



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 01:16 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

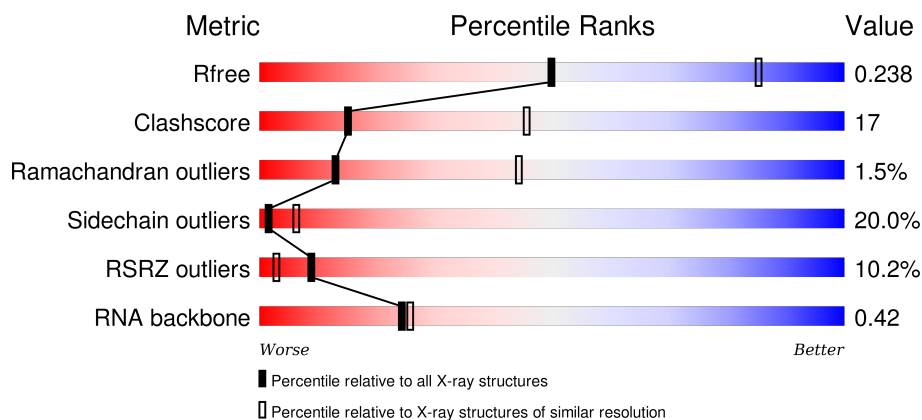
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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. 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>

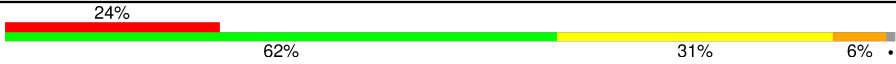

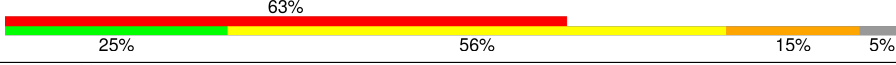

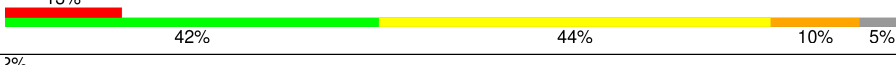
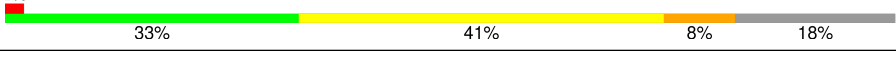
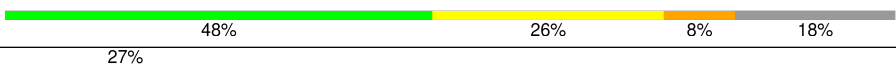
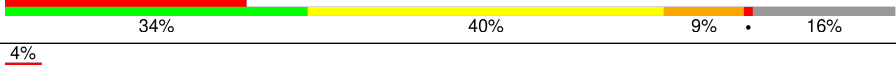
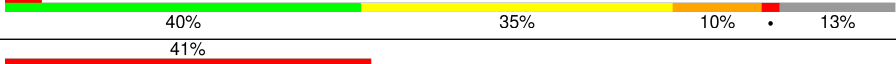



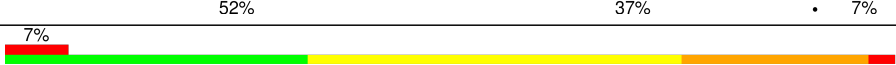
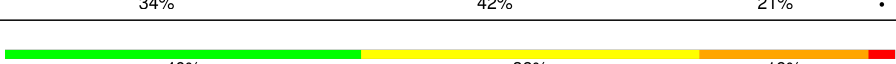
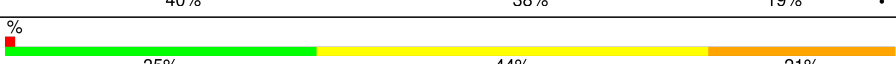
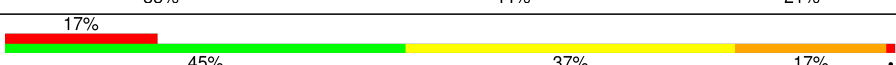
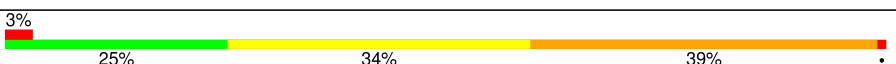
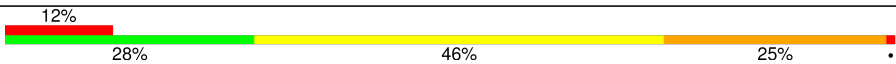
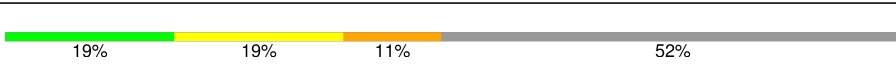

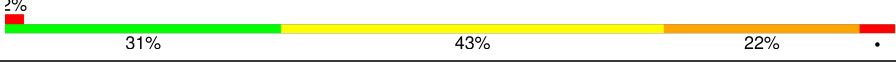
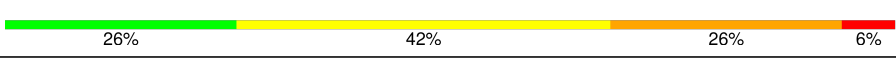

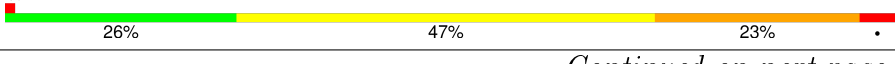

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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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	1602	-	-	-	X
56	MG	13	1621	-	-	-	X
56	MG	13	1641	-	-	-	X
56	MG	13	1652	-	-	-	X
56	MG	13	1664	-	-	-	X
56	MG	13	1666	-	-	-	X
56	MG	13	1680	-	-	-	X
56	MG	13	1686	-	-	-	X
56	MG	13	1689	-	-	-	X
56	MG	13	1706	-	-	-	X
56	MG	13	1721	-	-	-	X
56	MG	13	1752	-	-	-	X
56	MG	14	3007	-	-	-	X
56	MG	14	3055	-	-	-	X
56	MG	14	3060	-	-	-	X
56	MG	14	3091	-	-	-	X
56	MG	14	3146	-	-	-	X
56	MG	14	3169	-	-	-	X
56	MG	14	3170	-	-	-	X
56	MG	14	3194	-	-	-	X
56	MG	14	3195	-	-	-	X
56	MG	14	3199	-	-	-	X
56	MG	14	3202	-	-	-	X
56	MG	14	3205	-	-	-	X
56	MG	14	3209	-	-	-	X
56	MG	14	3211	-	-	-	X
56	MG	14	3216	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3217	-	-	-	X
56	MG	14	3227	-	-	-	X
56	MG	14	3233	-	-	-	X
56	MG	14	3248	-	-	-	X
56	MG	14	3253	-	-	-	X
56	MG	14	3254	-	-	-	X
56	MG	14	3264	-	-	-	X
56	MG	14	3266	-	-	-	X
56	MG	14	3272	-	-	-	X
56	MG	14	3274	-	-	-	X
56	MG	14	3306	-	-	-	X
56	MG	14	3308	-	-	-	X
56	MG	14	3382	-	-	-	X
56	MG	16	206	-	-	-	X
56	MG	16	207	-	-	-	X
56	MG	16	209	-	-	-	X
56	MG	1G	1614	-	-	-	X
56	MG	1G	1627	-	-	-	X
56	MG	1G	1645	-	-	-	X
56	MG	1G	1659	-	-	-	X
56	MG	1G	1660	-	-	-	X
56	MG	1G	1664	-	-	-	X
56	MG	1H	3004	-	-	-	X
56	MG	1H	3011	-	-	-	X
56	MG	1H	3013	-	-	-	X
56	MG	1H	3025	-	-	-	X
56	MG	1H	3037	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3056	-	-	-	X
56	MG	1H	3063	-	-	-	X
56	MG	1H	3069	-	-	-	X
56	MG	1H	3081	-	-	-	X
56	MG	1H	3084	-	-	-	X
56	MG	1H	3089	-	-	-	X
56	MG	1H	3110	-	-	-	X
56	MG	1H	3116	-	-	-	X
56	MG	1H	3139	-	-	-	X
56	MG	1H	3160	-	-	-	X
56	MG	1H	3170	-	-	-	X
56	MG	1H	3173	-	-	-	X
56	MG	1H	3178	-	-	-	X
56	MG	1H	3186	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3219	-	-	-	X
56	MG	1H	3222	-	-	-	X
56	MG	1H	3234	-	-	-	X
56	MG	1H	3235	-	-	-	X
56	MG	1H	3240	-	-	-	X
56	MG	1H	3245	-	-	-	X
56	MG	1H	3254	-	-	-	X
56	MG	1H	3255	-	-	-	X
56	MG	1H	3258	-	-	-	X
56	MG	1H	3260	-	-	-	X
56	MG	1H	3277	-	-	-	X
56	MG	1H	3298	-	-	-	X
56	MG	1H	3304	-	-	-	X
56	MG	1H	3332	-	-	-	X
56	MG	1J	207	-	-	-	X
56	MG	29	301	-	-	-	X
56	MG	2K	105	-	-	-	X
56	MG	39	303	-	-	-	X
56	MG	L8	101	-	-	-	X
57	ZN	32	302	-	-	-	X
57	ZN	3E	301	-	-	-	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 1	Zn 1	0	0
57	3E	1	Total 1	Zn 1	0	0
57	5I	1	Total 1	Zn 1	0	0
57	5A	1	Total 1	Zn 1	0	0
57	G8	1	Total 1	Zn 1	0	0
57	C5	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	164	Total 164	O 164	0	0
58	3E	1	Total 1	O 1	0	0
58	4E	1	Total 1	O 1	0	0
58	1I	1	Total 1	O 1	0	0
58	3I	1	Total 1	O 1	0	0
58	5I	1	Total 1	O 1	0	0
58	6I	1	Total 1	O 1	0	0
58	7I	1	Total 1	O 1	0	0
58	4K	1	Total 1	O 1	0	0
58	1H	920	Total 920	O 920	0	0
58	16	6	Total 6	O 6	0	0
58	11	9	Total 9	O 9	0	0
58	21	5	Total 5	O 5	0	0
58	31	7	Total 7	O 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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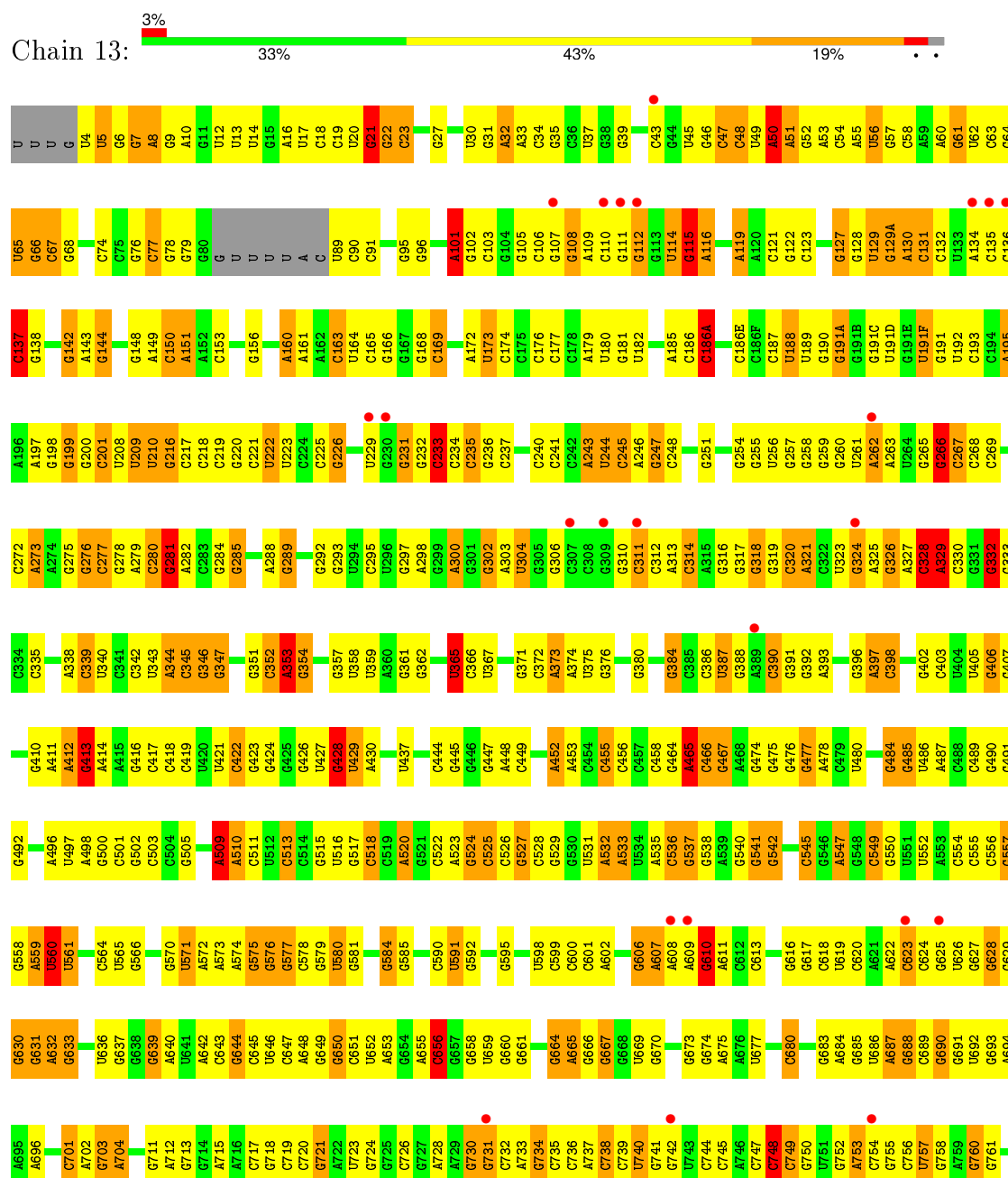
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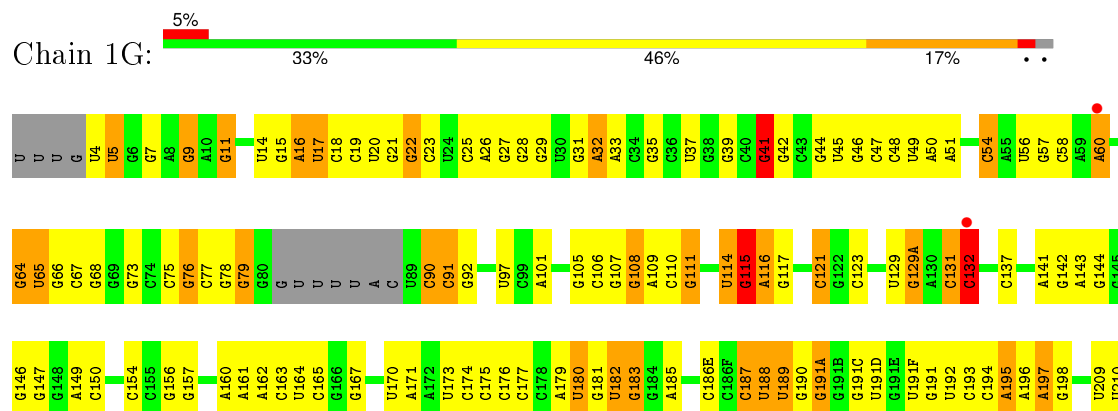
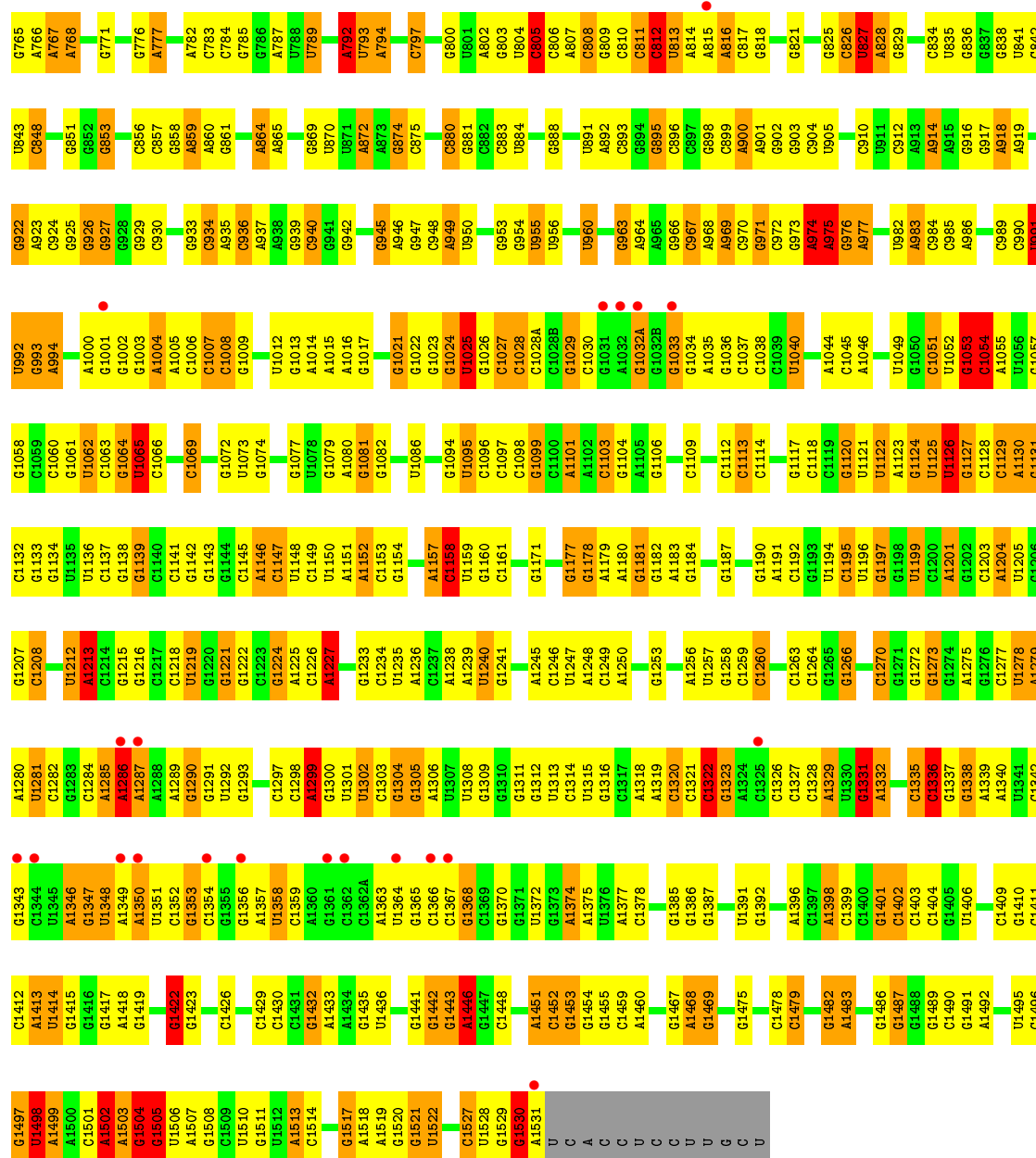
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	L5	2	Total	O	0	0
			2	2		

### 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 errors 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.

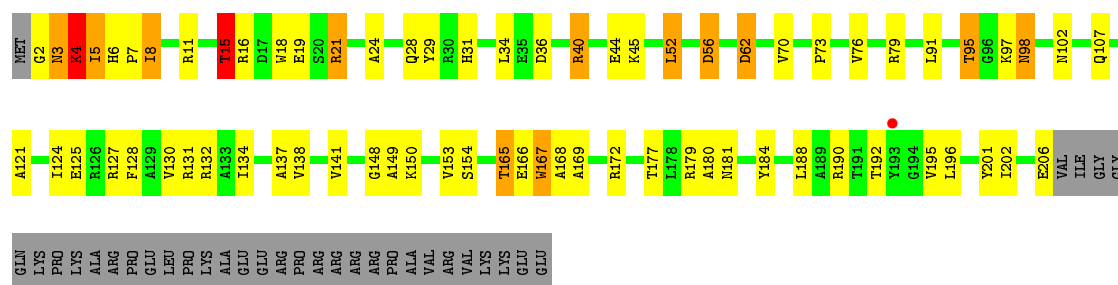
- Molecule 1: 16S ribosomal RNA



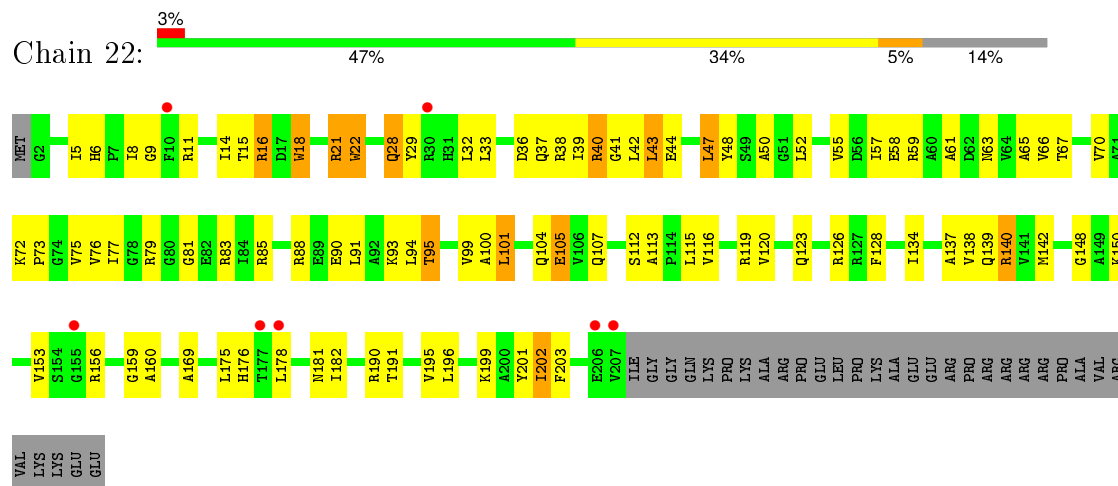


G1207	G1143	G1074	A1015	U950	G880	G811	G731	G660	G594	G521	C442	U367	G297	G216
C1208	G1144	G1078	A1016	G951	G881	C811	C735	G661	G595	C522	C443	G371	A298	C217
C1209	C1145	U1079	G1017	U952	G882	U813	C736	G662	C586	A523		G372	G299	C218
C1210	A1146	G1079	C1018	G953	C883	U813	C736	A663	G587	G524	G446	C371	A300	
U1211	A1147	A1080	C1019	G954	U884	A814	A814	G664	C588	C525	A447	A373	G302	U222
U1212	U1148	G1081	U1020	U955	G885	A815	C738	A665	C589	C526	A448	A374	G303	U223
A1213	U1149	G1082	G1021	U956	G886	A816	C739	G666	C590	G527	C449	U375	A303	
C1214	U1150	U1083	G1024	U957	G887	C817	C742	G667	U591	C528	G450	G376	U304	G230
C1215	A1151	U1084	U1025	A958	G888	G818	G742	G668		G529	A451	G377		
C1218	A1152	U1085	G1026	A959	G889	A819	U743		C596	G530	A452		G308	G236
U1219	C1153	U1086	C1027	U960	G890	U820	U744		G531	U531	A453	G380	G309	C237
G1220	G1154	G1094	U1028	U961	C893	G821	C745	U672	G600	A532	C454	G381		G238
U1221	G1155	U1095	C1028A	C962	G894	G822	A746	G673	G601	A533	C455	A382	C312	
G1222	G1156	C1028B	C1028B	G963		G823	C747	A675	A602	U534	C456	A383	A313	C241
C1223	A1157	G1029	G1029	A964	G898	C824	C748	A676	U603	A535	C457		C314	C242
C1224	C1158	C1030	C1030	A965	G899	G825	C749	G677	G604	C536	C458	C386	A315	A243
G1225	U1159	G1031	U1031	G966	C899	C826	G750	U678	U605	G537	C464	U387	G316	U244
A1226	U1160	A1032	A1032	C967	A900	U827	G751	C679	G606	G538	A465	G388	G317	C245
C1226	C1161	G1032A	G1032A	A968	A901	A828	C754	C680	A607	A539	C466	A389	A246	
A1227	C1162	G1032B	G1032B	A969	G829	G829	G755		A608	G540	A467	C390	G247	
C1228	C1163	G1033	G1033	C970	G830	U831	G760		A611	G541	A468	G391	A321	A250
U1232	G1166	G1103	G1034	G971	U905	G836	G761	G684	G612	G542	G474	A397	C322	G251
C1233	A1167	G1104	A1035	C972	G906		C762	G685	C613		G475	U323	U323	
G1234	A1169	A1105	G1036	G973	A909	G837	G762	U686	G614	C545	G476	C398	G326	G254
U1235	A1170	G1106	C1037	A974	C910	G838	G763	G687	G615	G546	G477	C399	A327	G255
A1236	G1171	C1107	C1038	A975	U911	U841	C764	G688	G616	A547	A478	C400	G327	U256
C1237	C1172	C1109	U1040	G976	U911	C842		G689	G617	G550	C479	C403	C328	
A1238	G1173	A1110		A977	C912	U843	U772	G690	G618	G551	U480	C403	C330	G257
A1239	G1174	A1111	C1043	A978	A913	U843	U773	G691	U619	U552	G481	G406	G331	U261
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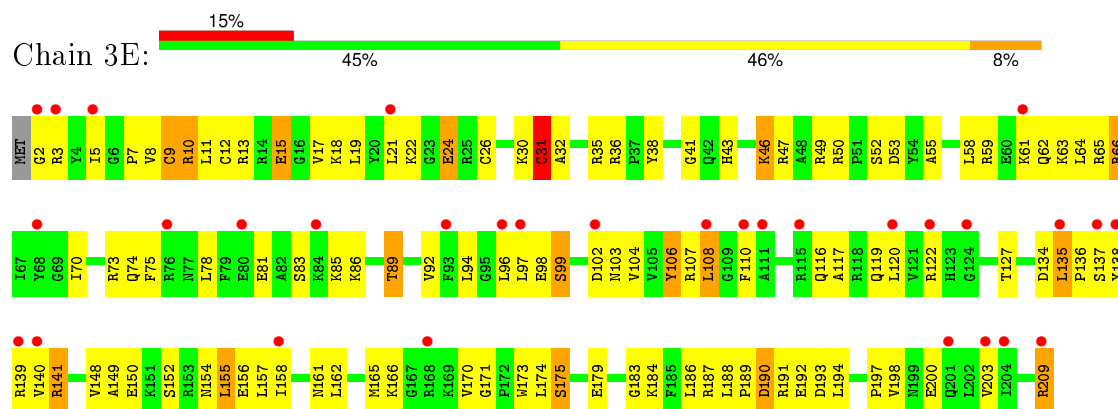




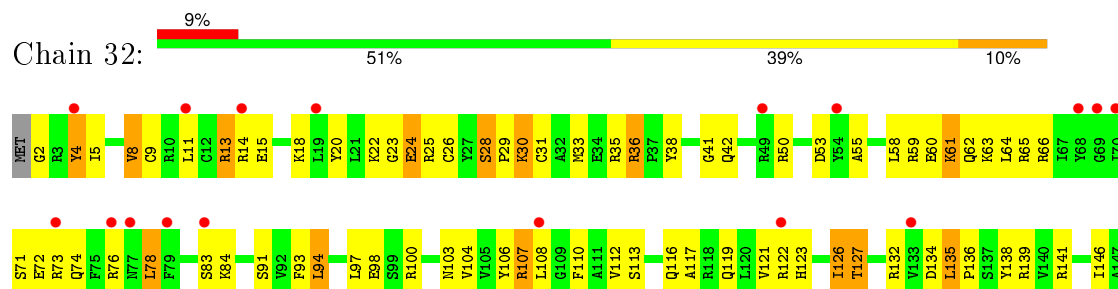
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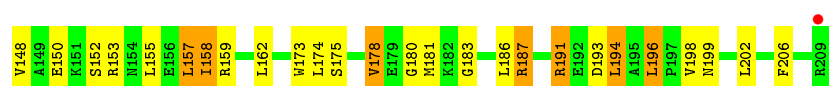


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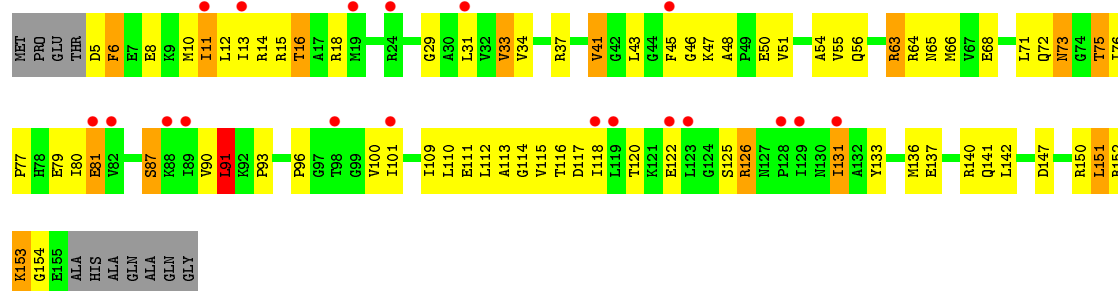


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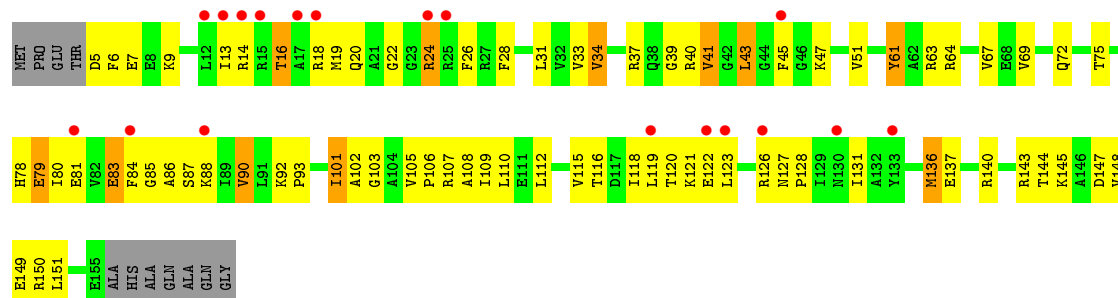




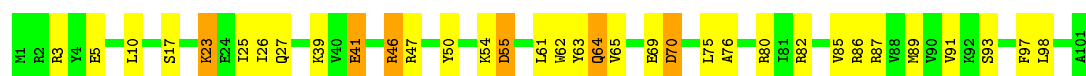
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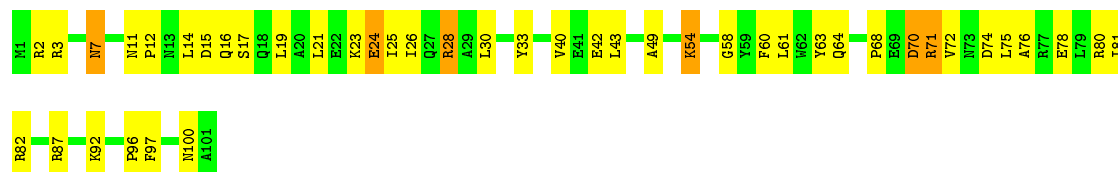
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

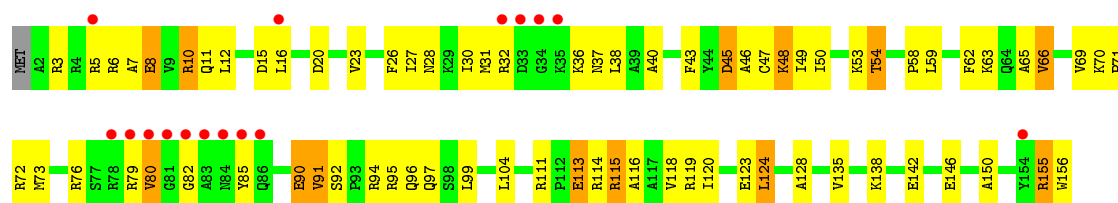


- Molecule 6: 30S ribosomal protein S6

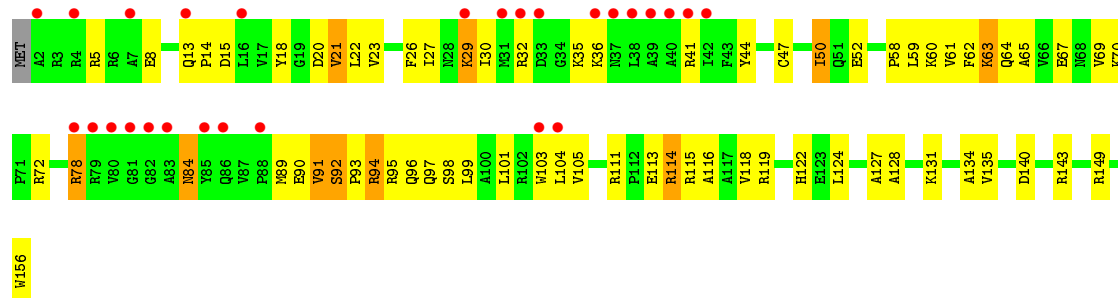


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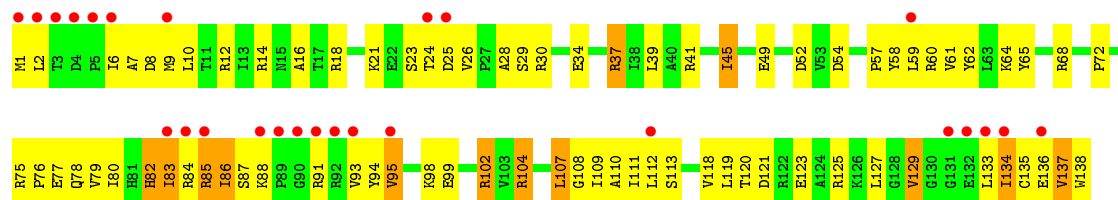
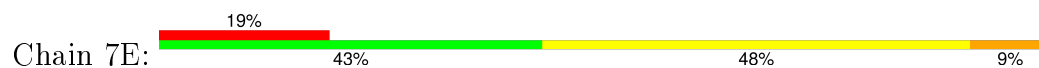




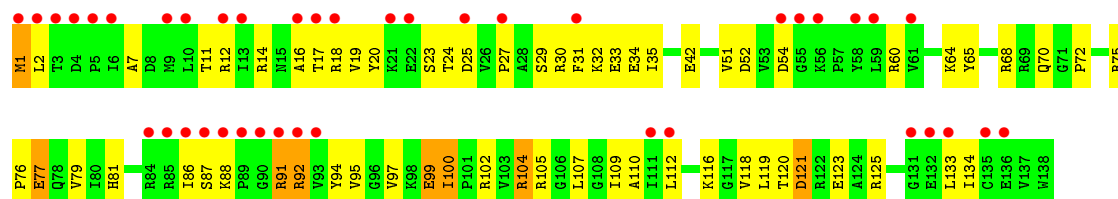
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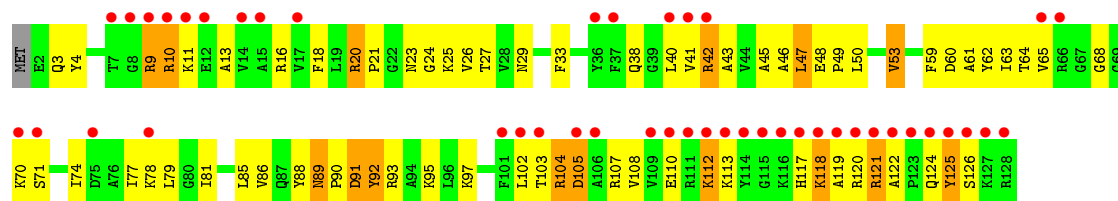
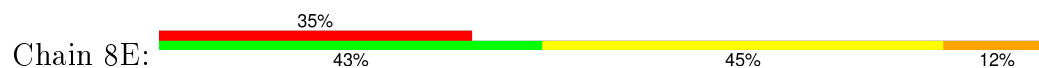
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

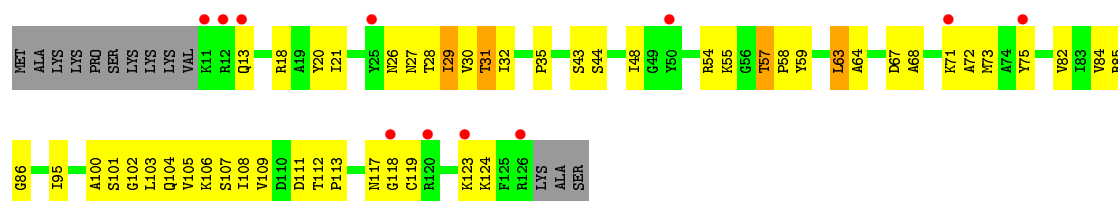


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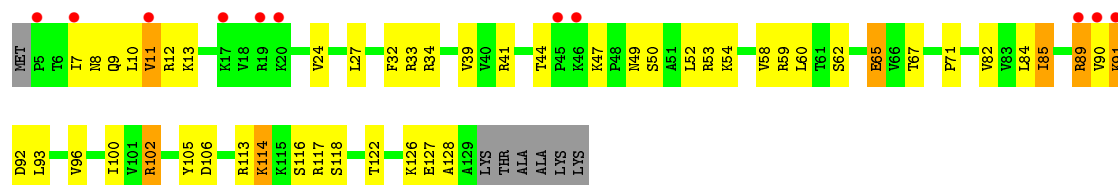




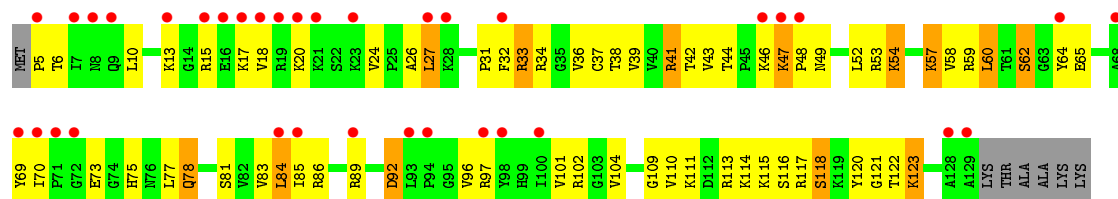
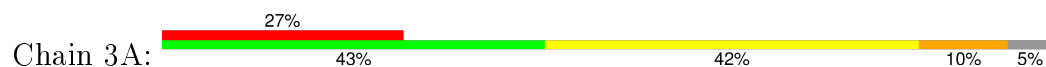
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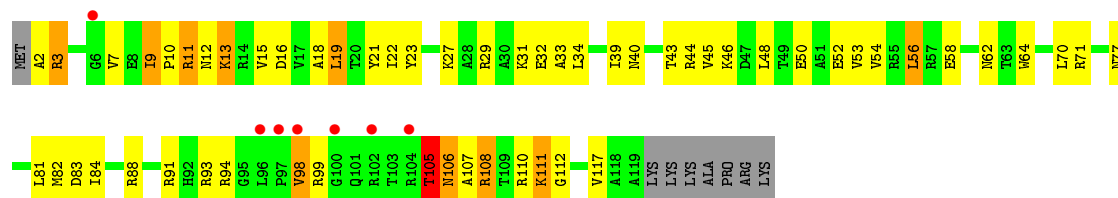
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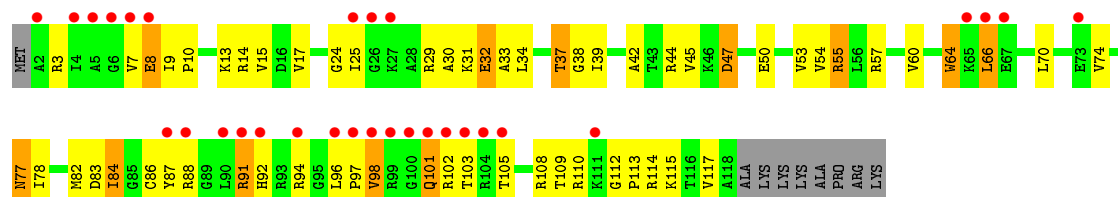
• Molecule 12: 30S ribosomal protein S12



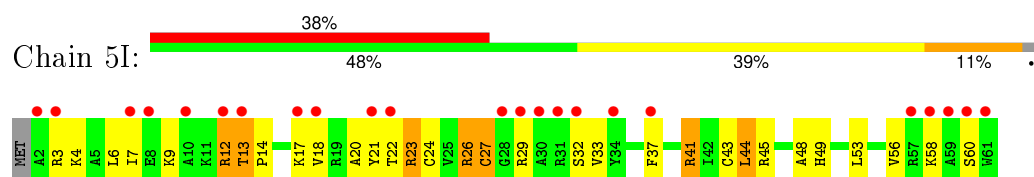
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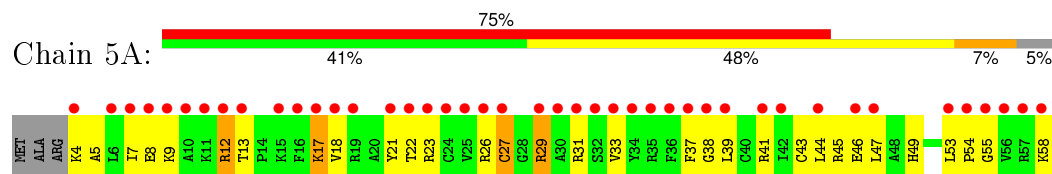
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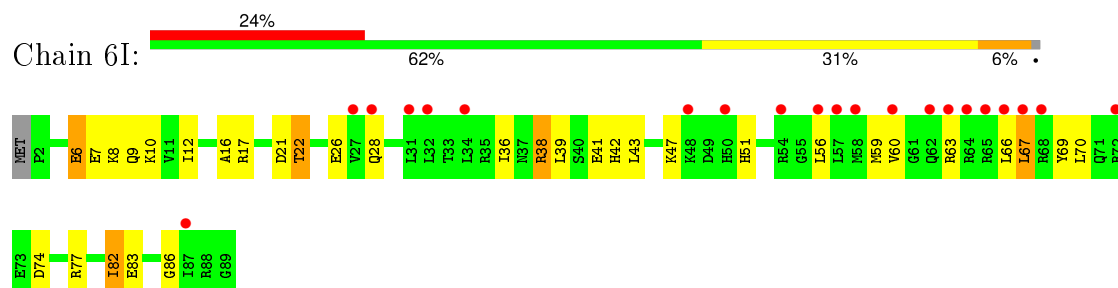
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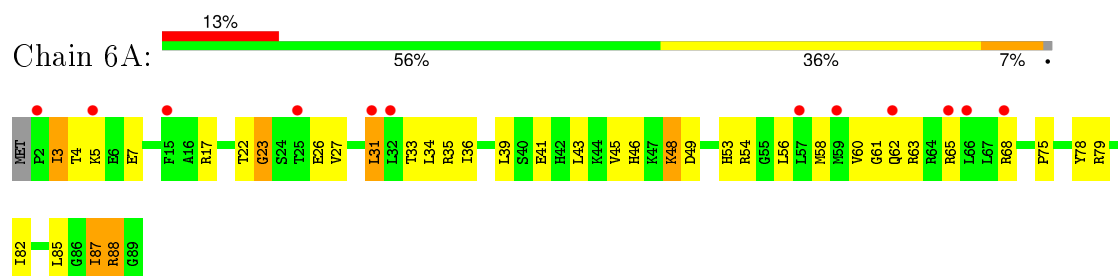
- Molecule 14: 30S ribosomal protein S14 type Z



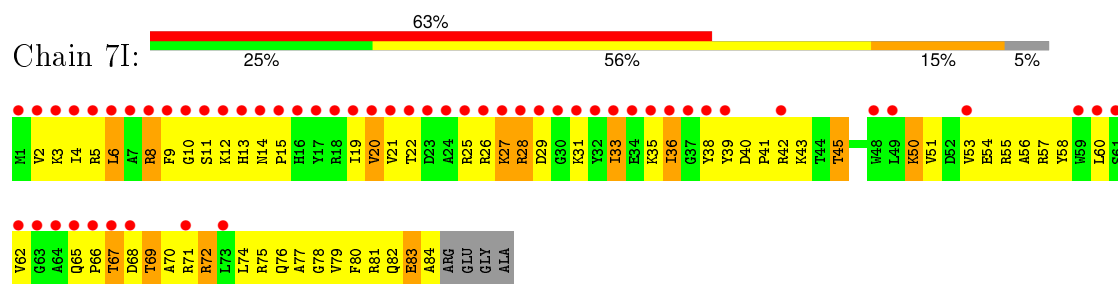
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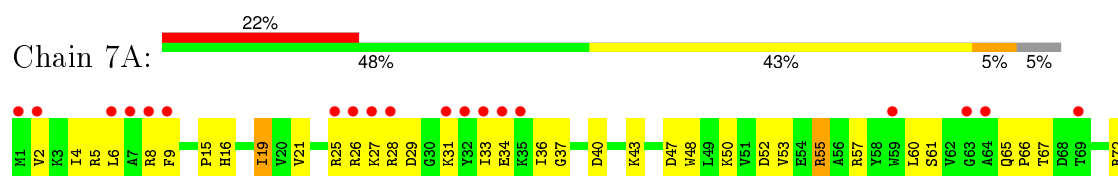
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

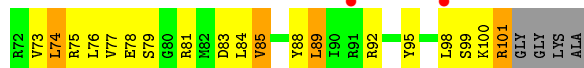
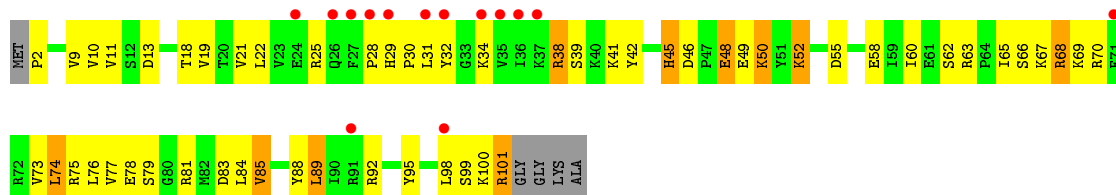


- Molecule 16: 30S ribosomal protein S16

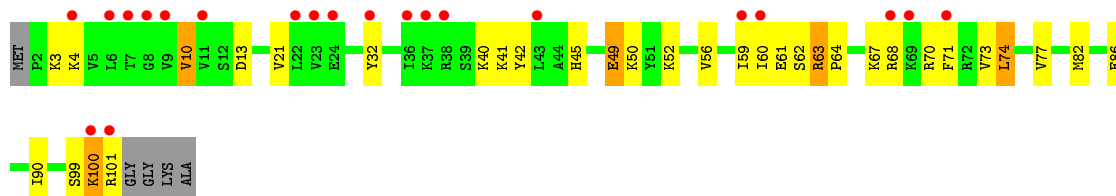




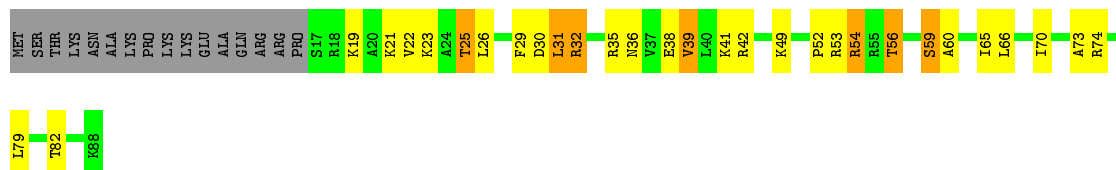
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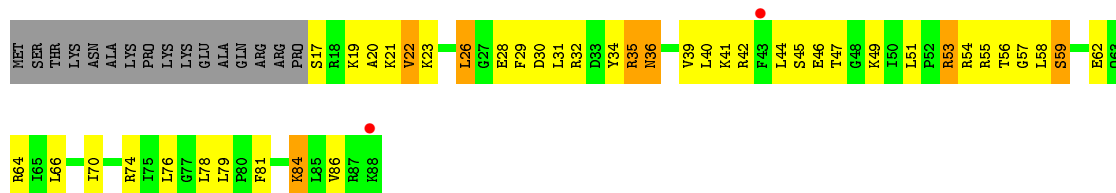
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



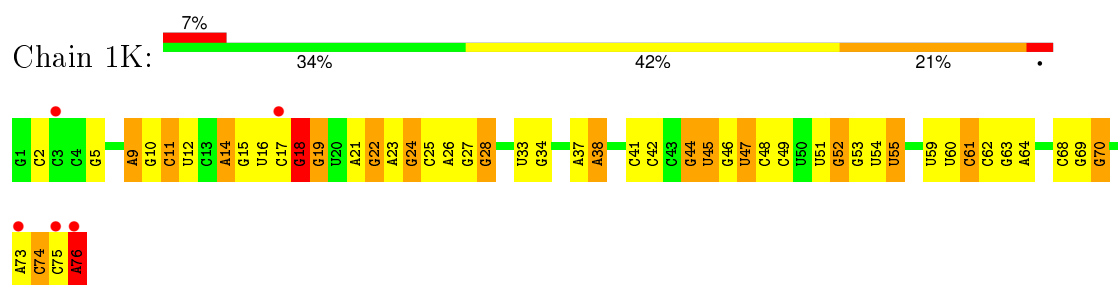
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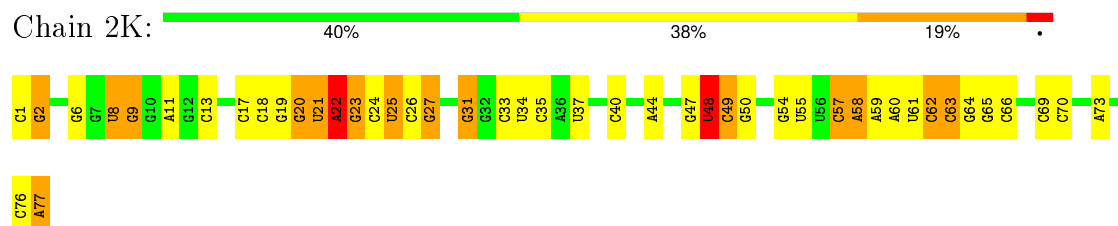
- Molecule 19: 30S ribosomal protein S19



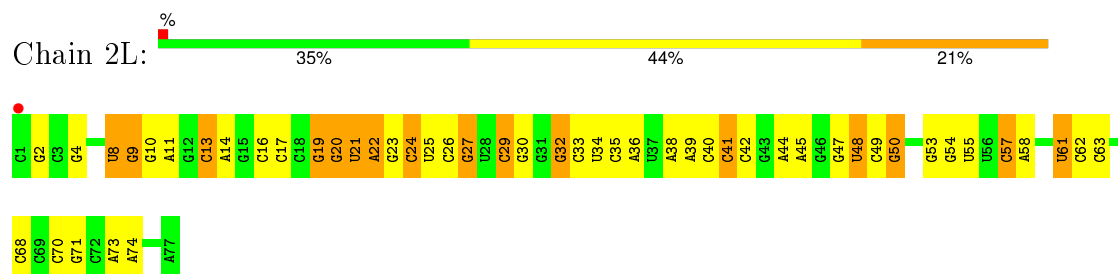




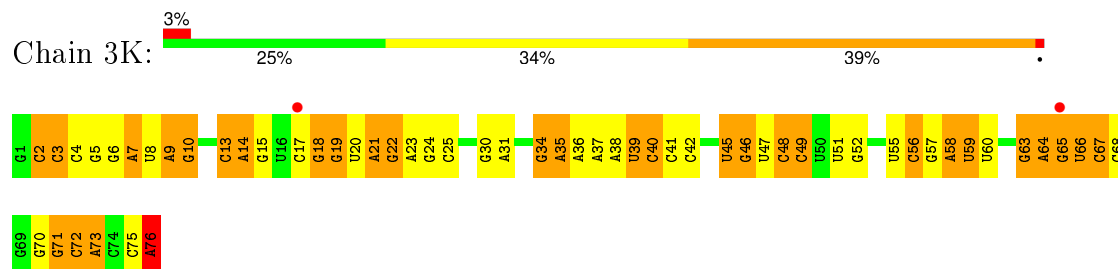
- Molecule 23: tRNA-fMet



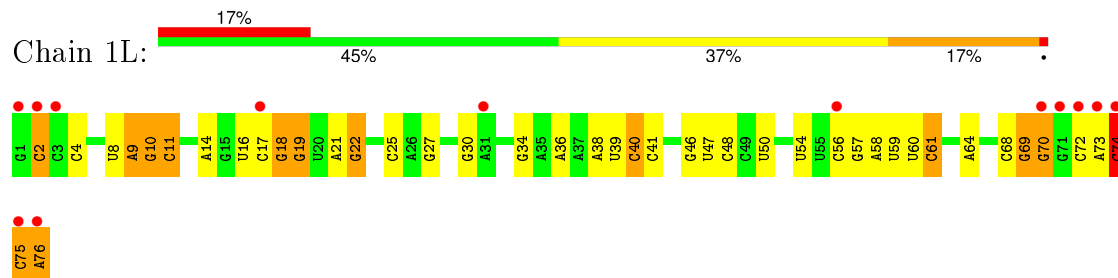
- Molecule 23: tRNA-fMet



- Molecule 24: tRNA-Phe

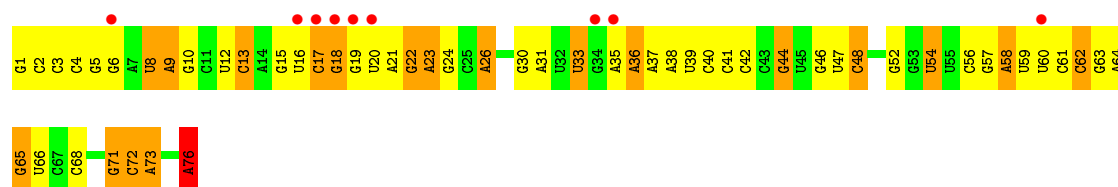


- Molecule 24: tRNA-Phe



- Molecule 24: tRNA-Phe





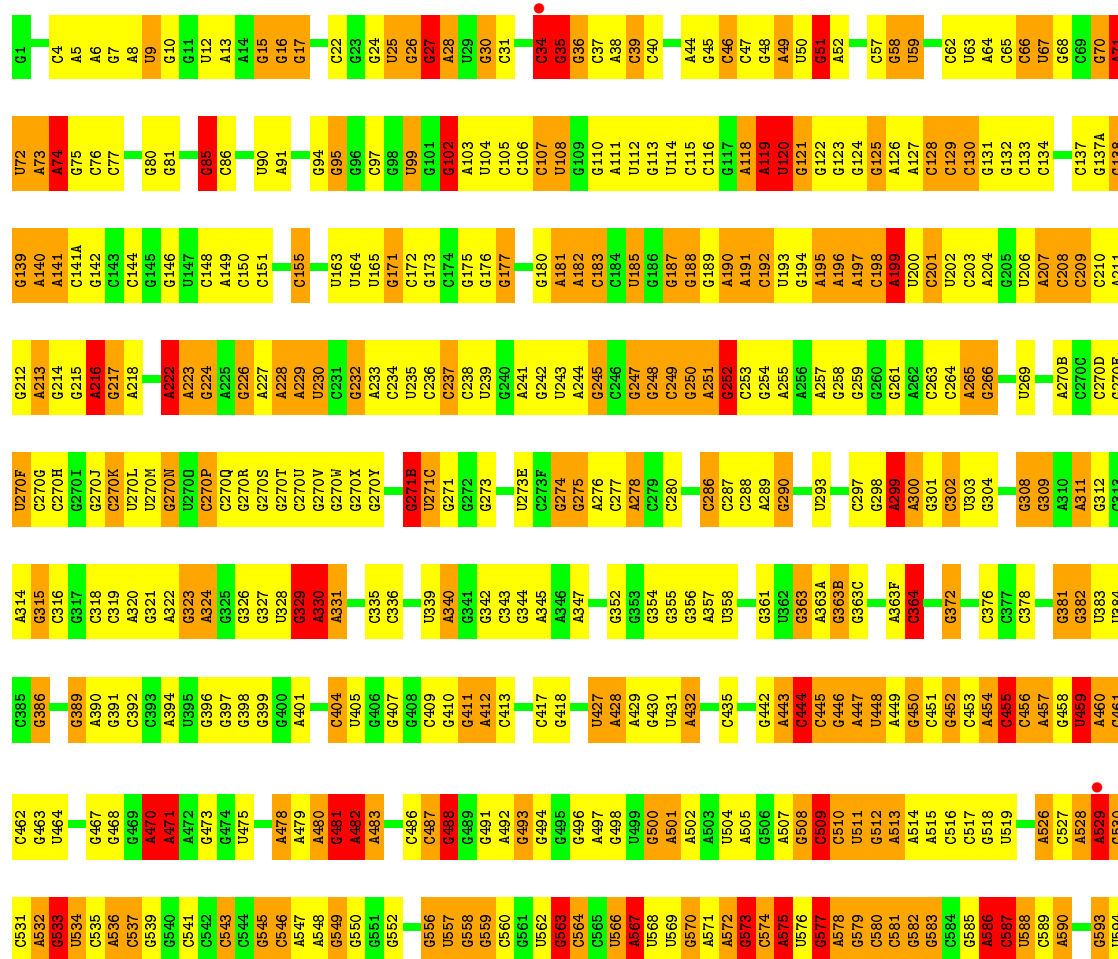
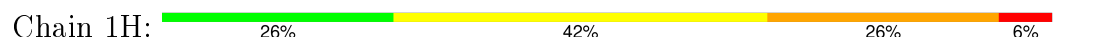
• Molecule 25: mRNA



• Molecule 25: mRNA



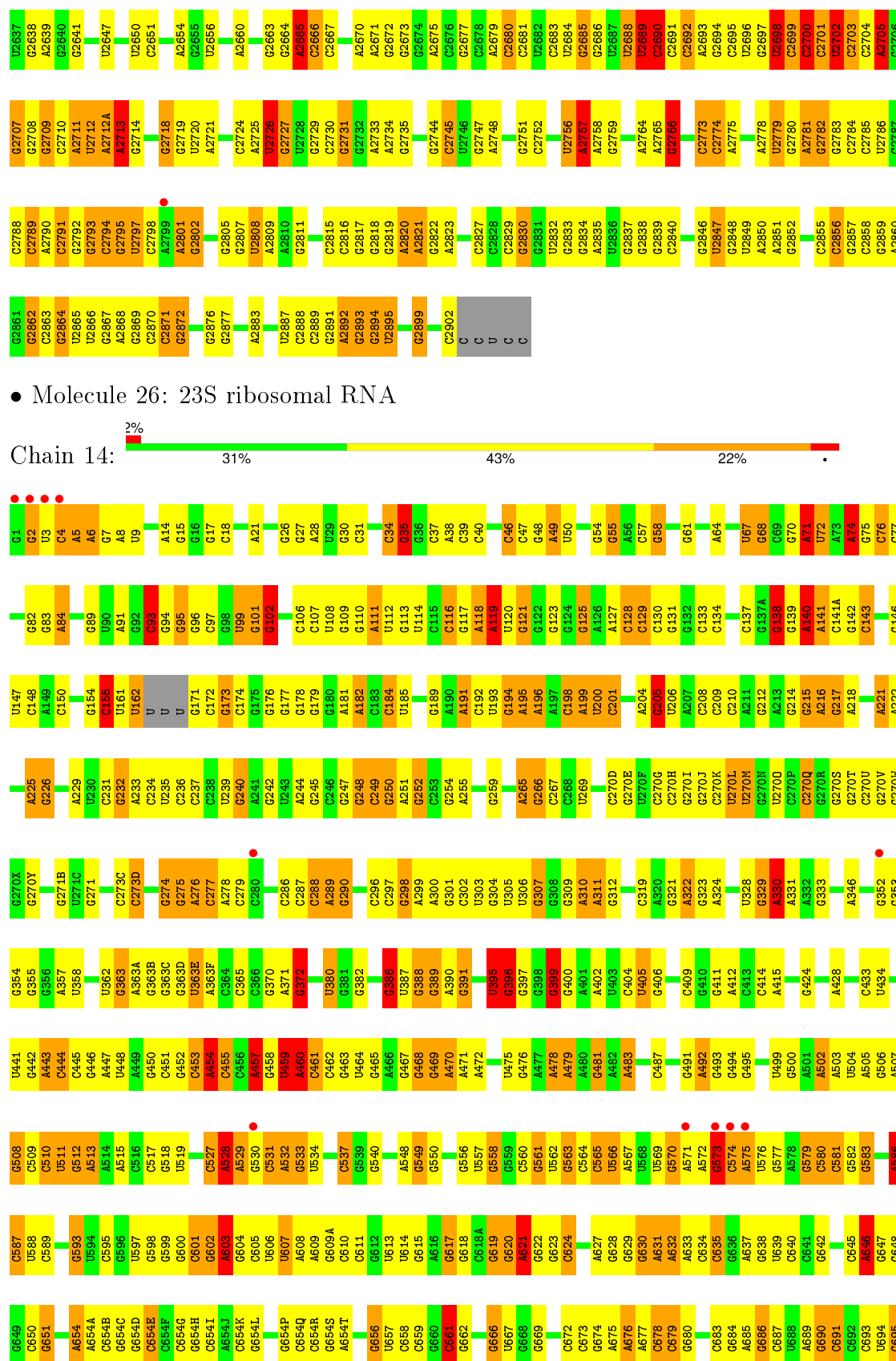
• Molecule 26: 23S ribosomal RNA





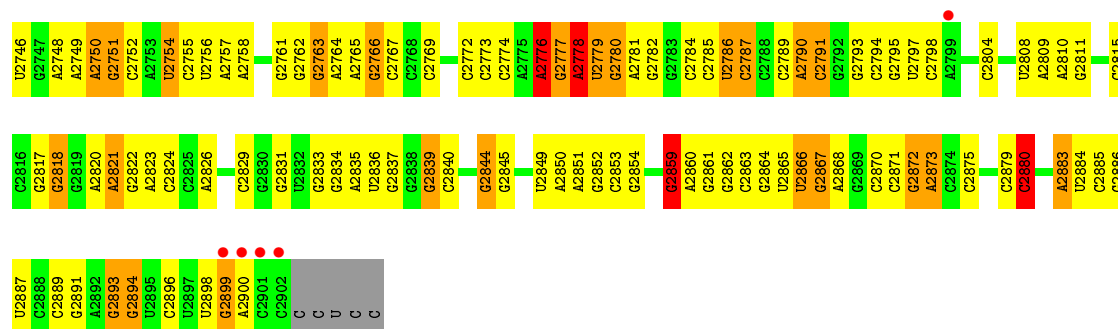


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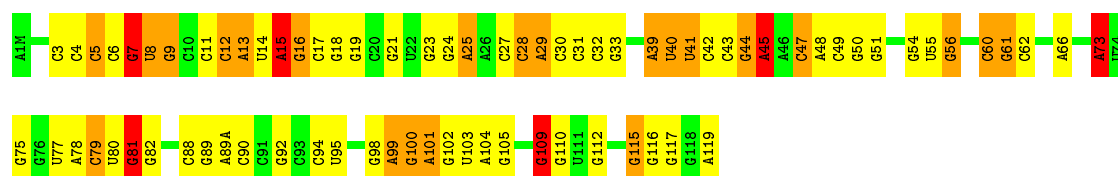
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U2070	A2071	G2072	G2073	U2074	U2075	U2076	U2077	U2078	U2079	G2080	G2081	G2082	G2083	G2084	U2085	U2086	G2087	U2093	U2096	C2097	U2098	G2099	G2100	G2101	U2102	C2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	U2124	G2125	A2126	G2127	G2128	G2129	U2130	G2131	U2132	G2133	A2134	A2135																																																																																																																																																																																																																																																																																																																																						
C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	U2150	C2151	G2152	C2153	C2154	G2157	A2158	G2159	G2160	C2161	G2162	C2163	C2164	G2165	U2166	U2167	G2168	C2169	A2170	U2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	G2184	C2185	G2186	G2187	C2188	U2189	G2190	G2191	G2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	U2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	U2503	U2504	U2505	U2506	U2507	U2508	U2509	U2510	U2511	U2512	U2513	U2514	U2515	U2516	U2517	U2518	U2519	U2520	U2521	U2522	U2523	U2524	U2525	U2526	U2527



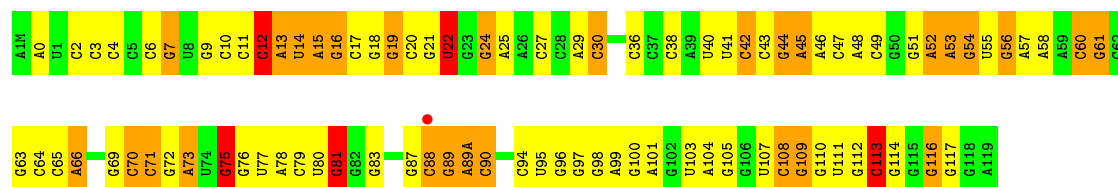
● Molecule 27: 5S ribosomal RNA

Chain 16: 38% 39% 18% 5%



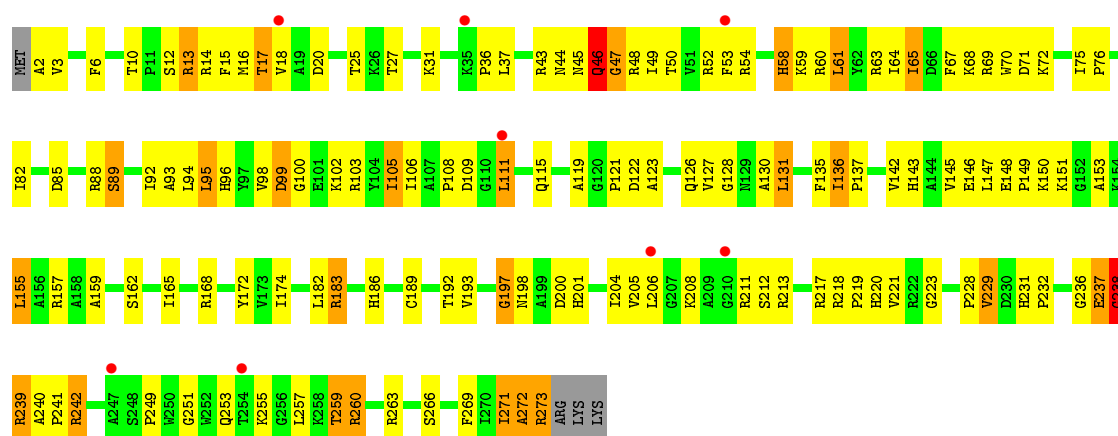
● Molecule 27: 5S ribosomal RNA

Chain 1J: 26% 47% 23% .



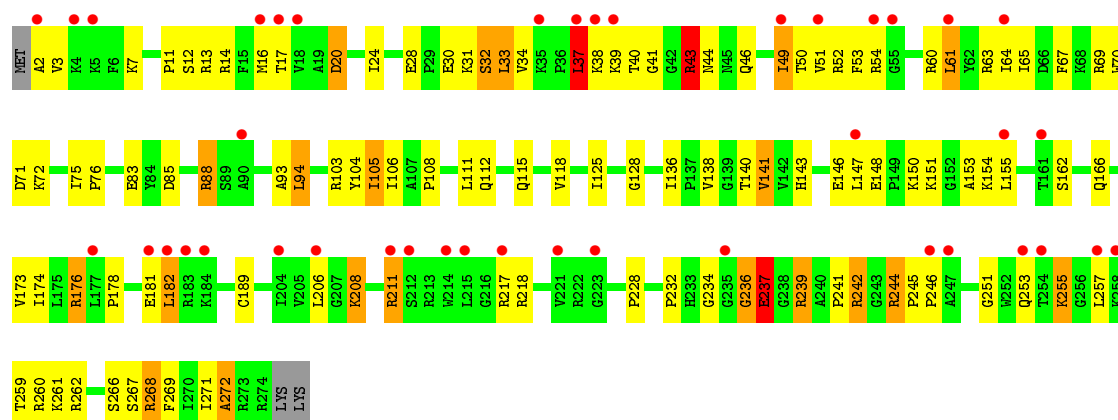
● Molecule 28: 50S ribosomal protein L2

Chain 11: 3% 48% 41% 9% ..

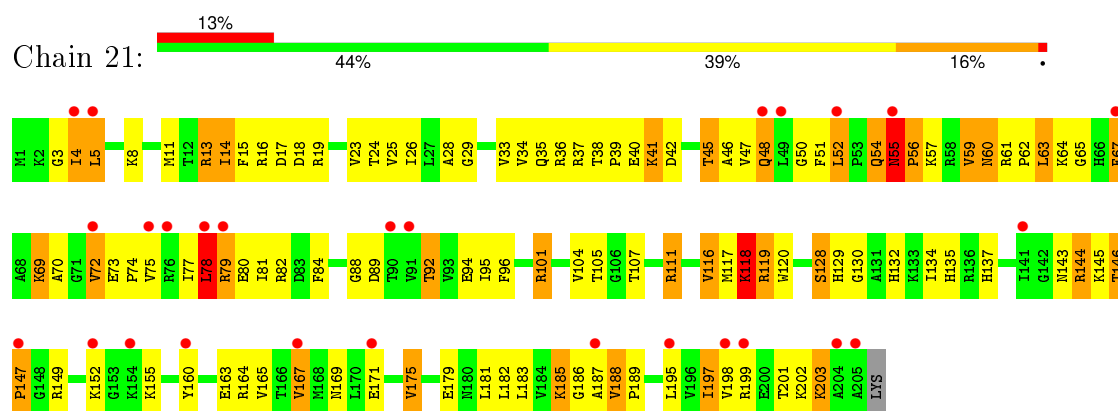


● Molecule 28: 50S ribosomal protein L2

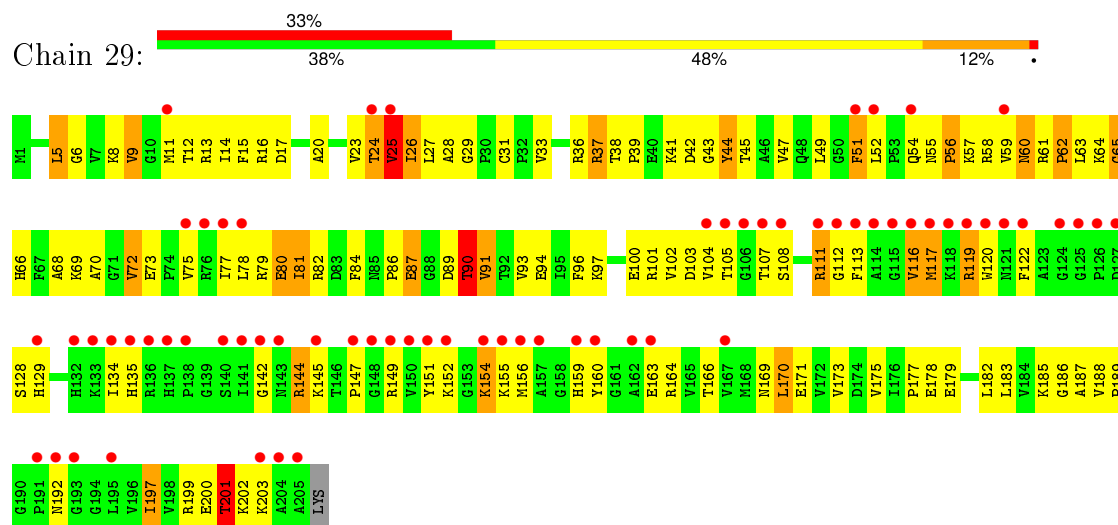
Chain 19: 15% 59% 32% 7% ..



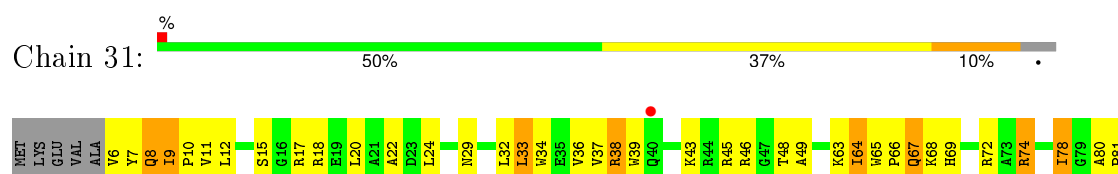
• Molecule 29: 50S ribosomal protein L3

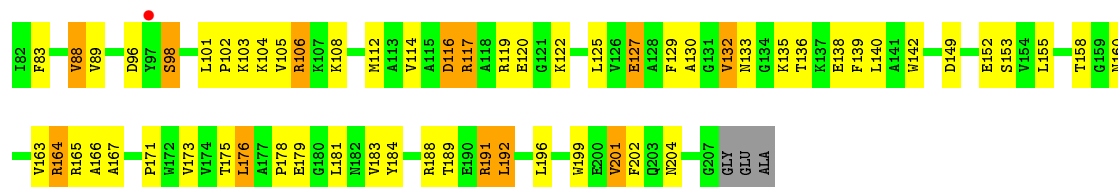


• Molecule 29: 50S ribosomal protein L3

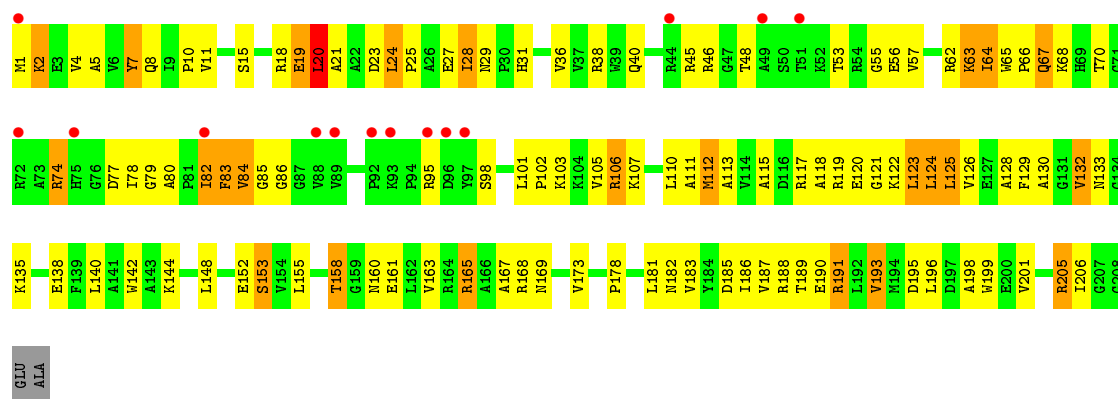


• Molecule 30: 50S ribosomal protein L4

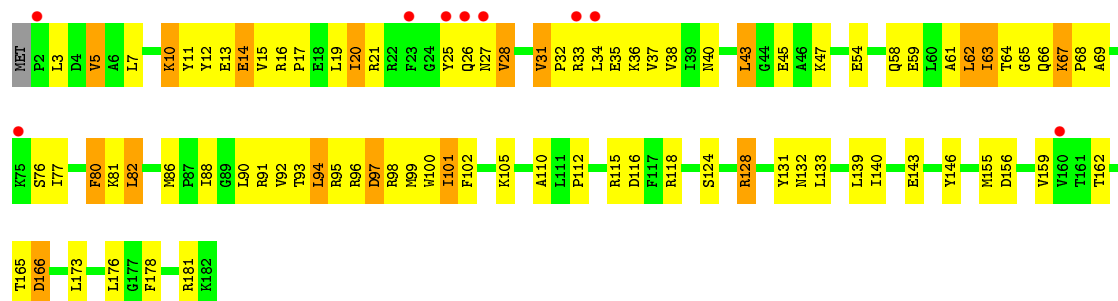




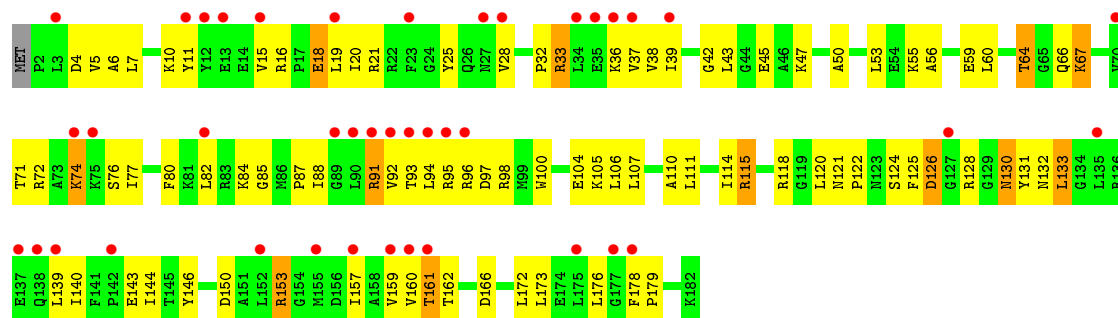
• Molecule 30: 50S ribosomal protein L4



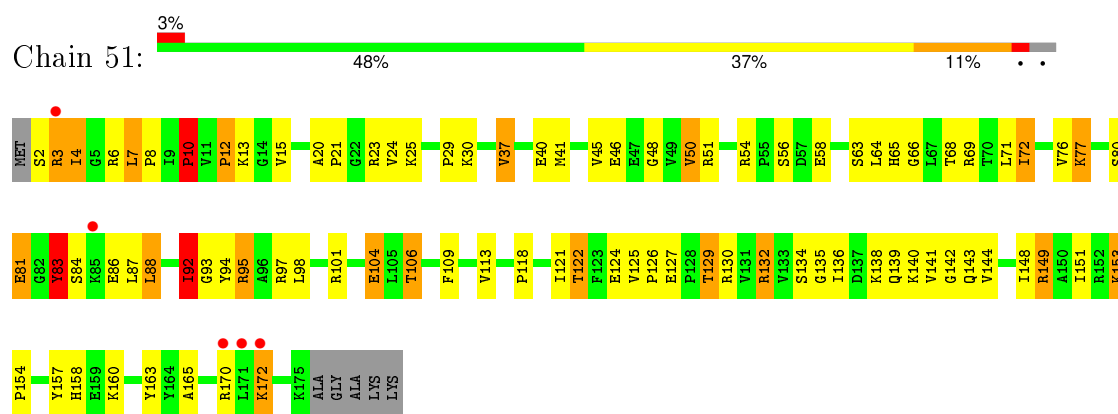
• Molecule 31: 50S ribosomal protein L5



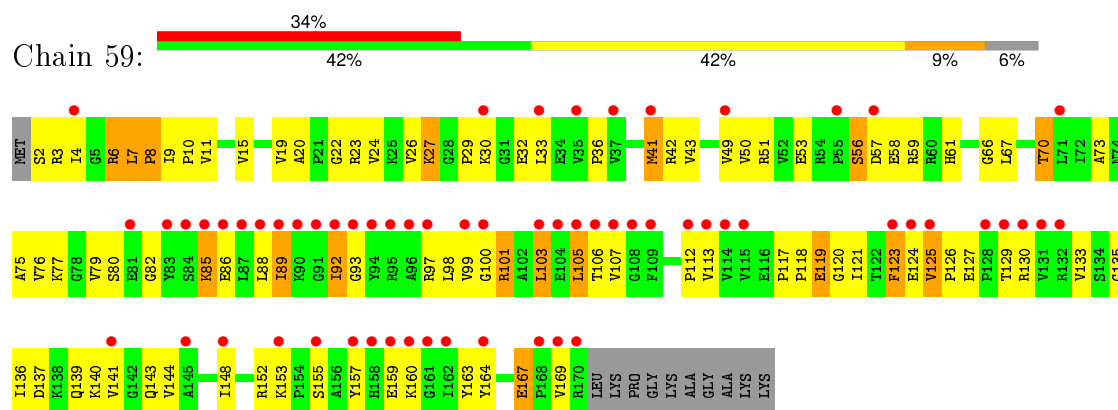
• Molecule 31: 50S ribosomal protein L5



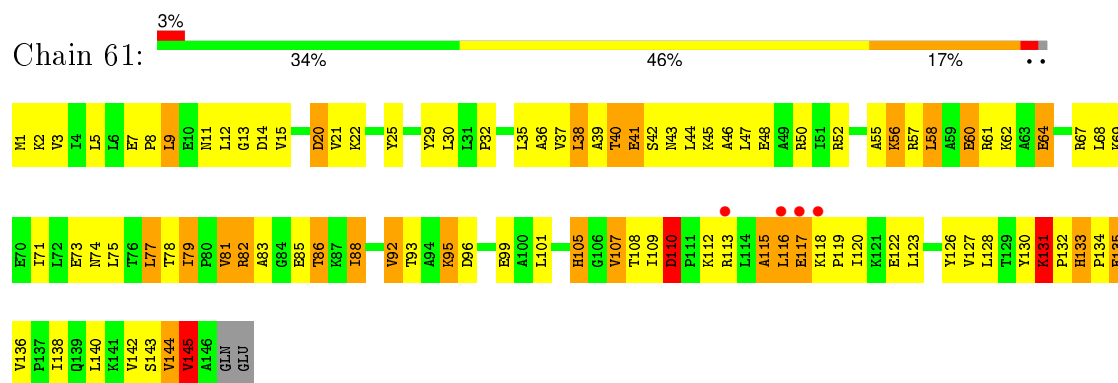
• Molecule 32: 50S ribosomal protein L6



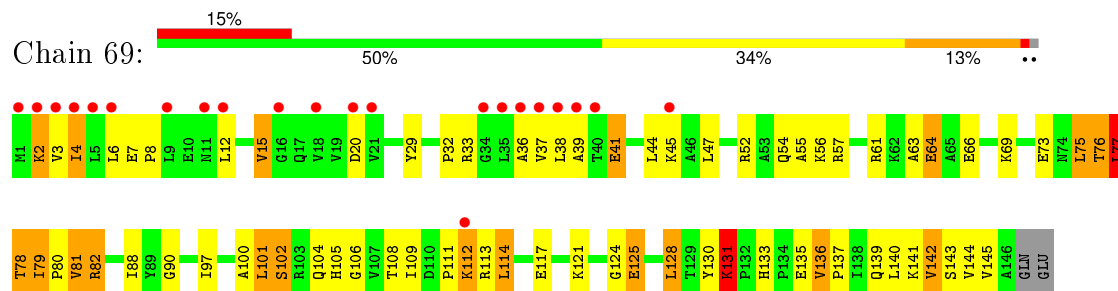
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9

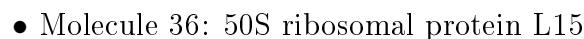
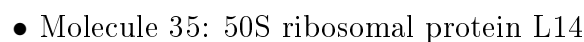
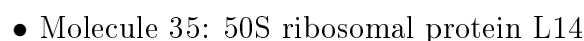
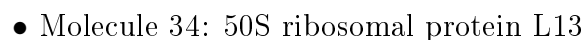


• Molecule 33: 50S ribosomal protein L9



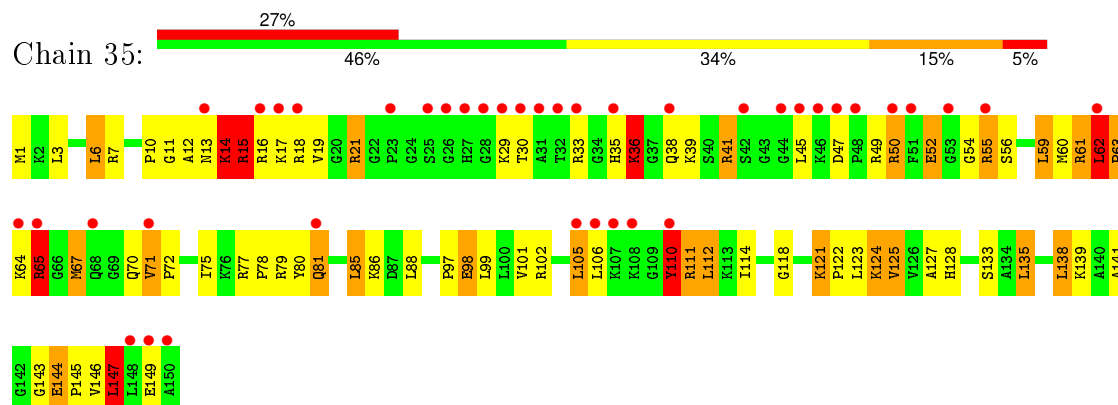
• Molecule 34: 50S ribosomal protein L13



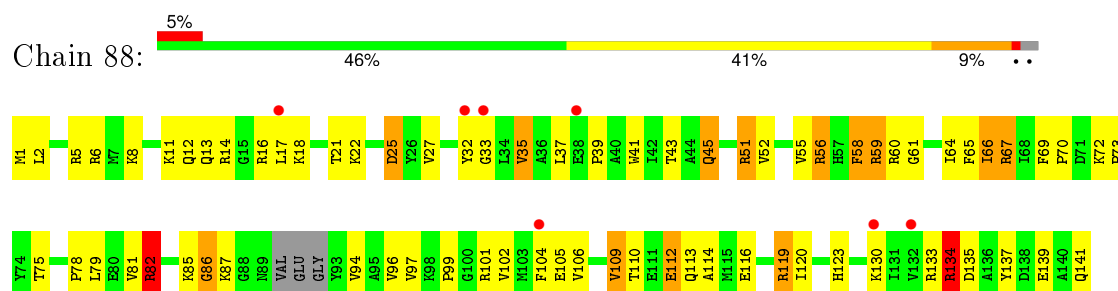




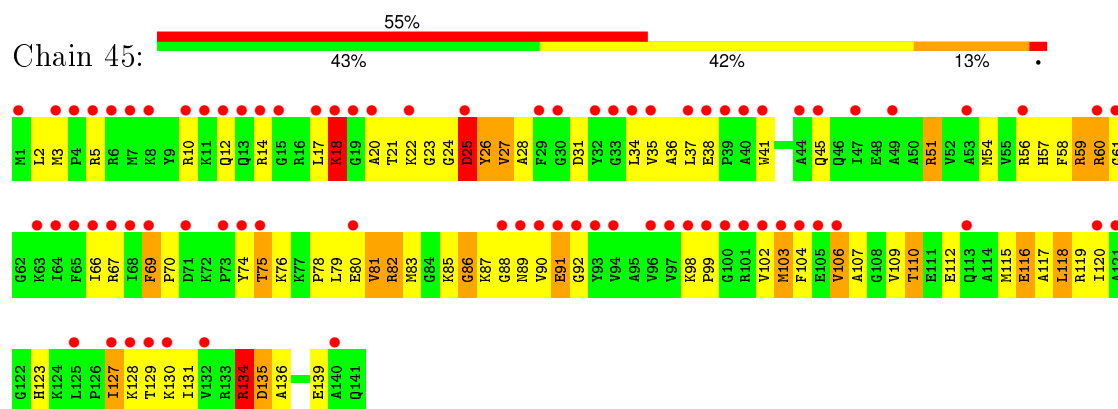
- Molecule 36: 50S ribosomal protein L15



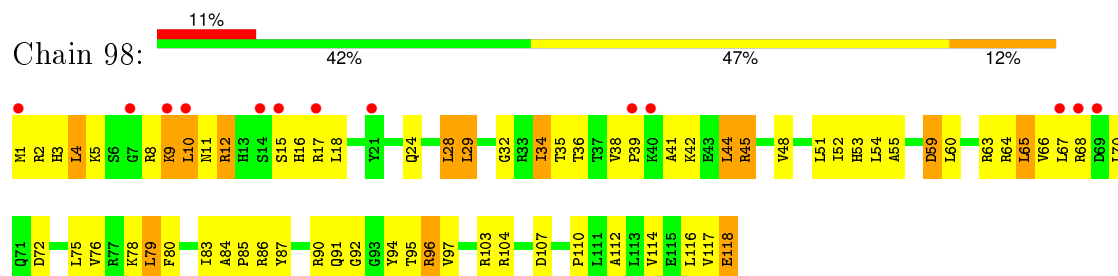
- Molecule 37: 50S ribosomal protein L16



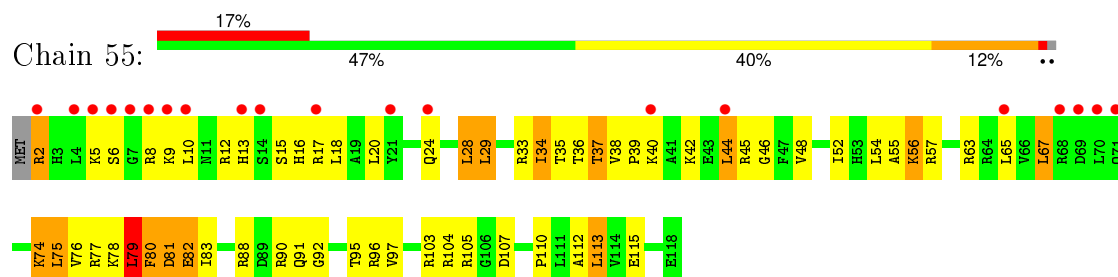
- Molecule 37: 50S ribosomal protein L16



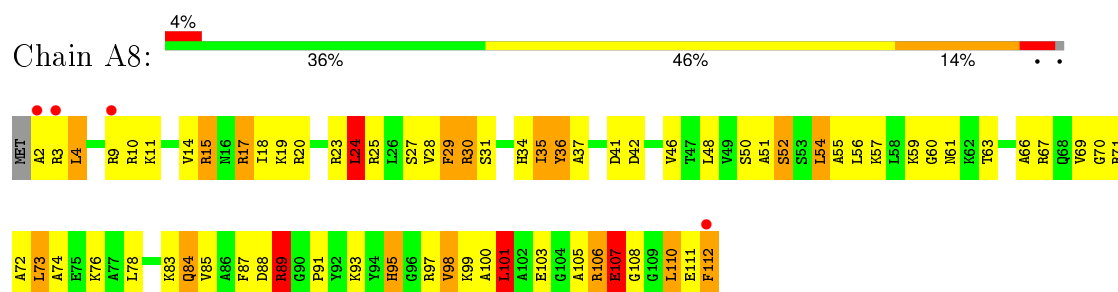
- Molecule 38: 50S ribosomal protein L17



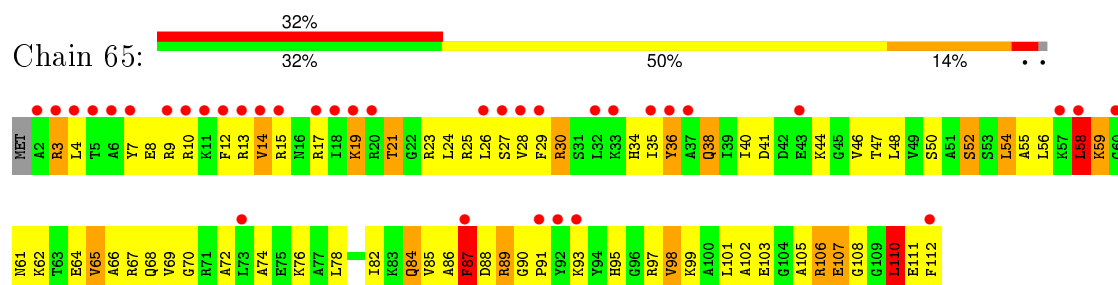
- Molecule 38: 50S ribosomal protein L17



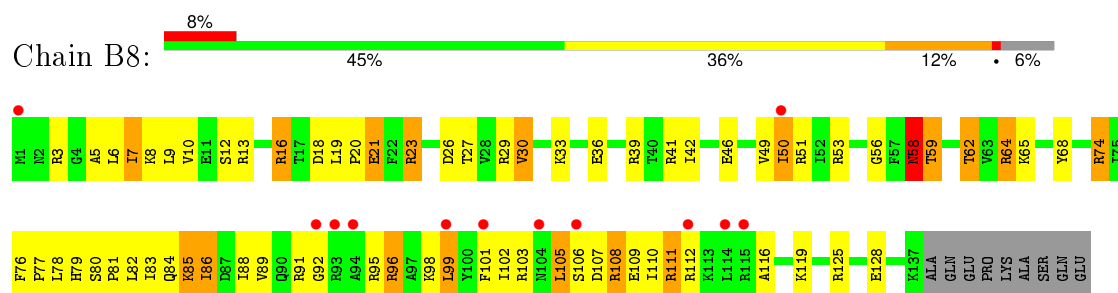
- Molecule 39: 50S ribosomal protein L18



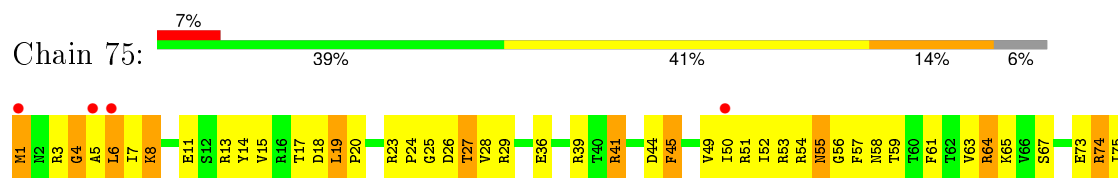
- Molecule 39: 50S ribosomal protein L18

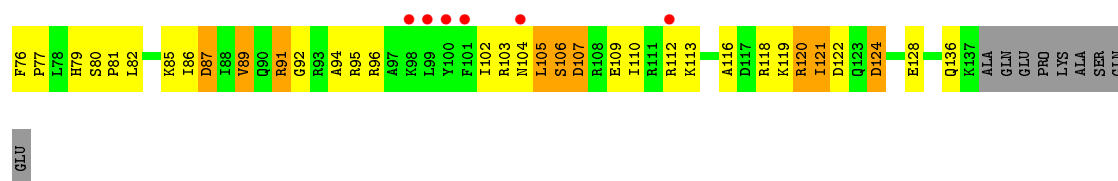


- Molecule 40: 50S ribosomal protein L19

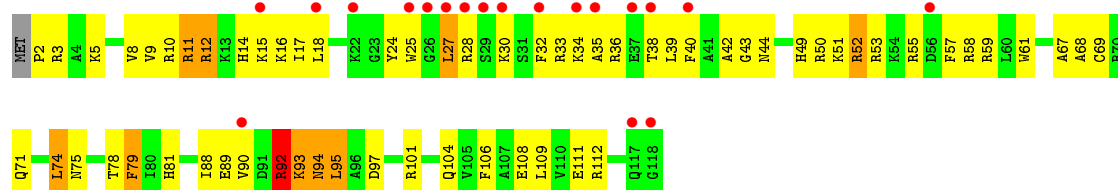


- Molecule 40: 50S ribosomal protein L19

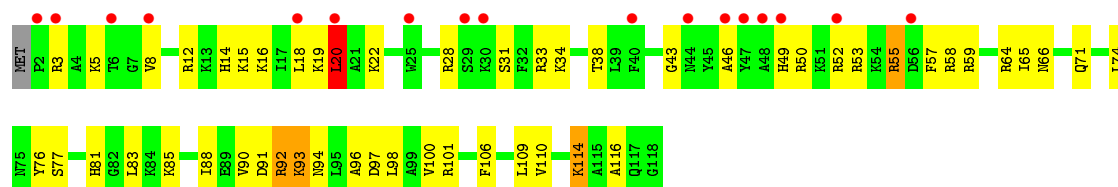




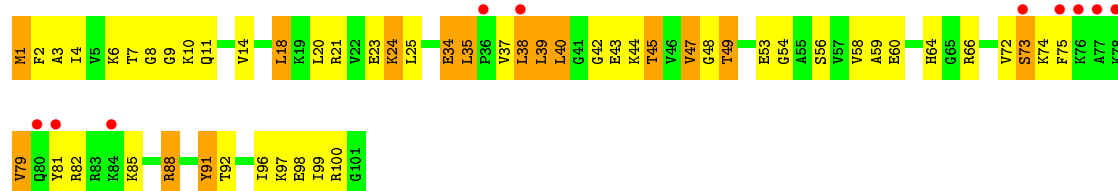
- Molecule 41: 50S ribosomal protein L20



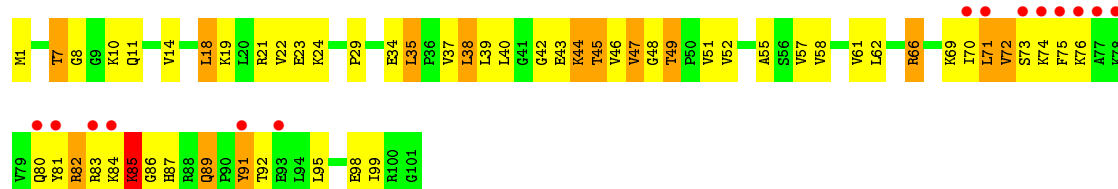
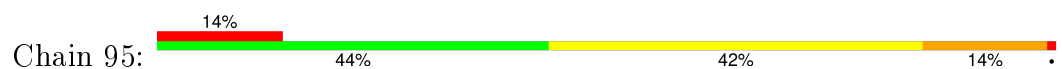
- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

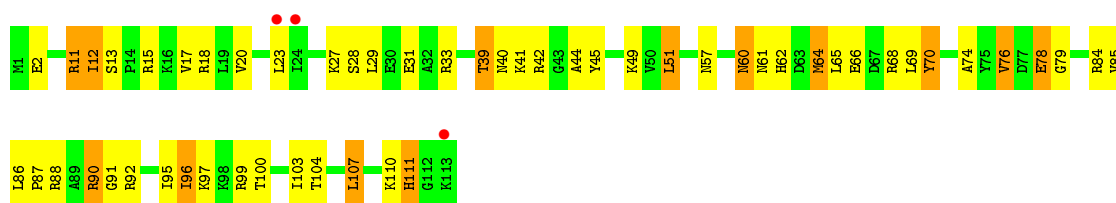


- Molecule 42: 50S ribosomal protein L21

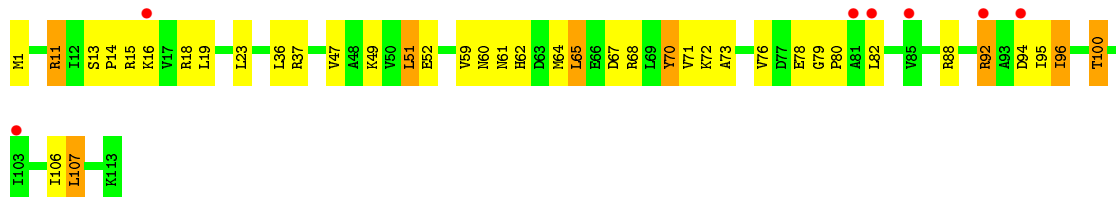


- Molecule 43: 50S ribosomal protein L22

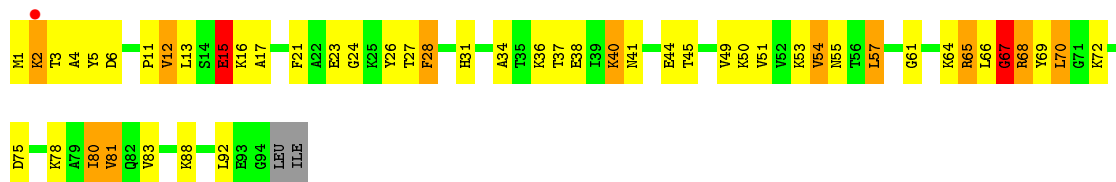




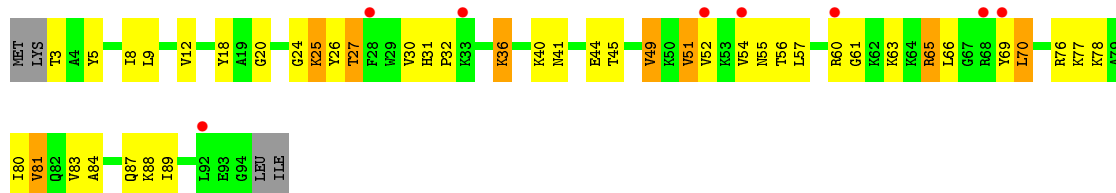
• Molecule 43: 50S ribosomal protein L22



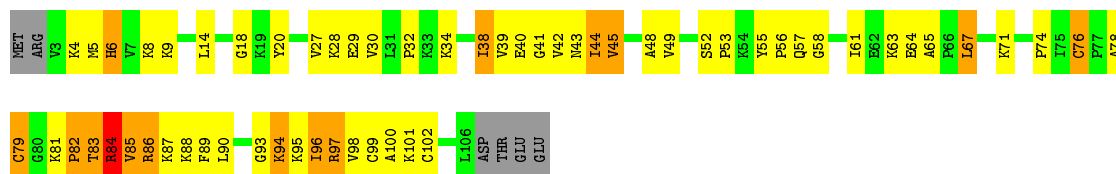
• Molecule 44: 50S ribosomal protein L23



• Molecule 44: 50S ribosomal protein L23

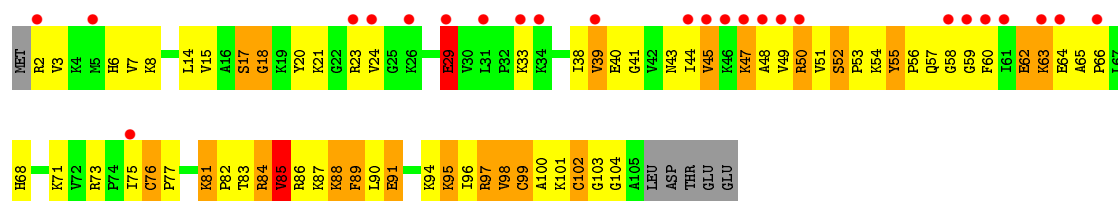


• Molecule 45: 50S ribosomal protein L24



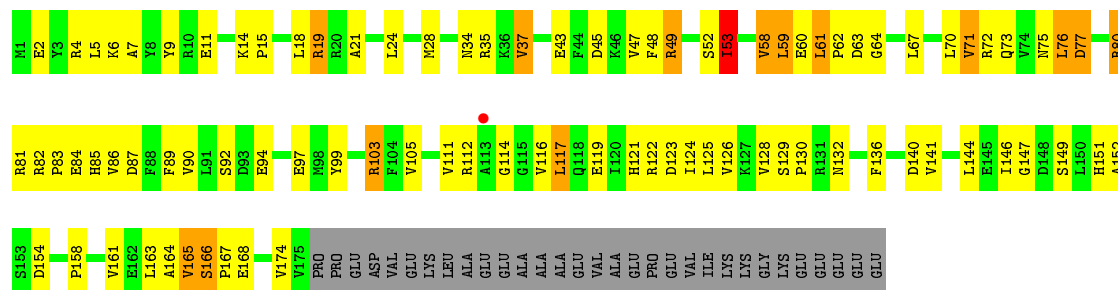
• Molecule 45: 50S ribosomal protein L24





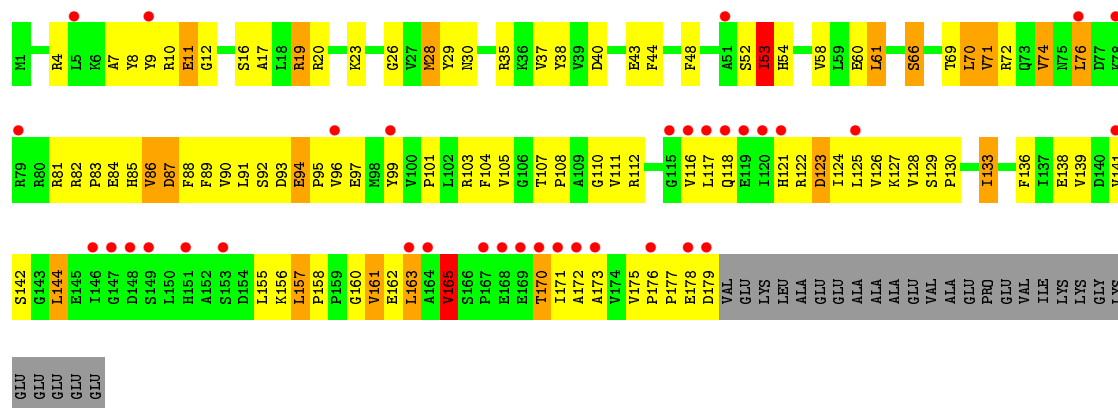
• Molecule 46: 50S ribosomal protein L25

Chain H8: 41% 36% 7% 15%



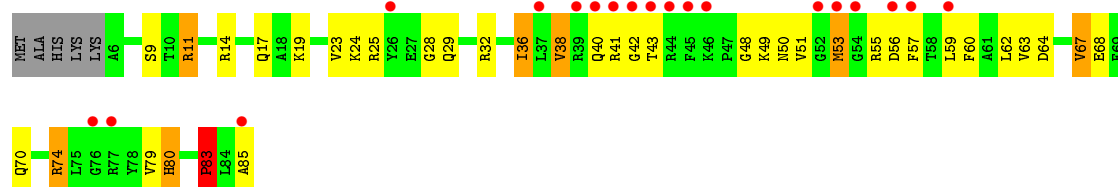
• Molecule 46: 50S ribosomal protein L25

Chain D5: 17% 38% 39% 9% 13%



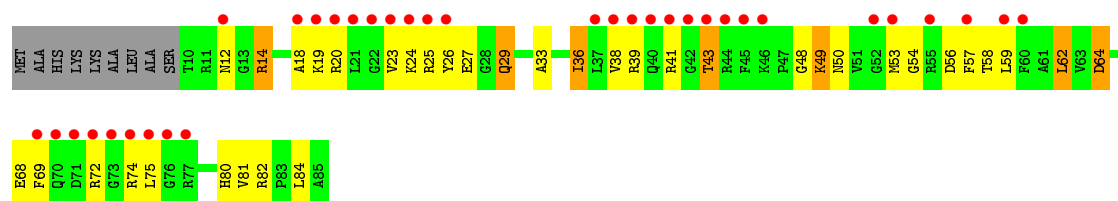
• Molecule 47: 50S ribosomal protein L27

Chain I8: 22% 49% 35% 8% 6%

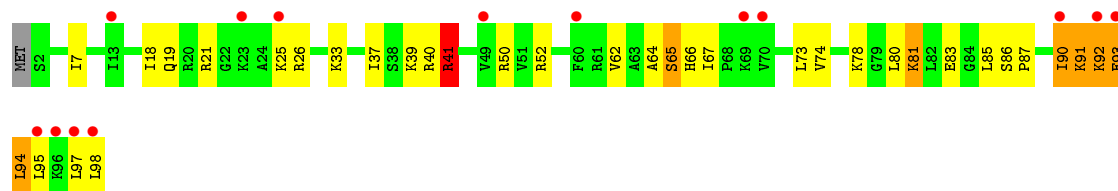


• Molecule 47: 50S ribosomal protein L27

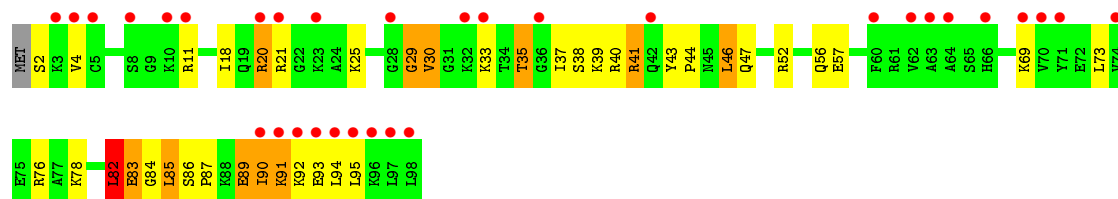
Chain E5: 41% 46% 35% 8% 11%



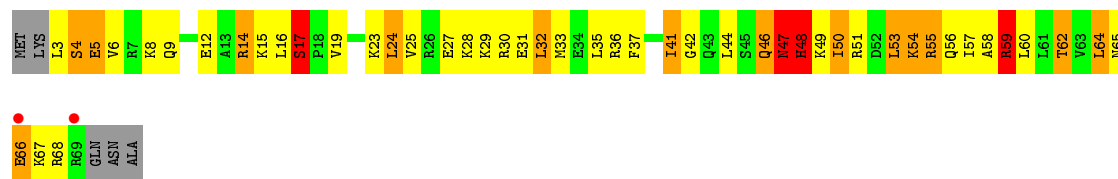
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28



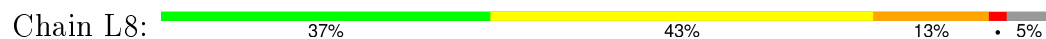
- Molecule 49: 50S ribosomal protein L29



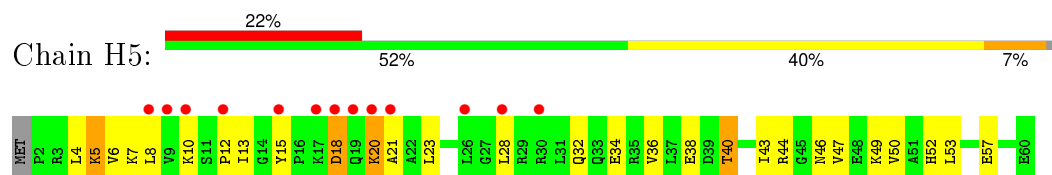
- Molecule 49: 50S ribosomal protein L29



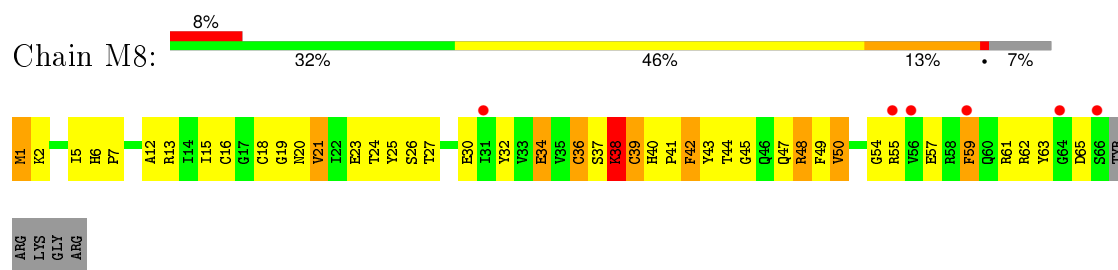
- Molecule 50: 50S ribosomal protein L30



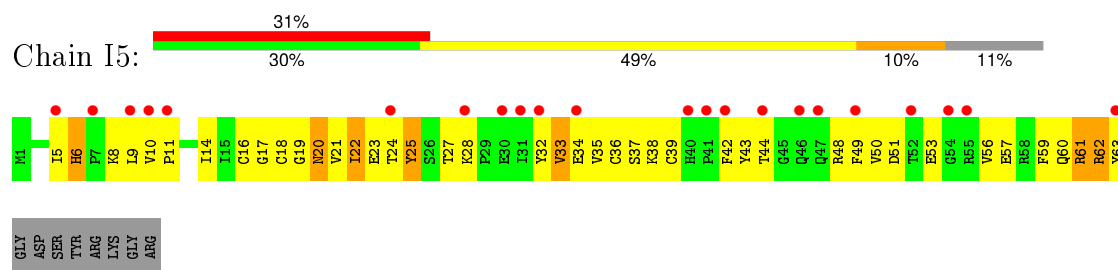
- Molecule 50: 50S ribosomal protein L30



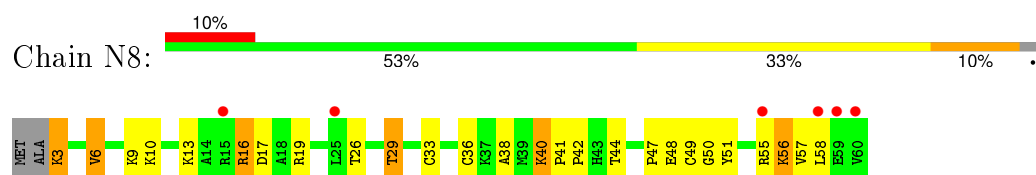
- Molecule 51: 50S ribosomal protein L31



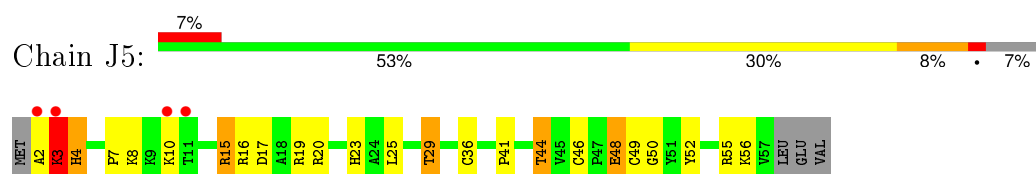
- Molecule 51: 50S ribosomal protein L31



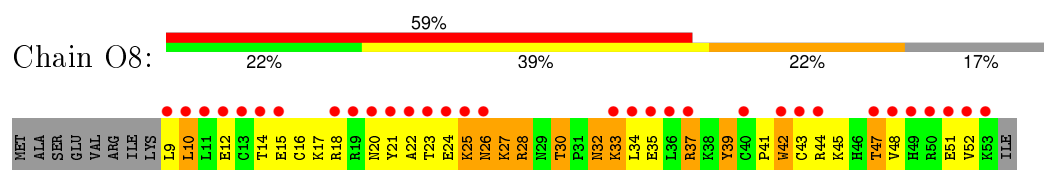
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32

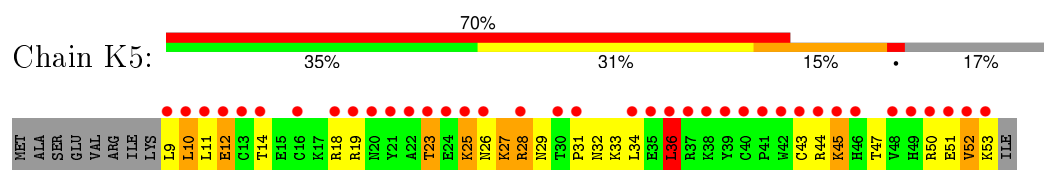


- Molecule 53: 50S ribosomal protein L33

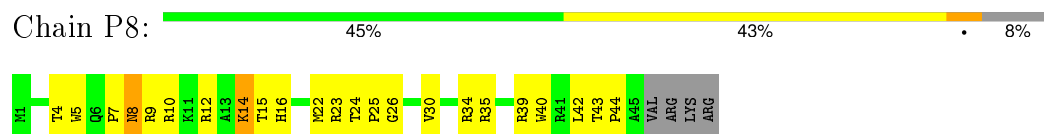


- Molecule 53: 50S ribosomal protein L33

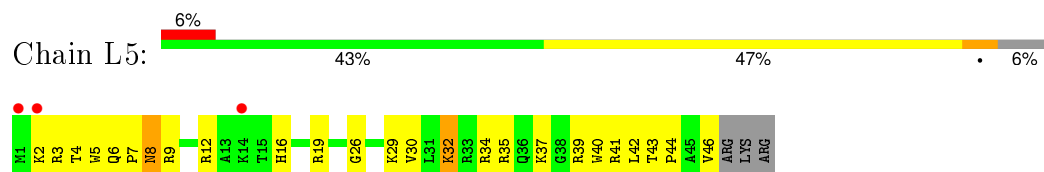




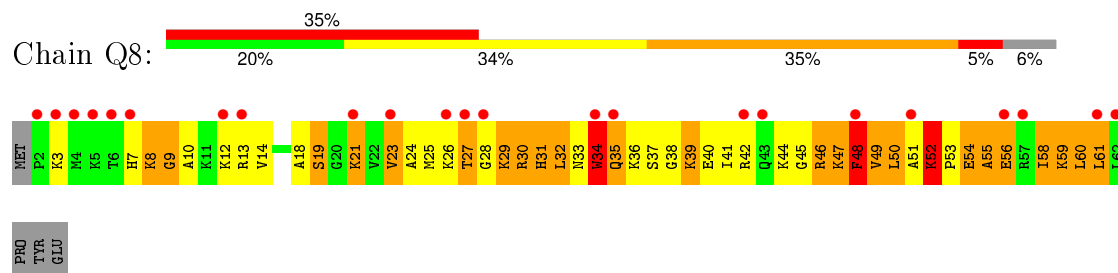
- Molecule 54: 50S ribosomal protein L34



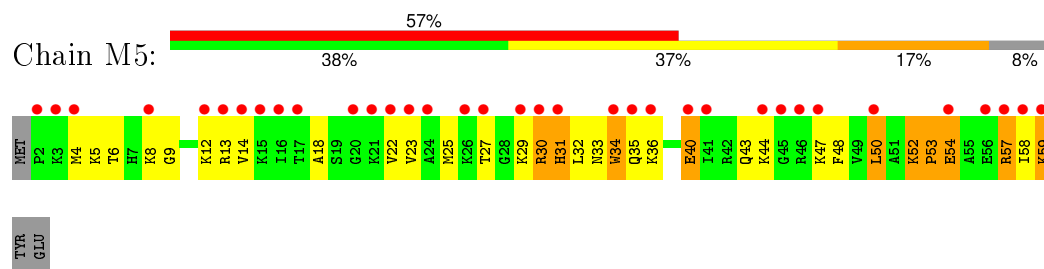
- Molecule 54: 50S ribosomal protein L34



- 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>	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.199 , (Not available) 0.201 , 0.238	Depositor DCC
$R_{free}$ test set	1998 reflections (0.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 89.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1097157 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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%)	15	48
2	1E	235/256 (92%)	199 (85%)	30 (13%)	6 (3%)	7	29
3	22	204/239 (85%)	178 (87%)	26 (13%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	14 (7%)	3 (2%)	13	44
4	32	206/209 (99%)	179 (87%)	27 (13%)	0	100	100
4	3E	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	13	44
5	42	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	26	64
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	26	64
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%)	26	64
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%)	21	58
11	2I	114/129 (88%)	101 (89%)	12 (10%)	1 (1%)	21	58
12	3A	123/132 (93%)	101 (82%)	18 (15%)	4 (3%)	5	24
12	3I	123/132 (93%)	104 (85%)	19 (15%)	0	100	100
13	4A	115/126 (91%)	95 (83%)	19 (16%)	1 (1%)	21	58
13	4I	116/126 (92%)	95 (82%)	20 (17%)	1 (1%)	21	58
14	5A	56/61 (92%)	47 (84%)	8 (14%)	1 (2%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	5	23
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%)	14	46
18	9I	70/88 (80%)	62 (89%)	6 (9%)	2 (3%)	6	27
19	AA	76/93 (82%)	60 (79%)	14 (18%)	2 (3%)	7	29
19	AI	79/93 (85%)	68 (86%)	8 (10%)	3 (4%)	4	21
20	BA	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	19	56
20	BI	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	19	56
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%)	8	34
28	19	271/276 (98%)	252 (93%)	16 (6%)	3 (1%)	17	53
29	21	203/206 (98%)	166 (82%)	29 (14%)	8 (4%)	4	20
29	29	203/206 (98%)	160 (79%)	32 (16%)	11 (5%)	2	13
30	31	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	34	70
30	39	206/210 (98%)	174 (84%)	28 (14%)	4 (2%)	10	38
31	41	179/182 (98%)	155 (87%)	20 (11%)	4 (2%)	8	34
31	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	17	53
32	51	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	6	27
32	59	167/180 (93%)	136 (81%)	28 (17%)	3 (2%)	11	39
33	61	144/148 (97%)	118 (82%)	21 (15%)	5 (4%)	4	23
33	69	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	9	35
34	15	136/140 (97%)	122 (90%)	14 (10%)	0	100	100
34	58	136/140 (97%)	114 (84%)	19 (14%)	3 (2%)	8	34
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%)	9	36
36	78	148/150 (99%)	115 (78%)	25 (17%)	8 (5%)	2	13
37	45	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	6	27
37	88	134/141 (95%)	112 (84%)	18 (13%)	4 (3%)	5	26
38	55	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	21	58
39	65	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	6	28
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	58
40	75	135/146 (92%)	113 (84%)	21 (16%)	1 (1%)	26	64
40	B8	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
41	85	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	21	58
41	C8	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	21	58
42	95	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	5	26
42	D8	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	19	56
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%)	17	53
44	F8	92/96 (96%)	83 (90%)	6 (6%)	3 (3%)	5	24
45	C5	102/110 (93%)	73 (72%)	24 (24%)	5 (5%)	3	15
45	G8	102/110 (93%)	84 (82%)	14 (14%)	4 (4%)	4	20
46	D5	177/206 (86%)	136 (77%)	31 (18%)	10 (6%)	2	12
46	H8	173/206 (84%)	142 (82%)	27 (16%)	4 (2%)	8	32
47	E5	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	15	48
48	F5	95/98 (97%)	83 (87%)	11 (12%)	1 (1%)	17	53
48	J8	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
49	G5	64/72 (89%)	57 (89%)	5 (8%)	2 (3%)	5	25
49	K8	65/72 (90%)	56 (86%)	7 (11%)	2 (3%)	5	25
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	49 (89%)	5 (9%)	1 (2%)	11	39
51	I5	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	M8	64/71 (90%)	45 (70%)	16 (25%)	3 (5%)	3	16
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%)	11	41
55	Q8	59/65 (91%)	39 (66%)	16 (27%)	4 (7%)	1	8
All	All	11325/12054 (94%)	9841 (87%)	1312 (12%)	172 (2%)	13	44

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%)	2	8
2	1E	205/220 (93%)	167 (82%)	38 (18%)	2	8
3	22	160/188 (85%)	132 (82%)	28 (18%)	2	9
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2	9
4	32	180/181 (99%)	148 (82%)	32 (18%)	2	9
4	3E	180/181 (99%)	147 (82%)	33 (18%)	2	8
5	42	116/123 (94%)	93 (80%)	23 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4E	116/123 (94%)	87 (75%)	29 (25%)	1	2
6	52	90/90 (100%)	76 (84%)	14 (16%)	3	13
6	5E	90/90 (100%)	78 (87%)	12 (13%)	5	19
7	62	126/127 (99%)	105 (83%)	21 (17%)	3	10
7	6E	126/127 (99%)	103 (82%)	23 (18%)	2	8
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	10
8	7E	119/119 (100%)	97 (82%)	22 (18%)	2	8
9	82	98/99 (99%)	81 (83%)	17 (17%)	2	10
9	8E	98/99 (99%)	76 (78%)	22 (22%)	1	4
10	1A	89/92 (97%)	81 (91%)	8 (9%)	12	39
10	1I	89/92 (97%)	78 (88%)	11 (12%)	6	22
11	2A	88/99 (89%)	76 (86%)	12 (14%)	5	18
11	2I	88/99 (89%)	75 (85%)	13 (15%)	4	15
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	4
12	3I	104/109 (95%)	88 (85%)	16 (15%)	3	13
13	4A	94/101 (93%)	79 (84%)	15 (16%)	3	12
13	4I	94/101 (93%)	75 (80%)	19 (20%)	1	6
14	5A	48/50 (96%)	41 (85%)	7 (15%)	4	15
14	5I	49/50 (98%)	37 (76%)	12 (24%)	1	2
15	6A	79/80 (99%)	70 (89%)	9 (11%)	7	26
15	6I	79/80 (99%)	71 (90%)	8 (10%)	9	32
16	7A	72/74 (97%)	58 (81%)	14 (19%)	2	7
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	4
17	8A	95/97 (98%)	83 (87%)	12 (13%)	5	21
17	8I	95/97 (98%)	81 (85%)	14 (15%)	4	15
18	9A	63/77 (82%)	49 (78%)	14 (22%)	1	4
18	9I	63/77 (82%)	53 (84%)	10 (16%)	3	12
19	AA	67/80 (84%)	52 (78%)	15 (22%)	1	4
19	AI	70/80 (88%)	49 (70%)	21 (30%)	0	1
20	BA	76/82 (93%)	61 (80%)	15 (20%)	1	7
20	BI	76/82 (93%)	62 (82%)	14 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1B	20/22 (91%)	18 (90%)	2 (10%)	9	32
21	1F	20/22 (91%)	19 (95%)	1 (5%)	30	66
28	11	214/218 (98%)	171 (80%)	43 (20%)	1	6
28	19	214/218 (98%)	180 (84%)	34 (16%)	3	12
29	21	165/166 (99%)	122 (74%)	43 (26%)	0	1
29	29	165/166 (99%)	134 (81%)	31 (19%)	2	7
30	31	161/166 (97%)	130 (81%)	31 (19%)	2	7
30	39	165/166 (99%)	132 (80%)	33 (20%)	1	6
31	41	155/156 (99%)	128 (83%)	27 (17%)	2	10
31	49	155/156 (99%)	132 (85%)	23 (15%)	4	15
32	51	145/148 (98%)	114 (79%)	31 (21%)	1	5
32	59	141/148 (95%)	112 (79%)	29 (21%)	1	6
33	61	122/124 (98%)	88 (72%)	34 (28%)	0	1
33	69	122/124 (98%)	93 (76%)	29 (24%)	1	3
34	15	117/119 (98%)	95 (81%)	22 (19%)	2	7
34	58	117/119 (98%)	94 (80%)	23 (20%)	1	7
35	25	100/100 (100%)	77 (77%)	23 (23%)	1	4
35	68	100/100 (100%)	84 (84%)	16 (16%)	3	12
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%)	1	2
37	88	104/111 (94%)	81 (78%)	23 (22%)	1	4
38	55	100/101 (99%)	78 (78%)	22 (22%)	1	4
38	98	101/101 (100%)	81 (80%)	20 (20%)	1	6
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	3
40	B8	120/127 (94%)	89 (74%)	31 (26%)	0	2
41	85	93/94 (99%)	80 (86%)	13 (14%)	4	17
41	C8	93/94 (99%)	76 (82%)	17 (18%)	2	8
42	95	82/82 (100%)	57 (70%)	25 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	D8	82/82 (100%)	61 (74%)	21 (26%)	0	2
43	A5	92/92 (100%)	78 (85%)	14 (15%)	3	14
43	E8	92/92 (100%)	72 (78%)	20 (22%)	1	5
44	B5	74/78 (95%)	57 (77%)	17 (23%)	1	4
44	F8	76/78 (97%)	59 (78%)	17 (22%)	1	4
45	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
45	G8	85/91 (93%)	67 (79%)	18 (21%)	1	5
46	D5	158/179 (88%)	131 (83%)	27 (17%)	2	10
46	H8	154/179 (86%)	123 (80%)	31 (20%)	1	6
47	E5	61/67 (91%)	52 (85%)	9 (15%)	4	15
47	I8	61/67 (91%)	52 (85%)	9 (15%)	4	15
48	F5	82/83 (99%)	67 (82%)	15 (18%)	2	8
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	6
49	G5	62/67 (92%)	53 (86%)	9 (14%)	4	16
49	K8	62/67 (92%)	41 (66%)	21 (34%)	0	0
50	H5	51/52 (98%)	42 (82%)	9 (18%)	2	9
50	L8	49/52 (94%)	40 (82%)	9 (18%)	2	8
51	I5	57/63 (90%)	47 (82%)	10 (18%)	2	9
51	M8	59/63 (94%)	44 (75%)	15 (25%)	1	2
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	4
52	N8	51/52 (98%)	38 (74%)	13 (26%)	1	2
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	9
54	P8	38/42 (90%)	32 (84%)	6 (16%)	3	12
55	M5	49/55 (89%)	37 (76%)	12 (24%)	1	2
55	Q8	50/55 (91%)	32 (64%)	18 (36%)	0	0
All	All	9556/9998 (96%)	7642 (80%)	1914 (20%)	1	6

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	32	22	15,21,22	1.01	1 (6%)	16,30,33	2.05	2 (12%)
22	MIA	1K	37	22	22,31,32	0.89	1 (4%)	26,44,47	1.73	6 (23%)
22	PSU	1K	39	22	15,21,22	0.98	1 (6%)	16,30,33	2.02	4 (25%)
22	7MG	1K	46	22	20,26,27	3.26	6 (30%)	23,39,42	2.23	5 (21%)
22	5MU	1K	54	22	13,22,23	1.70	2 (15%)	16,32,35	1.54	1 (6%)
22	PSU	1K	55	22	15,21,22	1.19	1 (6%)	16,30,33	2.30	3 (18%)
22	4SU	1K	8	22	12,21,22	3.26	2 (16%)	15,30,33	1.07	1 (6%)
23	OMC	2K	33	23	15,22,23	2.16	4 (26%)	20,31,34	1.58	2 (10%)
23	7MG	2K	47	23	20,26,27	3.30	6 (30%)	23,39,42	2.28	9 (39%)
23	5MU	2K	55	23	13,22,23	1.62	2 (15%)	16,32,35	1.29	1 (6%)
23	PSU	2K	56	23	15,21,22	0.98	1 (6%)	16,30,33	1.76	4 (25%)
23	4SU	2K	8	23	12,21,22	3.11	2 (16%)	15,30,33	1.02	1 (6%)
23	OMC	2L	33	23	15,22,23	2.23	4 (26%)	20,31,34	2.16	4 (20%)
23	7MG	2L	47	23	20,26,27	3.34	5 (25%)	23,39,42	2.12	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	5MU	2L	55	23	13,22,23	1.68	2 (15%)	16,32,35	1.18	1 (6%)
23	PSU	2L	56	23	15,21,22	1.11	1 (6%)	16,30,33	1.85	3 (18%)
23	4SU	2L	8	23	12,21,22	3.32	2 (16%)	15,30,33	1.23	1 (6%)

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

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C5-C4	-5.99	1.23	1.39
23	2L	47	7MG	C5-C4	-5.75	1.23	1.39
22	1K	46	7MG	C5-C4	-5.32	1.25	1.39
23	2K	55	5MU	C4-N3	-3.15	1.27	1.33
23	2L	55	5MU	C4-N3	-3.15	1.27	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	47	7MG	C5-C4-N3	-6.34	120.29	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	46	7MG	C5-C4-N3	-6.25	120.38	126.74
22	1K	37	MIA	C5-C6-N1	-4.81	115.70	120.58
23	2L	8	4SU	C5-C4-N3	-4.25	119.05	123.56
23	2K	47	7MG	C5-C4-N3	-3.90	122.77	126.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
1	13	1498/1522 (98%)	0.21	44 (2%) 55 29	73, 122, 204, 309	0
1	1G	1497/1522 (98%)	0.24	72 (4%) 34 15	92, 145, 218, 318	0
2	12	237/256 (92%)	0.20	17 (7%) 18 6	168, 199, 220, 228	0
2	1E	237/256 (92%)	0.12	8 (3%) 49 23	132, 167, 193, 205	0
3	22	206/239 (86%)	0.04	7 (3%) 49 23	161, 182, 205, 218	0
3	2E	205/239 (85%)	-0.02	1 (0%) 91 81	103, 128, 161, 170	0
4	32	208/209 (99%)	0.59	18 (8%) 13 4	122, 144, 165, 174	0
4	3E	208/209 (99%)	0.78	31 (14%) 3 1	102, 129, 151, 165	0
5	42	151/162 (93%)	0.52	18 (11%) 6 2	136, 154, 171, 203	0
5	4E	151/162 (93%)	0.57	19 (12%) 5 2	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%) 2 1	136, 154, 182, 207	0
7	6E	155/156 (99%)	0.49	16 (10%) 9 3	124, 139, 168, 193	0
8	72	138/138 (100%)	1.27	41 (29%) 1 0	130, 158, 174, 179	0
8	7E	138/138 (100%)	0.89	26 (18%) 2 0	105, 129, 141, 149	0
9	82	127/128 (99%)	3.26	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%) 1 0	102, 155, 187, 192	0
11	2A	116/129 (89%)	0.51	11 (9%) 10 4	111, 137, 158, 182	0
11	2I	116/129 (89%)	0.27	8 (6%) 20 7	90, 127, 153, 180	0
12	3A	125/132 (94%)	1.25	35 (28%) 1 0	109, 134, 160, 185	0
12	3I	125/132 (94%)	0.45	11 (8%) 12 4	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%) 1 0	140, 184, 206, 216	0
13	4I	118/126 (93%)	0.25	7 (5%) 26 10	101, 139, 159, 170	0
14	5A	58/61 (95%)	4.96	46 (79%) 0 0	164, 179, 194, 201	0
14	5I	60/61 (98%)	1.88	23 (38%) 0 0	106, 118, 137, 147	0
15	6A	88/89 (98%)	0.81	12 (13%) 4 1	118, 139, 155, 159	0
15	6I	88/89 (98%)	1.01	21 (23%) 1 0	98, 125, 142, 154	0
16	7A	84/88 (95%)	1.03	19 (22%) 1 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%) 4 1	108, 127, 140, 145	0
18	9A	72/88 (81%)	0.05	2 (2%) 56 30	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%) 1 0	172, 203, 216, 222	0
19	AI	81/93 (87%)	0.47	4 (4%) 33 14	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%)	6.09	23 (92%) 0 0	147, 163, 179, 196	0
21	1F	25/27 (92%)	4.76	22 (88%) 0 0	114, 126, 139, 164	0
22	1K	69/76 (90%)	0.13	5 (7%) 18 6	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%)	-0.41	1 (1%) 78 57	96, 136, 166, 170	0
24	1L	76/76 (100%)	0.82	13 (17%) 2 1	147, 264, 289, 295	0
24	3K	76/76 (100%)	-0.06	2 (2%) 59 33	92, 255, 286, 289	0
24	3L	76/76 (100%)	0.50	9 (11%) 6 2	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%)	0.60	0 100 100	121, 154, 165, 175	0
26	14	2909/2917 (99%)	0.21	70 (2%) 62 37	67, 105, 270, 378	0
26	1H	2912/2917 (99%)	0.28	12 (0%) 93 84	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%)	-0.14	1 (0%) 87 72	107, 152, 174, 226	0
28	11	272/276 (98%)	0.50	8 (2%) 55 29	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%)	0.91	41 (15%) 3 1	67, 94, 110, 125	0
29	21	205/206 (99%)	0.90	27 (13%) 4 1	66, 109, 151, 165	0
29	29	205/206 (99%)	1.29	67 (32%) 1 0	76, 113, 159, 183	0
30	31	202/210 (96%)	0.32	2 (0%) 84 66	60, 94, 130, 150	0
30	39	208/210 (99%)	0.43	14 (6%) 21 7	76, 123, 179, 199	0
31	41	181/182 (99%)	0.30	9 (4%) 32 13	100, 121, 159, 172	0
31	49	181/182 (99%)	1.07	41 (22%) 1 0	148, 169, 198, 209	0
32	51	174/180 (96%)	0.12	5 (2%) 55 29	99, 122, 139, 150	0
32	59	169/180 (93%)	1.63	62 (36%) 0 0	169, 218, 243, 258	0
33	61	146/148 (98%)	-0.02	4 (2%) 58 32	98, 155, 170, 175	0
33	69	146/148 (98%)	0.71	22 (15%) 3 1	102, 146, 170, 175	0
34	15	138/140 (98%)	1.27	35 (25%) 1 0	98, 129, 161, 185	0
34	58	138/140 (98%)	0.79	15 (10%) 7 2	81, 109, 148, 163	0
35	25	122/122 (100%)	0.51	9 (7%) 17 6	85, 107, 125, 135	0
35	68	122/122 (100%)	0.41	3 (2%) 61 35	75, 92, 111, 124	0
36	35	150/150 (100%)	1.13	40 (26%) 1 0	77, 128, 162, 198	0
36	78	150/150 (100%)	0.56	11 (7%) 18 6	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	7 (5%) 32 13	70, 95, 115, 147	0
38	55	117/118 (99%)	0.97	20 (17%) 2 1	77, 97, 113, 133	0
38	98	118/118 (100%)	0.82	13 (11%) 7 2	79, 102, 125, 139	0
39	65	111/112 (99%)	1.38	36 (32%) 1 0	118, 145, 162, 172	0
39	A8	111/112 (99%)	0.35	4 (3%) 46 21	92, 107, 130, 144	0
40	75	137/146 (93%)	0.31	10 (7%) 18 6	96, 115, 173, 208	0
40	B8	137/146 (93%)	0.49	12 (8%) 12 4	86, 111, 170, 202	0
41	85	117/118 (99%)	0.79	17 (14%) 3 1	86, 115, 155, 180	0
41	C8	117/118 (99%)	0.87	19 (16%) 3 1	71, 98, 136, 147	0
42	95	101/101 (100%)	0.51	14 (13%) 4 1	86, 143, 161, 177	0
42	D8	101/101 (100%)	0.31	10 (9%) 9 3	73, 123, 149, 162	0
43	A5	113/113 (100%)	0.42	7 (6%) 24 9	77, 94, 124, 183	0
43	E8	113/113 (100%)	0.38	3 (2%) 58 32	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%) 13 4	85, 102, 129, 133	0
44	F8	94/96 (97%)	0.29	1 (1%) 82 63	69, 88, 113, 128	0
45	C5	104/110 (94%)	1.29	25 (24%) 1 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%) 90 78	97, 139, 228, 236	0
47	E5	76/85 (89%)	1.89	35 (46%) 0 0	85, 111, 130, 169	0
47	I8	80/85 (94%)	1.09	19 (23%) 1 0	71, 90, 122, 131	0
48	F5	97/98 (98%)	1.74	32 (32%) 0 0	79, 102, 146, 163	0
48	J8	97/98 (98%)	1.14	14 (14%) 3 1	69, 91, 145, 176	0
49	G5	66/72 (91%)	0.19	2 (3%) 54 27	101, 121, 141, 167	0
49	K8	67/72 (93%)	0.39	2 (2%) 54 27	76, 96, 119, 154	0
50	H5	59/60 (98%)	1.04	13 (22%) 1 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%)	0.44	6 (9%) 11 4	128, 174, 203, 214	0
52	J5	56/60 (93%)	0.38	4 (7%) 19 6	77, 103, 150, 162	0
52	N8	58/60 (96%)	0.93	6 (10%) 9 3	68, 115, 186, 191	0
53	K5	45/54 (83%)	7.08	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%) 22 8	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%)	2.19	37 (61%) 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	2138 (10%) 9 3	56, 122, 214, 378	0

The worst 5 of 2138 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	16.9
7	62	82	GLY	16.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	PSU	1K	39	20/21	0.94	0.17	-	96,108,116,119	0
23	4SU	2K	8	20/21	0.94	0.21	-	100,108,123,123	0
22	PSU	1K	32	20/21	0.89	0.32	-	113,119,123,123	0
23	OMC	2L	33	21/22	0.96	0.20	-	124,127,132,137	0
22	PSU	1K	55	20/21	0.78	0.11	-	153,172,191,191	0
23	OMC	2K	33	21/22	0.98	0.32	-	88,94,101,106	0
23	4SU	2L	8	20/21	0.88	0.14	-	128,140,143,147	0
23	PSU	2K	56	20/21	0.96	0.14	-	109,113,120,127	0
22	4SU	1K	8	20/21	0.80	0.14	-	184,192,200,205	0
23	5MU	2L	55	21/22	0.95	0.11	-	138,142,147,151	0
22	7MG	1K	46	24/25	0.87	0.12	-	175,197,203,209	0
23	7MG	2K	47	24/25	0.95	0.17	-	110,120,128,137	0
23	PSU	2L	56	20/21	0.90	0.09	-	128,135,142,148	0
23	5MU	2K	55	21/22	0.97	0.15	-	99,116,125,136	0
22	5MU	1K	54	21/22	0.93	0.10	-	142,157,168,172	0
23	7MG	2L	47	24/25	0.95	0.12	-	140,151,156,161	0
22	MIA	1K	37	29/30	0.94	0.30	-	89,100,118,123	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	13	1641	1/1	0.76	0.35	34.96	88,88,88,88	0
56	MG	1H	3173	1/1	0.95	0.36	28.63	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3277	1/1	0.90	0.47	18.53	109,109,109,109	0
56	MG	13	1621	1/1	0.87	0.39	16.07	115,115,115,115	0
56	MG	1H	3025	1/1	0.95	0.48	15.77	78,78,78,78	0
56	MG	14	3217	1/1	0.90	0.80	15.55	82,82,82,82	0
56	MG	2K	105	1/1	0.80	0.38	14.78	107,107,107,107	0
56	MG	1H	3084	1/1	0.98	0.31	14.73	61,61,61,61	0
56	MG	1H	3037	1/1	0.97	0.37	14.32	76,76,76,76	0
56	MG	1H	3245	1/1	0.89	0.38	13.50	96,96,96,96	0
56	MG	1H	3069	1/1	0.96	0.37	11.34	89,89,89,89	0
56	MG	1H	3298	1/1	0.85	0.33	11.24	92,92,92,92	0
56	MG	1H	3304	1/1	0.90	0.39	11.21	114,114,114,114	0
56	MG	1H	3011	1/1	0.95	0.51	10.37	91,91,91,91	0
56	MG	16	206	1/1	0.86	0.25	9.60	102,102,102,102	0
56	MG	14	3274	1/1	0.72	0.25	9.53	122,122,122,122	0
56	MG	13	1686	1/1	0.92	0.29	8.88	134,134,134,134	0
56	MG	14	3169	1/1	0.82	0.29	8.48	93,93,93,93	0
56	MG	1H	3255	1/1	0.63	0.45	8.39	117,117,117,117	0
56	MG	1H	3056	1/1	0.92	0.30	8.23	72,72,72,72	0
56	MG	1H	3234	1/1	0.98	0.29	8.18	91,91,91,91	0
56	MG	13	1689	1/1	0.74	0.25	8.16	98,98,98,98	0
56	MG	14	3170	1/1	0.75	0.60	8.02	77,77,77,77	0
56	MG	1H	3013	1/1	0.80	0.41	8.01	104,104,104,104	0
56	MG	1H	3222	1/1	0.87	0.30	7.88	79,79,79,79	0
56	MG	14	3199	1/1	0.96	0.35	7.78	126,126,126,126	0
56	MG	1H	3170	1/1	0.95	0.33	7.71	100,100,100,100	0
56	MG	16	207	1/1	0.90	0.37	7.65	84,84,84,84	0
56	MG	1G	1660	1/1	0.93	0.43	7.50	97,97,97,97	0
56	MG	14	3055	1/1	0.91	0.42	7.25	85,85,85,85	0
56	MG	14	3233	1/1	0.88	0.30	7.09	118,118,118,118	0
56	MG	1H	3160	1/1	0.93	0.31	7.06	84,84,84,84	0
56	MG	1G	1614	1/1	0.93	0.25	7.03	140,140,140,140	0
56	MG	1H	3258	1/1	0.85	0.31	6.54	93,93,93,93	0
56	MG	1H	3110	1/1	0.97	0.31	6.50	67,67,67,67	0
56	MG	1H	3186	1/1	0.70	0.35	6.20	93,93,93,93	0
56	MG	14	3216	1/1	0.95	0.43	5.98	111,111,111,111	0
56	MG	L8	101	1/1	0.79	0.43	5.82	85,85,85,85	0
56	MG	14	3306	1/1	0.90	0.30	5.76	93,93,93,93	0
56	MG	14	3091	1/1	0.93	0.29	5.74	87,87,87,87	0
56	MG	14	3272	1/1	0.71	0.32	5.72	95,95,95,95	0
56	MG	1H	3063	1/1	0.98	0.28	5.57	83,83,83,83	0
56	MG	14	3195	1/1	0.86	0.38	5.47	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3116	1/1	0.80	0.29	5.41	70,70,70,70	0
56	MG	14	3253	1/1	0.83	0.29	5.36	82,82,82,82	0
56	MG	14	3227	1/1	0.70	0.33	5.22	97,97,97,97	0
56	MG	14	3211	1/1	0.82	0.40	5.14	93,93,93,93	0
56	MG	1H	3235	1/1	0.95	0.25	4.93	75,75,75,75	0
56	MG	14	3202	1/1	0.84	0.26	4.91	100,100,100,100	0
56	MG	1H	3254	1/1	0.82	0.37	4.86	80,80,80,80	0
56	MG	39	303	1/1	0.66	0.67	4.80	87,87,87,87	0
56	MG	1H	3178	1/1	0.86	0.27	4.68	76,76,76,76	0
56	MG	14	3194	1/1	0.97	0.23	4.27	97,97,97,97	0
56	MG	1H	3219	1/1	0.83	0.39	4.23	65,65,65,65	0
56	MG	1H	3089	1/1	0.97	0.27	3.98	58,58,58,58	0
56	MG	1H	3004	1/1	0.99	0.30	3.86	68,68,68,68	0
56	MG	14	3205	1/1	0.97	0.45	3.80	72,72,72,72	0
56	MG	13	1664	1/1	0.65	0.28	3.68	103,103,103,103	0
56	MG	1H	3081	1/1	0.84	0.25	3.53	77,77,77,77	0
56	MG	1H	3332	1/1	0.63	0.42	3.50	90,90,90,90	0
56	MG	13	1706	1/1	0.88	0.91	3.50	103,103,103,103	0
56	MG	29	301	1/1	0.74	0.64	3.50	101,101,101,101	0
56	MG	14	3209	1/1	0.85	0.33	3.49	71,71,71,71	0
56	MG	13	1602	1/1	0.94	0.31	3.43	87,87,87,87	0
56	MG	1G	1659	1/1	0.81	0.30	3.35	102,102,102,102	0
56	MG	14	3382	1/1	0.97	0.29	3.28	86,86,86,86	0
56	MG	13	1652	1/1	0.88	0.23	3.20	98,98,98,98	0
56	MG	1G	1645	1/1	0.68	0.31	3.18	113,113,113,113	0
56	MG	1H	3052	1/1	0.95	0.30	3.15	80,80,80,80	0
56	MG	14	3308	1/1	0.85	0.21	3.09	106,106,106,106	0
56	MG	14	3264	1/1	0.76	0.30	2.72	89,89,89,89	0
56	MG	1J	207	1/1	0.87	0.27	2.71	147,147,147,147	0
56	MG	1H	3260	1/1	0.86	0.29	2.57	76,76,76,76	0
56	MG	14	3266	1/1	0.86	0.38	2.55	80,80,80,80	0
56	MG	1H	3139	1/1	0.96	0.40	2.49	79,79,79,79	0
56	MG	14	3007	1/1	0.95	0.23	2.47	94,94,94,94	0
56	MG	1H	3240	1/1	0.96	0.25	2.43	94,94,94,94	0
56	MG	13	1680	1/1	0.88	0.19	2.33	124,124,124,124	0
56	MG	14	3248	1/1	0.80	0.26	2.33	85,85,85,85	0
56	MG	1G	1664	1/1	0.67	0.27	2.30	116,116,116,116	0
56	MG	13	1666	1/1	0.71	0.32	2.29	105,105,105,105	0
56	MG	16	209	1/1	0.96	0.21	2.25	88,88,88,88	0
56	MG	14	3060	1/1	0.95	0.27	2.23	83,83,83,83	0
56	MG	14	3146	1/1	0.93	0.19	2.22	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1G	1627	1/1	0.97	0.23	2.20	116,116,116,116	0
57	ZN	32	302	1/1	0.99	0.39	2.09	131,131,131,131	0
56	MG	14	3254	1/1	0.81	0.17	2.09	87,87,87,87	0
56	MG	14	3165	1/1	0.96	0.33	1.96	70,70,70,70	0
56	MG	13	1712	1/1	0.97	0.20	1.94	99,99,99,99	0
56	MG	14	3073	1/1	0.96	0.26	1.93	74,74,74,74	0
56	MG	1H	3230	1/1	0.79	0.24	1.89	91,91,91,91	0
56	MG	13	1603	1/1	0.94	0.21	1.86	97,97,97,97	0
56	MG	1H	3205	1/1	0.99	0.23	1.64	64,64,64,64	0
56	MG	14	3049	1/1	0.95	0.25	1.59	87,87,87,87	0
56	MG	16	214	1/1	0.78	0.22	1.55	109,109,109,109	0
56	MG	13	1721	1/1	0.77	0.63	1.53	101,101,101,101	0
56	MG	14	3150	1/1	0.66	0.33	1.50	80,80,80,80	0
56	MG	13	1604	1/1	0.98	0.27	1.50	108,108,108,108	0
56	MG	1H	3064	1/1	0.96	0.27	1.45	76,76,76,76	0
56	MG	41	202	1/1	0.79	0.29	1.40	96,96,96,96	0
56	MG	1H	3088	1/1	0.97	0.33	1.24	52,52,52,52	0
56	MG	I8	101	1/1	0.81	0.27	1.24	84,84,84,84	0
56	MG	14	3220	1/1	0.96	0.32	1.19	94,94,94,94	0
56	MG	1H	3216	1/1	0.92	0.22	1.05	77,77,77,77	0
56	MG	14	3262	1/1	0.54	0.29	1.02	81,81,81,81	0
56	MG	1H	3288	1/1	0.84	0.28	0.99	87,87,87,87	0
56	MG	14	3267	1/1	0.83	0.16	0.93	110,110,110,110	0
56	MG	13	1648	1/1	0.96	0.26	0.92	76,76,76,76	0
56	MG	14	3119	1/1	0.98	0.32	0.89	66,66,66,66	0
56	MG	1H	3001	1/1	0.98	0.29	0.89	64,64,64,64	0
56	MG	14	3268	1/1	0.89	0.19	0.84	100,100,100,100	0
56	MG	14	3058	1/1	0.85	0.15	0.84	128,128,128,128	0
56	MG	1H	3172	1/1	0.97	0.26	0.83	98,98,98,98	0
57	ZN	G8	202	1/1	0.87	0.31	0.82	192,192,192,192	0
56	MG	16	205	1/1	0.53	0.20	0.80	91,91,91,91	0
56	MG	13	1601	1/1	0.98	0.27	0.79	74,74,74,74	0
57	ZN	3E	301	1/1	0.98	0.41	0.79	115,115,115,115	0
56	MG	1H	3273	1/1	0.68	0.25	0.76	84,84,84,84	0
56	MG	14	3260	1/1	0.63	0.17	0.75	119,119,119,119	0
56	MG	14	3110	1/1	0.98	0.23	0.71	61,61,61,61	0
56	MG	13	1612	1/1	0.96	0.27	0.66	89,89,89,89	0
56	MG	13	1618	1/1	0.90	0.26	0.66	86,86,86,86	0
56	MG	14	3411	1/1	0.84	0.30	0.65	104,104,104,104	0
56	MG	14	3053	1/1	0.92	0.17	0.62	98,98,98,98	0
56	MG	1H	3241	1/1	0.91	0.21	0.59	80,80,80,80	0
56	MG	14	3128	1/1	0.97	0.21	0.57	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3252	1/1	0.93	0.21	0.55	69,69,69,69	0
56	MG	1H	3077	1/1	0.90	0.25	0.53	67,67,67,67	0
56	MG	13	1625	1/1	0.95	0.30	0.52	77,77,77,77	0
56	MG	1H	3076	1/1	0.99	0.26	0.43	73,73,73,73	0
56	MG	14	3014	1/1	0.99	0.27	0.43	73,73,73,73	0
56	MG	14	3256	1/1	0.83	0.19	0.42	97,97,97,97	0
56	MG	14	3118	1/1	0.98	0.24	0.42	71,71,71,71	0
56	MG	14	3098	1/1	0.92	0.28	0.42	74,74,74,74	0
56	MG	14	3121	1/1	0.94	0.23	0.38	84,84,84,84	0
56	MG	13	1752	1/1	0.89	0.51	0.38	92,92,92,92	0
56	MG	14	3106	1/1	0.94	0.20	0.37	89,89,89,89	0
56	MG	1G	1623	1/1	0.83	0.24	0.35	122,122,122,122	0
56	MG	13	1607	1/1	0.89	0.19	0.34	78,78,78,78	0
56	MG	13	1682	1/1	0.83	0.28	0.31	116,116,116,116	0
56	MG	16	203	1/1	0.97	0.18	0.26	107,107,107,107	0
56	MG	1G	1655	1/1	0.91	0.21	0.25	111,111,111,111	0
56	MG	1H	3244	1/1	0.96	0.20	0.23	90,90,90,90	0
56	MG	14	3278	1/1	0.86	0.26	0.21	85,85,85,85	0
56	MG	14	3154	1/1	0.91	0.23	0.19	86,86,86,86	0
56	MG	1H	3203	1/1	0.94	0.35	-0.07	73,73,73,73	0
56	MG	1H	3184	1/1	0.90	0.19	-0.09	107,107,107,107	0
56	MG	13	1667	1/1	0.92	0.30	-0.12	147,147,147,147	0
56	MG	14	3040	1/1	0.96	0.20	-0.12	79,79,79,79	0
56	MG	J8	101	1/1	0.94	0.26	-0.13	78,78,78,78	0
56	MG	1G	1607	1/1	0.93	0.28	-0.20	98,98,98,98	0
56	MG	14	3252	1/1	0.74	0.15	-0.20	105,105,105,105	0
56	MG	13	1620	1/1	0.94	0.28	-0.21	119,119,119,119	0
56	MG	85	201	1/1	0.95	0.28	-0.22	93,93,93,93	0
56	MG	14	3062	1/1	0.97	0.29	-0.23	85,85,85,85	0
56	MG	14	3052	1/1	0.94	0.21	-0.25	110,110,110,110	0
56	MG	14	3138	1/1	0.95	0.20	-0.28	73,73,73,73	0
56	MG	1H	3155	1/1	0.87	0.17	-0.29	78,78,78,78	0
56	MG	1H	3315	1/1	0.94	0.39	-0.32	105,105,105,105	0
56	MG	1H	3130	1/1	0.98	0.24	-0.33	78,78,78,78	0
56	MG	1G	1628	1/1	0.83	0.21	-0.34	118,118,118,118	0
56	MG	14	3219	1/1	0.95	0.20	-0.39	102,102,102,102	0
56	MG	14	3107	1/1	0.92	0.21	-0.42	80,80,80,80	0
56	MG	14	3103	1/1	0.78	0.38	-0.44	90,90,90,90	0
56	MG	14	3238	1/1	0.97	0.16	-0.46	110,110,110,110	0
56	MG	1H	3470	1/1	0.93	0.23	-0.47	99,99,99,99	0
56	MG	1G	1635	1/1	0.87	0.39	-0.48	118,118,118,118	0
56	MG	1H	3085	1/1	0.98	0.22	-0.49	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3008	1/1	0.98	0.25	-0.50	78,78,78,78	0
56	MG	13	1728	1/1	0.94	0.13	-0.51	131,131,131,131	0
56	MG	14	3244	1/1	0.97	0.23	-0.60	99,99,99,99	0
56	MG	13	1675	1/1	0.71	0.19	-0.65	121,121,121,121	0
56	MG	14	3215	1/1	0.99	0.15	-0.65	104,104,104,104	0
56	MG	1G	1644	1/1	0.59	0.19	-0.66	115,115,115,115	0
56	MG	1H	3324	1/1	0.95	0.15	-0.70	107,107,107,107	0
56	MG	13	1611	1/1	0.99	0.18	-0.71	95,95,95,95	0
56	MG	88	201	1/1	0.95	0.22	-0.72	95,95,95,95	0
56	MG	13	1743	1/1	0.77	0.18	-0.76	108,108,108,108	0
56	MG	13	1751	1/1	0.96	0.16	-0.77	94,94,94,94	0
56	MG	1J	204	1/1	0.82	0.12	-0.78	113,113,113,113	0
57	ZN	5I	101	1/1	0.97	0.20	-0.81	114,114,114,114	0
56	MG	14	3079	1/1	0.99	0.23	-0.82	84,84,84,84	0
56	MG	13	1608	1/1	0.97	0.20	-0.85	91,91,91,91	0
56	MG	14	3051	1/1	0.98	0.21	-0.85	100,100,100,100	0
56	MG	3I	201	1/1	0.95	0.19	-0.86	81,81,81,81	0
56	MG	14	3084	1/1	0.96	0.22	-0.86	78,78,78,78	0
56	MG	1H	3009	1/1	0.90	0.20	-0.87	69,69,69,69	0
56	MG	14	3171	1/1	0.95	0.19	-0.87	73,73,73,73	0
56	MG	11	301	1/1	0.92	0.31	-0.88	62,62,62,62	0
56	MG	14	3137	1/1	0.78	0.18	-0.88	80,80,80,80	0
56	MG	14	3009	1/1	0.96	0.24	-0.93	65,65,65,65	0
56	MG	14	3115	1/1	0.95	0.18	-0.95	100,100,100,100	0
56	MG	1G	1653	1/1	0.86	0.11	-0.96	106,106,106,106	0
56	MG	14	3425	1/1	0.94	0.28	-0.97	92,92,92,92	0
56	MG	2K	101	1/1	0.97	0.22	-0.99	76,76,76,76	0
56	MG	13	1671	1/1	0.94	0.24	-1.00	102,102,102,102	0
56	MG	14	3070	1/1	0.96	0.19	-1.01	66,66,66,66	0
56	MG	1H	3421	1/1	0.94	0.18	-1.06	62,62,62,62	0
56	MG	2L	101	1/1	0.97	0.18	-1.06	98,98,98,98	0
56	MG	1H	3053	1/1	0.94	0.17	-1.12	92,92,92,92	0
56	MG	1H	3101	1/1	0.92	0.21	-1.14	49,49,49,49	0
56	MG	1G	1667	1/1	0.67	0.24	-1.15	119,119,119,119	0
56	MG	39	301	1/1	0.93	0.19	-1.16	111,111,111,111	0
56	MG	14	3208	1/1	0.85	0.10	-1.16	84,84,84,84	0
56	MG	1H	3020	1/1	0.93	0.15	-1.17	90,90,90,90	0
56	MG	1H	3054	1/1	0.96	0.19	-1.17	71,71,71,71	0
56	MG	1G	1680	1/1	0.82	0.11	-1.20	140,140,140,140	0
56	MG	45	201	1/1	0.86	0.18	-1.22	113,113,113,113	0
56	MG	13	1668	1/1	0.80	0.19	-1.25	94,94,94,94	0
56	MG	14	3120	1/1	0.98	0.17	-1.25	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3456	1/1	0.94	0.18	-1.31	79,79,79,79	0
56	MG	1H	3166	1/1	0.93	0.17	-1.32	73,73,73,73	0
56	MG	14	3221	1/1	0.88	0.20	-1.34	87,87,87,87	0
57	ZN	5A	101	1/1	0.95	0.13	-1.36	172,172,172,172	0
56	MG	13	1655	1/1	0.96	0.14	-1.36	89,89,89,89	0
56	MG	13	1660	1/1	0.93	0.14	-1.39	94,94,94,94	0
56	MG	1H	3209	1/1	0.90	0.15	-1.41	82,82,82,82	0
56	MG	1H	3006	1/1	0.98	0.17	-1.42	91,91,91,91	0
56	MG	1G	1688	1/1	0.91	0.13	-1.44	117,117,117,117	0
56	MG	41	201	1/1	0.95	0.16	-1.44	89,89,89,89	0
56	MG	49	201	1/1	0.88	0.10	-1.44	143,143,143,143	0
56	MG	14	3041	1/1	0.94	0.16	-1.46	80,80,80,80	0
56	MG	14	3310	1/1	0.97	0.20	-1.47	96,96,96,96	0
56	MG	14	3076	1/1	0.90	0.11	-1.48	93,93,93,93	0
56	MG	1J	201	1/1	0.95	0.15	-1.48	123,123,123,123	0
56	MG	1H	3368	1/1	0.99	0.17	-1.50	79,79,79,79	0
56	MG	1G	1601	1/1	0.98	0.19	-1.57	109,109,109,109	0
56	MG	1H	3003	1/1	0.93	0.21	-1.58	75,75,75,75	0
56	MG	1H	3040	1/1	0.99	0.21	-1.61	78,78,78,78	0
56	MG	14	3246	1/1	0.92	0.21	-1.65	75,75,75,75	0
56	MG	1H	3067	1/1	0.94	0.16	-1.65	84,84,84,84	0
56	MG	14	3379	1/1	0.90	0.09	-1.66	77,77,77,77	0
56	MG	14	3198	1/1	0.97	0.11	-1.67	88,88,88,88	0
56	MG	14	3072	1/1	0.93	0.18	-1.67	90,90,90,90	0
56	MG	21	302	1/1	0.96	0.16	-1.67	82,82,82,82	0
56	MG	14	3016	1/1	0.99	0.24	-1.69	71,71,71,71	0
56	MG	14	3082	1/1	0.94	0.22	-1.70	71,71,71,71	0
56	MG	1H	3148	1/1	0.65	0.18	-1.76	79,79,79,79	0
56	MG	1H	3393	1/1	0.98	0.17	-1.76	60,60,60,60	0
56	MG	1H	3361	1/1	0.98	0.16	-1.80	56,56,56,56	0
56	MG	13	1723	1/1	0.98	0.14	-1.84	105,105,105,105	0
56	MG	14	3332	1/1	0.99	0.12	-1.85	72,72,72,72	0
56	MG	1H	3180	1/1	0.96	0.17	-1.89	84,84,84,84	0
56	MG	14	3095	1/1	0.97	0.20	-1.89	78,78,78,78	0
56	MG	14	3153	1/1	0.90	0.17	-1.89	70,70,70,70	0
56	MG	1H	3351	1/1	0.98	0.18	-1.91	65,65,65,65	0
56	MG	14	3369	1/1	0.88	0.18	-1.92	105,105,105,105	0
56	MG	14	3300	1/1	0.97	0.15	-1.93	98,98,98,98	0
56	MG	1G	1674	1/1	0.92	0.15	-1.94	111,111,111,111	0
56	MG	1H	3132	1/1	0.80	0.19	-1.94	74,74,74,74	0
56	MG	14	3393	1/1	0.95	0.14	-1.95	80,80,80,80	0
56	MG	14	3390	1/1	0.95	0.18	-1.96	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3094	1/1	0.92	0.20	-1.96	83,83,83,83	0
56	MG	14	3033	1/1	0.98	0.18	-1.99	66,66,66,66	0
56	MG	14	3189	1/1	0.98	0.12	-2.00	83,83,83,83	0
56	MG	14	3010	1/1	0.98	0.19	-2.04	65,65,65,65	0
56	MG	14	3257	1/1	0.99	0.20	-2.04	84,84,84,84	0
56	MG	1H	3024	1/1	0.94	0.23	-2.06	102,102,102,102	0
56	MG	13	1647	1/1	0.86	0.17	-2.07	93,93,93,93	0
56	MG	13	1679	1/1	0.88	0.19	-2.11	98,98,98,98	0
56	MG	1H	3403	1/1	0.97	0.16	-2.13	73,73,73,73	0
56	MG	1H	3055	1/1	0.83	0.16	-2.16	82,82,82,82	0
56	MG	14	3235	1/1	0.69	0.14	-2.20	83,83,83,83	0
56	MG	1H	3366	1/1	0.90	0.12	-2.24	60,60,60,60	0
56	MG	14	3337	1/1	0.87	0.12	-2.27	76,76,76,76	0
56	MG	14	3365	1/1	0.92	0.10	-2.28	80,80,80,80	0
56	MG	1G	1625	1/1	0.76	0.12	-2.28	131,131,131,131	0
56	MG	1G	1679	1/1	0.88	0.09	-2.30	108,108,108,108	0
56	MG	1H	3353	1/1	0.98	0.11	-2.35	77,77,77,77	0
56	MG	1H	3044	1/1	0.99	0.20	-2.36	68,68,68,68	0
56	MG	1H	3233	1/1	0.98	0.19	-2.38	65,65,65,65	0
56	MG	14	3206	1/1	0.96	0.08	-2.41	83,83,83,83	0
57	ZN	C5	202	1/1	0.89	0.11	-2.42	189,189,189,189	0
56	MG	1H	3145	1/1	0.98	0.20	-2.44	57,57,57,57	0
56	MG	1H	3163	1/1	0.92	0.20	-2.44	88,88,88,88	0
56	MG	1H	3489	1/1	0.85	0.12	-2.46	69,69,69,69	0
56	MG	1H	3096	1/1	0.97	0.17	-2.48	57,57,57,57	0
56	MG	1H	3237	1/1	0.89	0.17	-2.48	70,70,70,70	0
56	MG	1H	3215	1/1	0.95	0.14	-2.49	81,81,81,81	0
56	MG	14	3353	1/1	0.97	0.15	-2.49	91,91,91,91	0
56	MG	1H	3390	1/1	0.94	0.17	-2.52	83,83,83,83	0
56	MG	13	1713	1/1	0.91	0.12	-2.53	119,119,119,119	0
56	MG	1H	3005	1/1	0.92	0.20	-2.55	70,70,70,70	0
56	MG	1H	3087	1/1	0.69	0.18	-2.55	69,69,69,69	0
56	MG	14	3069	1/1	0.95	0.08	-2.62	63,63,63,63	0
56	MG	14	3357	1/1	0.99	0.13	-2.63	80,80,80,80	0
56	MG	14	3387	1/1	0.90	0.10	-2.69	76,76,76,76	0
56	MG	1H	3082	1/1	0.93	0.17	-2.71	77,77,77,77	0
56	MG	13	1650	1/1	0.86	0.15	-2.72	87,87,87,87	0
56	MG	1H	3431	1/1	0.65	0.11	-2.73	163,163,163,163	0
56	MG	13	1729	1/1	0.97	0.12	-2.76	109,109,109,109	0
56	MG	1H	3360	1/1	0.96	0.14	-2.77	58,58,58,58	0
56	MG	1G	1662	1/1	0.95	0.16	-2.83	155,155,155,155	0
56	MG	1H	3124	1/1	0.71	0.19	-2.88	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3204	1/1	0.83	0.13	-2.89	80,80,80,80	0
56	MG	1G	1682	1/1	0.88	0.09	-2.90	141,141,141,141	0
56	MG	13	1642	1/1	0.95	0.11	-2.91	98,98,98,98	0
56	MG	1H	3364	1/1	0.96	0.12	-2.92	80,80,80,80	0
56	MG	1H	3042	1/1	0.96	0.18	-2.93	53,53,53,53	0
56	MG	14	3044	1/1	0.95	0.14	-2.96	78,78,78,78	0
56	MG	1G	1678	1/1	0.96	0.13	-2.97	108,108,108,108	0
56	MG	13	1732	1/1	0.98	0.09	-3.02	81,81,81,81	0
56	MG	14	3005	1/1	0.95	0.18	-3.06	66,66,66,66	0
56	MG	13	1694	1/1	0.80	0.10	-3.07	121,121,121,121	0
56	MG	14	3192	1/1	0.88	0.14	-3.10	84,84,84,84	0
56	MG	14	3322	1/1	0.97	0.14	-3.17	90,90,90,90	0
56	MG	1H	3388	1/1	0.97	0.14	-3.22	65,65,65,65	0
56	MG	1H	3356	1/1	0.97	0.10	-3.30	58,58,58,58	0
56	MG	1H	3159	1/1	0.94	0.17	-3.33	77,77,77,77	0
56	MG	1H	3211	1/1	0.91	0.14	-3.34	76,76,76,76	0
56	MG	1H	3120	1/1	0.97	0.13	-3.35	80,80,80,80	0
56	MG	1H	3125	1/1	0.98	0.16	-3.35	68,68,68,68	0
56	MG	1H	3113	1/1	0.94	0.14	-3.36	64,64,64,64	0
56	MG	13	1643	1/1	0.94	0.09	-3.41	78,78,78,78	0
56	MG	1G	1609	1/1	0.91	0.12	-3.43	97,97,97,97	0
56	MG	13	1638	1/1	0.97	0.09	-3.44	115,115,115,115	0
56	MG	1G	1608	1/1	0.98	0.14	-3.47	98,98,98,98	0
56	MG	1H	3379	1/1	0.98	0.12	-3.47	74,74,74,74	0
56	MG	14	3358	1/1	0.98	0.09	-3.50	85,85,85,85	0
56	MG	14	3111	1/1	0.97	0.17	-3.51	72,72,72,72	0
56	MG	14	3336	1/1	0.95	0.14	-3.61	88,88,88,88	0
56	MG	14	3344	1/1	0.92	0.11	-3.66	82,82,82,82	0
56	MG	13	1662	1/1	0.91	0.11	-3.67	94,94,94,94	0
56	MG	14	3061	1/1	0.98	0.15	-3.68	79,79,79,79	0
56	MG	1G	1618	1/1	0.94	0.12	-3.68	104,104,104,104	0
56	MG	13	1738	1/1	0.98	0.13	-3.75	77,77,77,77	0
56	MG	13	1695	1/1	0.82	0.15	-3.79	112,112,112,112	0
56	MG	1G	1622	1/1	0.93	0.12	-3.79	89,89,89,89	0
56	MG	14	3047	1/1	0.91	0.14	-3.84	66,66,66,66	0
56	MG	1H	3369	1/1	0.97	0.15	-3.84	92,92,92,92	0
56	MG	1H	3471	1/1	0.88	0.11	-3.86	128,128,128,128	0
56	MG	1H	3385	1/1	0.95	0.14	-3.89	75,75,75,75	0
56	MG	14	3236	1/1	0.71	0.10	-3.95	99,99,99,99	0
56	MG	13	1617	1/1	0.96	0.08	-3.96	106,106,106,106	0
56	MG	1H	3350	1/1	0.96	0.14	-3.98	64,64,64,64	0
56	MG	1H	3362	1/1	0.99	0.14	-4.02	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3251	1/1	0.72	0.15	-4.03	93,93,93,93	0
56	MG	13	1630	1/1	0.83	0.12	-4.08	74,74,74,74	0
56	MG	1H	3414	1/1	0.98	0.15	-4.08	65,65,65,65	0
56	MG	1H	3349	1/1	0.96	0.16	-4.16	69,69,69,69	0
56	MG	1H	3057	1/1	0.96	0.19	-4.19	72,72,72,72	0
56	MG	1H	3105	1/1	0.94	0.09	-4.25	76,76,76,76	0
56	MG	1H	3112	1/1	0.94	0.14	-4.38	55,55,55,55	0
56	MG	14	3130	1/1	0.89	0.10	-4.39	71,71,71,71	0
56	MG	14	3334	1/1	0.96	0.11	-4.42	91,91,91,91	0
56	MG	14	3100	1/1	0.95	0.12	-4.43	87,87,87,87	0
56	MG	1H	3207	1/1	0.98	0.18	-4.48	60,60,60,60	0
56	MG	1H	3452	1/1	0.99	0.14	-4.51	65,65,65,65	0
56	MG	14	3218	1/1	0.92	0.13	-4.51	75,75,75,75	0
56	MG	1H	3389	1/1	0.98	0.16	-4.52	69,69,69,69	0
56	MG	13	1722	1/1	0.82	0.10	-4.55	85,85,85,85	0
56	MG	14	3351	1/1	0.98	0.12	-4.56	60,60,60,60	0
56	MG	1H	3491	1/1	0.73	0.16	-4.61	93,93,93,93	0
56	MG	1H	3206	1/1	0.77	0.14	-4.63	53,53,53,53	0
56	MG	14	3352	1/1	0.84	0.12	-4.68	74,74,74,74	0
56	MG	14	3423	1/1	0.91	0.10	-4.72	133,133,133,133	0
56	MG	1H	3358	1/1	0.91	0.15	-4.75	76,76,76,76	0
56	MG	14	3056	1/1	0.92	0.12	-4.81	92,92,92,92	0
56	MG	14	3347	1/1	0.97	0.07	-4.84	85,85,85,85	0
56	MG	1H	3347	1/1	0.95	0.13	-4.84	57,57,57,57	0
56	MG	14	3258	1/1	0.92	0.13	-4.87	104,104,104,104	0
56	MG	14	3312	1/1	0.68	0.12	-4.88	93,93,93,93	0
56	MG	1H	3136	1/1	0.88	0.15	-4.90	71,71,71,71	0
56	MG	14	3067	1/1	0.96	0.18	-4.92	73,73,73,73	0
56	MG	1H	3239	1/1	0.97	0.17	-4.93	88,88,88,88	0
56	MG	1H	3439	1/1	0.86	0.15	-4.93	92,92,92,92	0
56	MG	13	1632	1/1	0.91	0.16	-5.20	64,64,64,64	0
56	MG	14	3348	1/1	0.97	0.10	-5.20	71,71,71,71	0
56	MG	1H	3383	1/1	0.97	0.10	-5.20	67,67,67,67	0
56	MG	1H	3416	1/1	0.94	0.07	-5.25	78,78,78,78	0
56	MG	14	3240	1/1	0.94	0.10	-5.27	76,76,76,76	0
56	MG	1H	3371	1/1	0.97	0.08	-5.29	91,91,91,91	0
56	MG	1H	3404	1/1	0.94	0.09	-5.67	62,62,62,62	0
56	MG	14	3214	1/1	0.96	0.14	-5.70	70,70,70,70	0
56	MG	13	1724	1/1	0.91	0.06	-5.82	102,102,102,102	0
56	MG	1H	3411	1/1	0.99	0.12	-5.84	80,80,80,80	0
56	MG	1H	3440	1/1	0.99	0.10	-5.91	83,83,83,83	0
56	MG	1H	3352	1/1	0.98	0.14	-5.93	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3380	1/1	0.92	0.09	-5.98	97,97,97,97	0
56	MG	1H	3372	1/1	0.82	0.10	-6.28	79,79,79,79	0
56	MG	14	3105	1/1	0.97	0.14	-6.48	74,74,74,74	0
56	MG	14	3333	1/1	0.98	0.12	-6.53	73,73,73,73	0
56	MG	14	3018	1/1	0.91	0.13	-6.55	70,70,70,70	0
56	MG	1H	3443	1/1	0.99	0.17	-6.56	76,76,76,76	0
56	MG	14	3373	1/1	0.96	0.08	-6.61	81,81,81,81	0
56	MG	1H	3481	1/1	0.97	0.11	-6.74	70,70,70,70	0
56	MG	1H	3476	1/1	0.79	0.13	-7.08	93,93,93,93	0
56	MG	14	3350	1/1	0.94	0.08	-7.17	80,80,80,80	0
56	MG	14	3346	1/1	0.88	0.11	-7.40	92,92,92,92	0
56	MG	14	3412	1/1	0.85	0.08	-8.02	108,108,108,108	0
56	MG	1H	3412	1/1	0.99	0.12	-8.27	64,64,64,64	0
56	MG	14	3341	1/1	0.93	0.07	-8.39	78,78,78,78	0
56	MG	1H	3427	1/1	0.98	0.09	-8.44	75,75,75,75	0
56	MG	1H	3103	1/1	0.97	0.15	-8.99	60,60,60,60	0
56	MG	1G	1677	1/1	0.97	0.08	-9.02	91,91,91,91	0
56	MG	1H	3417	1/1	0.93	0.12	-9.21	90,90,90,90	0
56	MG	1H	3392	1/1	0.97	0.13	-9.26	65,65,65,65	0
56	MG	1H	3438	1/1	0.92	0.05	-9.42	82,82,82,82	0
56	MG	14	3335	1/1	0.99	0.12	-9.46	73,73,73,73	0
56	MG	1H	3212	1/1	0.95	0.14	-9.50	61,61,61,61	0
56	MG	1H	3384	1/1	0.95	0.07	-9.52	59,59,59,59	0
56	MG	14	3388	1/1	0.91	0.12	-10.69	85,85,85,85	0
56	MG	1H	3454	1/1	0.94	0.06	-11.11	85,85,85,85	0
56	MG	1H	3376	1/1	0.95	0.04	-14.20	96,96,96,96	0
56	MG	1H	3451	1/1	0.96	0.11	-14.82	87,87,87,87	0
56	MG	1H	3333	1/1	0.92	0.34	-	91,91,91,91	0
56	MG	13	1690	1/1	0.76	0.19	-	108,108,108,108	0
56	MG	1H	3008	1/1	0.97	0.41	-	79,79,79,79	0
56	MG	1H	3280	1/1	0.80	0.70	-	100,100,100,100	0
56	MG	1H	3144	1/1	0.88	0.23	-	80,80,80,80	0
56	MG	1H	3497	1/1	0.96	0.10	-	119,119,119,119	0
56	MG	1H	3119	1/1	0.35	0.52	-	101,101,101,101	0
56	MG	1H	3225	1/1	0.89	0.21	-	69,69,69,69	0
56	MG	14	3222	1/1	0.95	0.24	-	99,99,99,99	0
56	MG	1J	209	1/1	0.90	0.07	-	125,125,125,125	0
56	MG	1H	3450	1/1	0.96	0.12	-	66,66,66,66	0
56	MG	14	3022	1/1	0.90	0.48	-	107,107,107,107	0
56	MG	16	201	1/1	0.83	0.23	-	79,79,79,79	0
56	MG	1H	3503	1/1	0.83	0.12	-	116,116,116,116	0
56	MG	13	1644	1/1	0.90	0.12	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3302	1/1	0.93	0.23	-	90,90,90,90	0
56	MG	1H	3146	1/1	0.85	0.32	-	83,83,83,83	0
56	MG	1H	3375	1/1	0.93	0.18	-	76,76,76,76	0
56	MG	14	3386	1/1	0.98	0.25	-	105,105,105,105	0
56	MG	14	3004	1/1	0.96	0.25	-	64,64,64,64	0
56	MG	1H	3227	1/1	0.97	0.26	-	123,123,123,123	0
56	MG	16	213	1/1	0.95	0.43	-	85,85,85,85	0
56	MG	1H	3140	1/1	0.82	0.52	-	101,101,101,101	0
56	MG	14	3147	1/1	0.79	0.19	-	97,97,97,97	0
56	MG	1H	3380	1/1	0.99	0.16	-	61,61,61,61	0
56	MG	13	1622	1/1	0.87	0.32	-	102,102,102,102	0
56	MG	1G	1647	1/1	0.89	0.32	-	86,86,86,86	0
56	MG	1H	3023	1/1	0.67	0.37	-	100,100,100,100	0
56	MG	13	1696	1/1	0.90	0.29	-	108,108,108,108	0
56	MG	1H	3493	1/1	0.85	0.25	-	130,130,130,130	0
56	MG	1H	3329	1/1	0.90	0.34	-	99,99,99,99	0
56	MG	1H	3095	1/1	0.95	0.43	-	74,74,74,74	0
56	MG	1G	1642	1/1	0.70	0.22	-	102,102,102,102	0
56	MG	14	3143	1/1	0.70	0.43	-	100,100,100,100	0
56	MG	1H	3357	1/1	0.98	0.07	-	57,57,57,57	0
56	MG	1H	3370	1/1	0.99	0.16	-	84,84,84,84	0
56	MG	1H	3265	1/1	0.75	0.27	-	96,96,96,96	0
56	MG	1H	3310	1/1	0.92	0.37	-	96,96,96,96	0
56	MG	13	1700	1/1	0.93	0.24	-	109,109,109,109	0
56	MG	1H	3019	1/1	0.97	0.28	-	54,54,54,54	0
56	MG	1H	3473	1/1	0.90	0.21	-	127,127,127,127	0
56	MG	13	1747	1/1	0.97	0.28	-	103,103,103,103	0
56	MG	1G	1637	1/1	0.93	0.16	-	104,104,104,104	0
56	MG	1H	3341	1/1	0.95	0.27	-	100,100,100,100	0
56	MG	14	3345	1/1	0.94	0.10	-	84,84,84,84	0
56	MG	1H	3402	1/1	0.96	0.12	-	81,81,81,81	0
56	MG	1H	3467	1/1	0.77	0.10	-	106,106,106,106	0
56	MG	13	1663	1/1	0.86	0.16	-	87,87,87,87	0
56	MG	1H	3453	1/1	0.98	0.15	-	70,70,70,70	0
56	MG	1H	3396	1/1	0.96	0.17	-	87,87,87,87	0
56	MG	1H	3367	1/1	0.95	0.13	-	82,82,82,82	0
56	MG	14	3013	1/1	0.90	0.17	-	88,88,88,88	0
56	MG	14	3319	1/1	0.71	0.29	-	118,118,118,118	0
56	MG	14	3338	1/1	0.96	0.09	-	68,68,68,68	0
56	MG	14	3313	1/1	0.75	0.19	-	124,124,124,124	0
56	MG	14	3407	1/1	0.88	0.08	-	116,116,116,116	0
56	MG	1H	3138	1/1	0.90	0.40	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3212	1/1	0.98	0.16	-	104,104,104,104	0
56	MG	13	1657	1/1	0.95	0.24	-	104,104,104,104	0
56	MG	14	3376	1/1	0.71	0.13	-	119,119,119,119	0
56	MG	88	202	1/1	0.87	0.30	-	77,77,77,77	0
56	MG	14	3109	1/1	0.91	0.32	-	89,89,89,89	0
56	MG	1H	3462	1/1	0.96	0.11	-	75,75,75,75	0
56	MG	14	3168	1/1	0.84	0.23	-	67,67,67,67	0
56	MG	14	3131	1/1	0.96	0.20	-	56,56,56,56	0
56	MG	13	1748	1/1	0.69	0.09	-	140,140,140,140	0
56	MG	1H	3218	1/1	0.95	0.17	-	78,78,78,78	0
56	MG	1H	3281	1/1	0.57	0.30	-	85,85,85,85	0
56	MG	E5	101	1/1	0.66	0.23	-	98,98,98,98	0
56	MG	13	1665	1/1	0.87	0.12	-	91,91,91,91	0
56	MG	14	3349	1/1	0.96	0.14	-	71,71,71,71	0
56	MG	1H	3399	1/1	0.87	0.09	-	59,59,59,59	0
56	MG	13	1719	1/1	0.86	0.13	-	95,95,95,95	0
56	MG	1H	3129	1/1	0.79	0.41	-	90,90,90,90	0
56	MG	1H	3458	1/1	0.93	0.13	-	93,93,93,93	0
56	MG	14	3401	1/1	0.94	0.06	-	120,120,120,120	0
56	MG	13	1717	1/1	0.63	0.28	-	114,114,114,114	0
56	MG	13	1736	1/1	0.99	0.17	-	102,102,102,102	0
56	MG	1H	3153	1/1	0.73	0.40	-	98,98,98,98	0
56	MG	3I	202	1/1	0.83	0.45	-	101,101,101,101	0
56	MG	1H	3488	1/1	0.85	0.15	-	114,114,114,114	0
56	MG	1H	3198	1/1	0.87	0.38	-	90,90,90,90	0
56	MG	52	201	1/1	0.83	0.12	-	107,107,107,107	0
56	MG	1H	3034	1/1	0.80	0.33	-	96,96,96,96	0
56	MG	1H	3446	1/1	0.98	0.12	-	74,74,74,74	0
56	MG	1H	3271	1/1	0.98	0.46	-	93,93,93,93	0
56	MG	1H	3386	1/1	0.94	0.16	-	82,82,82,82	0
56	MG	1H	3026	1/1	0.73	0.34	-	94,94,94,94	0
56	MG	29	302	1/1	0.56	0.35	-	108,108,108,108	0
56	MG	14	3375	1/1	0.91	0.06	-	102,102,102,102	0
56	MG	1H	3109	1/1	0.95	0.19	-	84,84,84,84	0
56	MG	13	1676	1/1	0.90	0.18	-	111,111,111,111	0
56	MG	14	3301	1/1	0.82	0.29	-	83,83,83,83	0
56	MG	1J	203	1/1	0.75	0.16	-	114,114,114,114	0
56	MG	1H	3036	1/1	0.99	0.46	-	61,61,61,61	0
56	MG	14	3421	1/1	0.94	0.05	-	130,130,130,130	0
56	MG	1H	3188	1/1	0.93	0.51	-	100,100,100,100	0
56	MG	14	3303	1/1	0.90	0.12	-	100,100,100,100	0
56	MG	14	3230	1/1	0.97	0.27	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1675	1/1	0.86	0.47	-	99,99,99,99	0
56	MG	1H	3496	1/1	0.91	0.04	-	131,131,131,131	0
56	MG	1H	3339	1/1	0.86	0.33	-	90,90,90,90	0
56	MG	1H	3214	1/1	0.96	0.13	-	103,103,103,103	0
56	MG	14	3132	1/1	0.93	0.22	-	94,94,94,94	0
56	MG	14	3403	1/1	0.70	0.09	-	122,122,122,122	0
56	MG	1H	3015	1/1	0.87	0.24	-	71,71,71,71	0
56	MG	14	3207	1/1	0.91	0.14	-	68,68,68,68	0
56	MG	14	3068	1/1	0.85	0.38	-	86,86,86,86	0
56	MG	14	3383	1/1	0.90	0.16	-	98,98,98,98	0
56	MG	14	3113	1/1	0.93	0.35	-	80,80,80,80	0
56	MG	21	301	1/1	0.98	0.23	-	75,75,75,75	0
56	MG	1H	3322	1/1	0.52	0.22	-	96,96,96,96	0
56	MG	16	210	1/1	0.95	0.45	-	107,107,107,107	0
56	MG	1H	3210	1/1	0.89	0.17	-	69,69,69,69	0
56	MG	1H	3286	1/1	0.84	0.26	-	85,85,85,85	0
56	MG	1G	1663	1/1	0.83	0.20	-	92,92,92,92	0
56	MG	13	1677	1/1	0.91	0.39	-	98,98,98,98	0
56	MG	1H	3466	1/1	0.90	0.12	-	94,94,94,94	0
56	MG	14	3031	1/1	0.96	0.29	-	76,76,76,76	0
56	MG	1H	3290	1/1	0.86	0.49	-	92,92,92,92	0
56	MG	2K	102	1/1	0.94	0.23	-	97,97,97,97	0
56	MG	1H	3083	1/1	0.87	0.32	-	92,92,92,92	0
56	MG	15	201	1/1	0.84	0.54	-	102,102,102,102	0
56	MG	1H	3419	1/1	0.95	0.16	-	94,94,94,94	0
56	MG	14	3114	1/1	0.95	0.39	-	97,97,97,97	0
56	MG	5E	201	1/1	0.87	0.20	-	104,104,104,104	0
56	MG	1G	1611	1/1	0.92	0.18	-	105,105,105,105	0
56	MG	1H	3262	1/1	0.81	0.30	-	89,89,89,89	0
56	MG	1G	1643	1/1	0.74	0.30	-	104,104,104,104	0
56	MG	14	3287	1/1	0.90	0.20	-	95,95,95,95	0
56	MG	1G	1613	1/1	0.92	0.22	-	117,117,117,117	0
56	MG	25	202	1/1	0.87	0.33	-	125,125,125,125	0
56	MG	14	3190	1/1	0.94	0.22	-	124,124,124,124	0
56	MG	1H	3060	1/1	0.98	0.23	-	74,74,74,74	0
56	MG	14	3224	1/1	0.93	0.09	-	80,80,80,80	0
56	MG	14	3203	1/1	0.70	0.29	-	81,81,81,81	0
56	MG	14	3389	1/1	0.96	0.17	-	72,72,72,72	0
56	MG	14	3173	1/1	0.82	0.28	-	87,87,87,87	0
56	MG	14	3422	1/1	0.79	0.09	-	132,132,132,132	0
56	MG	1H	3309	1/1	0.61	0.45	-	96,96,96,96	0
56	MG	13	1750	1/1	0.45	0.35	-	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3124	1/1	0.97	0.26	-	85,85,85,85	0
56	MG	1H	3469	1/1	0.90	0.07	-	106,106,106,106	0
56	MG	1H	3338	1/1	0.92	0.27	-	110,110,110,110	0
56	MG	14	3149	1/1	0.89	0.21	-	79,79,79,79	0
56	MG	1G	1668	1/1	0.83	0.22	-	111,111,111,111	0
56	MG	1G	1616	1/1	0.95	0.18	-	149,149,149,149	0
56	MG	1G	1672	1/1	0.95	0.26	-	126,126,126,126	0
56	MG	14	3039	1/1	0.92	0.26	-	68,68,68,68	0
56	MG	1G	1612	1/1	0.95	0.15	-	110,110,110,110	0
56	MG	13	1681	1/1	0.96	0.25	-	107,107,107,107	0
56	MG	1H	3293	1/1	0.93	0.17	-	85,85,85,85	0
56	MG	13	1606	1/1	0.60	0.33	-	115,115,115,115	0
56	MG	45	202	1/1	0.88	0.53	-	82,82,82,82	0
56	MG	14	3026	1/1	0.68	0.39	-	92,92,92,92	0
56	MG	1H	3195	1/1	0.97	0.11	-	94,94,94,94	0
56	MG	1H	3061	1/1	0.85	0.34	-	85,85,85,85	0
56	MG	1H	3038	1/1	0.96	0.26	-	58,58,58,58	0
56	MG	13	1645	1/1	0.93	0.38	-	86,86,86,86	0
56	MG	16	202	1/1	0.94	0.28	-	73,73,73,73	0
56	MG	1G	1652	1/1	0.88	0.26	-	103,103,103,103	0
56	MG	13	1634	1/1	0.98	0.30	-	85,85,85,85	0
56	MG	1H	3185	1/1	0.84	0.38	-	88,88,88,88	0
56	MG	1G	1610	1/1	0.91	0.13	-	115,115,115,115	0
56	MG	14	3324	1/1	0.82	0.40	-	96,96,96,96	0
56	MG	1H	3179	1/1	0.72	0.40	-	96,96,96,96	0
56	MG	1G	1632	1/1	0.77	0.41	-	116,116,116,116	0
56	MG	14	3201	1/1	0.63	0.30	-	111,111,111,111	0
56	MG	14	3321	1/1	0.92	0.26	-	99,99,99,99	0
56	MG	1H	3442	1/1	0.93	0.12	-	57,57,57,57	0
56	MG	14	3161	1/1	0.90	0.19	-	104,104,104,104	0
56	MG	14	3193	1/1	0.83	0.09	-	89,89,89,89	0
56	MG	1H	3435	1/1	0.99	0.15	-	72,72,72,72	0
56	MG	14	3126	1/1	0.95	0.29	-	103,103,103,103	0
56	MG	1H	3492	1/1	0.86	0.23	-	120,120,120,120	0
56	MG	1H	3226	1/1	0.97	0.26	-	88,88,88,88	0
56	MG	14	3366	1/1	0.99	0.15	-	88,88,88,88	0
56	MG	1G	1683	1/1	0.96	0.14	-	129,129,129,129	0
56	MG	1H	3336	1/1	0.93	0.30	-	102,102,102,102	0
56	MG	78	201	1/1	0.92	0.15	-	67,67,67,67	0
56	MG	14	3417	1/1	0.93	0.06	-	148,148,148,148	0
56	MG	13	1740	1/1	0.85	0.17	-	106,106,106,106	0
56	MG	1H	3337	1/1	0.65	0.42	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	11	302	1/1	0.90	0.25	-	66,66,66,66	0
56	MG	1H	3264	1/1	0.93	0.29	-	96,96,96,96	0
56	MG	1H	3426	1/1	0.91	0.13	-	92,92,92,92	0
56	MG	1H	3395	1/1	0.65	0.17	-	118,118,118,118	0
56	MG	1H	3035	1/1	0.93	0.20	-	55,55,55,55	0
56	MG	14	3034	1/1	0.98	0.23	-	69,69,69,69	0
56	MG	1G	1676	1/1	0.95	0.35	-	121,121,121,121	0
56	MG	14	3191	1/1	0.97	0.21	-	92,92,92,92	0
56	MG	14	3316	1/1	0.87	0.54	-	103,103,103,103	0
56	MG	14	3108	1/1	0.96	0.15	-	92,92,92,92	0
56	MG	1H	3016	1/1	0.98	0.31	-	66,66,66,66	0
56	MG	1H	3482	1/1	0.94	0.10	-	119,119,119,119	0
56	MG	1H	3031	1/1	0.89	0.33	-	89,89,89,89	0
56	MG	1H	3263	1/1	0.86	0.22	-	106,106,106,106	0
56	MG	1H	3247	1/1	0.93	0.28	-	81,81,81,81	0
56	MG	1H	3236	1/1	0.95	0.26	-	77,77,77,77	0
56	MG	32	301	1/1	0.76	0.46	-	120,120,120,120	0
56	MG	1H	3191	1/1	0.91	0.34	-	87,87,87,87	0
56	MG	1H	3348	1/1	0.97	0.14	-	84,84,84,84	0
56	MG	14	3196	1/1	0.77	0.34	-	99,99,99,99	0
56	MG	14	3250	1/1	0.89	0.23	-	86,86,86,86	0
56	MG	1H	3093	1/1	0.96	0.16	-	81,81,81,81	0
56	MG	1G	1631	1/1	0.95	0.23	-	113,113,113,113	0
56	MG	13	1669	1/1	0.70	0.27	-	110,110,110,110	0
56	MG	14	3286	1/1	0.69	0.15	-	92,92,92,92	0
56	MG	1H	3480	1/1	0.87	0.14	-	109,109,109,109	0
56	MG	G8	201	1/1	0.95	0.11	-	83,83,83,83	0
56	MG	6A	101	1/1	0.84	0.21	-	138,138,138,138	0
56	MG	1H	3122	1/1	0.84	0.30	-	94,94,94,94	0
56	MG	14	3177	1/1	0.89	0.32	-	111,111,111,111	0
56	MG	1H	3422	1/1	0.94	0.15	-	91,91,91,91	0
56	MG	1H	3343	1/1	0.68	0.36	-	92,92,92,92	0
56	MG	13	1702	1/1	0.79	0.23	-	109,109,109,109	0
56	MG	1H	3199	1/1	0.84	0.51	-	99,99,99,99	0
56	MG	1H	3253	1/1	0.97	0.19	-	91,91,91,91	0
56	MG	13	1636	1/1	0.62	0.30	-	100,100,100,100	0
56	MG	1G	1658	1/1	0.95	0.21	-	110,110,110,110	0
56	MG	14	3367	1/1	0.92	0.06	-	111,111,111,111	0
56	MG	14	3135	1/1	0.93	0.31	-	101,101,101,101	0
56	MG	14	3400	1/1	0.93	0.22	-	95,95,95,95	0
56	MG	13	1624	1/1	0.87	0.22	-	95,95,95,95	0
56	MG	13	1673	1/1	0.95	0.28	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3400	1/1	0.94	0.10	-	61,61,61,61	0
56	MG	13	1734	1/1	0.81	0.15	-	133,133,133,133	0
56	MG	1H	3312	1/1	0.91	0.37	-	79,79,79,79	0
56	MG	1H	3413	1/1	0.97	0.15	-	77,77,77,77	0
56	MG	1H	3167	1/1	0.93	0.15	-	92,92,92,92	0
56	MG	1G	1646	1/1	0.96	0.15	-	102,102,102,102	0
56	MG	1G	1606	1/1	0.90	0.27	-	129,129,129,129	0
56	MG	13	1744	1/1	0.68	0.41	-	132,132,132,132	0
56	MG	13	1739	1/1	0.47	0.20	-	120,120,120,120	0
56	MG	14	3281	1/1	0.75	0.55	-	105,105,105,105	0
56	MG	1H	3460	1/1	0.94	0.11	-	110,110,110,110	0
56	MG	1H	3455	1/1	0.94	0.22	-	99,99,99,99	0
56	MG	14	3093	1/1	0.85	0.51	-	103,103,103,103	0
56	MG	14	3251	1/1	0.71	0.10	-	105,105,105,105	0
56	MG	14	3320	1/1	0.79	0.22	-	96,96,96,96	0
56	MG	14	3054	1/1	0.96	0.12	-	93,93,93,93	0
56	MG	14	3241	1/1	0.94	0.31	-	92,92,92,92	0
56	MG	14	3339	1/1	0.99	0.12	-	74,74,74,74	0
56	MG	13	1714	1/1	0.70	0.22	-	101,101,101,101	0
56	MG	1H	3295	1/1	0.88	0.50	-	92,92,92,92	0
56	MG	1H	3217	1/1	0.93	0.12	-	91,91,91,91	0
56	MG	1H	3118	1/1	0.88	0.29	-	76,76,76,76	0
56	MG	14	3402	1/1	0.96	0.11	-	99,99,99,99	0
56	MG	13	1687	1/1	0.84	0.28	-	109,109,109,109	0
56	MG	1H	3465	1/1	0.98	0.10	-	83,83,83,83	0
56	MG	14	3134	1/1	0.97	0.10	-	103,103,103,103	0
56	MG	14	3166	1/1	0.89	0.14	-	106,106,106,106	0
56	MG	13	1745	1/1	0.61	0.39	-	121,121,121,121	0
56	MG	14	3006	1/1	0.94	0.21	-	99,99,99,99	0
56	MG	1G	1686	1/1	0.82	0.07	-	129,129,129,129	0
56	MG	14	3200	1/1	0.85	0.18	-	85,85,85,85	0
56	MG	14	3099	1/1	0.95	0.14	-	106,106,106,106	0
56	MG	1H	3090	1/1	0.95	0.46	-	91,91,91,91	0
56	MG	14	3360	1/1	0.91	0.06	-	92,92,92,92	0
56	MG	14	3164	1/1	0.88	0.21	-	91,91,91,91	0
56	MG	14	3298	1/1	0.95	0.42	-	115,115,115,115	0
56	MG	14	3085	1/1	0.97	0.18	-	81,81,81,81	0
56	MG	14	3282	1/1	0.88	0.31	-	90,90,90,90	0
56	MG	1H	3423	1/1	0.84	0.14	-	102,102,102,102	0
56	MG	1H	3424	1/1	0.94	0.09	-	119,119,119,119	0
56	MG	14	3025	1/1	0.62	0.17	-	116,116,116,116	0
56	MG	14	3405	1/1	0.81	0.22	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3088	1/1	0.96	0.23	-	66,66,66,66	0
56	MG	13	1720	1/1	0.43	0.24	-	104,104,104,104	0
56	MG	1H	3365	1/1	0.98	0.14	-	69,69,69,69	0
56	MG	14	3012	1/1	0.92	0.23	-	94,94,94,94	0
56	MG	1H	3079	1/1	0.99	0.33	-	83,83,83,83	0
56	MG	1H	3373	1/1	0.98	0.12	-	63,63,63,63	0
56	MG	1H	3278	1/1	0.92	0.29	-	101,101,101,101	0
56	MG	1H	3072	1/1	0.79	0.29	-	80,80,80,80	0
56	MG	1H	3468	1/1	0.97	0.07	-	95,95,95,95	0
56	MG	14	3075	1/1	0.98	0.23	-	81,81,81,81	0
56	MG	1H	3059	1/1	0.98	0.49	-	92,92,92,92	0
56	MG	1H	3028	1/1	0.49	0.43	-	115,115,115,115	0
56	MG	1H	3483	1/1	0.94	0.07	-	110,110,110,110	0
56	MG	14	3331	1/1	0.99	0.29	-	112,112,112,112	0
56	MG	1J	206	1/1	0.82	0.12	-	123,123,123,123	0
56	MG	1H	3049	1/1	0.93	0.33	-	60,60,60,60	0
56	MG	13	1715	1/1	0.94	0.30	-	108,108,108,108	0
56	MG	1H	3161	1/1	0.94	0.36	-	82,82,82,82	0
56	MG	1H	3405	1/1	0.95	0.13	-	86,86,86,86	0
56	MG	14	3063	1/1	0.93	0.18	-	104,104,104,104	0
56	MG	1H	3335	1/1	0.87	0.42	-	85,85,85,85	0
56	MG	1H	3409	1/1	0.99	0.18	-	76,76,76,76	0
56	MG	1H	3246	1/1	0.84	0.22	-	78,78,78,78	0
56	MG	14	3101	1/1	0.98	0.15	-	80,80,80,80	0
56	MG	1G	1617	1/1	0.92	0.27	-	110,110,110,110	0
56	MG	14	3354	1/1	0.88	0.06	-	126,126,126,126	0
56	MG	14	3083	1/1	0.92	0.26	-	81,81,81,81	0
56	MG	14	3234	1/1	0.94	0.55	-	98,98,98,98	0
56	MG	1H	3354	1/1	0.92	0.14	-	64,64,64,64	0
56	MG	14	3152	1/1	0.86	0.23	-	80,80,80,80	0
56	MG	1H	3238	1/1	0.90	0.32	-	84,84,84,84	0
56	MG	1H	3111	1/1	0.83	0.43	-	91,91,91,91	0
56	MG	14	3249	1/1	0.87	0.27	-	97,97,97,97	0
56	MG	P8	101	1/1	0.85	0.41	-	84,84,84,84	0
56	MG	14	3288	1/1	0.56	0.53	-	107,107,107,107	0
56	MG	1H	3092	1/1	0.85	0.30	-	70,70,70,70	0
56	MG	14	3133	1/1	0.68	0.13	-	97,97,97,97	0
56	MG	1H	3018	1/1	0.97	0.40	-	79,79,79,79	0
56	MG	14	3326	1/1	0.81	0.39	-	117,117,117,117	0
56	MG	1H	3317	1/1	0.86	0.79	-	85,85,85,85	0
56	MG	13	1633	1/1	0.98	0.15	-	75,75,75,75	0
56	MG	1H	3142	1/1	0.41	0.41	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3187	1/1	0.96	0.24	-	89,89,89,89	0
56	MG	14	3145	1/1	0.97	0.25	-	105,105,105,105	0
56	MG	1H	3231	1/1	0.93	0.49	-	90,90,90,90	0
56	MG	1H	3283	1/1	0.84	0.38	-	112,112,112,112	0
56	MG	1H	3106	1/1	0.76	0.34	-	95,95,95,95	0
56	MG	1G	1649	1/1	0.73	0.27	-	105,105,105,105	0
56	MG	14	3175	1/1	0.83	0.38	-	99,99,99,99	0
56	MG	1H	3192	1/1	0.96	0.11	-	78,78,78,78	0
56	MG	14	3330	1/1	0.83	0.20	-	105,105,105,105	0
56	MG	14	3046	1/1	0.97	0.24	-	88,88,88,88	0
56	MG	13	1615	1/1	0.94	0.24	-	100,100,100,100	0
56	MG	1H	3022	1/1	0.99	0.38	-	64,64,64,64	0
56	MG	13	1688	1/1	0.72	0.33	-	93,93,93,93	0
56	MG	14	3297	1/1	0.72	0.24	-	96,96,96,96	0
56	MG	1H	3391	1/1	0.84	0.09	-	96,96,96,96	0
56	MG	14	3112	1/1	0.90	0.12	-	98,98,98,98	0
56	MG	14	3424	1/1	0.91	0.43	-	116,116,116,116	0
56	MG	1H	3313	1/1	0.57	0.24	-	93,93,93,93	0
56	MG	1H	3100	1/1	0.91	0.27	-	86,86,86,86	0
56	MG	2K	103	1/1	0.95	0.10	-	98,98,98,98	0
56	MG	1H	3050	1/1	0.93	0.27	-	80,80,80,80	0
56	MG	1H	3308	1/1	0.90	0.25	-	90,90,90,90	0
56	MG	1H	3306	1/1	0.68	0.61	-	81,81,81,81	0
56	MG	1H	3318	1/1	0.84	0.30	-	87,87,87,87	0
56	MG	1H	3223	1/1	0.87	0.18	-	82,82,82,82	0
56	MG	14	3129	1/1	0.96	0.20	-	78,78,78,78	0
56	MG	1H	3345	1/1	0.89	0.31	-	100,100,100,100	0
56	MG	14	3309	1/1	0.92	0.49	-	87,87,87,87	0
56	MG	14	3066	1/1	0.87	0.30	-	96,96,96,96	0
56	MG	14	3391	1/1	0.46	0.10	-	124,124,124,124	0
56	MG	1H	3200	1/1	0.57	0.35	-	104,104,104,104	0
56	MG	14	3187	1/1	0.88	0.36	-	100,100,100,100	0
56	MG	14	3117	1/1	0.80	0.45	-	98,98,98,98	0
56	MG	1G	1654	1/1	0.94	0.38	-	94,94,94,94	0
56	MG	1H	3194	1/1	0.92	0.20	-	104,104,104,104	0
56	MG	14	3342	1/1	0.99	0.12	-	80,80,80,80	0
56	MG	1H	3284	1/1	0.87	0.26	-	70,70,70,70	0
56	MG	1H	3296	1/1	0.75	0.21	-	86,86,86,86	0
56	MG	1H	3221	1/1	0.94	0.38	-	99,99,99,99	0
56	MG	14	3414	1/1	0.98	0.06	-	93,93,93,93	0
56	MG	14	3087	1/1	0.96	0.16	-	82,82,82,82	0
56	MG	14	3263	1/1	0.93	0.25	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3208	1/1	0.94	0.09	-	63,63,63,63	0
56	MG	14	3104	1/1	0.84	0.27	-	81,81,81,81	0
56	MG	1H	3268	1/1	0.90	0.50	-	125,125,125,125	0
56	MG	14	3125	1/1	0.89	0.27	-	101,101,101,101	0
56	MG	14	3148	1/1	0.86	0.11	-	117,117,117,117	0
56	MG	1G	1670	1/1	0.64	0.40	-	138,138,138,138	0
56	MG	13	1698	1/1	0.94	0.35	-	95,95,95,95	0
56	MG	1G	1669	1/1	0.84	0.28	-	112,112,112,112	0
56	MG	14	3239	1/1	0.90	0.23	-	166,166,166,166	0
56	MG	1H	3196	1/1	0.95	0.70	-	110,110,110,110	0
56	MG	1H	3276	1/1	0.65	0.44	-	99,99,99,99	0
56	MG	13	1716	1/1	0.68	0.18	-	111,111,111,111	0
56	MG	1H	3080	1/1	0.94	0.31	-	86,86,86,86	0
56	MG	14	3275	1/1	0.79	0.28	-	105,105,105,105	0
56	MG	1H	3157	1/1	0.71	0.51	-	104,104,104,104	0
56	MG	13	1626	1/1	0.94	0.20	-	109,109,109,109	0
56	MG	1H	3330	1/1	0.69	0.56	-	104,104,104,104	0
56	MG	14	3092	1/1	0.94	0.16	-	109,109,109,109	0
56	MG	1H	3323	1/1	0.87	0.11	-	110,110,110,110	0
56	MG	1H	3485	1/1	0.82	0.08	-	121,121,121,121	0
56	MG	1H	3012	1/1	0.84	0.50	-	93,93,93,93	0
56	MG	1H	3039	1/1	0.97	0.39	-	55,55,55,55	0
56	MG	14	3355	1/1	0.90	0.18	-	102,102,102,102	0
56	MG	1H	3058	1/1	0.94	0.20	-	107,107,107,107	0
56	MG	1G	1665	1/1	0.87	0.30	-	110,110,110,110	0
56	MG	1H	3499	1/1	0.81	0.11	-	110,110,110,110	0
56	MG	14	3136	1/1	0.84	0.10	-	112,112,112,112	0
56	MG	14	3017	1/1	0.90	0.15	-	91,91,91,91	0
56	MG	1H	3032	1/1	0.93	0.25	-	78,78,78,78	0
56	MG	14	3396	1/1	0.91	0.16	-	119,119,119,119	0
56	MG	1G	1619	1/1	0.96	0.21	-	72,72,72,72	0
56	MG	1H	3299	1/1	0.97	0.17	-	71,71,71,71	0
56	MG	14	3183	1/1	0.51	0.32	-	110,110,110,110	0
56	MG	14	3178	1/1	0.78	0.44	-	95,95,95,95	0
56	MG	14	3397	1/1	0.97	0.13	-	101,101,101,101	0
56	MG	14	3181	1/1	0.61	0.21	-	100,100,100,100	0
56	MG	14	3019	1/1	0.66	0.22	-	96,96,96,96	0
56	MG	14	3285	1/1	0.75	0.30	-	91,91,91,91	0
56	MG	1H	3436	1/1	0.96	0.10	-	79,79,79,79	0
56	MG	1H	3007	1/1	0.86	0.33	-	97,97,97,97	0
56	MG	1G	1684	1/1	0.84	0.12	-	124,124,124,124	0
56	MG	1H	3229	1/1	0.96	0.23	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1749	1/1	0.70	0.23	-	121,121,121,121	0
56	MG	31	301	1/1	0.86	0.10	-	92,92,92,92	0
56	MG	13	1661	1/1	0.93	0.29	-	91,91,91,91	0
56	MG	1H	3494	1/1	0.87	0.36	-	121,121,121,121	0
56	MG	14	3226	1/1	0.96	0.21	-	123,123,123,123	0
56	MG	1H	3070	1/1	0.98	0.54	-	125,125,125,125	0
56	MG	1J	208	1/1	0.81	0.11	-	121,121,121,121	0
56	MG	1H	3319	1/1	0.93	0.27	-	90,90,90,90	0
56	MG	14	3188	1/1	0.98	0.31	-	91,91,91,91	0
56	MG	14	3361	1/1	0.97	0.17	-	86,86,86,86	0
56	MG	13	1727	1/1	0.89	0.24	-	121,121,121,121	0
56	MG	14	3050	1/1	0.96	0.13	-	60,60,60,60	0
56	MG	1G	1604	1/1	0.77	0.23	-	142,142,142,142	0
56	MG	1H	3429	1/1	0.94	0.08	-	102,102,102,102	0
56	MG	14	3023	1/1	0.88	0.15	-	86,86,86,86	0
56	MG	14	3255	1/1	0.77	0.41	-	99,99,99,99	0
56	MG	1H	3374	1/1	0.93	0.16	-	71,71,71,71	0
56	MG	14	3036	1/1	0.97	0.15	-	67,67,67,67	0
56	MG	13	1699	1/1	0.84	0.50	-	102,102,102,102	0
56	MG	14	3043	1/1	0.98	0.21	-	101,101,101,101	0
56	MG	14	3317	1/1	0.73	0.28	-	98,98,98,98	0
56	MG	1H	3303	1/1	0.93	0.30	-	76,76,76,76	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	3062	1/1	0.74	0.23	-	101,101,101,101	0
56	MG	1H	3021	1/1	0.95	0.32	-	79,79,79,79	0
56	MG	14	3280	1/1	0.81	0.31	-	95,95,95,95	0
56	MG	1H	3506	1/1	0.96	0.33	-	57,57,57,57	0
56	MG	14	3315	1/1	0.75	0.12	-	92,92,92,92	0
56	MG	14	3356	1/1	0.71	0.25	-	118,118,118,118	0
56	MG	1H	3224	1/1	0.98	0.28	-	82,82,82,82	0
56	MG	1H	3502	1/1	0.89	0.29	-	118,118,118,118	0
56	MG	1H	3030	1/1	0.86	0.19	-	79,79,79,79	0
56	MG	14	3294	1/1	0.72	0.14	-	91,91,91,91	0
56	MG	1H	3201	1/1	0.93	0.32	-	121,121,121,121	0
56	MG	14	3343	1/1	0.88	0.12	-	89,89,89,89	0
56	MG	1H	3137	1/1	0.73	0.53	-	87,87,87,87	0
56	MG	1H	3344	1/1	0.85	0.42	-	95,95,95,95	0
56	MG	1H	3505	1/1	0.71	0.15	-	112,112,112,112	0
56	MG	1H	3325	1/1	0.94	0.13	-	86,86,86,86	0
56	MG	14	3035	1/1	0.99	0.27	-	79,79,79,79	0
56	MG	13	1672	1/1	0.88	0.20	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1627	1/1	0.66	0.28	-	101,101,101,101	0
56	MG	1H	3478	1/1	0.87	0.09	-	118,118,118,118	0
56	MG	14	3086	1/1	0.96	0.28	-	84,84,84,84	0
56	MG	14	3028	1/1	0.90	0.14	-	98,98,98,98	0
56	MG	14	3003	1/1	0.94	0.13	-	73,73,73,73	0
56	MG	1H	3074	1/1	0.80	0.41	-	80,80,80,80	0
56	MG	14	3378	1/1	0.96	0.16	-	101,101,101,101	0
56	MG	1H	3420	1/1	0.92	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	1638	1/1	0.84	0.42	-	95,95,95,95	0
56	MG	14	3158	1/1	0.77	0.15	-	93,93,93,93	0
56	MG	1H	3418	1/1	0.93	0.06	-	134,134,134,134	0
56	MG	1H	3433	1/1	0.95	0.09	-	76,76,76,76	0
56	MG	1H	3394	1/1	0.97	0.09	-	62,62,62,62	0
56	MG	13	1646	1/1	0.90	0.24	-	104,104,104,104	0
56	MG	14	3408	1/1	0.98	0.08	-	79,79,79,79	0
56	MG	1H	3407	1/1	0.77	0.07	-	115,115,115,115	0
56	MG	14	3377	1/1	0.98	0.08	-	82,82,82,82	0
56	MG	14	3029	1/1	0.69	0.22	-	97,97,97,97	0
56	MG	14	3030	1/1	0.74	0.22	-	115,115,115,115	0
56	MG	14	3283	1/1	0.87	0.21	-	98,98,98,98	0
56	MG	14	3077	1/1	0.99	0.28	-	80,80,80,80	0
56	MG	I8	102	1/1	0.90	0.41	-	64,64,64,64	0
56	MG	78	202	1/1	0.93	0.20	-	97,97,97,97	0
56	MG	13	1693	1/1	0.78	0.21	-	103,103,103,103	0
56	MG	13	1670	1/1	0.86	0.33	-	88,88,88,88	0
56	MG	13	1629	1/1	0.62	0.45	-	106,106,106,106	0
56	MG	1H	3428	1/1	0.75	0.06	-	123,123,123,123	0
56	MG	14	3399	1/1	0.94	0.08	-	78,78,78,78	0
56	MG	1H	3183	1/1	0.93	0.29	-	83,83,83,83	0
56	MG	1H	3274	1/1	0.90	0.57	-	100,100,100,100	0
56	MG	14	3127	1/1	0.94	0.06	-	87,87,87,87	0
56	MG	14	3151	1/1	0.83	0.24	-	91,91,91,91	0
56	MG	1H	3495	1/1	0.92	0.32	-	91,91,91,91	0
56	MG	1H	3501	1/1	0.92	0.17	-	107,107,107,107	0
56	MG	1H	3363	1/1	0.96	0.21	-	71,71,71,71	0
56	MG	1H	3346	1/1	0.75	0.61	-	106,106,106,106	0
56	MG	1H	3149	1/1	0.92	0.54	-	99,99,99,99	0
56	MG	1H	3182	1/1	0.85	0.36	-	74,74,74,74	0
56	MG	14	3024	1/1	0.93	0.28	-	73,73,73,73	0
56	MG	1G	1629	1/1	0.55	0.18	-	124,124,124,124	0
56	MG	1H	3381	1/1	0.88	0.09	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3096	1/1	0.99	0.15	-	77,77,77,77	0
56	MG	14	3140	1/1	0.92	0.34	-	93,93,93,93	0
56	MG	13	1683	1/1	0.57	0.28	-	106,106,106,106	0
56	MG	1G	1605	1/1	0.90	0.17	-	98,98,98,98	0
56	MG	14	3277	1/1	0.88	0.20	-	90,90,90,90	0
56	MG	13	1658	1/1	0.57	0.44	-	117,117,117,117	0
56	MG	1H	3397	1/1	0.97	0.15	-	77,77,77,77	0
56	MG	1H	3415	1/1	0.75	0.07	-	99,99,99,99	0
56	MG	13	1730	1/1	0.95	0.03	-	113,113,113,113	0
56	MG	14	3302	1/1	0.91	0.19	-	92,92,92,92	0
56	MG	1H	3279	1/1	0.90	0.25	-	80,80,80,80	0
56	MG	13	1616	1/1	0.95	0.10	-	82,82,82,82	0
56	MG	14	3311	1/1	0.76	0.17	-	89,89,89,89	0
56	MG	1G	1648	1/1	0.83	0.23	-	100,100,100,100	0
56	MG	14	3273	1/1	0.88	0.14	-	87,87,87,87	0
56	MG	14	3210	1/1	0.91	0.37	-	98,98,98,98	0
56	MG	13	1610	1/1	0.97	0.20	-	79,79,79,79	0
56	MG	1H	3065	1/1	0.96	0.27	-	71,71,71,71	0
56	MG	14	3144	1/1	0.81	0.35	-	93,93,93,93	0
56	MG	1H	3291	1/1	0.92	0.29	-	77,77,77,77	0
56	MG	1H	3010	1/1	0.95	0.34	-	83,83,83,83	0
56	MG	1G	1602	1/1	0.85	0.38	-	118,118,118,118	0
56	MG	14	3291	1/1	0.71	0.18	-	115,115,115,115	0
56	MG	1H	3398	1/1	0.94	0.09	-	92,92,92,92	0
56	MG	1H	3305	1/1	0.80	0.61	-	104,104,104,104	0
56	MG	1G	1666	1/1	0.90	0.36	-	89,89,89,89	0
56	MG	1H	3406	1/1	0.98	0.16	-	77,77,77,77	0
56	MG	25	201	1/1	0.83	0.43	-	111,111,111,111	0
56	MG	C5	201	1/1	0.86	0.23	-	123,123,123,123	0
56	MG	13	1691	1/1	0.87	0.30	-	95,95,95,95	0
56	MG	14	3089	1/1	0.97	0.21	-	85,85,85,85	0
56	MG	13	1692	1/1	0.56	0.22	-	102,102,102,102	0
56	MG	14	3305	1/1	0.87	0.14	-	79,79,79,79	0
56	MG	1H	3047	1/1	0.95	0.30	-	65,65,65,65	0
56	MG	1H	3474	1/1	0.94	0.20	-	124,124,124,124	0
56	MG	14	3374	1/1	0.83	0.08	-	113,113,113,113	0
56	MG	14	3027	1/1	0.93	0.20	-	84,84,84,84	0
56	MG	14	3159	1/1	0.91	0.13	-	112,112,112,112	0
56	MG	1H	3202	1/1	0.78	0.37	-	93,93,93,93	0
56	MG	1H	3175	1/1	0.77	0.35	-	93,93,93,93	0
56	MG	14	3276	1/1	0.74	1.34	-	103,103,103,103	0
56	MG	14	3179	1/1	0.95	0.31	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3487	1/1	0.83	0.29	-	126,126,126,126	0
56	MG	1H	3174	1/1	0.85	0.31	-	78,78,78,78	0
56	MG	14	3185	1/1	0.84	0.20	-	90,90,90,90	0
56	MG	1J	210	1/1	0.94	0.06	-	109,109,109,109	0
56	MG	13	1705	1/1	0.98	0.14	-	98,98,98,98	0
56	MG	1H	3073	1/1	0.94	0.24	-	88,88,88,88	0
56	MG	13	1653	1/1	0.95	0.21	-	78,78,78,78	0
56	MG	1H	3334	1/1	0.91	0.50	-	99,99,99,99	0
56	MG	14	3123	1/1	0.87	0.16	-	75,75,75,75	0
56	MG	14	3037	1/1	0.90	0.20	-	79,79,79,79	0
56	MG	14	3213	1/1	0.93	0.17	-	113,113,113,113	0
56	MG	13	1746	1/1	0.97	0.07	-	110,110,110,110	0
56	MG	1H	3267	1/1	0.79	0.34	-	84,84,84,84	0
56	MG	1H	3311	1/1	0.68	0.48	-	109,109,109,109	0
56	MG	1H	3282	1/1	0.88	0.14	-	107,107,107,107	0
56	MG	1J	202	1/1	0.86	0.12	-	157,157,157,157	0
56	MG	14	3410	1/1	0.94	0.30	-	96,96,96,96	0
56	MG	1H	3134	1/1	0.96	0.13	-	57,57,57,57	0
56	MG	14	3059	1/1	0.94	0.27	-	74,74,74,74	0
56	MG	14	3295	1/1	0.61	0.62	-	95,95,95,95	0
56	MG	13	1631	1/1	0.51	0.70	-	102,102,102,102	0
56	MG	1H	3086	1/1	0.87	0.39	-	72,72,72,72	0
56	MG	1G	1661	1/1	0.90	0.26	-	105,105,105,105	0
56	MG	2K	104	1/1	0.87	0.44	-	90,90,90,90	0
56	MG	1H	3484	1/1	0.98	0.09	-	79,79,79,79	0
56	MG	1G	1615	1/1	0.86	0.23	-	115,115,115,115	0
56	MG	1H	3126	1/1	0.82	0.32	-	79,79,79,79	0
56	MG	14	3174	1/1	0.88	0.18	-	93,93,93,93	0
56	MG	1H	3135	1/1	0.70	0.26	-	111,111,111,111	0
56	MG	1H	3158	1/1	0.62	0.46	-	104,104,104,104	0
56	MG	14	3292	1/1	0.93	0.17	-	90,90,90,90	0
56	MG	13	1605	1/1	0.86	0.18	-	93,93,93,93	0
56	MG	14	3225	1/1	0.94	0.20	-	65,65,65,65	0
56	MG	14	3325	1/1	0.83	0.34	-	89,89,89,89	0
56	MG	14	3167	1/1	0.79	0.27	-	110,110,110,110	0
56	MG	14	3245	1/1	0.96	0.18	-	71,71,71,71	0
56	MG	13	1656	1/1	0.74	0.42	-	103,103,103,103	0
56	MG	14	3359	1/1	0.95	0.13	-	114,114,114,114	0
56	MG	1H	3321	1/1	0.85	0.27	-	99,99,99,99	0
56	MG	14	3384	1/1	0.95	0.14	-	60,60,60,60	0
56	MG	14	3020	1/1	0.54	0.51	-	92,92,92,92	0
56	MG	14	3372	1/1	0.70	0.12	-	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3316	1/1	0.90	0.57	-	94,94,94,94	0
56	MG	1H	3498	1/1	0.39	0.20	-	119,119,119,119	0
56	MG	M5	101	1/1	0.56	0.25	-	94,94,94,94	0
56	MG	1H	3143	1/1	0.70	0.44	-	99,99,99,99	0
56	MG	13	1709	1/1	0.94	0.28	-	141,141,141,141	0
56	MG	39	302	1/1	0.78	0.30	-	118,118,118,118	0
56	MG	1H	3285	1/1	0.84	0.39	-	88,88,88,88	0
56	MG	13	1649	1/1	0.97	0.27	-	85,85,85,85	0
56	MG	14	3416	1/1	0.71	0.43	-	126,126,126,126	0
56	MG	13	1710	1/1	0.45	0.30	-	98,98,98,98	0
56	MG	14	3160	1/1	0.92	0.32	-	85,85,85,85	0
56	MG	14	3261	1/1	0.82	0.34	-	83,83,83,83	0
56	MG	1H	3410	1/1	0.93	0.12	-	73,73,73,73	0
56	MG	1H	3041	1/1	0.92	0.33	-	67,67,67,67	0
56	MG	14	3141	1/1	0.94	0.19	-	80,80,80,80	0
56	MG	1H	3071	1/1	0.90	0.12	-	94,94,94,94	0
56	MG	1H	3141	1/1	0.85	0.44	-	89,89,89,89	0
56	MG	1H	3102	1/1	0.86	0.28	-	67,67,67,67	0
56	MG	1H	3297	1/1	0.92	0.10	-	86,86,86,86	0
56	MG	1H	3437	1/1	0.93	0.06	-	109,109,109,109	0
56	MG	1H	3441	1/1	0.94	0.10	-	122,122,122,122	0
56	MG	14	3385	1/1	0.99	0.12	-	73,73,73,73	0
56	MG	14	3364	1/1	0.95	0.07	-	87,87,87,87	0
56	MG	14	3413	1/1	0.87	0.31	-	110,110,110,110	0
56	MG	14	3182	1/1	0.70	0.27	-	98,98,98,98	0
56	MG	13	1678	1/1	0.94	0.09	-	111,111,111,111	0
56	MG	1G	1651	1/1	0.97	0.20	-	138,138,138,138	0
56	MG	1H	3002	1/1	0.93	0.23	-	76,76,76,76	0
56	MG	14	3419	1/1	0.90	0.25	-	112,112,112,112	0
56	MG	13	1623	1/1	0.96	0.15	-	84,84,84,84	0
56	MG	1H	3408	1/1	0.95	0.09	-	87,87,87,87	0
56	MG	14	3370	1/1	0.82	0.12	-	110,110,110,110	0
56	MG	1H	3248	1/1	0.93	0.23	-	76,76,76,76	0
56	MG	13	1742	1/1	0.98	0.10	-	82,82,82,82	0
56	MG	13	1704	1/1	0.85	0.69	-	118,118,118,118	0
56	MG	1H	3045	1/1	0.98	0.20	-	63,63,63,63	0
56	MG	1J	205	1/1	0.86	0.23	-	101,101,101,101	0
56	MG	1H	3099	1/1	0.95	0.33	-	69,69,69,69	0
56	MG	2K	106	1/1	0.82	0.42	-	115,115,115,115	0
56	MG	14	3415	1/1	0.90	0.40	-	107,107,107,107	0
56	MG	1H	3131	1/1	0.97	0.17	-	56,56,56,56	0
56	MG	1H	3472	1/1	0.99	0.08	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3027	1/1	0.78	0.32	-	96,96,96,96	0
56	MG	14	3011	1/1	0.96	0.20	-	61,61,61,61	0
56	MG	14	3265	1/1	0.73	0.29	-	88,88,88,88	0
56	MG	1H	3266	1/1	0.72	0.58	-	95,95,95,95	0
56	MG	1H	3475	1/1	0.94	0.18	-	76,76,76,76	0
56	MG	14	3080	1/1	0.79	0.41	-	88,88,88,88	0
56	MG	13	1726	1/1	0.95	0.12	-	90,90,90,90	0
56	MG	1H	3228	1/1	0.93	0.55	-	94,94,94,94	0
56	MG	16	204	1/1	0.91	0.40	-	99,99,99,99	0
56	MG	1H	3289	1/1	0.96	0.22	-	93,93,93,93	0
56	MG	1H	3078	1/1	0.97	0.23	-	70,70,70,70	0
56	MG	14	3318	1/1	0.76	0.19	-	99,99,99,99	0
56	MG	1H	3432	1/1	0.92	0.06	-	113,113,113,113	0
56	MG	1H	3328	1/1	0.64	0.55	-	87,87,87,87	0
56	MG	14	3197	1/1	0.86	0.50	-	119,119,119,119	0
56	MG	1H	3152	1/1	0.76	0.30	-	93,93,93,93	0
56	MG	14	3406	1/1	0.94	0.07	-	99,99,99,99	0
56	MG	1H	3355	1/1	0.98	0.18	-	64,64,64,64	0
56	MG	14	3184	1/1	0.93	0.34	-	94,94,94,94	0
56	MG	1H	3464	1/1	0.68	0.14	-	133,133,133,133	0
56	MG	1G	1671	1/1	0.87	0.40	-	120,120,120,120	0
56	MG	13	1635	1/1	0.95	0.14	-	88,88,88,88	0
56	MG	1H	3275	1/1	0.95	0.30	-	97,97,97,97	0
56	MG	16	208	1/1	0.95	0.55	-	94,94,94,94	0
56	MG	14	3162	1/1	0.82	0.19	-	88,88,88,88	0
56	MG	1H	3479	1/1	0.81	0.16	-	126,126,126,126	0
56	MG	14	3304	1/1	0.91	0.33	-	121,121,121,121	0
56	MG	1H	3257	1/1	0.94	0.33	-	80,80,80,80	0
56	MG	13	1637	1/1	0.91	0.25	-	96,96,96,96	0
56	MG	14	3090	1/1	0.96	0.20	-	89,89,89,89	0
56	MG	1H	3127	1/1	0.81	0.29	-	92,92,92,92	0
56	MG	1H	3448	1/1	0.91	0.15	-	97,97,97,97	0
56	MG	1H	3189	1/1	0.77	0.30	-	81,81,81,81	0
56	MG	14	3242	1/1	0.96	0.16	-	94,94,94,94	0
56	MG	14	3279	1/1	0.84	0.25	-	87,87,87,87	0
56	MG	1H	3401	1/1	0.97	0.16	-	87,87,87,87	0
56	MG	14	3038	1/1	0.99	0.16	-	72,72,72,72	0
56	MG	1H	3176	1/1	0.95	0.30	-	91,91,91,91	0
56	MG	1H	3272	1/1	0.65	0.27	-	96,96,96,96	0
56	MG	14	3247	1/1	0.85	0.14	-	75,75,75,75	0
56	MG	1H	3269	1/1	0.96	0.52	-	90,90,90,90	0
56	MG	1H	3117	1/1	0.96	0.29	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3327	1/1	0.94	0.39	-	91,91,91,91	0
56	MG	14	3259	1/1	0.91	0.15	-	100,100,100,100	0
56	MG	13	1711	1/1	0.92	0.63	-	126,126,126,126	0
56	MG	16	211	1/1	0.94	0.40	-	79,79,79,79	0
56	MG	1H	3029	1/1	0.63	0.28	-	110,110,110,110	0
56	MG	1H	3457	1/1	0.89	0.05	-	113,113,113,113	0
56	MG	1H	3461	1/1	0.93	0.08	-	110,110,110,110	0
56	MG	14	3097	1/1	0.97	0.12	-	69,69,69,69	0
56	MG	1H	3270	1/1	0.62	0.48	-	98,98,98,98	0
56	MG	14	3296	1/1	0.89	0.20	-	107,107,107,107	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	1H	3326	1/1	0.69	0.54	-	117,117,117,117	0
56	MG	1H	3068	1/1	0.94	0.27	-	98,98,98,98	0
56	MG	14	3081	1/1	0.90	0.31	-	90,90,90,90	0
56	MG	14	3186	1/1	0.93	0.21	-	86,86,86,86	0
56	MG	13	1639	1/1	0.70	0.19	-	109,109,109,109	0
56	MG	1G	1633	1/1	0.49	0.32	-	93,93,93,93	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	16	212	1/1	0.96	0.43	-	99,99,99,99	0
56	MG	14	3299	1/1	0.93	0.58	-	84,84,84,84	0
56	MG	1G	1630	1/1	0.95	0.47	-	116,116,116,116	0
56	MG	14	3398	1/1	0.87	0.06	-	127,127,127,127	0
56	MG	1H	3292	1/1	0.81	0.23	-	72,72,72,72	0
56	MG	1H	3232	1/1	0.82	0.32	-	80,80,80,80	0
56	MG	13	1718	1/1	0.73	0.41	-	96,96,96,96	0
56	MG	14	3057	1/1	0.96	0.15	-	91,91,91,91	0
56	MG	13	1735	1/1	0.97	0.07	-	96,96,96,96	0
56	MG	1G	1624	1/1	0.97	0.17	-	93,93,93,93	0
56	MG	1H	3094	1/1	0.94	0.39	-	79,79,79,79	0
56	MG	14	3381	1/1	0.87	0.22	-	101,101,101,101	0
56	MG	13	1701	1/1	0.93	0.57	-	103,103,103,103	0
56	MG	1H	3387	1/1	0.96	0.17	-	70,70,70,70	0
56	MG	1H	3165	1/1	0.81	0.42	-	95,95,95,95	0
56	MG	1H	3075	1/1	0.96	0.08	-	59,59,59,59	0
56	MG	14	3032	1/1	0.98	0.20	-	52,52,52,52	0
56	MG	14	3102	1/1	0.92	0.36	-	93,93,93,93	0
56	MG	14	3176	1/1	0.79	0.39	-	101,101,101,101	0
56	MG	13	1628	1/1	0.96	0.35	-	102,102,102,102	0
56	MG	1H	3017	1/1	0.99	0.23	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3392	1/1	0.99	0.08	-	70,70,70,70	0
56	MG	14	3228	1/1	0.96	0.20	-	86,86,86,86	0
56	MG	14	3065	1/1	0.82	0.20	-	87,87,87,87	0
56	MG	14	3001	1/1	0.95	0.12	-	66,66,66,66	0
56	MG	1G	1639	1/1	0.86	0.17	-	89,89,89,89	0
56	MG	1H	3459	1/1	0.97	0.13	-	81,81,81,81	0
56	MG	1G	1626	1/1	0.97	0.27	-	102,102,102,102	0
56	MG	1H	3359	1/1	0.93	0.11	-	83,83,83,83	0
56	MG	1G	1634	1/1	0.87	0.48	-	120,120,120,120	0
56	MG	14	3157	1/1	0.94	0.31	-	76,76,76,76	0
56	MG	14	3071	1/1	0.94	0.12	-	94,94,94,94	0
56	MG	14	3328	1/1	0.87	0.12	-	111,111,111,111	0
56	MG	1H	3300	1/1	0.81	0.35	-	87,87,87,87	0
56	MG	1G	1657	1/1	0.79	0.25	-	106,106,106,106	0
56	MG	1H	3249	1/1	0.80	0.41	-	97,97,97,97	0
56	MG	14	3329	1/1	0.58	0.21	-	120,120,120,120	0
56	MG	13	1707	1/1	0.90	0.25	-	104,104,104,104	0
56	MG	14	3237	1/1	0.77	0.24	-	95,95,95,95	0
56	MG	1G	1641	1/1	0.88	0.29	-	90,90,90,90	0
56	MG	1H	3500	1/1	0.77	0.20	-	122,122,122,122	0
56	MG	14	3289	1/1	0.89	0.18	-	86,86,86,86	0
56	MG	14	3371	1/1	0.89	0.21	-	101,101,101,101	0
56	MG	1H	3177	1/1	0.84	0.44	-	98,98,98,98	0
56	MG	16	215	1/1	0.81	0.08	-	113,113,113,113	0
56	MG	14	3418	1/1	0.74	0.07	-	130,130,130,130	0
56	MG	1G	1681	1/1	0.94	0.18	-	133,133,133,133	0
56	MG	13	1619	1/1	0.93	0.58	-	103,103,103,103	0
56	MG	1G	1685	1/1	0.98	0.08	-	112,112,112,112	0
56	MG	1G	1603	1/1	0.86	0.17	-	118,118,118,118	0
56	MG	4K	101	1/1	0.94	0.19	-	90,90,90,90	0
56	MG	1H	3171	1/1	0.97	0.51	-	75,75,75,75	0
56	MG	14	3420	1/1	0.48	0.07	-	130,130,130,130	0
56	MG	1H	3261	1/1	0.95	0.48	-	99,99,99,99	0
56	MG	1H	3051	1/1	0.93	0.24	-	53,53,53,53	0
56	MG	1H	3490	1/1	0.83	0.13	-	125,125,125,125	0
56	MG	14	3290	1/1	0.94	0.26	-	113,113,113,113	0
56	MG	1H	3243	1/1	0.60	0.36	-	93,93,93,93	0
56	MG	1G	1621	1/1	0.98	0.11	-	88,88,88,88	0
56	MG	1H	3147	1/1	0.77	0.31	-	94,94,94,94	0
56	MG	1H	3342	1/1	0.84	0.17	-	92,92,92,92	0
56	MG	13	1741	1/1	0.94	0.08	-	118,118,118,118	0
56	MG	1G	1656	1/1	0.90	0.30	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3323	1/1	0.94	0.10	-	101,101,101,101	0
56	MG	14	3078	1/1	0.93	0.11	-	97,97,97,97	0
56	MG	13	1697	1/1	0.47	0.26	-	97,97,97,97	0
56	MG	14	3362	1/1	0.94	0.17	-	101,101,101,101	0
56	MG	1H	3168	1/1	0.83	0.30	-	83,83,83,83	0
56	MG	1H	3294	1/1	0.83	0.46	-	100,100,100,100	0
56	MG	13	1640	1/1	0.70	0.23	-	94,94,94,94	0
56	MG	1H	3256	1/1	0.85	0.26	-	88,88,88,88	0
56	MG	1G	1673	1/1	0.81	0.14	-	108,108,108,108	0
56	MG	14	3002	1/1	0.97	0.24	-	70,70,70,70	0
56	MG	1H	3425	1/1	0.94	0.06	-	95,95,95,95	0
56	MG	1H	3154	1/1	0.54	0.22	-	91,91,91,91	0
56	MG	14	3021	1/1	0.95	0.40	-	79,79,79,79	0
56	MG	13	1614	1/1	0.97	0.16	-	98,98,98,98	0
56	MG	1H	3463	1/1	0.95	0.04	-	113,113,113,113	0
56	MG	14	3042	1/1	0.94	0.21	-	87,87,87,87	0
56	MG	14	3156	1/1	0.93	0.18	-	99,99,99,99	0
56	MG	14	3142	1/1	0.84	0.46	-	100,100,100,100	0
56	MG	13	1703	1/1	0.92	0.37	-	96,96,96,96	0
56	MG	1H	3444	1/1	0.95	0.29	-	102,102,102,102	0
56	MG	1H	3331	1/1	0.70	0.83	-	106,106,106,106	0
56	MG	35	201	1/1	0.89	0.21	-	91,91,91,91	0
56	MG	1H	3430	1/1	0.90	0.10	-	116,116,116,116	0
56	MG	14	3271	1/1	0.91	0.12	-	87,87,87,87	0
56	MG	1H	3204	1/1	0.88	0.75	-	104,104,104,104	0
56	MG	1H	3213	1/1	0.95	0.27	-	113,113,113,113	0
56	MG	1H	3162	1/1	0.92	0.24	-	74,74,74,74	0
56	MG	14	3045	1/1	0.96	0.17	-	70,70,70,70	0
56	MG	1H	3181	1/1	0.91	0.34	-	74,74,74,74	0
56	MG	1H	3046	1/1	0.96	0.30	-	72,72,72,72	0
56	MG	14	3409	1/1	0.92	0.07	-	114,114,114,114	0
56	MG	13	1731	1/1	0.94	0.06	-	91,91,91,91	0
56	MG	1H	3150	1/1	0.93	0.36	-	86,86,86,86	0
56	MG	1H	3104	1/1	0.89	0.22	-	78,78,78,78	0
56	MG	13	1737	1/1	0.98	0.14	-	72,72,72,72	0
56	MG	14	3340	1/1	0.95	0.34	-	91,91,91,91	0
56	MG	1H	3287	1/1	0.81	0.42	-	92,92,92,92	0
56	MG	1H	3340	1/1	0.73	0.36	-	93,93,93,93	0
56	MG	1H	3107	1/1	0.81	0.28	-	85,85,85,85	0
56	MG	14	3116	1/1	0.97	0.21	-	73,73,73,73	0
56	MG	1G	1640	1/1	0.79	0.49	-	106,106,106,106	0
56	MG	1H	3382	1/1	0.99	0.10	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3133	1/1	0.91	0.14	-	84,84,84,84	0
56	MG	14	3074	1/1	0.95	0.13	-	79,79,79,79	0
56	MG	1H	3314	1/1	0.81	0.37	-	76,76,76,76	0
56	MG	14	3394	1/1	0.92	0.07	-	93,93,93,93	0
56	MG	14	3314	1/1	0.94	0.34	-	102,102,102,102	0
56	MG	1H	3014	1/1	0.98	0.42	-	57,57,57,57	0
56	MG	14	3284	1/1	0.57	0.30	-	100,100,100,100	0
56	MG	13	1659	1/1	0.97	0.31	-	109,109,109,109	0
56	MG	1H	3066	1/1	0.95	0.27	-	71,71,71,71	0
56	MG	14	3223	1/1	0.97	0.82	-	81,81,81,81	0
56	MG	1G	1620	1/1	0.73	0.20	-	107,107,107,107	0
56	MG	1H	3164	1/1	0.95	0.43	-	102,102,102,102	0
56	MG	13	1613	1/1	0.94	0.18	-	96,96,96,96	0
56	MG	13	1685	1/1	0.77	0.17	-	112,112,112,112	0
56	MG	1H	3434	1/1	0.86	0.19	-	130,130,130,130	0
56	MG	14	3015	1/1	0.97	0.08	-	81,81,81,81	0
56	MG	1H	3449	1/1	0.97	0.15	-	78,78,78,78	0
56	MG	14	3232	1/1	0.74	0.29	-	103,103,103,103	0
56	MG	1H	3307	1/1	0.78	0.28	-	99,99,99,99	0
56	MG	13	1684	1/1	0.82	0.33	-	106,106,106,106	0
56	MG	1H	3477	1/1	0.83	0.10	-	108,108,108,108	0
56	MG	1H	3378	1/1	0.93	0.09	-	94,94,94,94	0
56	MG	14	3231	1/1	0.89	0.21	-	93,93,93,93	0
56	MG	14	3139	1/1	0.95	0.19	-	67,67,67,67	0
56	MG	1H	3097	1/1	0.92	0.20	-	89,89,89,89	0
56	MG	1H	3197	1/1	0.96	0.41	-	89,89,89,89	0
56	MG	14	3269	1/1	0.90	0.31	-	102,102,102,102	0
56	MG	14	3307	1/1	0.52	0.25	-	87,87,87,87	0
56	MG	1H	3486	1/1	0.96	0.07	-	98,98,98,98	0
56	MG	14	3293	1/1	0.81	0.27	-	95,95,95,95	0
56	MG	14	3229	1/1	0.93	0.19	-	83,83,83,83	0
56	MG	1H	3123	1/1	0.99	0.24	-	68,68,68,68	0
56	MG	2L	102	1/1	0.70	0.26	-	89,89,89,89	0
56	MG	1H	3169	1/1	0.75	0.25	-	85,85,85,85	0
56	MG	1H	3114	1/1	0.96	0.42	-	82,82,82,82	0
56	MG	1H	3447	1/1	0.85	0.17	-	105,105,105,105	0
56	MG	14	3155	1/1	0.97	0.16	-	76,76,76,76	0
56	MG	14	3395	1/1	0.91	0.09	-	96,96,96,96	0
56	MG	14	3048	1/1	0.98	0.20	-	73,73,73,73	0
56	MG	1H	3445	1/1	0.97	0.12	-	83,83,83,83	0
56	MG	14	3368	1/1	0.76	0.12	-	117,117,117,117	0
56	MG	1H	3048	1/1	0.98	0.21	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3064	1/1	0.77	0.26	-	97,97,97,97	0
56	MG	1H	3320	1/1	0.92	0.73	-	106,106,106,106	0
56	MG	1H	3156	1/1	0.96	0.36	-	110,110,110,110	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	1H	3242	1/1	0.81	0.52	-	105,105,105,105	0
56	MG	1H	3091	1/1	0.97	0.36	-	70,70,70,70	0
56	MG	1H	3043	1/1	0.98	0.27	-	72,72,72,72	0
56	MG	1H	3190	1/1	0.84	0.17	-	77,77,77,77	0
56	MG	1H	3504	1/1	0.75	0.11	-	138,138,138,138	0
56	MG	2K	107	1/1	0.91	0.41	-	106,106,106,106	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	1H	3108	1/1	0.90	0.22	-	86,86,86,86	0
56	MG	14	3327	1/1	0.98	0.43	-	117,117,117,117	0
56	MG	14	3270	1/1	0.80	0.20	-	107,107,107,107	0
56	MG	14	3243	1/1	0.92	0.10	-	91,91,91,91	0
56	MG	13	1651	1/1	0.71	0.23	-	100,100,100,100	0
56	MG	13	1654	1/1	0.88	0.28	-	123,123,123,123	0
56	MG	1G	1687	1/1	0.84	0.30	-	135,135,135,135	0
56	MG	13	1609	1/1	0.96	0.19	-	83,83,83,83	0
56	MG	14	3180	1/1	0.95	0.31	-	83,83,83,83	0
56	MG	1G	1636	1/1	0.88	0.08	-	115,115,115,115	0
56	MG	14	3163	1/1	0.65	0.18	-	105,105,105,105	0
56	MG	13	1674	1/1	0.89	0.23	-	118,118,118,118	0
56	MG	2L	103	1/1	0.84	0.28	-	115,115,115,115	0
56	MG	1H	3301	1/1	0.94	0.24	-	79,79,79,79	0
56	MG	14	3363	1/1	0.88	0.06	-	117,117,117,117	0
56	MG	13	1708	1/1	0.61	0.34	-	119,119,119,119	0
56	MG	1H	3250	1/1	0.59	0.21	-	104,104,104,104	0
56	MG	1H	3220	1/1	0.94	0.29	-	124,124,124,124	0
56	MG	1H	3098	1/1	0.92	0.23	-	72,72,72,72	0
56	MG	14	3172	1/1	0.96	0.21	-	107,107,107,107	0
56	MG	1H	3259	1/1	0.98	0.52	-	105,105,105,105	0
56	MG	1H	3121	1/1	0.94	0.21	-	80,80,80,80	0

## 6.5 Other polymers

There are no such residues in this entry.