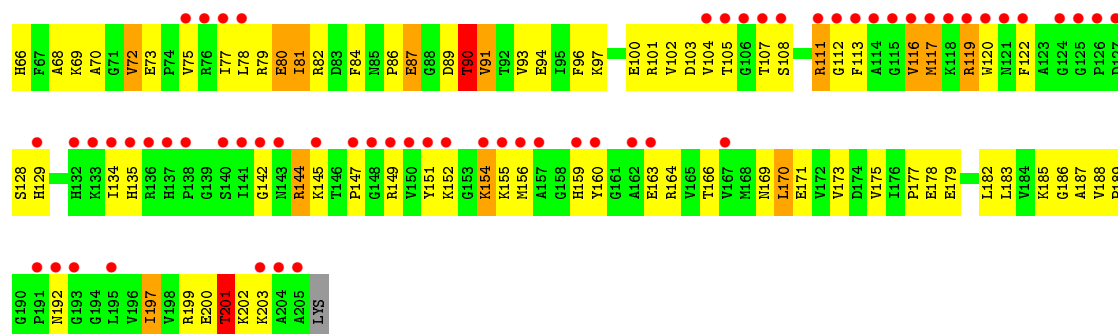


• Molecule 29: 50S ribosomal protein L3

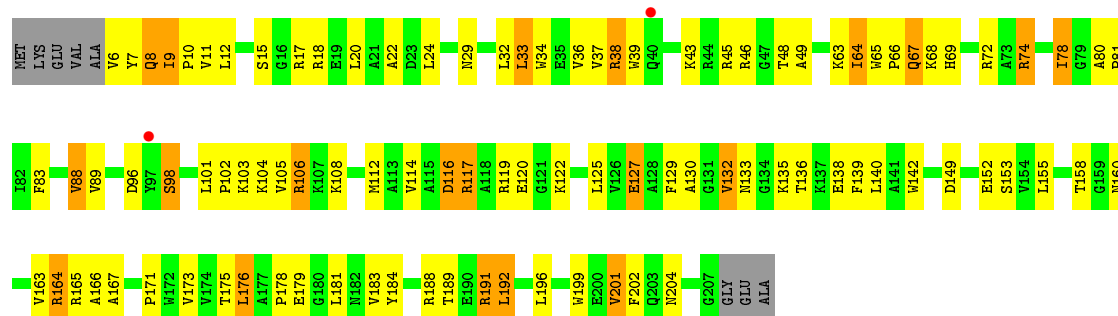


• Molecule 29: 50S ribosomal protein L3

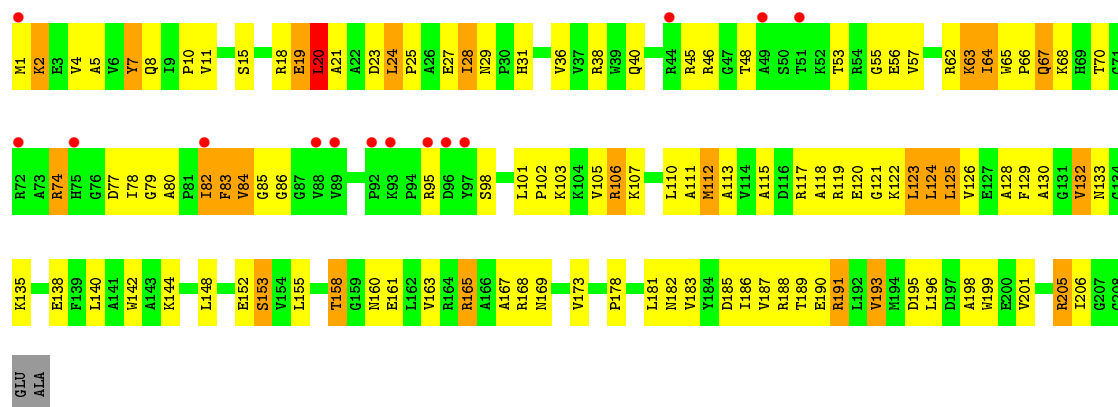




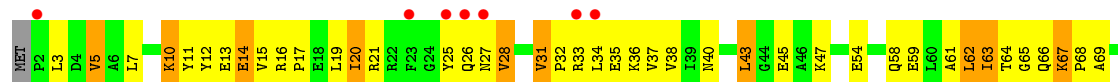
• Molecule 30: 50S ribosomal protein L4

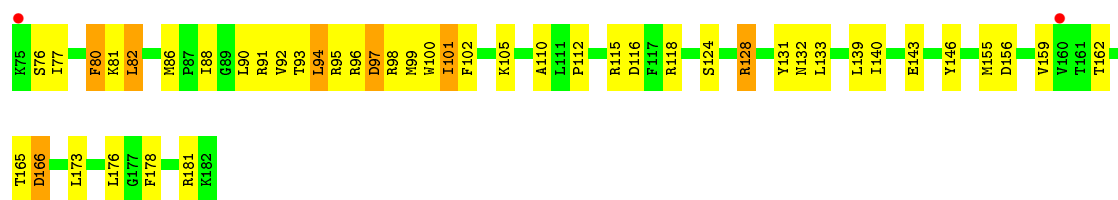


• Molecule 30: 50S ribosomal protein L4

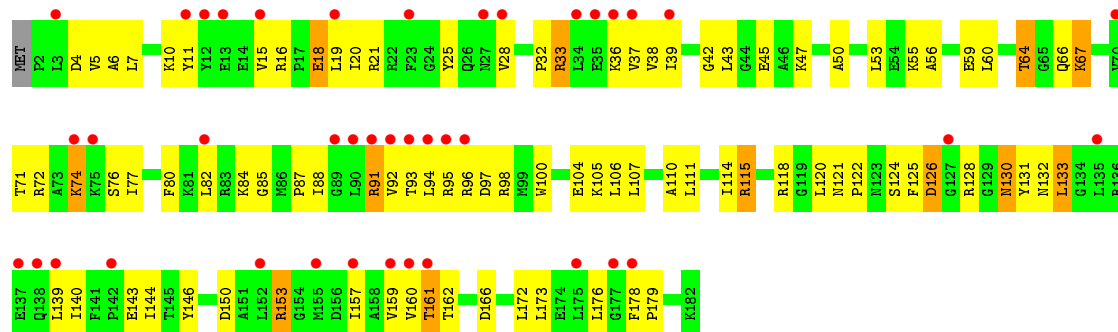


• Molecule 31: 50S ribosomal protein L5

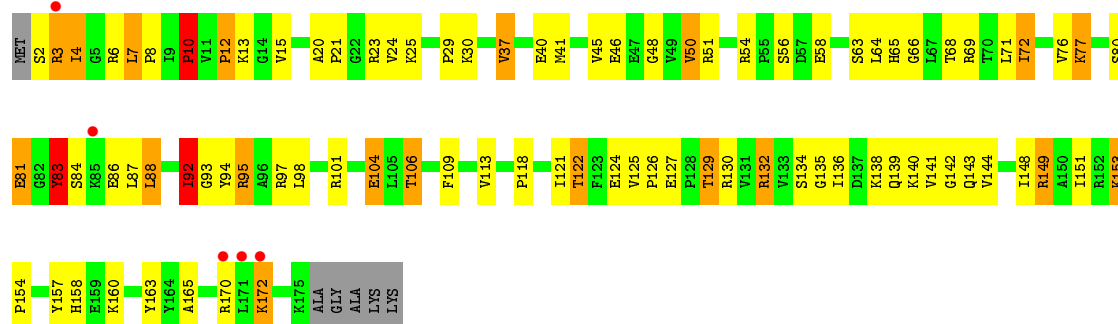




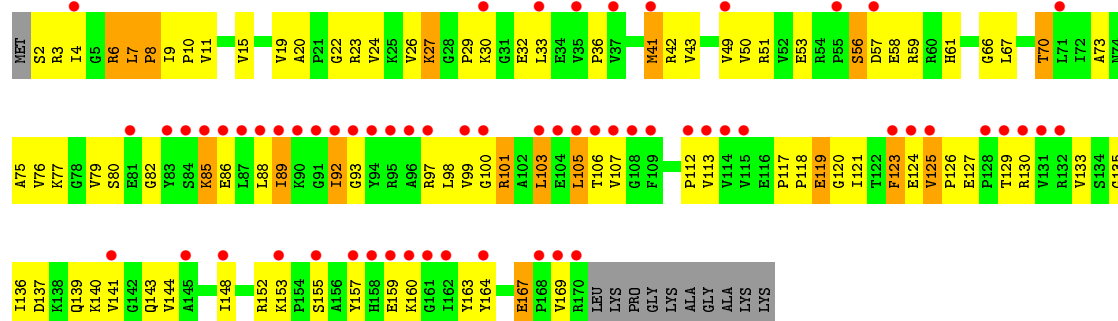
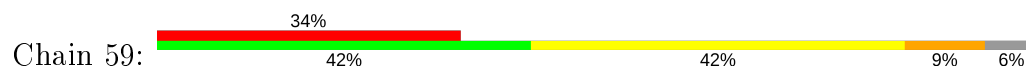
• Molecule 31: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L6

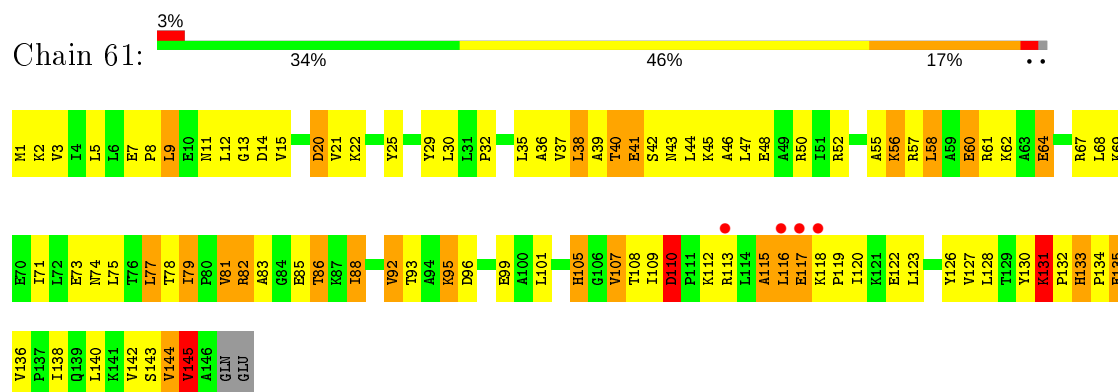


• Molecule 32: 50S ribosomal protein L6

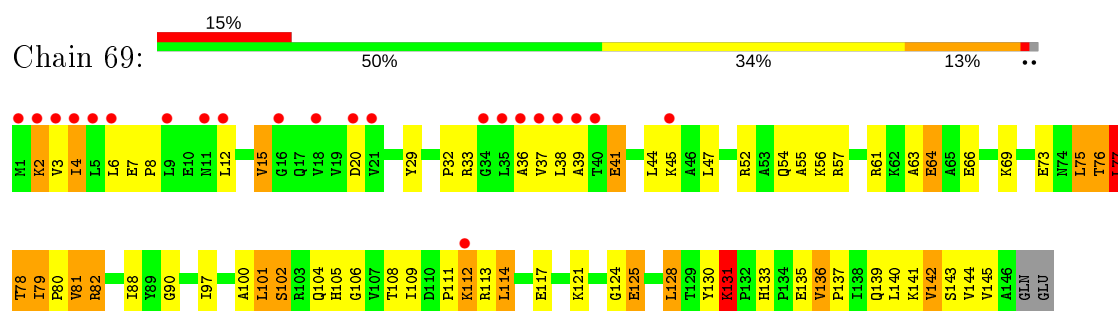




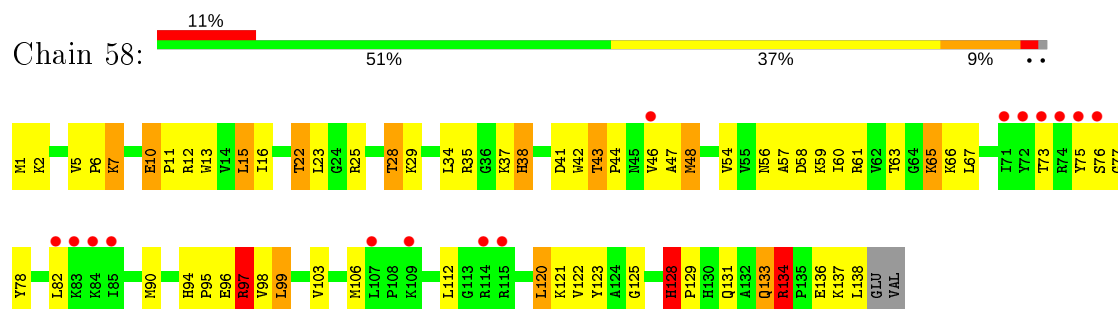
- Molecule 33: 50S ribosomal protein L9



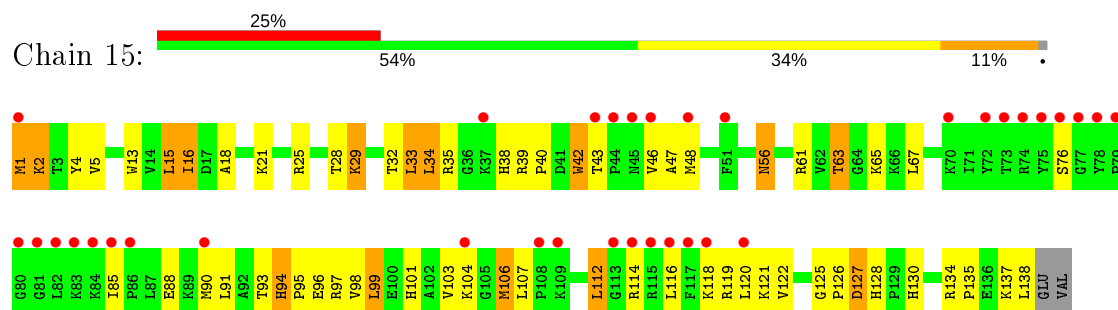
- Molecule 33: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L13

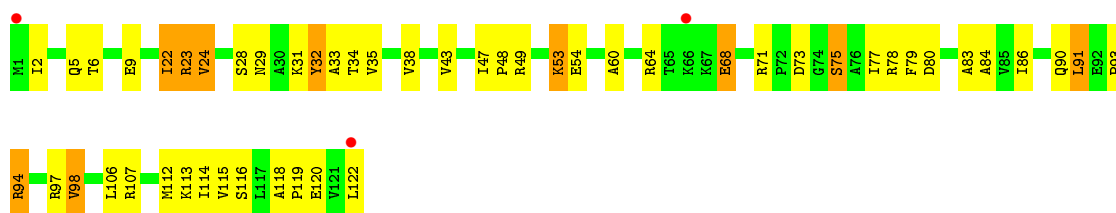


- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14

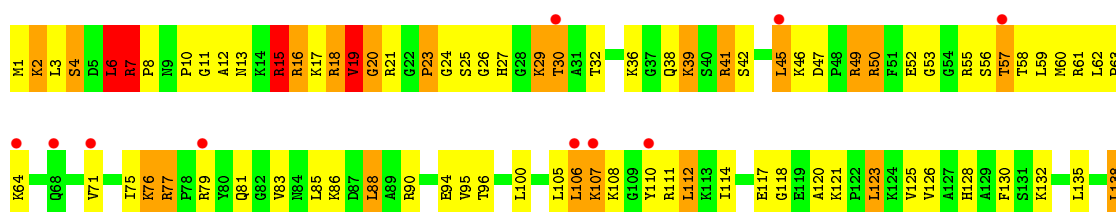




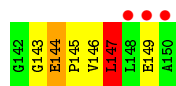
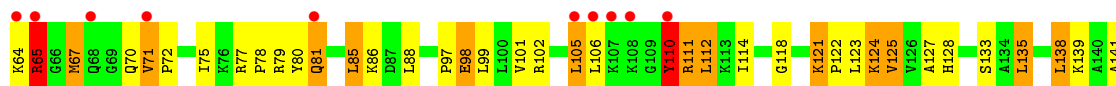
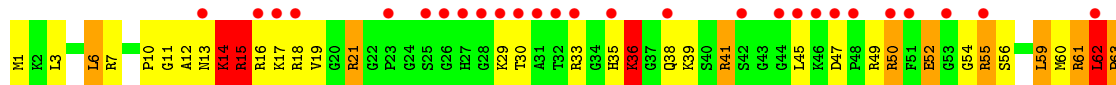
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15

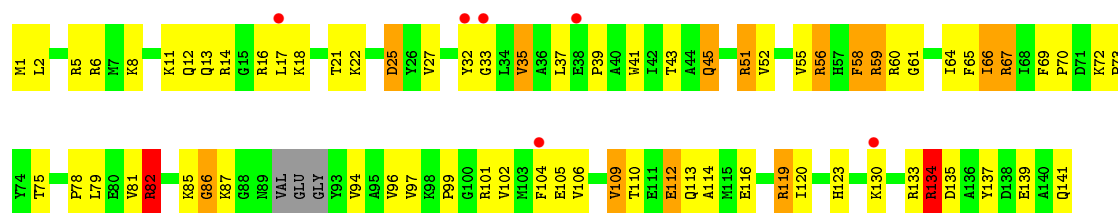


- Molecule 36: 50S ribosomal protein L15

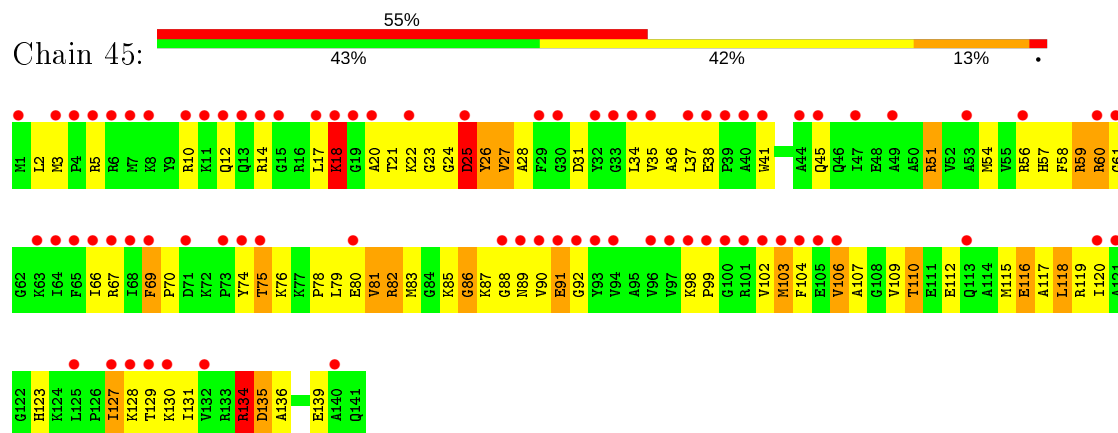


- Molecule 37: 50S ribosomal protein L16

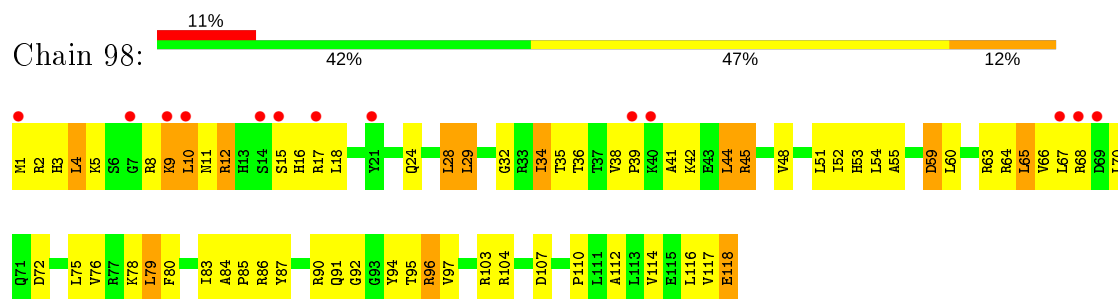




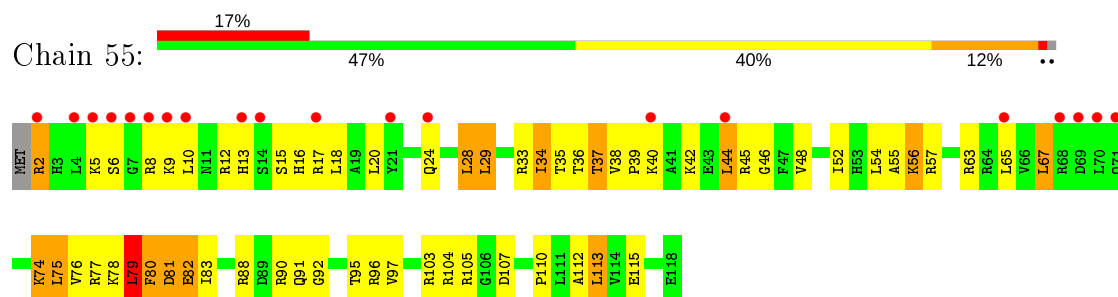
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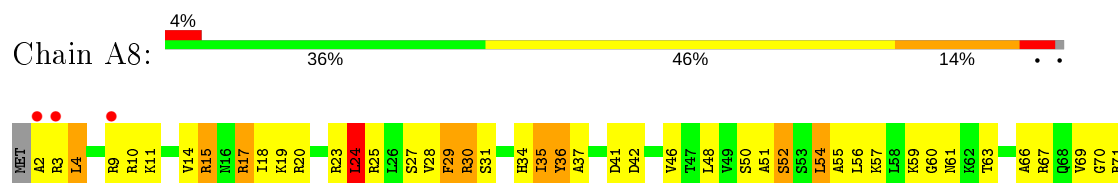
• Molecule 38: 50S ribosomal protein L17

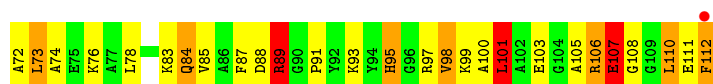


• Molecule 38: 50S ribosomal protein L17

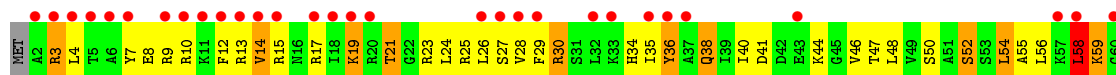


• Molecule 39: 50S ribosomal protein L18





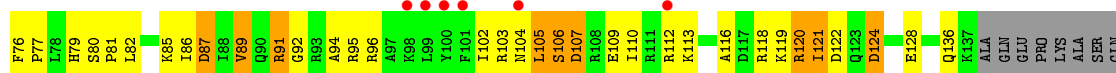
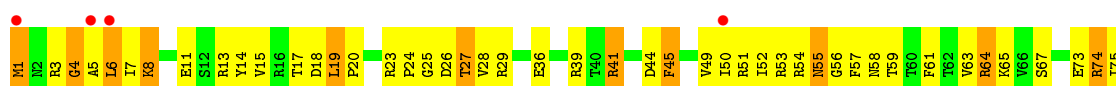
- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19

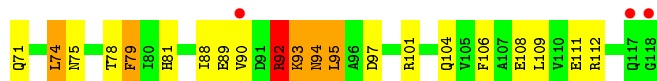
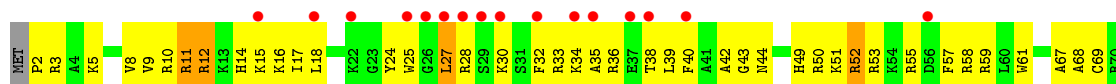


- Molecule 40: 50S ribosomal protein L19

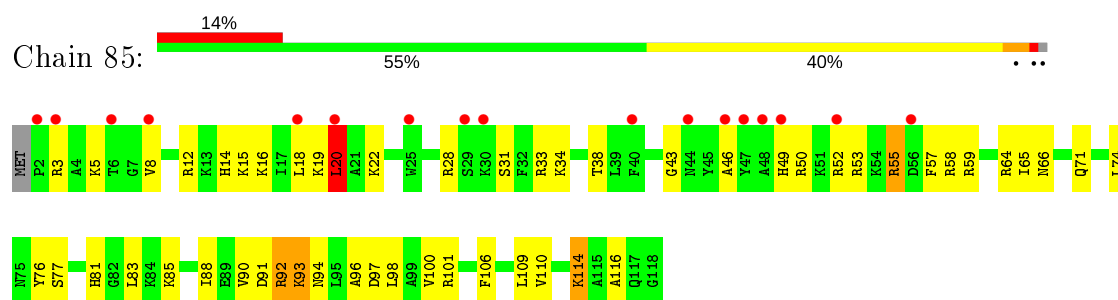


GLU

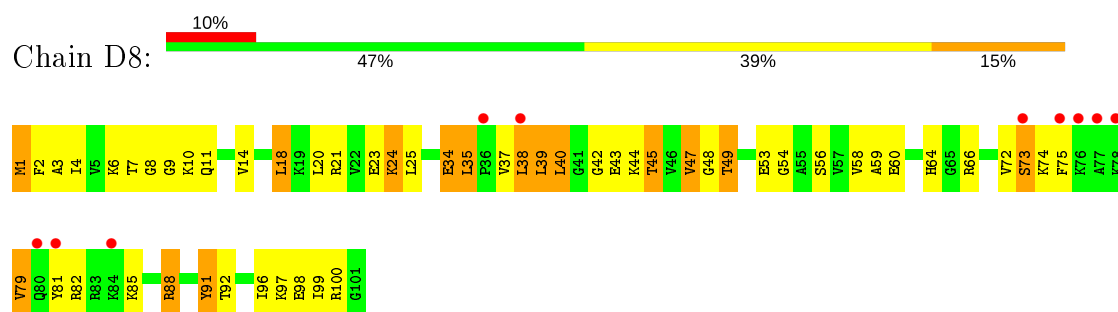
- Molecule 41: 50S ribosomal protein L20



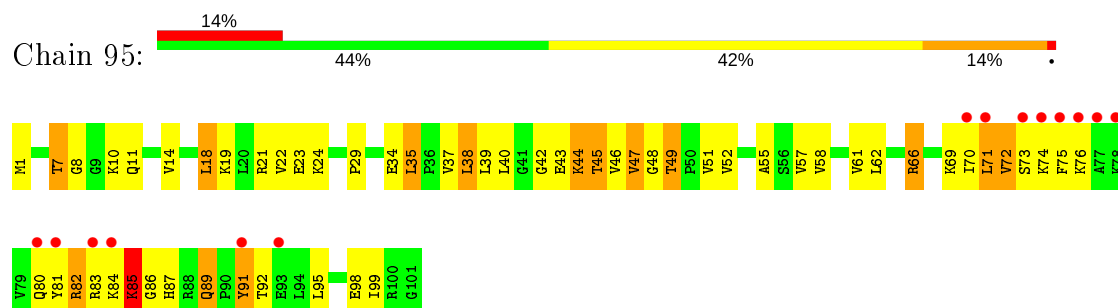
- Molecule 41: 50S ribosomal protein L20



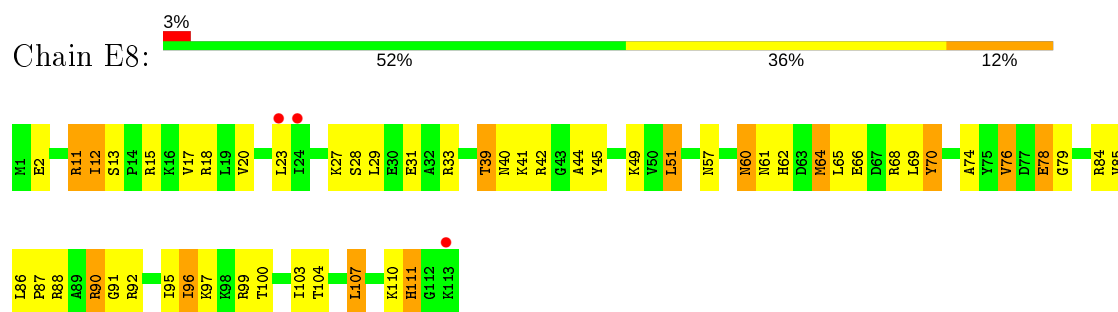
- Molecule 42: 50S ribosomal protein L21



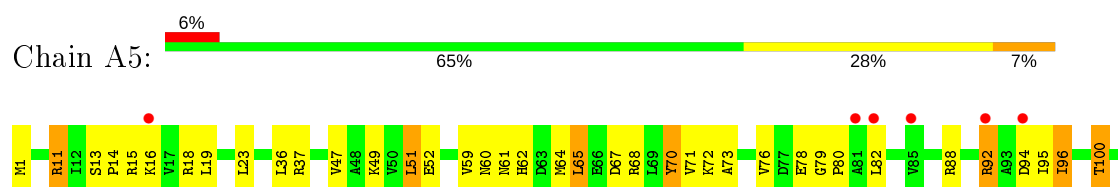
- Molecule 42: 50S ribosomal protein L21

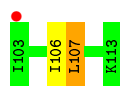


- Molecule 43: 50S ribosomal protein L22

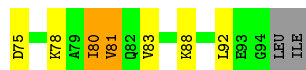


- Molecule 43: 50S ribosomal protein L22

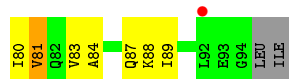




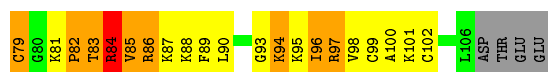
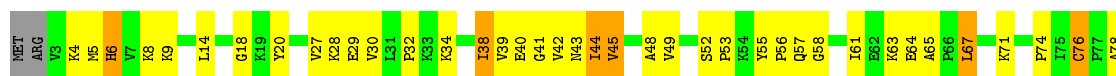
- Molecule 44: 50S ribosomal protein L23



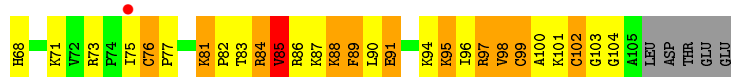
- Molecule 44: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L24

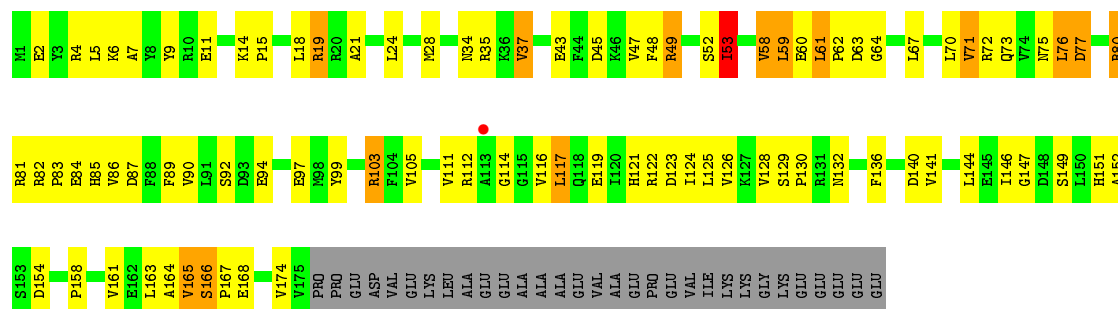


- Molecule 45: 50S ribosomal protein L24

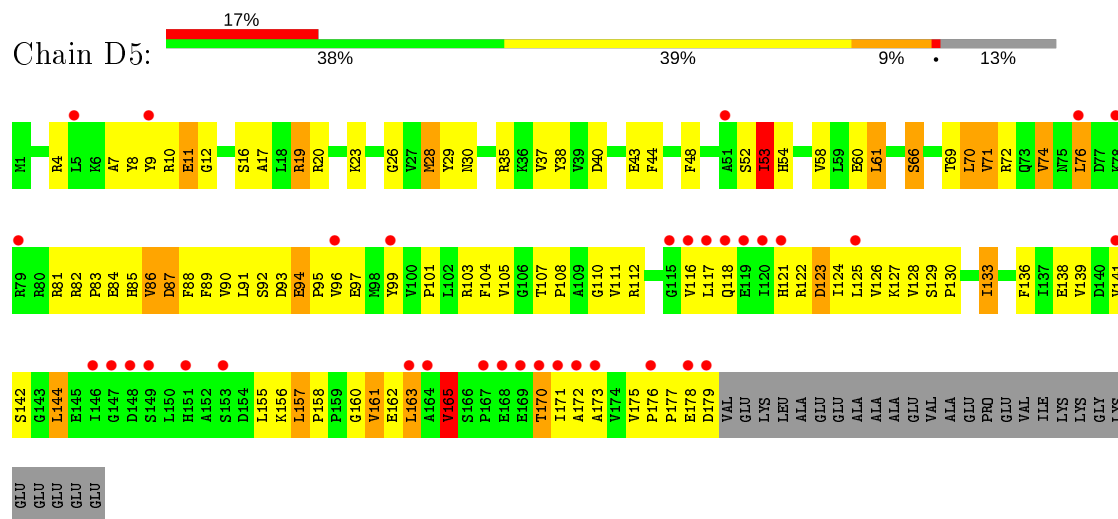


- Molecule 46: 50S ribosomal protein L25

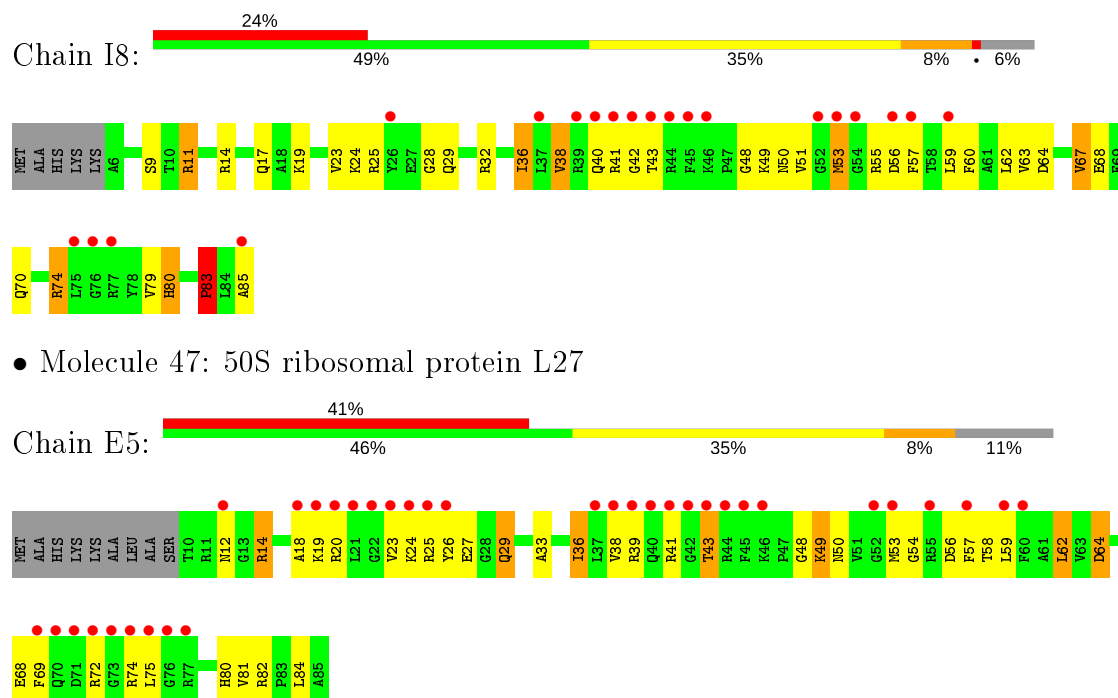




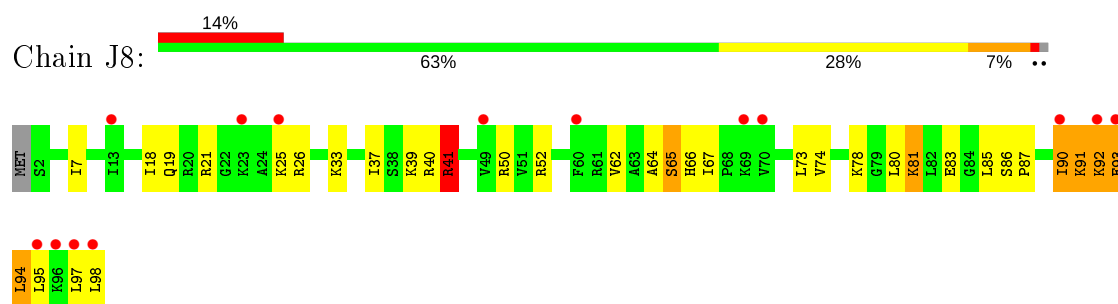
• Molecule 46: 50S ribosomal protein L25



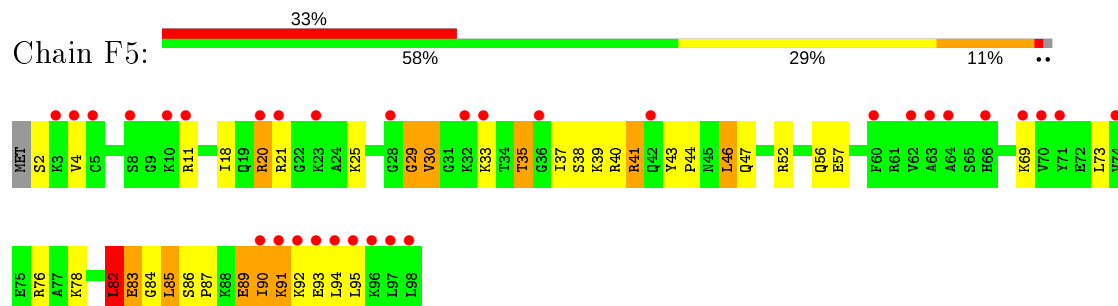
• Molecule 47: 50S ribosomal protein L27



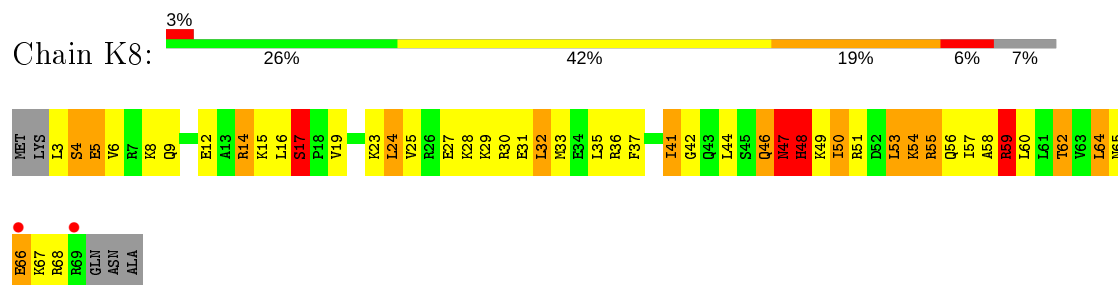
• Molecule 48: 50S ribosomal protein L28



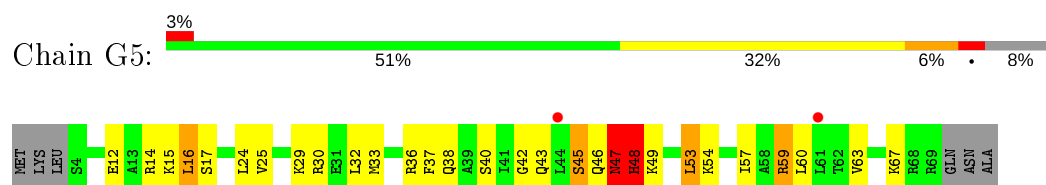
- Molecule 48: 50S ribosomal protein L28



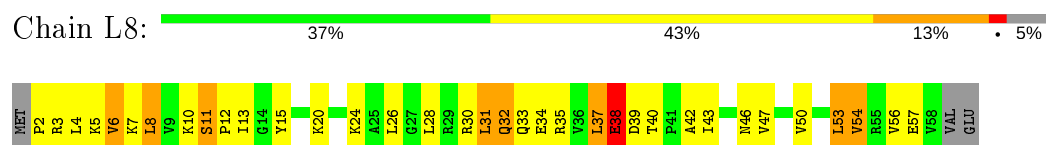
- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29



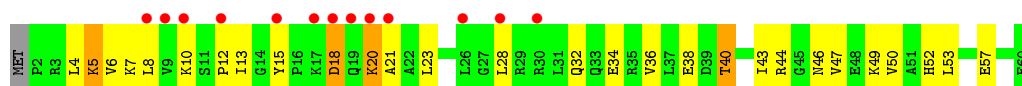
- Molecule 50: 50S ribosomal protein L30



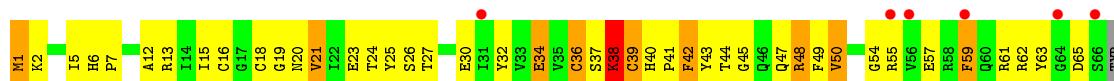
- Molecule 50: 50S ribosomal protein L30





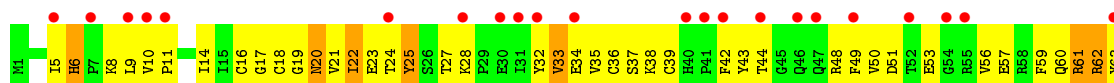


- Molecule 51: 50S ribosomal protein L31



ARG  
LYS  
GLY  
ARG

- Molecule 51: 50S ribosomal protein L31



GLY  
ASP  
SER  
TYR  
ARG  
LYS  
GLY  
ARG

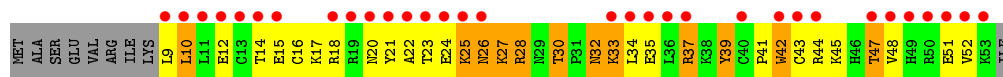
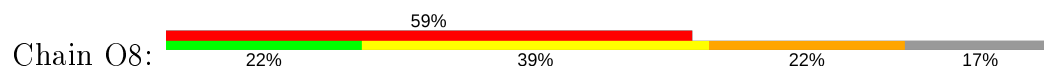
- Molecule 52: 50S ribosomal protein L32



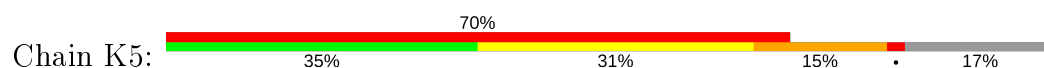
- Molecule 52: 50S ribosomal protein L32

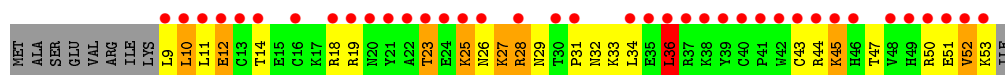


- Molecule 53: 50S ribosomal protein L33

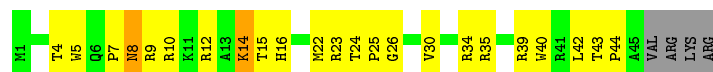


- Molecule 53: 50S ribosomal protein L33





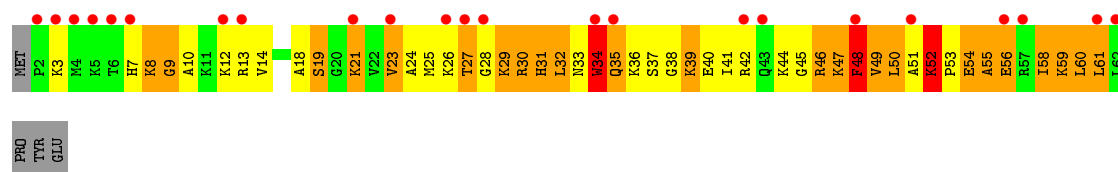
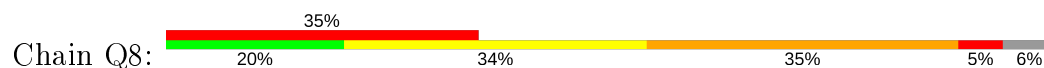
- Molecule 54: 50S ribosomal protein L34



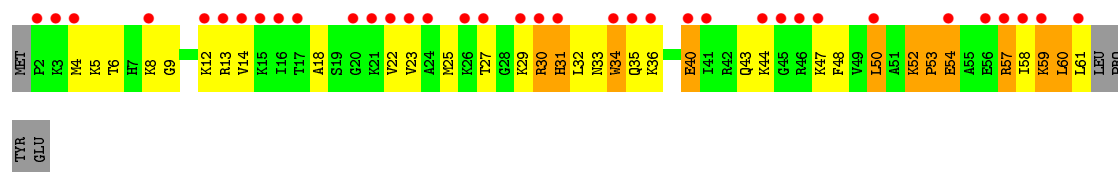
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



## 4 Data and refinement statistics

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, MIA, MG, 4SU, 7MG, PSU

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

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

## 5.2 Too-close contacts [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

## 5.3 Torsion angles ⓘ

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

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

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

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

5 of 172 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

Mol	Chain	Res	Type
46	H8	132	ASN

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Mol	Chain	Res	Type
4	32	50	ARG
44	B5	88	LYS
48	J8	86	SER
53	O8	52	VAL

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

Mol	Chain	Res	Type
2	12	19	HIS
30	39	203	GLN
51	I5	6	HIS
8	72	15	ASN
34	15	56	ASN

### 5.3.3 RNA ⓘ

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

5 of 2319 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	13	9	G

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2171	A
1	1G	328	C
26	14	2406	U
26	1H	2225	A
26	1H	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	PSU	1K	39	22	17,21,22	1.08	1 (5%)	20,30,33	3.44	6 (30%)
23	4SU	2K	8	23	14,21,22	3.23	2 (14%)	15,30,33	1.01	1 (6%)
22	PSU	1K	32	22	17,21,22	1.03	1 (5%)	20,30,33	3.58	4 (20%)
23	OMC	2L	33	23	15,22,23	2.28	4 (26%)	17,31,34	1.89	4 (23%)
22	PSU	1K	55	22	17,21,22	1.17	1 (5%)	20,30,33	3.60	5 (25%)
23	OMC	2K	33	23	15,22,23	2.19	4 (26%)	17,31,34	1.44	2 (11%)
23	4SU	2L	8	23	14,21,22	3.43	2 (14%)	15,30,33	1.37	2 (13%)
22	5MU	1K	54	22	15,22,23	2.16	3 (20%)	16,32,35	1.78	2 (12%)
23	5MU	2K	55	23	15,22,23	2.15	3 (20%)	16,32,35	1.97	2 (12%)
23	5MU	2L	55	23	15,22,23	2.15	3 (20%)	16,32,35	1.79	2 (12%)
22	7MG	1K	46	22	22,26,27	3.39	7 (31%)	28,39,42	2.57	10 (35%)
23	PSU	2K	56	23	17,21,22	1.05	1 (5%)	20,30,33	3.19	6 (30%)
23	7MG	2K	47	23	22,26,27	3.50	7 (31%)	28,39,42	2.57	13 (46%)
23	PSU	2L	56	23	17,21,22	1.11	1 (5%)	20,30,33	3.22	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	7MG	2L	47	23	22,26,27	3.50	7 (31%)	28,39,42	2.47	11 (39%)
22	4SU	1K	8	22	14,21,22	3.36	2 (14%)	15,30,33	1.28	2 (13%)
22	MIA	1K	37	22	24,31,32	2.55	4 (16%)	26,44,47	2.59	8 (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	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	3/5/25/26	0/2/2/2
22	PSU	1K	32	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/7/27/28	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
23	4SU	2L	8	23	-	2/5/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
22	7MG	1K	46	22	-	1/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	1/7/37/38	0/3/3/3
22	4SU	1K	8	22	-	0/5/25/26	0/2/2/2
22	MIA	1K	37	22	-	4/11/33/34	0/3/3/3

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C4-N3	10.94	1.48	1.34
22	1K	46	7MG	C4-N3	10.75	1.47	1.34
23	2K	47	7MG	C4-N3	10.47	1.47	1.34
23	2K	8	4SU	C5-C4	10.44	1.50	1.38
23	2L	8	4SU	C5-C4	10.27	1.50	1.38

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	32	PSU	N1-C2-N3	-12.92	118.16	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	39	PSU	N1-C2-N3	-12.37	118.60	128.43
22	1K	55	PSU	N1-C2-N3	-12.10	118.81	128.43
23	2L	56	PSU	N1-C2-N3	-11.17	119.55	128.43
23	2K	56	PSU	N1-C2-N3	-11.03	119.66	128.43

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2K	8	4SU	O4'-C4'-C5'-O5'
23	2L	33	OMC	C2'-C1'-N1-C6
23	2K	33	OMC	C2'-C1'-N1-C6
22	1K	37	MIA	N1-C2-S10-C11
22	1K	37	MIA	N3-C2-S10-C11

There are no ring outliers.

12 monomers are involved in 25 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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(Å²)	Q<0.9
1	13	1498/1522 (98%)	0.21	45 (3%)	50	25	73, 122, 204, 309	0
1	1G	1497/1522 (98%)	0.24	74 (4%)	29	13	92, 145, 218, 318	0
2	12	237/256 (92%)	0.20	17 (7%)	15	5	168, 199, 220, 228	0
2	1E	237/256 (92%)	0.13	8 (3%)	45	22	132, 167, 193, 205	0
3	22	206/239 (86%)	0.04	7 (3%)	45	22	161, 182, 205, 218	0
3	2E	205/239 (85%)	-0.02	1 (0%)	91	79	103, 128, 161, 170	0
4	32	208/209 (99%)	0.59	18 (8%)	10	3	122, 144, 165, 174	0
4	3E	208/209 (99%)	0.77	30 (14%)	2	1	102, 129, 151, 165	0
5	42	151/162 (93%)	0.52	18 (11%)	4	1	136, 154, 171, 203	0
5	4E	151/162 (93%)	0.57	19 (12%)	3	1	97, 120, 143, 176	0
6	52	101/101 (100%)	-0.27	0	100	100	106, 127, 147, 161	0
6	5E	101/101 (100%)	-0.07	0	100	100	101, 123, 148, 161	0
7	62	155/156 (99%)	0.92	27 (17%)	1	0	136, 154, 182, 207	0
7	6E	155/156 (99%)	0.49	16 (10%)	6	2	124, 139, 168, 193	0
8	72	138/138 (100%)	1.28	42 (30%)	0	0	130, 158, 174, 179	0
8	7E	138/138 (100%)	0.90	26 (18%)	1	0	105, 129, 141, 149	0
9	82	127/128 (99%)	3.27	75 (59%)	0	0	141, 183, 204, 208	0
9	8E	127/128 (99%)	1.66	45 (35%)	0	0	107, 156, 179, 193	0
10	1A	99/105 (94%)	1.96	39 (39%)	0	0	153, 184, 203, 210	0
10	1I	99/105 (94%)	1.40	32 (32%)	0	0	102, 155, 187, 192	0
11	2A	116/129 (89%)	0.50	11 (9%)	8	2	111, 137, 158, 182	0
11	2I	116/129 (89%)	0.27	8 (6%)	16	6	90, 127, 153, 180	0
12	3A	125/132 (94%)	1.24	35 (28%)	0	0	109, 134, 160, 185	0
12	3I	125/132 (94%)	0.44	11 (8%)	10	3	83, 96, 131, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	117/126 (92%)	1.15	30 (25%) 0 0	140, 184, 206, 216	0
13	4I	118/126 (93%)	0.25	7 (5%) 22 9	101, 139, 159, 170	0
14	5A	58/61 (95%)	4.97	46 (79%) 0 0	164, 179, 194, 201	0
14	5I	60/61 (98%)	1.88	24 (40%) 0 0	106, 118, 137, 147	0
15	6A	88/89 (98%)	0.81	12 (13%) 3 1	118, 139, 155, 159	0
15	6I	88/89 (98%)	1.02	21 (23%) 0 0	98, 125, 142, 154	0
16	7A	84/88 (95%)	1.04	19 (22%) 0 0	113, 132, 150, 174	0
16	7I	84/88 (95%)	3.10	55 (65%) 0 0	122, 135, 169, 187	0
17	8A	100/105 (95%)	1.17	21 (21%) 1 0	118, 138, 153, 176	0
17	8I	100/105 (95%)	0.66	14 (14%) 2 1	108, 127, 140, 145	0
18	9A	72/88 (81%)	0.04	2 (2%) 53 28	116, 142, 178, 198	0
18	9I	72/88 (81%)	0.10	0 100 100	109, 127, 162, 187	0
19	AA	78/93 (83%)	1.25	25 (32%) 0 0	172, 203, 216, 222	0
19	AI	81/93 (87%)	0.47	5 (6%) 20 8	109, 135, 160, 166	0
20	BA	99/106 (93%)	1.63	43 (43%) 0 0	108, 130, 158, 173	0
20	BI	99/106 (93%)	1.35	34 (34%) 0 0	129, 144, 177, 183	0
21	1B	25/27 (92%)	6.10	23 (92%) 0 0	147, 163, 179, 196	0
21	1F	25/27 (92%)	4.77	22 (88%) 0 0	114, 126, 139, 164	0
22	1K	69/76 (90%)	0.12	4 (5%) 23 9	101, 222, 265, 271	0
23	2K	72/77 (93%)	0.05	0 100 100	84, 108, 137, 146	0
23	2L	72/77 (93%)	-0.42	1 (1%) 75 53	96, 136, 166, 170	0
24	1L	76/76 (100%)	0.81	12 (15%) 2 0	147, 264, 289, 295	0
24	3K	76/76 (100%)	-0.06	2 (2%) 56 30	92, 255, 286, 289	0
24	3L	76/76 (100%)	0.49	9 (11%) 4 1	104, 264, 294, 299	0
25	4K	13/27 (48%)	0.92	0 100 100	88, 101, 151, 157	0
25	4L	9/27 (33%)	0.59	0 100 100	121, 154, 165, 175	0
26	14	2909/2917 (99%)	0.21	70 (2%) 59 34	67, 105, 270, 378	0
26	1H	2912/2917 (99%)	0.28	12 (0%) 92 82	56, 91, 253, 353	0
27	16	122/122 (100%)	-0.17	0 100 100	83, 111, 133, 217	0
27	1J	122/122 (100%)	-0.13	1 (0%) 86 70	107, 152, 174, 226	0
28	11	272/276 (98%)	0.50	8 (2%) 51 26	57, 83, 100, 110	0

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

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

The worst 5 of 2139 RSRZ outliers are listed below:

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

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	PSU	1K	55	20/21	0.78	0.12	153,172,191,191	0
22	4SU	1K	8	20/21	0.80	0.14	184,192,200,205	0
22	7MG	1K	46	24/25	0.87	0.12	175,197,203,209	0
23	4SU	2L	8	20/21	0.88	0.14	128,140,143,147	0
22	PSU	1K	32	20/21	0.89	0.32	113,119,123,123	0
23	PSU	2L	56	20/21	0.90	0.09	128,135,142,148	0
22	5MU	1K	54	21/22	0.93	0.10	142,157,168,172	0
23	4SU	2K	8	20/21	0.94	0.21	100,108,123,123	0
22	PSU	1K	39	20/21	0.94	0.17	96,108,116,119	0
22	MIA	1K	37	29/30	0.94	0.30	89,100,118,123	0
23	7MG	2K	47	24/25	0.95	0.17	110,120,128,137	0
23	7MG	2L	47	24/25	0.95	0.12	140,151,156,161	0
23	5MU	2L	55	21/22	0.95	0.11	138,142,147,151	0
23	OMC	2L	33	21/22	0.96	0.20	124,127,132,137	0
23	PSU	2K	56	20/21	0.96	0.14	109,113,120,127	0
23	5MU	2K	55	21/22	0.97	0.15	99,116,125,136	0
23	OMC	2K	33	21/22	0.98	0.32	88,94,101,106	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	1H	3119	1/1	0.35	0.52	101,101,101,101	0
56	MG	1H	3498	1/1	0.39	0.20	119,119,119,119	0
56	MG	1H	3142	1/1	0.41	0.41	88,88,88,88	0
56	MG	13	1720	1/1	0.43	0.24	104,104,104,104	0
56	MG	13	1710	1/1	0.45	0.30	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1750	1/1	0.45	0.35	131,131,131,131	0
56	MG	14	3391	1/1	0.46	0.10	124,124,124,124	0
56	MG	13	1739	1/1	0.47	0.20	120,120,120,120	0
56	MG	13	1697	1/1	0.47	0.26	97,97,97,97	0
56	MG	14	3420	1/1	0.48	0.07	130,130,130,130	0
56	MG	1G	1633	1/1	0.49	0.32	93,93,93,93	0
56	MG	1H	3028	1/1	0.49	0.43	115,115,115,115	0
56	MG	13	1631	1/1	0.51	0.70	102,102,102,102	0
56	MG	1H	3322	1/1	0.51	0.22	96,96,96,96	0
56	MG	14	3183	1/1	0.51	0.32	110,110,110,110	0
56	MG	14	3307	1/1	0.52	0.25	87,87,87,87	0
56	MG	16	205	1/1	0.53	0.20	91,91,91,91	0
56	MG	14	3262	1/1	0.54	0.29	81,81,81,81	0
56	MG	1H	3154	1/1	0.54	0.22	91,91,91,91	0
56	MG	14	3020	1/1	0.54	0.51	92,92,92,92	0
56	MG	1G	1629	1/1	0.55	0.18	124,124,124,124	0
56	MG	29	302	1/1	0.56	0.35	108,108,108,108	0
56	MG	14	3288	1/1	0.56	0.53	107,107,107,107	0
56	MG	M5	101	1/1	0.56	0.25	94,94,94,94	0
56	MG	13	1683	1/1	0.56	0.28	106,106,106,106	0
56	MG	13	1692	1/1	0.56	0.22	102,102,102,102	0
56	MG	1H	3281	1/1	0.57	0.30	85,85,85,85	0
56	MG	1H	3200	1/1	0.57	0.35	104,104,104,104	0
56	MG	14	3284	1/1	0.57	0.30	100,100,100,100	0
56	MG	1H	3313	1/1	0.57	0.24	93,93,93,93	0
56	MG	13	1658	1/1	0.58	0.44	117,117,117,117	0
56	MG	14	3329	1/1	0.58	0.21	120,120,120,120	0
56	MG	1G	1644	1/1	0.59	0.19	115,115,115,115	0
56	MG	1H	3250	1/1	0.59	0.21	104,104,104,104	0
56	MG	13	1606	1/1	0.60	0.33	115,115,115,115	0
56	MG	1H	3243	1/1	0.60	0.36	93,93,93,93	0
56	MG	13	1745	1/1	0.61	0.39	121,121,121,121	0
56	MG	1H	3309	1/1	0.61	0.45	96,96,96,96	0
56	MG	14	3181	1/1	0.61	0.21	100,100,100,100	0
56	MG	13	1708	1/1	0.61	0.34	119,119,119,119	0
56	MG	14	3295	1/1	0.61	0.62	95,95,95,95	0
56	MG	1H	3158	1/1	0.62	0.46	104,104,104,104	0
56	MG	14	3025	1/1	0.62	0.17	116,116,116,116	0
56	MG	13	1629	1/1	0.62	0.45	106,106,106,106	0
56	MG	13	1636	1/1	0.62	0.30	100,100,100,100	0
56	MG	14	3260	1/1	0.63	0.17	119,119,119,119	0
56	MG	1H	3332	1/1	0.63	0.42	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3201	1/1	0.63	0.30	111,111,111,111	0
56	MG	13	1717	1/1	0.63	0.28	114,114,114,114	0
56	MG	1H	3255	1/1	0.63	0.45	117,117,117,117	0
56	MG	1H	3029	1/1	0.63	0.28	110,110,110,110	0
56	MG	1H	3270	1/1	0.63	0.48	98,98,98,98	0
56	MG	1H	3328	1/1	0.64	0.54	87,87,87,87	0
56	MG	1G	1670	1/1	0.64	0.40	138,138,138,138	0
56	MG	13	1664	1/1	0.65	0.28	103,103,103,103	0
56	MG	1H	3431	1/1	0.65	0.11	163,163,163,163	0
56	MG	1H	3395	1/1	0.65	0.17	118,118,118,118	0
56	MG	1H	3337	1/1	0.65	0.42	106,106,106,106	0
56	MG	1H	3272	1/1	0.65	0.27	96,96,96,96	0
56	MG	14	3163	1/1	0.65	0.18	105,105,105,105	0
56	MG	1H	3148	1/1	0.65	0.18	79,79,79,79	0
56	MG	13	1627	1/1	0.66	0.28	101,101,101,101	0
56	MG	1H	3276	1/1	0.66	0.44	99,99,99,99	0
56	MG	14	3150	1/1	0.66	0.33	80,80,80,80	0
56	MG	E5	101	1/1	0.66	0.23	98,98,98,98	0
56	MG	14	3019	1/1	0.66	0.22	96,96,96,96	0
56	MG	39	303	1/1	0.66	0.66	87,87,87,87	0
56	MG	1G	1664	1/1	0.67	0.27	116,116,116,116	0
56	MG	1G	1667	1/1	0.67	0.24	119,119,119,119	0
56	MG	1H	3023	1/1	0.67	0.37	100,100,100,100	0
56	MG	1H	3311	1/1	0.68	0.48	109,109,109,109	0
56	MG	14	3026	1/1	0.68	0.39	92,92,92,92	0
56	MG	1H	3273	1/1	0.68	0.25	84,84,84,84	0
56	MG	1G	1645	1/1	0.68	0.31	113,113,113,113	0
56	MG	14	3133	1/1	0.68	0.13	97,97,97,97	0
56	MG	1H	3464	1/1	0.68	0.14	133,133,133,133	0
56	MG	14	3312	1/1	0.68	0.12	93,93,93,93	0
56	MG	1H	3306	1/1	0.68	0.60	81,81,81,81	0
56	MG	13	1744	1/1	0.68	0.41	132,132,132,132	0
56	MG	13	1716	1/1	0.68	0.18	111,111,111,111	0
56	MG	1H	3343	1/1	0.68	0.36	92,92,92,92	0
56	MG	1H	3326	1/1	0.69	0.54	117,117,117,117	0
56	MG	14	3029	1/1	0.69	0.22	97,97,97,97	0
56	MG	1G	1642	1/1	0.69	0.22	102,102,102,102	0
56	MG	13	1748	1/1	0.69	0.09	140,140,140,140	0
56	MG	1H	3087	1/1	0.69	0.18	69,69,69,69	0
56	MG	1H	3330	1/1	0.69	0.56	104,104,104,104	0
56	MG	14	3235	1/1	0.69	0.14	83,83,83,83	0
56	MG	14	3286	1/1	0.69	0.15	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1640	1/1	0.69	0.23	94,94,94,94	0
56	MG	14	3182	1/1	0.70	0.27	98,98,98,98	0
56	MG	13	1639	1/1	0.70	0.19	109,109,109,109	0
56	MG	14	3143	1/1	0.70	0.43	100,100,100,100	0
56	MG	14	3403	1/1	0.70	0.09	122,122,122,122	0
56	MG	14	3372	1/1	0.70	0.12	134,134,134,134	0
56	MG	14	3227	1/1	0.70	0.33	97,97,97,97	0
56	MG	13	1669	1/1	0.70	0.27	110,110,110,110	0
56	MG	14	3203	1/1	0.70	0.29	81,81,81,81	0
56	MG	1H	3135	1/1	0.70	0.26	111,111,111,111	0
56	MG	14	3251	1/1	0.70	0.10	105,105,105,105	0
56	MG	1H	3331	1/1	0.70	0.82	106,106,106,106	0
56	MG	13	1714	1/1	0.70	0.22	101,101,101,101	0
56	MG	2L	102	1/1	0.70	0.26	89,89,89,89	0
56	MG	1H	3186	1/1	0.70	0.35	93,93,93,93	0
56	MG	1H	3143	1/1	0.70	0.44	99,99,99,99	0
56	MG	13	1749	1/1	0.70	0.23	121,121,121,121	0
56	MG	14	3319	1/1	0.71	0.29	118,118,118,118	0
56	MG	1H	3124	1/1	0.71	0.19	72,72,72,72	0
56	MG	14	3297	1/1	0.71	0.24	96,96,96,96	0
56	MG	14	3416	1/1	0.71	0.43	126,126,126,126	0
56	MG	13	1675	1/1	0.71	0.19	121,121,121,121	0
56	MG	13	1666	1/1	0.71	0.31	105,105,105,105	0
56	MG	14	3236	1/1	0.71	0.10	99,99,99,99	0
56	MG	1H	3157	1/1	0.71	0.51	104,104,104,104	0
56	MG	1H	3505	1/1	0.71	0.15	112,112,112,112	0
56	MG	14	3356	1/1	0.71	0.25	118,118,118,118	0
56	MG	14	3272	1/1	0.71	0.32	95,95,95,95	0
56	MG	13	1651	1/1	0.71	0.23	100,100,100,100	0
56	MG	14	3291	1/1	0.71	0.18	115,115,115,115	0
56	MG	14	3376	1/1	0.71	0.13	119,119,119,119	0
56	MG	1H	3251	1/1	0.72	0.15	93,93,93,93	0
56	MG	14	3274	1/1	0.72	0.25	122,122,122,122	0
56	MG	14	3294	1/1	0.72	0.14	91,91,91,91	0
56	MG	1H	3179	1/1	0.72	0.40	96,96,96,96	0
56	MG	1H	3266	1/1	0.72	0.58	95,95,95,95	0
56	MG	13	1688	1/1	0.72	0.33	93,93,93,93	0
56	MG	1H	3340	1/1	0.73	0.36	93,93,93,93	0
56	MG	1G	1649	1/1	0.73	0.27	105,105,105,105	0
56	MG	1H	3153	1/1	0.73	0.40	98,98,98,98	0
56	MG	1H	3026	1/1	0.73	0.34	94,94,94,94	0
56	MG	13	1718	1/1	0.73	0.41	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1620	1/1	0.73	0.20	107,107,107,107	0
56	MG	14	3232	1/1	0.73	0.29	103,103,103,103	0
56	MG	1H	3491	1/1	0.73	0.16	93,93,93,93	0
56	MG	14	3317	1/1	0.73	0.28	98,98,98,98	0
56	MG	1H	3137	1/1	0.73	0.53	87,87,87,87	0
56	MG	14	3265	1/1	0.73	0.29	88,88,88,88	0
56	MG	1H	3062	1/1	0.74	0.23	101,101,101,101	0
56	MG	14	3276	1/1	0.74	1.33	103,103,103,103	0
56	MG	13	1656	1/1	0.74	0.42	103,103,103,103	0
56	MG	14	3030	1/1	0.74	0.22	115,115,115,115	0
56	MG	14	3252	1/1	0.74	0.15	105,105,105,105	0
56	MG	14	3418	1/1	0.74	0.07	130,130,130,130	0
56	MG	13	1689	1/1	0.74	0.25	98,98,98,98	0
56	MG	1G	1643	1/1	0.74	0.30	104,104,104,104	0
56	MG	29	301	1/1	0.74	0.64	101,101,101,101	0
56	MG	1J	203	1/1	0.75	0.17	114,114,114,114	0
56	MG	1H	3265	1/1	0.75	0.27	96,96,96,96	0
56	MG	14	3281	1/1	0.75	0.55	105,105,105,105	0
56	MG	14	3313	1/1	0.75	0.19	124,124,124,124	0
56	MG	14	3285	1/1	0.75	0.30	91,91,91,91	0
56	MG	1H	3296	1/1	0.75	0.21	86,86,86,86	0
56	MG	1H	3346	1/1	0.75	0.61	106,106,106,106	0
56	MG	1H	3106	1/1	0.75	0.34	95,95,95,95	0
56	MG	1H	3428	1/1	0.75	0.06	123,123,123,123	0
56	MG	1H	3169	1/1	0.75	0.25	85,85,85,85	0
56	MG	1H	3504	1/1	0.75	0.11	138,138,138,138	0
56	MG	1H	3415	1/1	0.75	0.07	99,99,99,99	0
56	MG	14	3170	1/1	0.75	0.60	77,77,77,77	0
56	MG	14	3315	1/1	0.75	0.13	92,92,92,92	0
56	MG	1G	1625	1/1	0.76	0.12	131,131,131,131	0
56	MG	14	3318	1/1	0.76	0.19	99,99,99,99	0
56	MG	14	3264	1/1	0.76	0.30	89,89,89,89	0
56	MG	1H	3152	1/1	0.76	0.31	93,93,93,93	0
56	MG	14	3368	1/1	0.76	0.11	117,117,117,117	0
56	MG	13	1690	1/1	0.76	0.19	108,108,108,108	0
56	MG	14	3311	1/1	0.76	0.17	89,89,89,89	0
56	MG	13	1641	1/1	0.76	0.35	88,88,88,88	0
56	MG	32	301	1/1	0.76	0.46	120,120,120,120	0
56	MG	1H	3407	1/1	0.77	0.07	115,115,115,115	0
56	MG	13	1743	1/1	0.77	0.18	108,108,108,108	0
56	MG	1H	3147	1/1	0.77	0.32	94,94,94,94	0
56	MG	1H	3175	1/1	0.77	0.35	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3189	1/1	0.77	0.30	81,81,81,81	0
56	MG	1G	1632	1/1	0.77	0.41	116,116,116,116	0
56	MG	13	1721	1/1	0.77	0.64	101,101,101,101	0
56	MG	1G	1604	1/1	0.77	0.23	142,142,142,142	0
56	MG	13	1685	1/1	0.77	0.17	112,112,112,112	0
56	MG	14	3255	1/1	0.77	0.41	99,99,99,99	0
56	MG	1H	3307	1/1	0.77	0.28	99,99,99,99	0
56	MG	1H	3467	1/1	0.77	0.10	106,106,106,106	0
56	MG	1H	3500	1/1	0.77	0.20	122,122,122,122	0
56	MG	1H	3206	1/1	0.77	0.14	53,53,53,53	0
56	MG	14	3064	1/1	0.77	0.27	97,97,97,97	0
56	MG	14	3237	1/1	0.77	0.24	95,95,95,95	0
56	MG	16	214	1/1	0.77	0.22	109,109,109,109	0
56	MG	14	3196	1/1	0.77	0.34	99,99,99,99	0
56	MG	14	3158	1/1	0.77	0.15	93,93,93,93	0
56	MG	14	3137	1/1	0.78	0.19	80,80,80,80	0
56	MG	14	3103	1/1	0.78	0.38	90,90,90,90	0
56	MG	39	302	1/1	0.78	0.30	118,118,118,118	0
56	MG	1H	3027	1/1	0.78	0.32	96,96,96,96	0
56	MG	13	1693	1/1	0.78	0.21	103,103,103,103	0
56	MG	14	3178	1/1	0.78	0.44	95,95,95,95	0
56	MG	1H	3072	1/1	0.79	0.29	80,80,80,80	0
56	MG	13	1702	1/1	0.79	0.23	109,109,109,109	0
56	MG	1H	3129	1/1	0.79	0.41	90,90,90,90	0
56	MG	1G	1640	1/1	0.79	0.49	106,106,106,106	0
56	MG	14	3320	1/1	0.79	0.22	96,96,96,96	0
56	MG	14	3275	1/1	0.79	0.27	105,105,105,105	0
56	MG	14	3080	1/1	0.79	0.41	88,88,88,88	0
56	MG	1H	3230	1/1	0.79	0.24	91,91,91,91	0
56	MG	14	3147	1/1	0.79	0.19	97,97,97,97	0
56	MG	14	3176	1/1	0.79	0.39	101,101,101,101	0
56	MG	1H	3202	1/1	0.79	0.38	93,93,93,93	0
56	MG	1G	1657	1/1	0.79	0.25	106,106,106,106	0
56	MG	14	3167	1/1	0.79	0.27	110,110,110,110	0
56	MG	L8	101	1/1	0.79	0.43	85,85,85,85	0
56	MG	1H	3267	1/1	0.79	0.34	84,84,84,84	0
56	MG	1H	3476	1/1	0.79	0.12	93,93,93,93	0
56	MG	41	202	1/1	0.79	0.29	96,96,96,96	0
56	MG	14	3254	1/1	0.80	0.17	87,87,87,87	0
56	MG	1H	3034	1/1	0.80	0.34	96,96,96,96	0
56	MG	1H	3249	1/1	0.80	0.42	97,97,97,97	0
56	MG	13	1668	1/1	0.80	0.19	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3117	1/1	0.80	0.45	98,98,98,98	0
56	MG	1H	3074	1/1	0.80	0.41	80,80,80,80	0
56	MG	2K	105	1/1	0.80	0.38	107,107,107,107	0
56	MG	1H	3280	1/1	0.80	0.70	100,100,100,100	0
56	MG	14	3270	1/1	0.80	0.20	107,107,107,107	0
56	MG	1H	3132	1/1	0.80	0.18	74,74,74,74	0
56	MG	1H	3116	1/1	0.80	0.29	70,70,70,70	0
56	MG	1H	3305	1/1	0.80	0.61	104,104,104,104	0
56	MG	13	1694	1/1	0.80	0.10	121,121,121,121	0
56	MG	1H	3013	1/1	0.80	0.41	104,104,104,104	0
56	MG	14	3422	1/1	0.80	0.09	132,132,132,132	0
56	MG	1H	3300	1/1	0.81	0.35	87,87,87,87	0
56	MG	1H	3499	1/1	0.81	0.11	110,110,110,110	0
56	MG	1G	1673	1/1	0.81	0.14	108,108,108,108	0
56	MG	14	3326	1/1	0.81	0.39	117,117,117,117	0
56	MG	14	3405	1/1	0.81	0.22	102,102,102,102	0
56	MG	1H	3107	1/1	0.81	0.28	85,85,85,85	0
56	MG	1H	3127	1/1	0.81	0.29	92,92,92,92	0
56	MG	1H	3314	1/1	0.81	0.37	76,76,76,76	0
56	MG	16	215	1/1	0.81	0.08	113,113,113,113	0
56	MG	1G	1659	1/1	0.81	0.29	102,102,102,102	0
56	MG	18	101	1/1	0.81	0.27	84,84,84,84	0
56	MG	1H	3292	1/1	0.81	0.23	72,72,72,72	0
56	MG	1J	208	1/1	0.81	0.11	121,121,121,121	0
56	MG	13	1684	1/1	0.81	0.33	106,106,106,106	0
56	MG	14	3280	1/1	0.81	0.31	95,95,95,95	0
56	MG	14	3293	1/1	0.81	0.27	95,95,95,95	0
56	MG	14	3248	1/1	0.81	0.26	85,85,85,85	0
56	MG	1H	3262	1/1	0.81	0.30	89,89,89,89	0
56	MG	1J	204	1/1	0.81	0.12	113,113,113,113	0
56	MG	1H	3479	1/1	0.81	0.16	126,126,126,126	0
56	MG	1H	3242	1/1	0.81	0.52	105,105,105,105	0
56	MG	14	3144	1/1	0.81	0.35	93,93,93,93	0
56	MG	1H	3287	1/1	0.81	0.42	92,92,92,92	0
56	MG	1H	3165	1/1	0.81	0.42	95,95,95,95	0
56	MG	13	1734	1/1	0.81	0.15	133,133,133,133	0
56	MG	14	3162	1/1	0.82	0.19	88,88,88,88	0
56	MG	13	1722	1/1	0.82	0.10	85,85,85,85	0
56	MG	1J	206	1/1	0.82	0.12	123,123,123,123	0
56	MG	14	3324	1/1	0.82	0.40	96,96,96,96	0
56	MG	1H	3254	1/1	0.82	0.37	80,80,80,80	0
56	MG	1G	1680	1/1	0.82	0.11	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3126	1/1	0.82	0.32	79,79,79,79	0
56	MG	14	3065	1/1	0.82	0.20	87,87,87,87	0
56	MG	2K	106	1/1	0.82	0.42	115,115,115,115	0
56	MG	14	3169	1/1	0.82	0.29	93,93,93,93	0
56	MG	1H	3232	1/1	0.82	0.32	80,80,80,80	0
56	MG	1G	1686	1/1	0.82	0.07	129,129,129,129	0
56	MG	14	3261	1/1	0.82	0.34	83,83,83,83	0
56	MG	14	3301	1/1	0.82	0.29	83,83,83,83	0
56	MG	14	3370	1/1	0.82	0.13	110,110,110,110	0
56	MG	14	3211	1/1	0.82	0.40	93,93,93,93	0
56	MG	13	1695	1/1	0.82	0.15	112,112,112,112	0
56	MG	1H	3372	1/1	0.82	0.10	79,79,79,79	0
56	MG	1G	1628	1/1	0.82	0.21	118,118,118,118	0
56	MG	1H	3140	1/1	0.82	0.52	101,101,101,101	0
56	MG	14	3173	1/1	0.82	0.28	87,87,87,87	0
56	MG	1H	3490	1/1	0.82	0.13	125,125,125,125	0
56	MG	1H	3485	1/1	0.82	0.08	121,121,121,121	0
56	MG	1H	3168	1/1	0.83	0.30	83,83,83,83	0
56	MG	1H	3294	1/1	0.83	0.47	100,100,100,100	0
56	MG	14	3330	1/1	0.83	0.20	105,105,105,105	0
56	MG	13	1630	1/1	0.83	0.12	74,74,74,74	0
56	MG	1H	3055	1/1	0.83	0.16	82,82,82,82	0
56	MG	3I	202	1/1	0.83	0.45	101,101,101,101	0
56	MG	14	3325	1/1	0.83	0.34	89,89,89,89	0
56	MG	14	3151	1/1	0.83	0.24	91,91,91,91	0
56	MG	1G	1648	1/1	0.83	0.23	100,100,100,100	0
56	MG	1G	1668	1/1	0.83	0.22	111,111,111,111	0
56	MG	14	3267	1/1	0.83	0.16	110,110,110,110	0
56	MG	52	201	1/1	0.83	0.12	107,107,107,107	0
56	MG	16	201	1/1	0.83	0.23	79,79,79,79	0
56	MG	13	1682	1/1	0.83	0.28	116,116,116,116	0
56	MG	14	3253	1/1	0.83	0.29	82,82,82,82	0
56	MG	1H	3477	1/1	0.83	0.10	108,108,108,108	0
56	MG	1H	3111	1/1	0.83	0.43	91,91,91,91	0
56	MG	1H	3503	1/1	0.83	0.12	116,116,116,116	0
56	MG	14	3256	1/1	0.83	0.19	97,97,97,97	0
56	MG	1G	1623	1/1	0.83	0.24	122,122,122,122	0
56	MG	14	3193	1/1	0.83	0.09	89,89,89,89	0
56	MG	25	201	1/1	0.83	0.43	111,111,111,111	0
56	MG	1H	3128	1/1	0.83	0.21	88,88,88,88	0
56	MG	1H	3193	1/1	0.83	0.36	95,95,95,95	0
56	MG	14	3374	1/1	0.83	0.08	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3204	1/1	0.83	0.13	80,80,80,80	0
56	MG	1H	3219	1/1	0.83	0.39	65,65,65,65	0
56	MG	1G	1663	1/1	0.83	0.21	92,92,92,92	0
56	MG	14	3175	1/1	0.83	0.38	99,99,99,99	0
56	MG	1H	3122	1/1	0.84	0.30	94,94,94,94	0
56	MG	14	3168	1/1	0.84	0.23	67,67,67,67	0
56	MG	1H	3342	1/1	0.84	0.17	92,92,92,92	0
56	MG	1H	3199	1/1	0.84	0.51	99,99,99,99	0
56	MG	1H	3012	1/1	0.84	0.51	93,93,93,93	0
56	MG	1H	3185	1/1	0.84	0.38	88,88,88,88	0
56	MG	14	3142	1/1	0.84	0.46	100,100,100,100	0
56	MG	13	1687	1/1	0.84	0.28	109,109,109,109	0
56	MG	1H	3283	1/1	0.84	0.38	112,112,112,112	0
56	MG	1G	1684	1/1	0.84	0.12	124,124,124,124	0
56	MG	1G	1638	1/1	0.84	0.43	95,95,95,95	0
56	MG	1H	3258	1/1	0.84	0.31	93,93,93,93	0
56	MG	1H	3286	1/1	0.84	0.26	85,85,85,85	0
56	MG	14	3279	1/1	0.84	0.25	87,87,87,87	0
56	MG	13	1699	1/1	0.84	0.50	102,102,102,102	0
56	MG	14	3352	1/1	0.84	0.12	74,74,74,74	0
56	MG	15	201	1/1	0.84	0.54	102,102,102,102	0
56	MG	14	3185	1/1	0.84	0.21	90,90,90,90	0
56	MG	1H	3391	1/1	0.84	0.09	96,96,96,96	0
56	MG	2L	103	1/1	0.84	0.28	115,115,115,115	0
56	MG	1H	3285	1/1	0.84	0.39	88,88,88,88	0
56	MG	1H	3081	1/1	0.84	0.25	77,77,77,77	0
56	MG	1H	3423	1/1	0.84	0.14	102,102,102,102	0
56	MG	1H	3288	1/1	0.84	0.28	87,87,87,87	0
56	MG	14	3411	1/1	0.84	0.30	104,104,104,104	0
56	MG	14	3104	1/1	0.84	0.27	81,81,81,81	0
56	MG	14	3136	1/1	0.84	0.10	112,112,112,112	0
56	MG	1G	1669	1/1	0.84	0.28	112,112,112,112	0
56	MG	14	3202	1/1	0.84	0.26	100,100,100,100	0
56	MG	1H	3190	1/1	0.84	0.17	77,77,77,77	0
56	MG	1H	3177	1/1	0.84	0.44	98,98,98,98	0
56	MG	1H	3487	1/1	0.84	0.29	126,126,126,126	0
56	MG	1G	1687	1/1	0.84	0.30	135,135,135,135	0
56	MG	6A	101	1/1	0.84	0.21	138,138,138,138	0
56	MG	1H	3246	1/1	0.84	0.22	78,78,78,78	0
56	MG	14	3209	1/1	0.85	0.33	71,71,71,71	0
56	MG	1H	3256	1/1	0.85	0.26	88,88,88,88	0
56	MG	1H	3092	1/1	0.85	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3412	1/1	0.85	0.08	108,108,108,108	0
56	MG	1H	3141	1/1	0.85	0.44	89,89,89,89	0
56	MG	1G	1602	1/1	0.85	0.39	118,118,118,118	0
56	MG	14	3200	1/1	0.85	0.18	85,85,85,85	0
56	MG	1H	3146	1/1	0.85	0.32	83,83,83,83	0
56	MG	1G	1639	1/1	0.85	0.17	89,89,89,89	0
56	MG	14	3058	1/1	0.85	0.16	128,128,128,128	0
56	MG	13	1704	1/1	0.85	0.69	118,118,118,118	0
56	MG	1H	3344	1/1	0.85	0.42	95,95,95,95	0
56	MG	1H	3174	1/1	0.85	0.31	78,78,78,78	0
56	MG	1H	3061	1/1	0.85	0.34	85,85,85,85	0
56	MG	14	3308	1/1	0.85	0.21	106,106,106,106	0
56	MG	14	3068	1/1	0.85	0.39	86,86,86,86	0
56	MG	1H	3488	1/1	0.85	0.15	114,114,114,114	0
56	MG	1H	3447	1/1	0.85	0.17	105,105,105,105	0
56	MG	1H	3298	1/1	0.85	0.33	92,92,92,92	0
56	MG	14	3093	1/1	0.85	0.51	103,103,103,103	0
56	MG	P8	101	1/1	0.85	0.41	84,84,84,84	0
56	MG	1H	3182	1/1	0.85	0.36	74,74,74,74	0
56	MG	1H	3489	1/1	0.85	0.12	69,69,69,69	0
56	MG	1H	3493	1/1	0.85	0.25	130,130,130,130	0
56	MG	13	1740	1/1	0.85	0.17	106,106,106,106	0
56	MG	1H	3318	1/1	0.85	0.30	87,87,87,87	0
56	MG	14	3247	1/1	0.85	0.14	75,75,75,75	0
56	MG	1H	3321	1/1	0.85	0.27	99,99,99,99	0
56	MG	14	3208	1/1	0.85	0.10	84,84,84,84	0
56	MG	1G	1650	1/1	0.86	0.36	101,101,101,101	0
56	MG	1G	1653	1/1	0.86	0.11	106,106,106,106	0
56	MG	13	1719	1/1	0.86	0.13	95,95,95,95	0
56	MG	1H	3290	1/1	0.86	0.49	92,92,92,92	0
56	MG	1H	3439	1/1	0.86	0.15	92,92,92,92	0
56	MG	1H	3178	1/1	0.86	0.27	76,76,76,76	0
56	MG	1H	3339	1/1	0.86	0.33	90,90,90,90	0
56	MG	1G	1635	1/1	0.86	0.39	118,118,118,118	0
56	MG	1J	202	1/1	0.86	0.12	157,157,157,157	0
56	MG	1G	1615	1/1	0.86	0.23	115,115,115,115	0
56	MG	13	1670	1/1	0.86	0.33	88,88,88,88	0
56	MG	1H	3492	1/1	0.86	0.23	120,120,120,120	0
56	MG	13	1605	1/1	0.86	0.18	93,93,93,93	0
56	MG	1H	3007	1/1	0.86	0.33	97,97,97,97	0
56	MG	1H	3434	1/1	0.86	0.19	130,130,130,130	0
56	MG	14	3152	1/1	0.86	0.23	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1647	1/1	0.86	0.17	93,93,93,93	0
56	MG	31	301	1/1	0.86	0.10	92,92,92,92	0
56	MG	16	206	1/1	0.86	0.25	102,102,102,102	0
56	MG	1G	1675	1/1	0.86	0.47	99,99,99,99	0
56	MG	14	3266	1/1	0.86	0.38	80,80,80,80	0
56	MG	1H	3263	1/1	0.86	0.22	106,106,106,106	0
56	MG	1H	3102	1/1	0.86	0.28	67,67,67,67	0
56	MG	14	3278	1/1	0.86	0.26	85,85,85,85	0
56	MG	1H	3317	1/1	0.86	0.79	85,85,85,85	0
56	MG	13	1650	1/1	0.86	0.15	87,87,87,87	0
56	MG	45	201	1/1	0.86	0.18	113,113,113,113	0
56	MG	1G	1603	1/1	0.86	0.17	118,118,118,118	0
56	MG	1H	3030	1/1	0.86	0.19	79,79,79,79	0
56	MG	1J	205	1/1	0.86	0.23	101,101,101,101	0
56	MG	13	1663	1/1	0.86	0.16	87,87,87,87	0
56	MG	1H	3260	1/1	0.86	0.28	76,76,76,76	0
56	MG	14	3148	1/1	0.86	0.11	117,117,117,117	0
56	MG	C5	201	1/1	0.86	0.23	123,123,123,123	0
56	MG	14	3197	1/1	0.86	0.50	119,119,119,119	0
56	MG	14	3413	1/1	0.87	0.31	110,110,110,110	0
56	MG	1H	3494	1/1	0.87	0.36	121,121,121,121	0
56	MG	1H	3198	1/1	0.87	0.38	90,90,90,90	0
56	MG	25	202	1/1	0.87	0.33	125,125,125,125	0
56	MG	1H	3284	1/1	0.87	0.27	70,70,70,70	0
56	MG	1H	3335	1/1	0.87	0.42	85,85,85,85	0
56	MG	14	3249	1/1	0.87	0.27	97,97,97,97	0
56	MG	14	3316	1/1	0.87	0.54	103,103,103,103	0
56	MG	13	1691	1/1	0.87	0.30	95,95,95,95	0
57	ZN	G8	202	1/1	0.87	0.31	192,192,192,192	0
56	MG	1H	3086	1/1	0.87	0.39	72,72,72,72	0
56	MG	1H	3015	1/1	0.87	0.24	71,71,71,71	0
56	MG	14	3305	1/1	0.87	0.14	79,79,79,79	0
56	MG	14	3398	1/1	0.87	0.06	127,127,127,127	0
56	MG	14	3066	1/1	0.87	0.30	96,96,96,96	0
56	MG	14	3195	1/1	0.87	0.38	100,100,100,100	0
56	MG	1H	3155	1/1	0.87	0.17	78,78,78,78	0
56	MG	14	3123	1/1	0.87	0.16	75,75,75,75	0
56	MG	1G	1671	1/1	0.87	0.40	120,120,120,120	0
56	MG	1H	3222	1/1	0.87	0.30	79,79,79,79	0
56	MG	14	3174	1/1	0.87	0.18	93,93,93,93	0
56	MG	13	1622	1/1	0.87	0.32	102,102,102,102	0
56	MG	13	1624	1/1	0.87	0.22	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2K	104	1/1	0.87	0.44	90,90,90,90	0
56	MG	13	1665	1/1	0.87	0.12	91,91,91,91	0
56	MG	1H	3323	1/1	0.87	0.11	110,110,110,110	0
56	MG	14	3283	1/1	0.87	0.21	98,98,98,98	0
56	MG	13	1621	1/1	0.87	0.39	115,115,115,115	0
56	MG	1H	3399	1/1	0.87	0.09	59,59,59,59	0
56	MG	1G	1634	1/1	0.87	0.48	120,120,120,120	0
56	MG	14	3328	1/1	0.87	0.12	111,111,111,111	0
56	MG	14	3337	1/1	0.87	0.12	76,76,76,76	0
56	MG	1G	1665	1/1	0.87	0.30	110,110,110,110	0
56	MG	1H	3478	1/1	0.87	0.09	118,118,118,118	0
56	MG	14	3381	1/1	0.87	0.22	101,101,101,101	0
56	MG	1H	3223	1/1	0.87	0.18	82,82,82,82	0
56	MG	1H	3083	1/1	0.87	0.32	92,92,92,92	0
56	MG	1H	3480	1/1	0.87	0.14	109,109,109,109	0
56	MG	88	202	1/1	0.87	0.30	77,77,77,77	0
56	MG	1J	207	1/1	0.87	0.27	147,147,147,147	0
56	MG	5E	201	1/1	0.87	0.20	104,104,104,104	0
56	MG	14	3369	1/1	0.88	0.18	105,105,105,105	0
56	MG	1G	1682	1/1	0.88	0.09	141,141,141,141	0
56	MG	1H	3295	1/1	0.88	0.50	92,92,92,92	0
56	MG	1H	3118	1/1	0.88	0.30	76,76,76,76	0
56	MG	1H	3144	1/1	0.88	0.23	80,80,80,80	0
56	MG	14	3023	1/1	0.88	0.15	86,86,86,86	0
56	MG	1G	1652	1/1	0.88	0.26	103,103,103,103	0
56	MG	14	3273	1/1	0.88	0.14	87,87,87,87	0
56	MG	14	3233	1/1	0.88	0.30	118,118,118,118	0
56	MG	1H	3282	1/1	0.88	0.15	107,107,107,107	0
56	MG	1G	1641	1/1	0.88	0.29	90,90,90,90	0
56	MG	14	3192	1/1	0.88	0.14	84,84,84,84	0
56	MG	1H	3381	1/1	0.88	0.09	89,89,89,89	0
56	MG	1G	1679	1/1	0.88	0.09	108,108,108,108	0
56	MG	14	3164	1/1	0.88	0.21	91,91,91,91	0
56	MG	14	3282	1/1	0.88	0.31	90,90,90,90	0
56	MG	1H	3136	1/1	0.88	0.15	71,71,71,71	0
56	MG	13	1672	1/1	0.88	0.20	100,100,100,100	0
56	MG	1H	3471	1/1	0.88	0.11	128,128,128,128	0
56	MG	14	3221	1/1	0.88	0.20	87,87,87,87	0
56	MG	13	1706	1/1	0.88	0.91	103,103,103,103	0
56	MG	14	3343	1/1	0.88	0.12	89,89,89,89	0
56	MG	14	3346	1/1	0.88	0.11	92,92,92,92	0
56	MG	13	1679	1/1	0.88	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1652	1/1	0.88	0.23	98,98,98,98	0
56	MG	14	3354	1/1	0.88	0.06	126,126,126,126	0
56	MG	13	1680	1/1	0.88	0.19	124,124,124,124	0
56	MG	45	202	1/1	0.88	0.53	82,82,82,82	0
56	MG	14	3187	1/1	0.88	0.36	100,100,100,100	0
56	MG	13	1654	1/1	0.88	0.28	123,123,123,123	0
56	MG	14	3407	1/1	0.88	0.08	116,116,116,116	0
56	MG	1G	1636	1/1	0.88	0.08	115,115,115,115	0
56	MG	49	201	1/1	0.88	0.10	143,143,143,143	0
56	MG	14	3363	1/1	0.88	0.06	117,117,117,117	0
56	MG	35	201	1/1	0.88	0.21	91,91,91,91	0
56	MG	1H	3204	1/1	0.88	0.75	104,104,104,104	0
56	MG	14	3277	1/1	0.89	0.20	90,90,90,90	0
56	MG	1H	3210	1/1	0.89	0.17	69,69,69,69	0
56	MG	14	3250	1/1	0.89	0.23	86,86,86,86	0
56	MG	1H	3237	1/1	0.89	0.17	70,70,70,70	0
56	MG	14	3231	1/1	0.89	0.21	93,93,93,93	0
57	ZN	C5	202	1/1	0.89	0.11	189,189,189,189	0
56	MG	1H	3245	1/1	0.89	0.38	96,96,96,96	0
56	MG	13	1607	1/1	0.89	0.19	78,78,78,78	0
56	MG	13	1727	1/1	0.89	0.24	121,121,121,121	0
56	MG	14	3130	1/1	0.89	0.10	71,71,71,71	0
56	MG	14	3166	1/1	0.89	0.14	106,106,106,106	0
56	MG	13	1676	1/1	0.89	0.18	111,111,111,111	0
56	MG	1H	3502	1/1	0.89	0.29	118,118,118,118	0
56	MG	14	3149	1/1	0.89	0.21	79,79,79,79	0
56	MG	14	3371	1/1	0.89	0.21	101,101,101,101	0
56	MG	1H	3104	1/1	0.89	0.22	78,78,78,78	0
56	MG	11	302	1/1	0.89	0.25	66,66,66,66	0
56	MG	14	3268	1/1	0.89	0.19	100,100,100,100	0
56	MG	1G	1647	1/1	0.89	0.32	86,86,86,86	0
56	MG	14	3289	1/1	0.89	0.18	86,86,86,86	0
56	MG	1H	3345	1/1	0.89	0.31	100,100,100,100	0
56	MG	1H	3225	1/1	0.89	0.21	69,69,69,69	0
56	MG	1H	3031	1/1	0.89	0.33	89,89,89,89	0
56	MG	13	1674	1/1	0.89	0.23	118,118,118,118	0
56	MG	14	3177	1/1	0.89	0.32	111,111,111,111	0
56	MG	1H	3457	1/1	0.89	0.05	113,113,113,113	0
56	MG	13	1752	1/1	0.89	0.51	92,92,92,92	0
56	MG	14	3125	1/1	0.89	0.27	101,101,101,101	0
56	MG	1H	3279	1/1	0.90	0.25	80,80,80,80	0
56	MG	14	3355	1/1	0.90	0.18	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1656	1/1	0.90	0.30	103,103,103,103	0
56	MG	1H	3009	1/1	0.90	0.20	69,69,69,69	0
56	MG	1H	3277	1/1	0.90	0.47	109,109,109,109	0
56	MG	13	1696	1/1	0.90	0.29	108,108,108,108	0
56	MG	1H	3238	1/1	0.90	0.32	84,84,84,84	0
56	MG	14	3017	1/1	0.90	0.15	91,91,91,91	0
56	MG	14	3217	1/1	0.90	0.80	82,82,82,82	0
56	MG	1G	1605	1/1	0.90	0.17	98,98,98,98	0
56	MG	14	3415	1/1	0.90	0.40	107,107,107,107	0
56	MG	1H	3469	1/1	0.90	0.07	106,106,106,106	0
56	MG	13	1632	1/1	0.90	0.16	64,64,64,64	0
56	MG	1H	3430	1/1	0.90	0.10	116,116,116,116	0
56	MG	1H	3366	1/1	0.90	0.12	60,60,60,60	0
56	MG	1H	3473	1/1	0.90	0.21	127,127,127,127	0
56	MG	16	207	1/1	0.90	0.37	84,84,84,84	0
56	MG	13	1618	1/1	0.90	0.26	86,86,86,86	0
56	MG	14	3153	1/1	0.90	0.17	70,70,70,70	0
56	MG	14	3303	1/1	0.90	0.11	100,100,100,100	0
56	MG	1H	3466	1/1	0.90	0.12	94,94,94,94	0
56	MG	1G	1666	1/1	0.90	0.36	89,89,89,89	0
56	MG	13	1707	1/1	0.90	0.25	104,104,104,104	0
56	MG	1H	3077	1/1	0.90	0.25	67,67,67,67	0
56	MG	14	3013	1/1	0.90	0.17	88,88,88,88	0
56	MG	13	1644	1/1	0.90	0.12	96,96,96,96	0
56	MG	14	3306	1/1	0.90	0.30	93,93,93,93	0
56	MG	14	3112	1/1	0.90	0.12	98,98,98,98	0
56	MG	14	3383	1/1	0.90	0.16	98,98,98,98	0
56	MG	1H	3308	1/1	0.90	0.25	90,90,90,90	0
56	MG	14	3161	1/1	0.90	0.20	104,104,104,104	0
56	MG	14	3081	1/1	0.90	0.31	90,90,90,90	0
56	MG	14	3269	1/1	0.90	0.31	102,102,102,102	0
56	MG	14	3296	1/1	0.90	0.20	107,107,107,107	0
56	MG	1H	3138	1/1	0.90	0.40	94,94,94,94	0
56	MG	14	3037	1/1	0.90	0.20	79,79,79,79	0
56	MG	14	3028	1/1	0.90	0.14	98,98,98,98	0
56	MG	1G	1606	1/1	0.90	0.27	129,129,129,129	0
56	MG	1H	3304	1/1	0.90	0.39	114,114,114,114	0
56	MG	14	3076	1/1	0.90	0.11	93,93,93,93	0
56	MG	1H	3184	1/1	0.90	0.19	107,107,107,107	0
56	MG	1H	3268	1/1	0.90	0.50	125,125,125,125	0
56	MG	1G	1661	1/1	0.90	0.26	105,105,105,105	0
56	MG	1J	209	1/1	0.90	0.07	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3287	1/1	0.90	0.21	95,95,95,95	0
56	MG	1H	3209	1/1	0.90	0.15	82,82,82,82	0
56	MG	14	3239	1/1	0.90	0.23	166,166,166,166	0
56	MG	1H	3108	1/1	0.90	0.22	86,86,86,86	0
56	MG	13	1646	1/1	0.90	0.24	104,104,104,104	0
56	MG	14	3379	1/1	0.90	0.09	77,77,77,77	0
56	MG	14	3022	1/1	0.90	0.48	107,107,107,107	0
56	MG	I8	102	1/1	0.90	0.41	64,64,64,64	0
56	MG	1H	3316	1/1	0.90	0.57	94,94,94,94	0
56	MG	14	3387	1/1	0.90	0.10	76,76,76,76	0
56	MG	1H	3274	1/1	0.90	0.57	100,100,100,100	0
56	MG	14	3419	1/1	0.90	0.24	112,112,112,112	0
56	MG	1H	3071	1/1	0.90	0.12	94,94,94,94	0
56	MG	13	1713	1/1	0.91	0.12	119,119,119,119	0
56	MG	14	3159	1/1	0.91	0.13	112,112,112,112	0
56	MG	14	3154	1/1	0.91	0.23	86,86,86,86	0
56	MG	1H	3100	1/1	0.91	0.27	86,86,86,86	0
56	MG	1H	3133	1/1	0.91	0.14	84,84,84,84	0
56	MG	1H	3426	1/1	0.91	0.13	92,92,92,92	0
56	MG	13	1662	1/1	0.91	0.11	94,94,94,94	0
56	MG	14	3018	1/1	0.91	0.13	70,70,70,70	0
56	MG	1H	3334	1/1	0.91	0.50	99,99,99,99	0
56	MG	14	3207	1/1	0.91	0.14	68,68,68,68	0
56	MG	1H	3496	1/1	0.91	0.04	131,131,131,131	0
56	MG	1G	1688	1/1	0.91	0.13	117,117,117,117	0
56	MG	2K	107	1/1	0.91	0.41	106,106,106,106	0
56	MG	13	1724	1/1	0.91	0.06	102,102,102,102	0
56	MG	1G	1610	1/1	0.91	0.13	115,115,115,115	0
56	MG	1H	3191	1/1	0.91	0.34	87,87,87,87	0
56	MG	1H	3358	1/1	0.91	0.15	76,76,76,76	0
56	MG	14	3302	1/1	0.91	0.19	92,92,92,92	0
56	MG	14	3360	1/1	0.91	0.06	92,92,92,92	0
56	MG	1G	1655	1/1	0.91	0.21	111,111,111,111	0
56	MG	13	1677	1/1	0.91	0.39	98,98,98,98	0
56	MG	14	3396	1/1	0.91	0.16	119,119,119,119	0
56	MG	14	3271	1/1	0.91	0.12	87,87,87,87	0
56	MG	14	3109	1/1	0.91	0.32	89,89,89,89	0
56	MG	14	3304	1/1	0.91	0.33	121,121,121,121	0
56	MG	14	3395	1/1	0.91	0.09	96,96,96,96	0
56	MG	13	1637	1/1	0.91	0.26	96,96,96,96	0
56	MG	1H	3448	1/1	0.91	0.14	97,97,97,97	0
56	MG	14	3210	1/1	0.91	0.37	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3375	1/1	0.91	0.06	102,102,102,102	0
56	MG	1H	3329	1/1	0.91	0.34	99,99,99,99	0
56	MG	16	204	1/1	0.91	0.40	99,99,99,99	0
56	MG	1H	3241	1/1	0.91	0.21	80,80,80,80	0
56	MG	14	3259	1/1	0.91	0.15	100,100,100,100	0
56	MG	14	3388	1/1	0.91	0.12	85,85,85,85	0
56	MG	14	3424	1/1	0.91	0.43	116,116,116,116	0
56	MG	1H	3211	1/1	0.91	0.14	76,76,76,76	0
56	MG	14	3055	1/1	0.91	0.42	85,85,85,85	0
56	MG	1H	3312	1/1	0.91	0.37	79,79,79,79	0
56	MG	14	3423	1/1	0.91	0.10	133,133,133,133	0
56	MG	1H	3181	1/1	0.91	0.35	74,74,74,74	0
56	MG	14	3047	1/1	0.91	0.14	66,66,66,66	0
56	MG	1G	1609	1/1	0.91	0.12	97,97,97,97	0
56	MG	1H	3098	1/1	0.91	0.23	72,72,72,72	0
56	MG	1H	3354	1/1	0.92	0.14	64,64,64,64	0
56	MG	14	3160	1/1	0.92	0.32	85,85,85,85	0
56	MG	1H	3437	1/1	0.92	0.06	109,109,109,109	0
56	MG	1H	3438	1/1	0.92	0.05	82,82,82,82	0
56	MG	1H	3495	1/1	0.92	0.32	91,91,91,91	0
56	MG	1H	3162	1/1	0.92	0.24	74,74,74,74	0
56	MG	1H	3501	1/1	0.92	0.17	107,107,107,107	0
56	MG	14	3409	1/1	0.92	0.07	114,114,114,114	0
56	MG	14	3012	1/1	0.92	0.23	94,94,94,94	0
56	MG	13	1711	1/1	0.92	0.63	126,126,126,126	0
56	MG	1H	3149	1/1	0.92	0.54	99,99,99,99	0
56	MG	1H	3278	1/1	0.92	0.29	101,101,101,101	0
56	MG	14	3344	1/1	0.92	0.11	82,82,82,82	0
56	MG	13	1667	1/1	0.92	0.30	147,147,147,147	0
56	MG	14	3098	1/1	0.92	0.28	74,74,74,74	0
56	MG	1G	1611	1/1	0.92	0.18	105,105,105,105	0
56	MG	14	3394	1/1	0.92	0.07	93,93,93,93	0
56	MG	14	3309	1/1	0.92	0.48	87,87,87,87	0
56	MG	1H	3216	1/1	0.92	0.22	77,77,77,77	0
56	MG	14	3367	1/1	0.92	0.06	111,111,111,111	0
56	MG	1H	3101	1/1	0.92	0.21	49,49,49,49	0
56	MG	14	3102	1/1	0.92	0.36	93,93,93,93	0
56	MG	14	3094	1/1	0.92	0.20	83,83,83,83	0
56	MG	1H	3041	1/1	0.92	0.33	67,67,67,67	0
56	MG	1H	3194	1/1	0.92	0.20	104,104,104,104	0
56	MG	14	3053	1/1	0.92	0.17	98,98,98,98	0
56	MG	1G	1617	1/1	0.92	0.27	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3297	1/1	0.92	0.10	86,86,86,86	0
56	MG	1H	3097	1/1	0.92	0.20	89,89,89,89	0
56	MG	1G	1674	1/1	0.92	0.15	111,111,111,111	0
56	MG	1H	3291	1/1	0.92	0.29	77,77,77,77	0
56	MG	14	3321	1/1	0.92	0.27	99,99,99,99	0
56	MG	14	3218	1/1	0.92	0.13	75,75,75,75	0
56	MG	1H	3056	1/1	0.92	0.30	72,72,72,72	0
56	MG	14	3258	1/1	0.92	0.13	104,104,104,104	0
56	MG	14	3107	1/1	0.92	0.21	80,80,80,80	0
56	MG	1G	1613	1/1	0.92	0.22	117,117,117,117	0
56	MG	13	1686	1/1	0.92	0.29	134,134,134,134	0
56	MG	1H	3420	1/1	0.92	0.10	84,84,84,84	0
56	MG	78	201	1/1	0.92	0.15	67,67,67,67	0
56	MG	14	3056	1/1	0.92	0.11	92,92,92,92	0
56	MG	1H	3320	1/1	0.92	0.73	106,106,106,106	0
56	MG	14	3365	1/1	0.92	0.10	80,80,80,80	0
56	MG	1H	3163	1/1	0.92	0.20	88,88,88,88	0
56	MG	1H	3432	1/1	0.92	0.06	113,113,113,113	0
56	MG	14	3246	1/1	0.92	0.21	75,75,75,75	0
56	MG	14	3243	1/1	0.92	0.10	91,91,91,91	0
56	MG	11	301	1/1	0.92	0.32	62,62,62,62	0
56	MG	14	3380	1/1	0.92	0.09	97,97,97,97	0
56	MG	14	3140	1/1	0.92	0.34	93,93,93,93	0
56	MG	1H	3338	1/1	0.92	0.27	110,110,110,110	0
56	MG	1H	3333	1/1	0.92	0.34	91,91,91,91	0
56	MG	14	3039	1/1	0.92	0.26	68,68,68,68	0
56	MG	1H	3310	1/1	0.92	0.37	96,96,96,96	0
56	MG	1H	3005	1/1	0.92	0.20	70,70,70,70	0
56	MG	13	1703	1/1	0.92	0.37	96,96,96,96	0
56	MG	1H	3319	1/1	0.93	0.27	90,90,90,90	0
56	MG	1H	3293	1/1	0.93	0.17	85,85,85,85	0
56	MG	1G	1614	1/1	0.93	0.25	140,140,140,140	0
56	MG	14	3024	1/1	0.93	0.28	73,73,73,73	0
56	MG	39	301	1/1	0.93	0.19	111,111,111,111	0
56	MG	1H	3374	1/1	0.93	0.16	71,71,71,71	0
56	MG	14	3063	1/1	0.93	0.18	104,104,104,104	0
56	MG	1H	3228	1/1	0.93	0.55	94,94,94,94	0
56	MG	1H	3201	1/1	0.93	0.32	121,121,121,121	0
56	MG	1H	3303	1/1	0.93	0.30	76,76,76,76	0
56	MG	1H	3160	1/1	0.93	0.31	84,84,84,84	0
56	MG	14	3156	1/1	0.93	0.18	99,99,99,99	0
56	MG	14	3417	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
56	MG	13	1660	1/1	0.93	0.14	94,94,94,94	0
56	MG	1H	3417	1/1	0.93	0.12	90,90,90,90	0
56	MG	14	3027	1/1	0.93	0.20	84,84,84,84	0
56	MG	14	3184	1/1	0.93	0.34	94,94,94,94	0
56	MG	14	3146	1/1	0.93	0.19	128,128,128,128	0
56	MG	1H	3264	1/1	0.93	0.29	96,96,96,96	0
56	MG	1G	1660	1/1	0.93	0.43	97,97,97,97	0
56	MG	13	1700	1/1	0.93	0.24	109,109,109,109	0
56	MG	1H	3035	1/1	0.93	0.20	55,55,55,55	0
56	MG	1H	3150	1/1	0.93	0.36	86,86,86,86	0
56	MG	1H	3247	1/1	0.93	0.28	81,81,81,81	0
56	MG	1G	1622	1/1	0.93	0.12	89,89,89,89	0
56	MG	14	3224	1/1	0.93	0.09	80,80,80,80	0
56	MG	14	3072	1/1	0.93	0.17	90,90,90,90	0
56	MG	14	3213	1/1	0.93	0.17	113,113,113,113	0
56	MG	1G	1637	1/1	0.93	0.16	104,104,104,104	0
56	MG	1H	3327	1/1	0.93	0.39	91,91,91,91	0
56	MG	14	3113	1/1	0.93	0.35	80,80,80,80	0
56	MG	1H	3049	1/1	0.93	0.33	60,60,60,60	0
56	MG	1H	3167	1/1	0.93	0.15	92,92,92,92	0
56	MG	14	3186	1/1	0.93	0.21	86,86,86,86	0
56	MG	1H	3050	1/1	0.93	0.27	80,80,80,80	0
56	MG	1H	3166	1/1	0.93	0.17	73,73,73,73	0
56	MG	1G	1607	1/1	0.93	0.28	98,98,98,98	0
56	MG	78	202	1/1	0.93	0.20	97,97,97,97	0
56	MG	14	3299	1/1	0.93	0.58	84,84,84,84	0
56	MG	14	3292	1/1	0.93	0.17	90,90,90,90	0
56	MG	14	3083	1/1	0.93	0.26	81,81,81,81	0
56	MG	1H	3470	1/1	0.93	0.23	99,99,99,99	0
56	MG	1H	3378	1/1	0.93	0.09	94,94,94,94	0
56	MG	1H	3252	1/1	0.93	0.21	69,69,69,69	0
56	MG	13	1701	1/1	0.93	0.57	103,103,103,103	0
56	MG	1H	3183	1/1	0.93	0.29	83,83,83,83	0
56	MG	14	3341	1/1	0.93	0.07	78,78,78,78	0
56	MG	14	3132	1/1	0.93	0.22	94,94,94,94	0
56	MG	14	3229	1/1	0.93	0.20	83,83,83,83	0
56	MG	14	3078	1/1	0.93	0.11	97,97,97,97	0
56	MG	1H	3458	1/1	0.93	0.13	93,93,93,93	0
56	MG	14	3135	1/1	0.93	0.31	101,101,101,101	0
56	MG	1H	3359	1/1	0.93	0.10	83,83,83,83	0
56	MG	1H	3032	1/1	0.93	0.25	78,78,78,78	0
56	MG	1H	3003	1/1	0.93	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3442	1/1	0.93	0.12	57,57,57,57	0
56	MG	1H	3410	1/1	0.93	0.12	73,73,73,73	0
56	MG	14	3091	1/1	0.93	0.29	87,87,87,87	0
56	MG	13	1645	1/1	0.93	0.38	86,86,86,86	0
56	MG	1H	3375	1/1	0.93	0.18	76,76,76,76	0
56	MG	1H	3461	1/1	0.93	0.08	110,110,110,110	0
56	MG	14	3263	1/1	0.93	0.26	88,88,88,88	0
56	MG	1H	3231	1/1	0.93	0.49	90,90,90,90	0
56	MG	1H	3418	1/1	0.93	0.06	134,134,134,134	0
56	MG	13	1661	1/1	0.93	0.29	91,91,91,91	0
56	MG	1H	3336	1/1	0.93	0.30	102,102,102,102	0
56	MG	1H	3020	1/1	0.93	0.15	90,90,90,90	0
56	MG	1H	3082	1/1	0.93	0.17	77,77,77,77	0
56	MG	13	1619	1/1	0.93	0.57	103,103,103,103	0
56	MG	1H	3002	1/1	0.93	0.23	76,76,76,76	0
56	MG	1H	3302	1/1	0.93	0.23	90,90,90,90	0
56	MG	1H	3051	1/1	0.93	0.24	53,53,53,53	0
56	MG	1H	3217	1/1	0.93	0.12	91,91,91,91	0
56	MG	1H	3248	1/1	0.93	0.23	76,76,76,76	0
56	MG	1H	3315	1/1	0.94	0.39	105,105,105,105	0
56	MG	14	3345	1/1	0.94	0.10	84,84,84,84	0
56	MG	1H	3483	1/1	0.94	0.07	110,110,110,110	0
56	MG	J8	101	1/1	0.94	0.27	78,78,78,78	0
56	MG	13	1698	1/1	0.94	0.35	95,95,95,95	0
56	MG	14	3421	1/1	0.94	0.05	130,130,130,130	0
56	MG	1H	3188	1/1	0.94	0.51	100,100,100,100	0
56	MG	13	1709	1/1	0.94	0.28	141,141,141,141	0
56	MG	14	3234	1/1	0.94	0.54	98,98,98,98	0
56	MG	13	1643	1/1	0.94	0.09	78,78,78,78	0
56	MG	14	3399	1/1	0.94	0.08	78,78,78,78	0
56	MG	1H	3080	1/1	0.94	0.31	86,86,86,86	0
56	MG	4K	101	1/1	0.94	0.19	90,90,90,90	0
56	MG	1H	3161	1/1	0.94	0.36	82,82,82,82	0
56	MG	14	3141	1/1	0.94	0.19	80,80,80,80	0
56	MG	14	3106	1/1	0.94	0.20	89,89,89,89	0
56	MG	13	1626	1/1	0.94	0.20	109,109,109,109	0
56	MG	1H	3112	1/1	0.94	0.14	55,55,55,55	0
56	MG	14	3092	1/1	0.94	0.16	109,109,109,109	0
56	MG	1H	3422	1/1	0.94	0.15	91,91,91,91	0
56	MG	13	1741	1/1	0.94	0.08	118,118,118,118	0
56	MG	1H	3325	1/1	0.94	0.13	86,86,86,86	0
56	MG	14	3052	1/1	0.94	0.21	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1678	1/1	0.94	0.09	111,111,111,111	0
56	MG	14	3401	1/1	0.94	0.06	120,120,120,120	0
56	MG	13	1620	1/1	0.94	0.27	119,119,119,119	0
56	MG	1H	3058	1/1	0.94	0.20	107,107,107,107	0
56	MG	14	3121	1/1	0.94	0.23	84,84,84,84	0
56	MG	1H	3455	1/1	0.94	0.22	99,99,99,99	0
56	MG	1H	3425	1/1	0.94	0.06	95,95,95,95	0
56	MG	1H	3429	1/1	0.94	0.08	102,102,102,102	0
56	MG	16	202	1/1	0.94	0.28	73,73,73,73	0
56	MG	1H	3067	1/1	0.94	0.16	84,84,84,84	0
56	MG	14	3400	1/1	0.94	0.22	95,95,95,95	0
56	MG	1G	1618	1/1	0.94	0.12	104,104,104,104	0
56	MG	1H	3421	1/1	0.94	0.18	62,62,62,62	0
56	MG	1H	3454	1/1	0.94	0.06	85,85,85,85	0
56	MG	1H	3475	1/1	0.94	0.18	76,76,76,76	0
56	MG	13	1671	1/1	0.94	0.24	102,102,102,102	0
56	MG	1H	3400	1/1	0.94	0.10	61,61,61,61	0
56	MG	1H	3441	1/1	0.94	0.10	122,122,122,122	0
56	MG	13	1731	1/1	0.94	0.05	91,91,91,91	0
56	MG	1H	3398	1/1	0.94	0.09	92,92,92,92	0
56	MG	13	1603	1/1	0.94	0.21	97,97,97,97	0
56	MG	14	3241	1/1	0.94	0.31	92,92,92,92	0
56	MG	14	3082	1/1	0.94	0.23	71,71,71,71	0
56	MG	1G	1681	1/1	0.94	0.18	133,133,133,133	0
56	MG	14	3406	1/1	0.94	0.07	99,99,99,99	0
56	MG	1H	3203	1/1	0.94	0.35	73,73,73,73	0
56	MG	1H	3390	1/1	0.94	0.17	83,83,83,83	0
56	MG	14	3425	1/1	0.94	0.28	92,92,92,92	0
56	MG	14	3190	1/1	0.94	0.22	124,124,124,124	0
56	MG	14	3314	1/1	0.94	0.34	102,102,102,102	0
56	MG	14	3041	1/1	0.94	0.16	80,80,80,80	0
56	MG	14	3290	1/1	0.94	0.26	113,113,113,113	0
56	MG	14	3179	1/1	0.94	0.30	96,96,96,96	0
56	MG	1H	3159	1/1	0.94	0.17	77,77,77,77	0
56	MG	1H	3257	1/1	0.94	0.33	80,80,80,80	0
56	MG	13	1615	1/1	0.94	0.24	100,100,100,100	0
56	MG	1H	3474	1/1	0.94	0.20	124,124,124,124	0
56	MG	2K	102	1/1	0.94	0.23	97,97,97,97	0
56	MG	14	3323	1/1	0.94	0.10	101,101,101,101	0
56	MG	14	3006	1/1	0.94	0.21	99,99,99,99	0
56	MG	14	3362	1/1	0.94	0.17	101,101,101,101	0
56	MG	1H	3416	1/1	0.94	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3003	1/1	0.94	0.14	73,73,73,73	0
56	MG	1H	3404	1/1	0.94	0.09	62,62,62,62	0
56	MG	1H	3460	1/1	0.94	0.11	110,110,110,110	0
56	MG	1J	210	1/1	0.94	0.06	109,109,109,109	0
56	MG	1H	3073	1/1	0.94	0.24	88,88,88,88	0
56	MG	14	3042	1/1	0.94	0.21	87,87,87,87	0
56	MG	1H	3068	1/1	0.94	0.27	98,98,98,98	0
56	MG	1H	3113	1/1	0.94	0.14	64,64,64,64	0
56	MG	13	1715	1/1	0.94	0.31	108,108,108,108	0
56	MG	1H	3456	1/1	0.94	0.18	79,79,79,79	0
56	MG	1H	3053	1/1	0.94	0.17	92,92,92,92	0
56	MG	1H	3424	1/1	0.94	0.09	119,119,119,119	0
56	MG	13	1613	1/1	0.94	0.18	96,96,96,96	0
56	MG	1H	3094	1/1	0.94	0.39	79,79,79,79	0
56	MG	1H	3386	1/1	0.94	0.16	82,82,82,82	0
56	MG	14	3410	1/1	0.94	0.30	96,96,96,96	0
56	MG	14	3059	1/1	0.94	0.27	74,74,74,74	0
56	MG	14	3240	1/1	0.94	0.10	76,76,76,76	0
56	MG	1H	3024	1/1	0.94	0.23	102,102,102,102	0
56	MG	1H	3482	1/1	0.94	0.10	119,119,119,119	0
56	MG	1G	1654	1/1	0.94	0.38	94,94,94,94	0
56	MG	16	211	1/1	0.94	0.40	79,79,79,79	0
56	MG	14	3127	1/1	0.94	0.06	87,87,87,87	0
56	MG	1H	3221	1/1	0.94	0.38	99,99,99,99	0
56	MG	14	3350	1/1	0.94	0.08	80,80,80,80	0
56	MG	13	1728	1/1	0.94	0.13	131,131,131,131	0
56	MG	14	3157	1/1	0.94	0.31	76,76,76,76	0
56	MG	1H	3301	1/1	0.94	0.24	79,79,79,79	0
56	MG	14	3071	1/1	0.94	0.12	94,94,94,94	0
56	MG	1H	3105	1/1	0.94	0.09	76,76,76,76	0
56	MG	14	3225	1/1	0.94	0.20	65,65,65,65	0
56	MG	1H	3220	1/1	0.94	0.29	124,124,124,124	0
56	MG	1H	3208	1/1	0.94	0.09	63,63,63,63	0
56	MG	1H	3121	1/1	0.94	0.21	80,80,80,80	0
56	MG	1H	3099	1/1	0.95	0.33	69,69,69,69	0
56	MG	14	3298	1/1	0.95	0.42	115,115,115,115	0
56	MG	1H	3021	1/1	0.95	0.32	79,79,79,79	0
56	MG	14	3138	1/1	0.95	0.20	73,73,73,73	0
56	MG	14	3216	1/1	0.95	0.43	111,111,111,111	0
56	MG	13	1642	1/1	0.95	0.11	98,98,98,98	0
56	MG	1H	3047	1/1	0.95	0.30	65,65,65,65	0
56	MG	13	1726	1/1	0.95	0.12	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3069	1/1	0.95	0.08	63,63,63,63	0
56	MG	14	3393	1/1	0.95	0.14	80,80,80,80	0
56	MG	1G	1631	1/1	0.95	0.23	113,113,113,113	0
56	MG	1H	3212	1/1	0.95	0.14	61,61,61,61	0
56	MG	1H	3385	1/1	0.95	0.14	75,75,75,75	0
56	MG	14	3336	1/1	0.95	0.14	88,88,88,88	0
56	MG	14	3100	1/1	0.95	0.12	87,87,87,87	0
56	MG	14	3021	1/1	0.95	0.40	79,79,79,79	0
56	MG	3I	201	1/1	0.95	0.18	81,81,81,81	0
56	MG	1G	1672	1/1	0.95	0.26	126,126,126,126	0
56	MG	14	3049	1/1	0.95	0.25	87,87,87,87	0
56	MG	1H	3236	1/1	0.95	0.26	77,77,77,77	0
56	MG	14	3001	1/1	0.95	0.12	66,66,66,66	0
56	MG	1H	3025	1/1	0.95	0.48	78,78,78,78	0
56	MG	16	208	1/1	0.95	0.55	94,94,94,94	0
56	MG	13	1653	1/1	0.95	0.21	78,78,78,78	0
56	MG	1H	3170	1/1	0.95	0.33	100,100,100,100	0
56	MG	1H	3109	1/1	0.95	0.20	84,84,84,84	0
56	MG	1H	3213	1/1	0.95	0.27	113,113,113,113	0
56	MG	1G	1662	1/1	0.95	0.16	155,155,155,155	0
56	MG	14	3219	1/1	0.95	0.20	102,102,102,102	0
56	MG	1H	3463	1/1	0.95	0.04	113,113,113,113	0
56	MG	1H	3433	1/1	0.95	0.09	76,76,76,76	0
56	MG	G8	201	1/1	0.95	0.11	83,83,83,83	0
56	MG	1G	1616	1/1	0.95	0.18	149,149,149,149	0
56	MG	1H	3176	1/1	0.95	0.30	91,91,91,91	0
56	MG	14	3171	1/1	0.95	0.19	73,73,73,73	0
56	MG	1J	201	1/1	0.95	0.15	123,123,123,123	0
56	MG	1H	3196	1/1	0.95	0.70	110,110,110,110	0
56	MG	1H	3405	1/1	0.95	0.13	86,86,86,86	0
56	MG	14	3222	1/1	0.95	0.24	99,99,99,99	0
56	MG	1G	1612	1/1	0.95	0.15	110,110,110,110	0
56	MG	14	3074	1/1	0.95	0.13	79,79,79,79	0
56	MG	1H	3011	1/1	0.95	0.51	91,91,91,91	0
56	MG	1H	3367	1/1	0.95	0.13	82,82,82,82	0
56	MG	1H	3341	1/1	0.95	0.27	100,100,100,100	0
57	ZN	5A	101	1/1	0.95	0.13	172,172,172,172	0
56	MG	1H	3066	1/1	0.95	0.27	71,71,71,71	0
56	MG	1H	3173	1/1	0.95	0.36	98,98,98,98	0
56	MG	1H	3376	1/1	0.95	0.04	96,96,96,96	0
56	MG	1H	3215	1/1	0.95	0.14	81,81,81,81	0
56	MG	1G	1658	1/1	0.95	0.21	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3324	1/1	0.95	0.15	107,107,107,107	0
56	MG	13	1635	1/1	0.95	0.14	88,88,88,88	0
56	MG	1G	1630	1/1	0.95	0.47	116,116,116,116	0
56	MG	1H	3275	1/1	0.95	0.30	97,97,97,97	0
56	MG	13	1657	1/1	0.95	0.24	104,104,104,104	0
56	MG	13	1673	1/1	0.95	0.28	91,91,91,91	0
56	MG	14	3359	1/1	0.95	0.13	114,114,114,114	0
56	MG	1H	3444	1/1	0.95	0.28	102,102,102,102	0
56	MG	14	3139	1/1	0.95	0.19	67,67,67,67	0
56	MG	14	3384	1/1	0.95	0.14	60,60,60,60	0
56	MG	14	3390	1/1	0.95	0.18	94,94,94,94	0
56	MG	14	3060	1/1	0.95	0.27	83,83,83,83	0
56	MG	13	1625	1/1	0.95	0.30	77,77,77,77	0
56	MG	16	210	1/1	0.95	0.45	107,107,107,107	0
56	MG	1H	3164	1/1	0.95	0.43	102,102,102,102	0
56	MG	1H	3218	1/1	0.95	0.17	78,78,78,78	0
56	MG	16	213	1/1	0.95	0.43	85,85,85,85	0
56	MG	14	3044	1/1	0.95	0.14	78,78,78,78	0
56	MG	1H	3229	1/1	0.95	0.23	83,83,83,83	0
56	MG	14	3114	1/1	0.95	0.39	97,97,97,97	0
56	MG	14	3005	1/1	0.95	0.18	66,66,66,66	0
56	MG	13	1730	1/1	0.95	0.03	113,113,113,113	0
56	MG	14	3126	1/1	0.95	0.29	103,103,103,103	0
56	MG	14	3340	1/1	0.95	0.34	91,91,91,91	0
56	MG	13	1616	1/1	0.95	0.10	82,82,82,82	0
56	MG	13	1602	1/1	0.95	0.31	87,87,87,87	0
56	MG	1H	3347	1/1	0.95	0.13	57,57,57,57	0
56	MG	14	3007	1/1	0.95	0.23	94,94,94,94	0
56	MG	14	3364	1/1	0.95	0.07	87,87,87,87	0
56	MG	1H	3419	1/1	0.95	0.16	94,94,94,94	0
56	MG	1H	3384	1/1	0.95	0.07	59,59,59,59	0
56	MG	1G	1676	1/1	0.95	0.35	121,121,121,121	0
56	MG	1H	3235	1/1	0.95	0.25	75,75,75,75	0
56	MG	14	3180	1/1	0.95	0.32	83,83,83,83	0
56	MG	41	201	1/1	0.95	0.16	89,89,89,89	0
56	MG	88	201	1/1	0.95	0.22	95,95,95,95	0
56	MG	85	201	1/1	0.95	0.28	93,93,93,93	0
56	MG	1H	3010	1/1	0.95	0.34	83,83,83,83	0
56	MG	1H	3408	1/1	0.95	0.09	87,87,87,87	0
56	MG	2K	103	1/1	0.95	0.10	98,98,98,98	0
56	MG	14	3099	1/1	0.95	0.14	106,106,106,106	0
56	MG	1H	3090	1/1	0.95	0.47	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3095	1/1	0.95	0.43	74,74,74,74	0
56	MG	1H	3261	1/1	0.95	0.48	99,99,99,99	0
56	MG	1H	3052	1/1	0.95	0.30	80,80,80,80	0
56	MG	1H	3054	1/1	0.96	0.19	71,71,71,71	0
56	MG	1H	3134	1/1	0.96	0.13	57,57,57,57	0
56	MG	14	3402	1/1	0.96	0.11	99,99,99,99	0
56	MG	1G	1619	1/1	0.96	0.21	72,72,72,72	0
56	MG	14	3108	1/1	0.96	0.15	92,92,92,92	0
56	MG	13	1609	1/1	0.96	0.19	83,83,83,83	0
56	MG	1H	3192	1/1	0.96	0.11	78,78,78,78	0
56	MG	14	3090	1/1	0.96	0.20	89,89,89,89	0
56	MG	16	209	1/1	0.96	0.21	88,88,88,88	0
56	MG	1H	3364	1/1	0.96	0.12	80,80,80,80	0
56	MG	13	1623	1/1	0.96	0.15	84,84,84,84	0
56	MG	2K	101	1/1	0.96	0.22	76,76,76,76	0
56	MG	1H	3363	1/1	0.96	0.21	71,71,71,71	0
56	MG	14	3373	1/1	0.96	0.08	81,81,81,81	0
56	MG	14	3011	1/1	0.96	0.20	61,61,61,61	0
56	MG	1H	3117	1/1	0.96	0.29	87,87,87,87	0
56	MG	1H	3396	1/1	0.96	0.17	87,87,87,87	0
56	MG	1H	3451	1/1	0.96	0.11	87,87,87,87	0
56	MG	14	3045	1/1	0.96	0.17	70,70,70,70	0
56	MG	14	3129	1/1	0.96	0.20	78,78,78,78	0
56	MG	1H	3046	1/1	0.96	0.30	72,72,72,72	0
56	MG	1H	3244	1/1	0.96	0.20	90,90,90,90	0
56	MG	14	3226	1/1	0.96	0.21	123,123,123,123	0
56	MG	1H	3139	1/1	0.96	0.40	79,79,79,79	0
56	MG	14	3165	1/1	0.96	0.33	70,70,70,70	0
56	MG	1H	3497	1/1	0.96	0.10	119,119,119,119	0
56	MG	14	3067	1/1	0.96	0.18	73,73,73,73	0
56	MG	1H	3269	1/1	0.96	0.52	90,90,90,90	0
56	MG	14	3220	1/1	0.96	0.32	94,94,94,94	0
56	MG	13	1617	1/1	0.96	0.08	106,106,106,106	0
56	MG	1H	3350	1/1	0.96	0.14	64,64,64,64	0
56	MG	13	1681	1/1	0.96	0.25	107,107,107,107	0
56	MG	16	212	1/1	0.96	0.43	99,99,99,99	0
56	MG	1H	3093	1/1	0.96	0.16	81,81,81,81	0
56	MG	14	3088	1/1	0.96	0.23	66,66,66,66	0
56	MG	14	3199	1/1	0.96	0.35	126,126,126,126	0
56	MG	14	3070	1/1	0.96	0.19	66,66,66,66	0
56	MG	14	3057	1/1	0.96	0.15	91,91,91,91	0
56	MG	1H	3486	1/1	0.96	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3402	1/1	0.96	0.12	81,81,81,81	0
56	MG	14	3404	1/1	0.96	0.08	97,97,97,97	0
56	MG	1H	3377	1/1	0.96	0.17	97,97,97,97	0
56	MG	1H	3387	1/1	0.96	0.17	70,70,70,70	0
56	MG	1H	3065	1/1	0.96	0.27	71,71,71,71	0
56	MG	14	3242	1/1	0.96	0.16	94,94,94,94	0
56	MG	1H	3064	1/1	0.96	0.27	76,76,76,76	0
56	MG	1H	3042	1/1	0.96	0.19	53,53,53,53	0
56	MG	13	1628	1/1	0.96	0.35	102,102,102,102	0
56	MG	1H	3506	1/1	0.96	0.33	57,57,57,57	0
56	MG	14	3338	1/1	0.96	0.09	68,68,68,68	0
56	MG	1H	3038	1/1	0.96	0.26	58,58,58,58	0
56	MG	1H	3069	1/1	0.96	0.37	89,89,89,89	0
56	MG	14	3073	1/1	0.96	0.26	74,74,74,74	0
56	MG	13	1612	1/1	0.96	0.27	89,89,89,89	0
56	MG	14	3087	1/1	0.96	0.16	82,82,82,82	0
56	MG	14	3115	1/1	0.96	0.18	100,100,100,100	0
56	MG	1H	3450	1/1	0.96	0.13	66,66,66,66	0
56	MG	1H	3240	1/1	0.96	0.25	94,94,94,94	0
56	MG	14	3245	1/1	0.96	0.18	71,71,71,71	0
56	MG	14	3004	1/1	0.96	0.25	64,64,64,64	0
56	MG	14	3040	1/1	0.96	0.20	79,79,79,79	0
56	MG	1H	3114	1/1	0.96	0.42	82,82,82,82	0
56	MG	14	3086	1/1	0.96	0.28	84,84,84,84	0
56	MG	14	3031	1/1	0.96	0.29	76,76,76,76	0
56	MG	1H	3360	1/1	0.96	0.14	58,58,58,58	0
56	MG	14	3349	1/1	0.96	0.14	71,71,71,71	0
56	MG	13	1751	1/1	0.96	0.16	94,94,94,94	0
56	MG	13	1648	1/1	0.96	0.26	76,76,76,76	0
56	MG	1H	3156	1/1	0.96	0.36	110,110,110,110	0
56	MG	14	3009	1/1	0.96	0.24	65,65,65,65	0
56	MG	14	3389	1/1	0.96	0.17	72,72,72,72	0
56	MG	14	3378	1/1	0.96	0.16	101,101,101,101	0
56	MG	14	3206	1/1	0.96	0.08	83,83,83,83	0
56	MG	1H	3462	1/1	0.96	0.11	75,75,75,75	0
56	MG	14	3131	1/1	0.96	0.20	56,56,56,56	0
56	MG	1H	3151	1/1	0.96	0.17	110,110,110,110	0
56	MG	1H	3033	1/1	0.96	0.59	100,100,100,100	0
56	MG	13	1655	1/1	0.96	0.14	89,89,89,89	0
56	MG	1H	3057	1/1	0.96	0.19	72,72,72,72	0
56	MG	1H	3349	1/1	0.96	0.16	69,69,69,69	0
56	MG	1G	1678	1/1	0.96	0.13	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3084	1/1	0.96	0.22	78,78,78,78	0
56	MG	1G	1646	1/1	0.96	0.15	102,102,102,102	0
56	MG	14	3050	1/1	0.96	0.13	60,60,60,60	0
56	MG	1H	3187	1/1	0.96	0.24	89,89,89,89	0
56	MG	1H	3289	1/1	0.96	0.22	93,93,93,93	0
56	MG	1G	1683	1/1	0.96	0.14	129,129,129,129	0
56	MG	14	3334	1/1	0.96	0.11	91,91,91,91	0
56	MG	1H	3197	1/1	0.96	0.41	89,89,89,89	0
56	MG	14	3214	1/1	0.96	0.14	70,70,70,70	0
56	MG	1H	3436	1/1	0.96	0.10	79,79,79,79	0
56	MG	14	3054	1/1	0.96	0.12	93,93,93,93	0
56	MG	1H	3075	1/1	0.96	0.08	59,59,59,59	0
56	MG	1H	3214	1/1	0.96	0.13	103,103,103,103	0
56	MG	14	3228	1/1	0.96	0.20	86,86,86,86	0
56	MG	21	302	1/1	0.96	0.16	82,82,82,82	0
56	MG	14	3172	1/1	0.96	0.21	107,107,107,107	0
56	MG	1H	3180	1/1	0.96	0.17	84,84,84,84	0
56	MG	1H	3356	1/1	0.97	0.10	58,58,58,58	0
56	MG	1H	3008	1/1	0.97	0.41	79,79,79,79	0
56	MG	14	3111	1/1	0.97	0.17	72,72,72,72	0
56	MG	1H	3195	1/1	0.97	0.11	94,94,94,94	0
56	MG	14	3105	1/1	0.97	0.14	74,74,74,74	0
56	MG	13	1649	1/1	0.97	0.27	85,85,85,85	0
56	MG	14	3097	1/1	0.97	0.12	69,69,69,69	0
56	MG	1H	3037	1/1	0.97	0.37	76,76,76,76	0
56	MG	14	3191	1/1	0.97	0.21	92,92,92,92	0
56	MG	1H	3115	1/1	0.97	0.34	95,95,95,95	0
56	MG	13	1725	1/1	0.97	0.11	102,102,102,102	0
56	MG	14	3426	1/1	0.97	0.24	67,67,67,67	0
56	MG	14	3347	1/1	0.97	0.07	85,85,85,85	0
56	MG	16	203	1/1	0.97	0.17	107,107,107,107	0
57	ZN	5I	101	1/1	0.97	0.20	114,114,114,114	0
56	MG	1H	3403	1/1	0.97	0.16	73,73,73,73	0
56	MG	1H	3103	1/1	0.97	0.15	60,60,60,60	0
56	MG	1H	3369	1/1	0.97	0.15	92,92,92,92	0
56	MG	1H	3019	1/1	0.97	0.28	54,54,54,54	0
56	MG	1H	3172	1/1	0.97	0.26	98,98,98,98	0
56	MG	14	3116	1/1	0.97	0.21	73,73,73,73	0
56	MG	14	3300	1/1	0.97	0.15	98,98,98,98	0
56	MG	1H	3110	1/1	0.97	0.31	67,67,67,67	0
56	MG	1H	3088	1/1	0.97	0.33	52,52,52,52	0
56	MG	13	1747	1/1	0.97	0.28	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1627	1/1	0.97	0.23	116,116,116,116	0
56	MG	14	3238	1/1	0.97	0.16	110,110,110,110	0
56	MG	1G	1624	1/1	0.97	0.17	93,93,93,93	0
56	MG	1G	1651	1/1	0.97	0.20	138,138,138,138	0
56	MG	13	1659	1/1	0.97	0.31	109,109,109,109	0
56	MG	14	3089	1/1	0.97	0.21	85,85,85,85	0
56	MG	14	3223	1/1	0.97	0.82	81,81,81,81	0
56	MG	14	3095	1/1	0.97	0.20	78,78,78,78	0
56	MG	14	3134	1/1	0.97	0.10	103,103,103,103	0
56	MG	1H	3392	1/1	0.97	0.13	65,65,65,65	0
56	MG	1H	3348	1/1	0.97	0.14	84,84,84,84	0
56	MG	14	3322	1/1	0.97	0.14	90,90,90,90	0
56	MG	14	3015	1/1	0.97	0.08	81,81,81,81	0
56	MG	14	3145	1/1	0.97	0.25	105,105,105,105	0
56	MG	1H	3039	1/1	0.97	0.39	55,55,55,55	0
56	MG	13	1729	1/1	0.97	0.12	109,109,109,109	0
56	MG	1H	3459	1/1	0.97	0.14	81,81,81,81	0
56	MG	1G	1626	1/1	0.97	0.27	102,102,102,102	0
56	MG	14	3128	1/1	0.97	0.21	97,97,97,97	0
56	MG	1H	3120	1/1	0.97	0.13	80,80,80,80	0
56	MG	2L	101	1/1	0.97	0.18	98,98,98,98	0
56	MG	1H	3131	1/1	0.97	0.17	56,56,56,56	0
56	MG	1H	3394	1/1	0.97	0.09	62,62,62,62	0
56	MG	13	1610	1/1	0.97	0.20	79,79,79,79	0
56	MG	1H	3371	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3089	1/1	0.97	0.28	58,58,58,58	0
56	MG	14	3046	1/1	0.97	0.24	88,88,88,88	0
56	MG	1H	3299	1/1	0.97	0.17	71,71,71,71	0
56	MG	1H	3227	1/1	0.97	0.26	123,123,123,123	0
56	MG	14	3348	1/1	0.97	0.10	71,71,71,71	0
56	MG	14	3397	1/1	0.97	0.13	101,101,101,101	0
56	MG	14	3085	1/1	0.97	0.18	81,81,81,81	0
56	MG	1H	3078	1/1	0.97	0.23	70,70,70,70	0
56	MG	13	1746	1/1	0.97	0.07	110,110,110,110	0
56	MG	13	1712	1/1	0.97	0.19	99,99,99,99	0
56	MG	1H	3445	1/1	0.97	0.12	83,83,83,83	0
56	MG	14	3155	1/1	0.97	0.17	76,76,76,76	0
56	MG	14	3244	1/1	0.97	0.23	99,99,99,99	0
56	MG	14	3353	1/1	0.97	0.15	91,91,91,91	0
56	MG	1G	1621	1/1	0.97	0.11	88,88,88,88	0
56	MG	14	3205	1/1	0.97	0.45	72,72,72,72	0
56	MG	1H	3171	1/1	0.97	0.51	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3383	1/1	0.97	0.10	67,67,67,67	0
56	MG	1H	3091	1/1	0.97	0.36	70,70,70,70	0
56	MG	1H	3253	1/1	0.97	0.20	91,91,91,91	0
56	MG	1H	3239	1/1	0.97	0.17	88,88,88,88	0
56	MG	14	3194	1/1	0.97	0.23	97,97,97,97	0
56	MG	1H	3388	1/1	0.97	0.14	65,65,65,65	0
56	MG	14	3198	1/1	0.97	0.11	88,88,88,88	0
56	MG	1H	3096	1/1	0.97	0.17	57,57,57,57	0
56	MG	1H	3226	1/1	0.97	0.26	88,88,88,88	0
56	MG	14	3230	1/1	0.97	0.27	86,86,86,86	0
56	MG	1H	3468	1/1	0.97	0.07	95,95,95,95	0
56	MG	1G	1677	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3018	1/1	0.97	0.41	79,79,79,79	0
56	MG	14	3361	1/1	0.97	0.17	86,86,86,86	0
56	MG	13	1608	1/1	0.97	0.20	91,91,91,91	0
56	MG	14	3310	1/1	0.97	0.20	96,96,96,96	0
56	MG	13	1638	1/1	0.97	0.09	115,115,115,115	0
56	MG	14	3062	1/1	0.97	0.29	85,85,85,85	0
56	MG	14	3382	1/1	0.97	0.29	86,86,86,86	0
56	MG	1H	3401	1/1	0.97	0.16	87,87,87,87	0
56	MG	14	3002	1/1	0.97	0.24	70,70,70,70	0
56	MG	14	3124	1/1	0.97	0.26	85,85,85,85	0
56	MG	14	3036	1/1	0.97	0.15	67,67,67,67	0
56	MG	13	1614	1/1	0.97	0.16	98,98,98,98	0
56	MG	1H	3413	1/1	0.97	0.15	77,77,77,77	0
56	MG	1H	3481	1/1	0.97	0.11	70,70,70,70	0
56	MG	1H	3397	1/1	0.97	0.15	77,77,77,77	0
56	MG	1H	3449	1/1	0.97	0.15	78,78,78,78	0
56	MG	14	3414	1/1	0.98	0.06	93,93,93,93	0
56	MG	14	3327	1/1	0.98	0.43	117,117,117,117	0
56	MG	1H	3389	1/1	0.98	0.16	69,69,69,69	0
56	MG	1H	3271	1/1	0.98	0.46	93,93,93,93	0
56	MG	1H	3393	1/1	0.98	0.17	60,60,60,60	0
56	MG	14	3043	1/1	0.98	0.21	101,101,101,101	0
56	MG	1H	3484	1/1	0.98	0.09	79,79,79,79	0
56	MG	1H	3145	1/1	0.98	0.20	57,57,57,57	0
56	MG	13	1634	1/1	0.98	0.30	85,85,85,85	0
56	MG	1H	3406	1/1	0.98	0.17	77,77,77,77	0
56	MG	14	3110	1/1	0.98	0.23	61,61,61,61	0
56	MG	1H	3014	1/1	0.98	0.42	57,57,57,57	0
56	MG	1H	3353	1/1	0.98	0.11	77,77,77,77	0
56	MG	14	3010	1/1	0.98	0.19	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3465	1/1	0.98	0.10	83,83,83,83	0
56	MG	1H	3063	1/1	0.98	0.28	83,83,83,83	0
56	MG	1H	3207	1/1	0.98	0.18	60,60,60,60	0
56	MG	1H	3351	1/1	0.98	0.18	65,65,65,65	0
56	MG	1H	3125	1/1	0.98	0.16	68,68,68,68	0
56	MG	1H	3224	1/1	0.98	0.28	82,82,82,82	0
56	MG	14	3212	1/1	0.98	0.16	104,104,104,104	0
56	MG	1H	3070	1/1	0.98	0.54	125,125,125,125	0
56	MG	13	1604	1/1	0.98	0.27	108,108,108,108	0
56	MG	13	1633	1/1	0.98	0.15	75,75,75,75	0
56	MG	1H	3233	1/1	0.98	0.19	65,65,65,65	0
56	MG	14	3408	1/1	0.98	0.08	79,79,79,79	0
56	MG	1H	3379	1/1	0.98	0.12	74,74,74,74	0
56	MG	14	3377	1/1	0.98	0.08	82,82,82,82	0
56	MG	1G	1685	1/1	0.98	0.08	112,112,112,112	0
56	MG	1H	3060	1/1	0.98	0.24	74,74,74,74	0
56	MG	14	3333	1/1	0.98	0.12	73,73,73,73	0
56	MG	1G	1608	1/1	0.98	0.14	98,98,98,98	0
56	MG	14	3189	1/1	0.98	0.12	83,83,83,83	0
56	MG	1H	3352	1/1	0.98	0.14	61,61,61,61	0
56	MG	13	1742	1/1	0.98	0.10	82,82,82,82	0
56	MG	1H	3357	1/1	0.98	0.07	57,57,57,57	0
56	MG	1H	3006	1/1	0.98	0.17	91,91,91,91	0
56	MG	14	3118	1/1	0.98	0.24	71,71,71,71	0
56	MG	1H	3427	1/1	0.98	0.09	75,75,75,75	0
56	MG	14	3386	1/1	0.98	0.25	105,105,105,105	0
56	MG	1G	1601	1/1	0.98	0.19	109,109,109,109	0
56	MG	1H	3446	1/1	0.98	0.12	74,74,74,74	0
56	MG	14	3061	1/1	0.98	0.15	79,79,79,79	0
56	MG	14	3008	1/1	0.98	0.25	78,78,78,78	0
56	MG	14	3048	1/1	0.98	0.20	73,73,73,73	0
56	MG	1H	3373	1/1	0.98	0.12	63,63,63,63	0
56	MG	21	301	1/1	0.98	0.23	75,75,75,75	0
56	MG	1H	3048	1/1	0.98	0.21	65,65,65,65	0
56	MG	14	3358	1/1	0.98	0.09	85,85,85,85	0
56	MG	1H	3234	1/1	0.98	0.29	91,91,91,91	0
56	MG	1H	3085	1/1	0.98	0.22	62,62,62,62	0
56	MG	1H	3355	1/1	0.98	0.18	64,64,64,64	0
56	MG	14	3075	1/1	0.98	0.23	81,81,81,81	0
56	MG	14	3034	1/1	0.98	0.23	69,69,69,69	0
56	MG	14	3033	1/1	0.98	0.18	66,66,66,66	0
56	MG	1H	3043	1/1	0.98	0.27	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1738	1/1	0.98	0.13	77,77,77,77	0
56	MG	1H	3130	1/1	0.98	0.24	78,78,78,78	0
56	MG	1H	3365	1/1	0.98	0.13	69,69,69,69	0
56	MG	1H	3059	1/1	0.98	0.49	92,92,92,92	0
56	MG	14	3119	1/1	0.98	0.32	66,66,66,66	0
56	MG	13	1733	1/1	0.98	0.10	102,102,102,102	0
56	MG	14	3122	1/1	0.98	0.19	68,68,68,68	0
56	MG	13	1705	1/1	0.98	0.14	98,98,98,98	0
56	MG	14	3120	1/1	0.98	0.17	80,80,80,80	0
56	MG	1H	3084	1/1	0.98	0.31	61,61,61,61	0
56	MG	1H	3016	1/1	0.98	0.31	66,66,66,66	0
56	MG	1H	3045	1/1	0.98	0.20	63,63,63,63	0
56	MG	13	1601	1/1	0.98	0.27	74,74,74,74	0
56	MG	13	1735	1/1	0.98	0.07	96,96,96,96	0
57	ZN	3E	301	1/1	0.98	0.41	115,115,115,115	0
56	MG	1H	3001	1/1	0.98	0.29	64,64,64,64	0
56	MG	1H	3453	1/1	0.98	0.15	70,70,70,70	0
56	MG	14	3188	1/1	0.98	0.31	91,91,91,91	0
56	MG	13	1732	1/1	0.98	0.09	81,81,81,81	0
56	MG	14	3351	1/1	0.98	0.12	60,60,60,60	0
56	MG	1H	3361	1/1	0.98	0.16	56,56,56,56	0
56	MG	14	3032	1/1	0.98	0.20	52,52,52,52	0
56	MG	14	3101	1/1	0.98	0.15	80,80,80,80	0
56	MG	14	3051	1/1	0.98	0.20	100,100,100,100	0
56	MG	13	1737	1/1	0.98	0.14	72,72,72,72	0
56	MG	1H	3259	1/1	0.98	0.52	105,105,105,105	0
56	MG	1H	3414	1/1	0.98	0.15	65,65,65,65	0
56	MG	13	1723	1/1	0.99	0.14	105,105,105,105	0
56	MG	13	1611	1/1	0.99	0.18	95,95,95,95	0
56	MG	1H	3368	1/1	0.99	0.17	79,79,79,79	0
56	MG	14	3096	1/1	0.99	0.15	77,77,77,77	0
56	MG	14	3357	1/1	0.99	0.13	80,80,80,80	0
56	MG	14	3331	1/1	0.99	0.29	112,112,112,112	0
56	MG	1H	3409	1/1	0.99	0.18	76,76,76,76	0
56	MG	14	3335	1/1	0.99	0.12	73,73,73,73	0
56	MG	1H	3022	1/1	0.99	0.38	64,64,64,64	0
56	MG	1H	3443	1/1	0.99	0.17	76,76,76,76	0
56	MG	14	3016	1/1	0.99	0.24	71,71,71,71	0
56	MG	1H	3380	1/1	0.99	0.16	61,61,61,61	0
56	MG	1H	3382	1/1	0.99	0.10	58,58,58,58	0
56	MG	14	3339	1/1	0.99	0.12	74,74,74,74	0
56	MG	1H	3123	1/1	0.99	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3038	1/1	0.99	0.16	72,72,72,72	0
56	MG	14	3332	1/1	0.99	0.12	72,72,72,72	0
56	MG	1H	3079	1/1	0.99	0.33	83,83,83,83	0
56	MG	1H	3017	1/1	0.99	0.23	79,79,79,79	0
56	MG	1H	3412	1/1	0.99	0.12	64,64,64,64	0
56	MG	1H	3472	1/1	0.99	0.08	98,98,98,98	0
56	MG	1H	3040	1/1	0.99	0.21	78,78,78,78	0
56	MG	14	3077	1/1	0.99	0.28	80,80,80,80	0
56	MG	1H	3036	1/1	0.99	0.46	61,61,61,61	0
56	MG	1H	3452	1/1	0.99	0.14	65,65,65,65	0
57	ZN	32	302	1/1	0.99	0.39	131,131,131,131	0
56	MG	1H	3411	1/1	0.99	0.12	80,80,80,80	0
56	MG	14	3257	1/1	0.99	0.20	84,84,84,84	0
56	MG	14	3392	1/1	0.99	0.08	70,70,70,70	0
56	MG	1H	3004	1/1	0.99	0.30	68,68,68,68	0
56	MG	14	3014	1/1	0.99	0.27	73,73,73,73	0
56	MG	13	1736	1/1	0.99	0.17	102,102,102,102	0
56	MG	1H	3362	1/1	0.99	0.14	61,61,61,61	0
56	MG	1H	3435	1/1	0.99	0.16	72,72,72,72	0
56	MG	14	3079	1/1	0.99	0.23	84,84,84,84	0
56	MG	14	3035	1/1	0.99	0.27	79,79,79,79	0
56	MG	1H	3044	1/1	0.99	0.20	68,68,68,68	0
56	MG	1H	3370	1/1	0.99	0.16	84,84,84,84	0
56	MG	14	3366	1/1	0.99	0.15	88,88,88,88	0
56	MG	1H	3440	1/1	0.99	0.10	83,83,83,83	0
56	MG	1H	3205	1/1	0.99	0.23	64,64,64,64	0
56	MG	14	3385	1/1	0.99	0.12	73,73,73,73	0
56	MG	1H	3076	1/1	0.99	0.26	73,73,73,73	0
56	MG	14	3342	1/1	0.99	0.12	80,80,80,80	0
56	MG	14	3215	1/1	0.99	0.15	104,104,104,104	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.