



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 07:28 AM GMT

PDB ID : 4WRA  
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in the first position in the A-site and with antibiotic paromomycin.  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-23  
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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



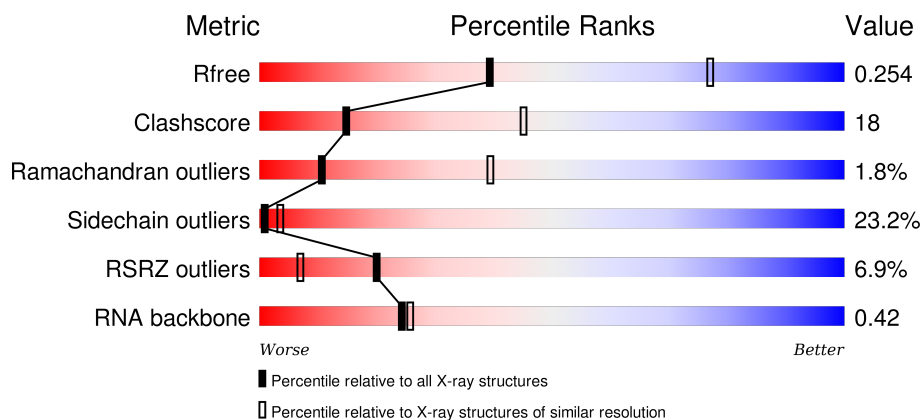
# 1 Overall quality at a glance

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>2%</div> <div>33% 44% 17% . .</div> </div>
1	1G	1522	<div> <div>2%</div> <div>38% 42% 17% . .</div> </div>
2	12	256	<div> <div>3%</div> <div>41% 39% 13% 7%</div> </div>
2	1E	256	<div> <div>2%</div> <div>39% 41% 12% 7%</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	85	
23	2K	77	
23	2L	77	
24	1L	85	
24	3K	85	
25	4K	30	
25	4L	30	
26	14	2918	
26	1H	2918	
27	16	122	
27	1J	122	
28	11	276	

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Mol	Chain	Length	Quality of chain
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	
40	B8	146	

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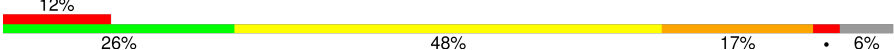
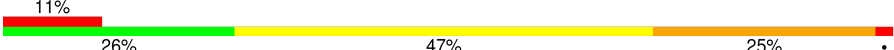
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Mol	Chain	Length	Quality of chain
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1611	-	-	-	X
56	MG	13	1613	-	-	-	X
56	MG	13	1625	-	-	-	X
56	MG	13	1649	-	-	-	X
56	MG	13	1654	-	-	-	X
56	MG	13	1680	-	-	-	X
56	MG	13	1696	-	-	-	X
56	MG	13	1705	-	-	-	X
56	MG	14	3031	-	-	-	X
56	MG	14	3045	-	-	-	X
56	MG	14	3078	-	-	-	X
56	MG	14	3092	-	-	-	X
56	MG	14	3117	-	-	-	X
56	MG	14	3126	-	-	-	X
56	MG	14	3136	-	-	-	X
56	MG	14	3138	-	-	-	X
56	MG	14	3142	-	-	-	X
56	MG	14	3159	-	-	-	X
56	MG	14	3186	-	-	-	X
56	MG	14	3192	-	-	-	X
56	MG	14	3197	-	-	-	X
56	MG	14	3202	-	-	-	X
56	MG	14	3224	-	-	-	X
56	MG	14	3235	-	-	-	X
56	MG	14	3253	-	-	-	X
56	MG	14	3281	-	-	-	X
56	MG	14	3291	-	-	-	X
56	MG	14	3299	-	-	-	X
56	MG	14	3301	-	-	-	X
56	MG	14	3305	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3391	-	-	-	X
56	MG	16	201	-	-	-	X
56	MG	16	205	-	-	-	X
56	MG	1G	1610	-	-	-	X
56	MG	1G	1637	-	-	-	X
56	MG	1G	1642	-	-	-	X
56	MG	1G	1655	-	-	-	X
56	MG	1H	3007	-	-	-	X
56	MG	1H	3014	-	-	-	X
56	MG	1H	3022	-	-	-	X
56	MG	1H	3028	-	-	-	X
56	MG	1H	3046	-	-	-	X
56	MG	1H	3049	-	-	-	X
56	MG	1H	3050	-	-	-	X
56	MG	1H	3075	-	-	-	X
56	MG	1H	3081	-	-	-	X
56	MG	1H	3084	-	-	-	X
56	MG	1H	3089	-	-	-	X
56	MG	1H	3094	-	-	-	X
56	MG	1H	3095	-	-	-	X
56	MG	1H	3118	-	-	-	X
56	MG	1H	3122	-	-	-	X
56	MG	1H	3128	-	-	-	X
56	MG	1H	3141	-	-	-	X
56	MG	1H	3144	-	-	-	X
56	MG	1H	3148	-	-	-	X
56	MG	1H	3149	-	-	-	X
56	MG	1H	3153	-	-	-	X
56	MG	1H	3161	-	-	-	X
56	MG	1H	3175	-	-	-	X
56	MG	1H	3177	-	-	-	X
56	MG	1H	3193	-	-	-	X
56	MG	1H	3205	-	-	-	X
56	MG	1H	3206	-	-	-	X
56	MG	1H	3221	-	-	-	X
56	MG	1H	3241	-	-	-	X
56	MG	1H	3265	-	-	-	X
56	MG	1H	3297	-	-	-	X
56	MG	1H	3299	-	-	-	X
56	MG	1H	3306	-	-	-	X
56	MG	1H	3310	-	-	-	X
56	MG	1H	3315	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3357	-	-	-	X
56	MG	1H	3366	-	-	-	X
56	MG	1H	3367	-	-	-	X
56	MG	2K	102	-	-	-	X
56	MG	41	201	-	-	-	X
58	ZN	32	301	-	-	-	X



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 299607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1505	Total	C	N	O	P	0	0	0
			32352	14399	5994	10454	1505			
1	1G	1504	Total	C	N	O	P	0	0	0
			32327	14389	5989	10446	1503			

- 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	152	Total	C	N	O	S	0	0	0
			1243	774	249	214	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			480	306	100	70	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	71	Total	C	N	O	0	0	0
			581	370	115	96			

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

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

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

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

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



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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 25 is a RNA chain called mRNA.

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	654A	A	G	conflict	GB 48268
1H	654E	C	G	conflict	GB 48268
1H	654P	G	C	conflict	GB 48268
1H	654T	A	C	conflict	GB 48268
1H	1058	U	G	conflict	GB 48268
1H	1080	A	C	conflict	GB 48268
1H	1228	G	-	insertion	GB 48268
14	158	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	654A	A	G	conflict	GB 48268
14	654E	C	G	conflict	GB 48268
14	654P	G	C	conflict	GB 48268
14	654T	A	C	conflict	GB 48268
14	1058	U	G	conflict	GB 48268
14	1080	A	C	conflict	GB 48268
14	1228	G	-	insertion	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	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	173	Total	C	N	O	S	0	0	0
			1321	837	248	235	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	93	Total	C	N	O	0	0	0
			730	474	132	124			
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	138	Total	C	N	O	S	0	0	0
			1139	732	205	199	3			

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	45	1	Total 1	Mg 1	0	0
56	P8	1	Total 1	Mg 1	0	0
56	85	1	Total 1	Mg 1	0	0
56	C5	1	Total 1	Mg 1	0	0
56	13	146	Total 146	Mg 146	0	0
56	1J	6	Total 6	Mg 6	0	0
56	35	1	Total 1	Mg 1	0	0
56	16	12	Total 12	Mg 12	0	0
56	25	1	Total 1	Mg 1	0	0
56	21	2	Total 2	Mg 2	0	0
56	31	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0
56	3I	1	Total 1	Mg 1	0	0
56	I8	1	Total 1	Mg 1	0	0
56	L5	1	Total 1	Mg 1	0	0
56	5E	1	Total 1	Mg 1	0	0
56	29	3	Total 3	Mg 3	0	0
56	2K	7	Total 7	Mg 7	0	0
56	39	1	Total 1	Mg 1	0	0
56	1G	86	Total 86	Mg 86	0	0
56	11	2	Total 2	Mg 2	0	0

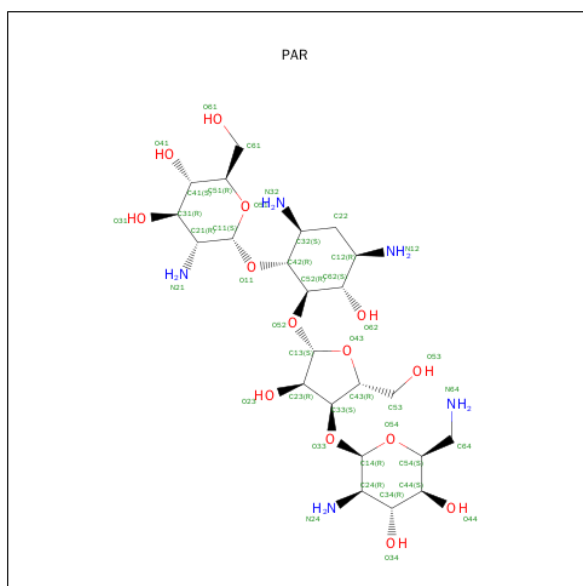
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1H	481	Total	Mg	0	0
			481	481		
56	88	1	Total	Mg	0	0
			1	1		
56	14	391	Total	Mg	0	0
			391	391		
56	78	1	Total	Mg	0	0
			1	1		
56	3E	1	Total	Mg	0	0
			1	1		
56	1K	1	Total	Mg	0	0
			1	1		
56	41	1	Total	Mg	0	0
			1	1		
56	2L	4	Total	Mg	0	0
			4	4		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	13	1	Total	C	N	O	0	0
			42	23	5	14		
57	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).



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

- Molecule 59 is water.

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

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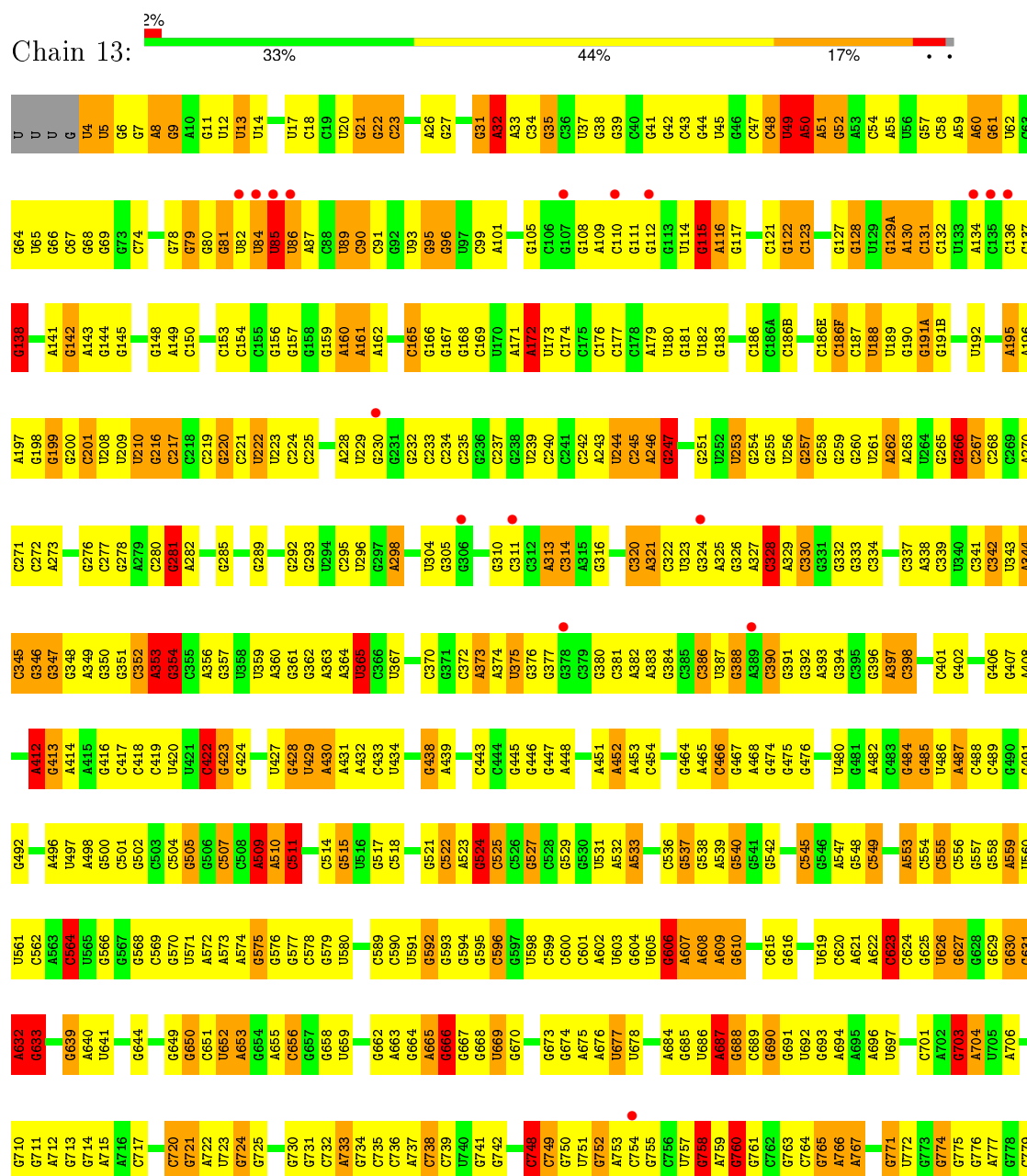
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	F8	1	Total 1	O 1	0	0
59	G8	2	Total 2	O 2	0	0
59	J8	1	Total 1	O 1	0	0
59	L8	2	Total 2	O 2	0	0
59	1G	87	Total 87	O 87	0	0
59	5A	1	Total 1	O 1	0	0
59	6A	1	Total 1	O 1	0	0
59	BA	1	Total 1	O 1	0	0
59	14	474	Total 474	O 474	0	0
59	1J	6	Total 6	O 6	0	0
59	19	9	Total 9	O 9	0	0
59	29	3	Total 3	O 3	0	0
59	39	5	Total 5	O 5	0	0
59	55	1	Total 1	O 1	0	0
59	75	1	Total 1	O 1	0	0
59	85	1	Total 1	O 1	0	0
59	A5	1	Total 1	O 1	0	0
59	M5	2	Total 2	O 2	0	0



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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







Frequency	Percentage
Never	2%
Once a week	38%
Several times a week	42%
Every day	17%



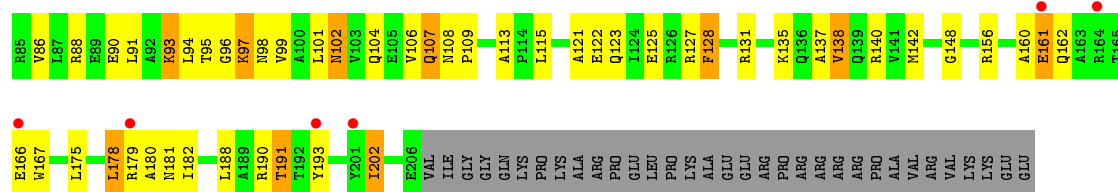


A1286	G1087	A1151	G1087	A1015	G947	G856	G765	G691	C615	C543	A478	A397	G322	C235
A1287	G1088	G1154	G1088	A1016	C948	G867	A766	A696	G616	G944	G479	C398	G323	G236
A1288	G1089	G1155	G1089	C1017	G951	U870	A767	U697	G617	C545	U480	G406	G326	C237
G1291	A1092	G1156	A1092	C1018	G954	A872	G771	A702	U619	A547	G484	G407	A243	U244
G1292	A1093	G1157	A1093	C1019	U955	A873	U772	G703	C620	G550	G485	G408	C328	U245
G1293	G1094	G1158	G1094	G1020	U956	A874	U777	A704	A621	G553	G486	G409	C245	C246
G1294	U1095	G1159	U1095	G1021	U957	C875	G778	G705	C623	A553	A487	G410	C330	G247
G1295	U1096	G1160	U1096	G1022	A958	G876	G779	A706	G624	C554	C488	G411	G331	A250
G1296	C1097	G1161	C1097	G1023	A959	C877	G780	A707	G625	C555	C489	A412	G332	U251
G1297	A1101	G1162	A1101	U1024	U960	G878	A780	C708	U626	C556	G490	G413	C337	U252
G1298	G1163	G1167	G1163	G1025	U961	G879	G781	C709	U627	C557	G491	G416	A338	U253
G1299	A1164	G1168	A1164	G1026	U962	C880	G784	G710	C628	A559	G492	C417	C339	U254
G1300	G1165	G1169	G1165	C1027	C963	G881	G785	G711	G629	U560	G493	C418	A344	G255
U1301	A1170	G1170	A1170	C1028	A964	C882	G786	G712	G630	U561	U494	G419	A345	U256
U1302	G1171	G1172	G1171	C1028A	A965	C883	A787	G713	G631	C562	U495	U420	C346	U257
C1303	C1172	G1173	C1172	G1029	A966	C884	G788	G714	G632	A563	A496	U421	G345	
G1304	G1174	G1176	G1174	G1030	G967	C885	G789	G715	G633	C564	U497	C422	G347	
G1305	C1175	G1177	C1175	C1031	C967	G886	G791	G716	C634	U565	U498	G423	U261	
U1308	A1178	G1178	A1178	A1032	A968	G888	G792	G717	C635	A572	G500	G424	A262	
G1309	G1179	G1179	G1179	G1032A	A969	A889	A793	G718	G636	A573	G501	G425	G350	
G1310	A1180	G1180	A1180	G1032B	C970	G890	A794	A722	U636	A574	C502	G426	G351	
G1311	G1181	G1181	G1181	G1033	G971	U891	G795	U723		G575	G503	G427	G352	
G1312	G1182	G1182	G1182	G1034	C972	A892	G799	G724	G649	G576	C504	U428	A353	
U1313	A1183	G1183	A1183	A1035	G973	C893	G800	G725	G650	G577	C505	U429	G354	
C1314	G1184	G1184	G1184	G1036	A974	G894	U801	C726	G651	C578	G506	U430	U359	
U1315	G1185	G1185	G1185	C1037	A975	G895	A802	G727	U652	G581	G507	A431	A360	
G1316	G1186	G1186	G1186	G1038	G976	C896	G803	A728	A653	G582	C508	A432	G361	
G1317	G1187	G1187	G1187	U1039	A977	G898	G811	G729		G583	C509	A433	G362	
G1318	A1188	G1188	A1188	A1041	C978	A900	C812	G730	G656	G584	U516	C436	A363	
A1319	C1189	G1189	C1189	G1042	C980	A901	U813	G731	G657	C578	G517	C437	G277	
A1320	G1190	G1190	G1190	G1043	U981	C904	G735	C735	U659		G518	U438	G278	
U1321	A1191	G1191	A1191	G1050	U982	U905	G736	C736	A665	G582	C519	G445	G279	
G1322	G1192	G1192	G1192	C1051	A983	G906	A737	A737	G660	G583	A520	G446	A298	
G1323	U1193	G1193	U1193	G1052	C984	A907	C738	C738	G661	G584	G521	G447	C299	
A1324	G1194	G1194	G1194	A1053	G985	A908	G821	U740	G662	A583	C522	A448	A300	
G1325	C1195	G1195	C1195	A1054	A986	A909	C822	G741	G663	G584	A523	C449	G301	
C1326	U1196	G1196	U1196	A1055	G987	A910	G825	U742	G664		C526	G450	G305	
G1327	G1197	G1197	G1197	U1056	U987	A911	C826	G743	A666	G585	G527	A451	G306	
G1328	G1198	G1198	G1198	C1059	C990	A912	U827	U744	G667	G586	C528	A452	G307	
U1329	A1199	G1199	A1199	G1060	U991	A913	U828	C745	G668	G587	G529	A453	G310	
G1330	G1200	G1200	G1200	C1061	U992	A914	A828	G747	U672	G588	G530	C456	G311	
A1331	A1201	G1201	A1201	U1062	G993	U920	G836	C748	G673	G589	G531	C457	C312	
A1332	G1202	G1202	G1202	C1063	A994	U921	G837	C749	G674	G590	G532	C458	C313	
G1333	C1203	G1203	C1203	G1064	C998A	G922	G838	G750	A675	G591	C523	G459	A314	
G1334	A1204	G1204	A1204	G1065	U999	A923	U841	U751	A676	G592	G533	C460	A315	
G1335	U1205	G1205	U1205	C1066	A1000	A924	C942	G752	U677	G593	G534	C461	A316	
G1336	G1206	G1206	G1206	G1067	G1001	G926	U843	A753	G680	U598	G535	C462	G317	
G1337	C1207	G1207	C1207	G1072	U1002	G927	C948	G754	G683	G599	G536	C463	G318	
G1338	G1208	G1208	G1208	U1073	G1003	G928	C949	C755	G684	G600	C537	C464	G319	
C1342	U1212	G1212	U1212	G1074	A1004	G933	U950	G756	G685	G601	C538	G465	G320	
G1343	G1143	G1143	G1143	C1075	A1005	C934	C949	C757	A684	G604	C539	G466	C314	
U1345	G1144	G1144	G1144	G1076	C1006	A935	G853	U758	G686	G605	C540	C467	A317	
G1346	C1145	G1145	C1145	U1078	G1007	C936	G854	A759	U686	G606	C541	G468	G319	
G1347	G1146	G1146	G1146	G1079	U1008	A937	G855	G760	A687	G607	C542	G469	G320	
U1348	C1147	G1147	C1147	A1080	G1009	A937	A859	C761	G688	A608	G543	G470	G321	
G1349	U1148	G1148	U1148	G1081	G1013	G942	A865	C762	G689	A614	G544	G471	G322	
A1349	U1150	G1150	A1150	U1086	A1014				G690		G545	G472	G323	

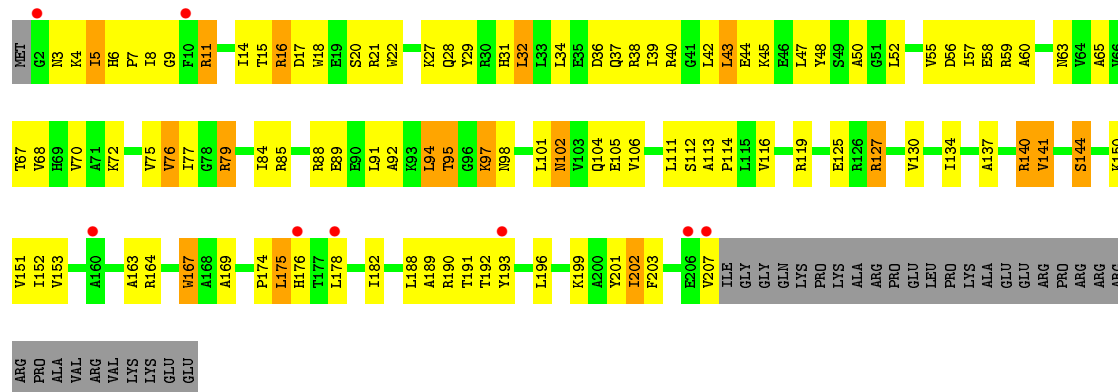




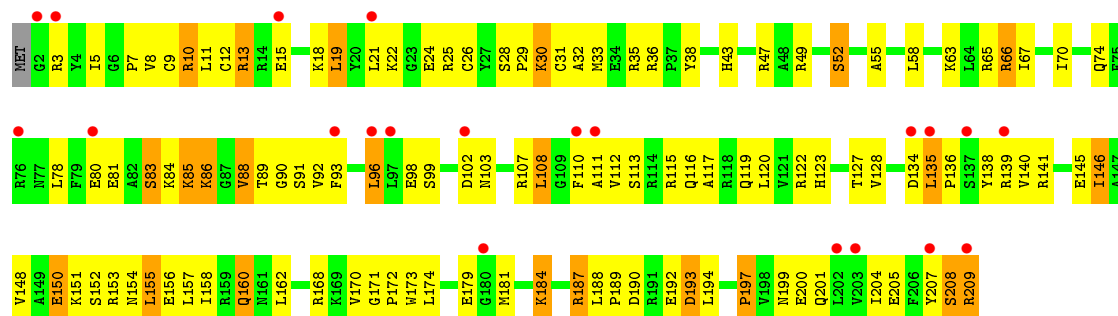




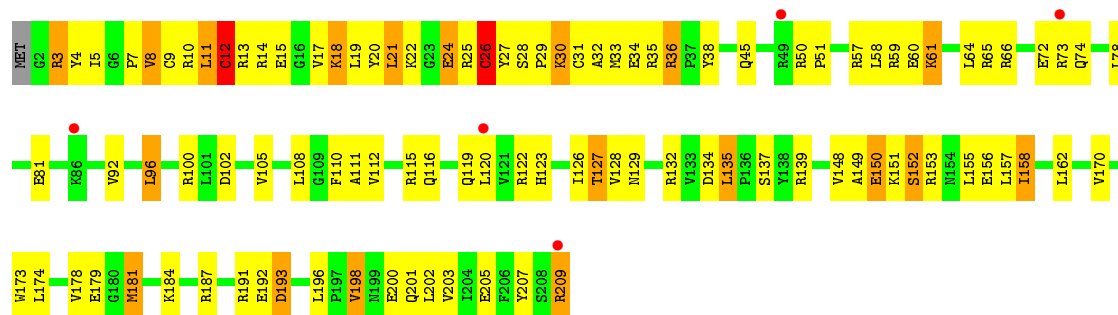
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• Molecule 4: 30S ribosomal protein S4

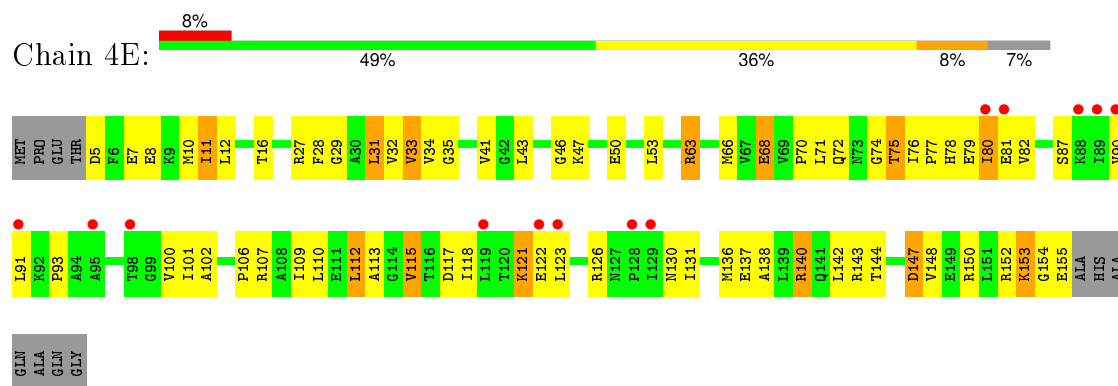


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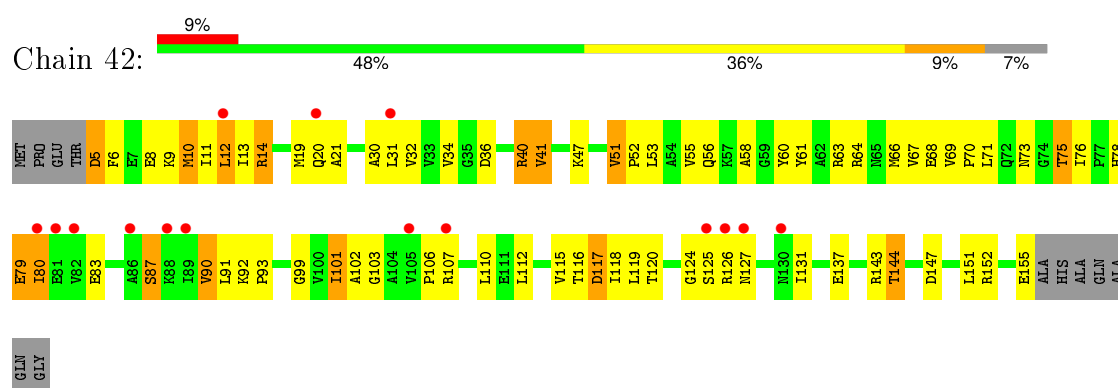




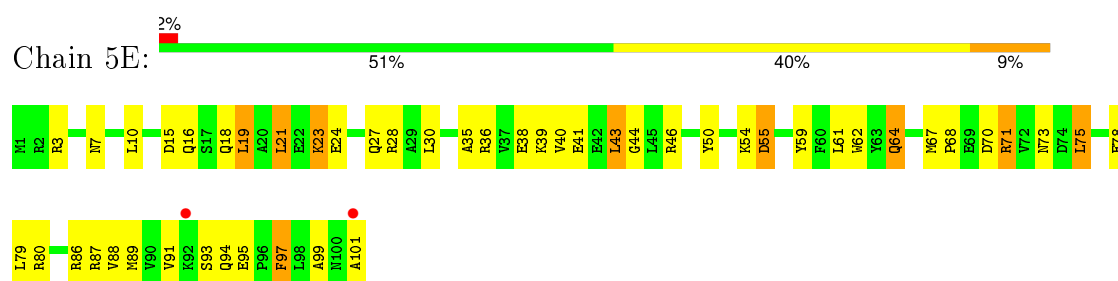
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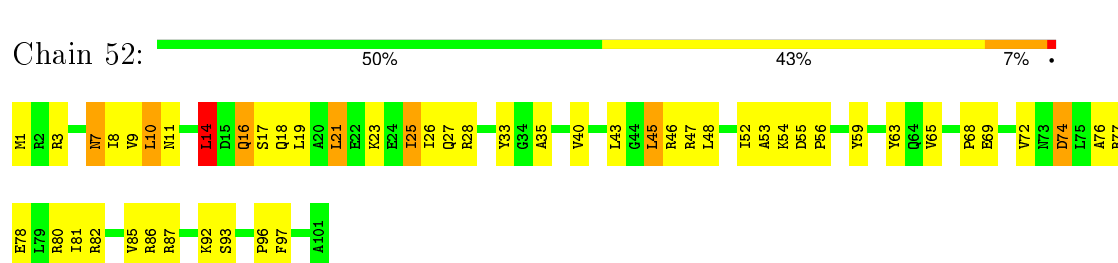
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- Molecule 6: 30S ribosomal protein S6



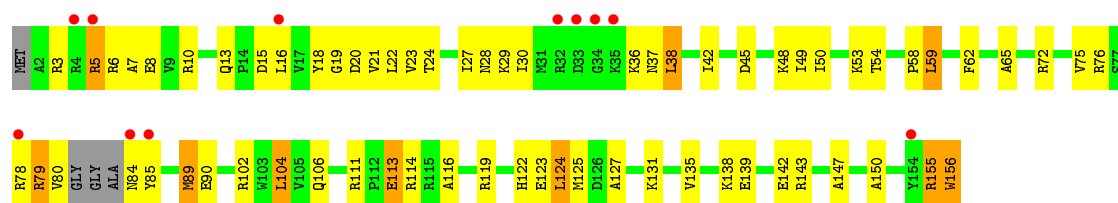
- Molecule 6: 30S ribosomal protein S6



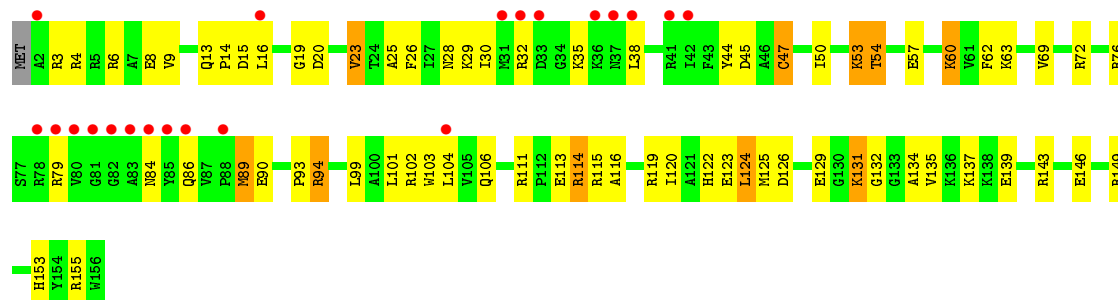
- Molecule 7: 30S ribosomal protein S7



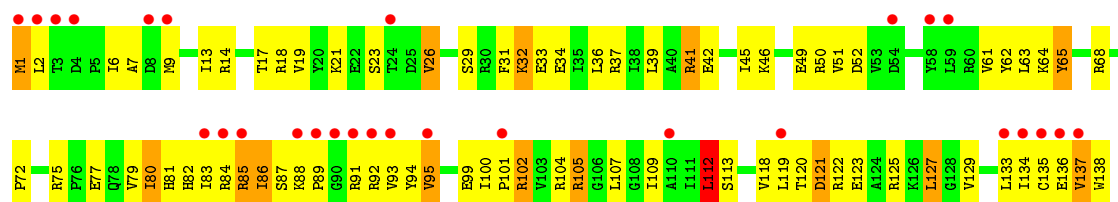




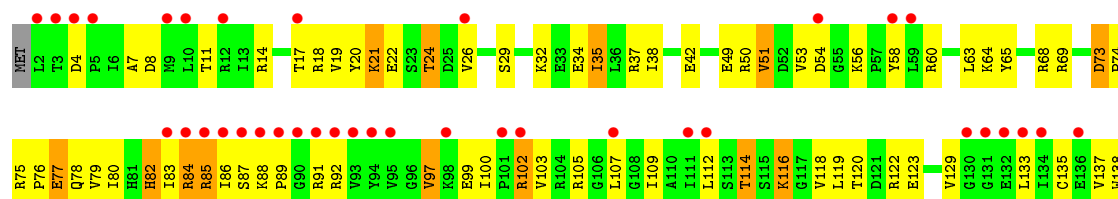
• Molecule 7: 30S ribosomal protein S7



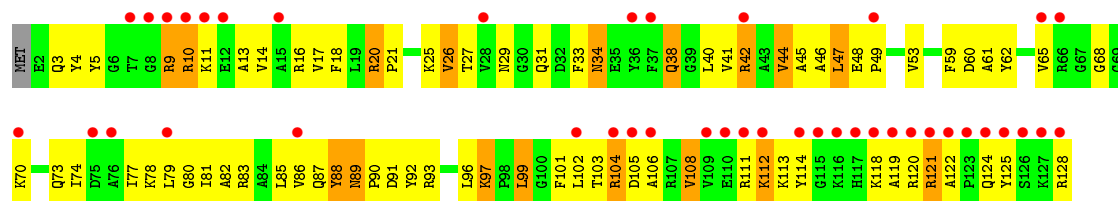
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8



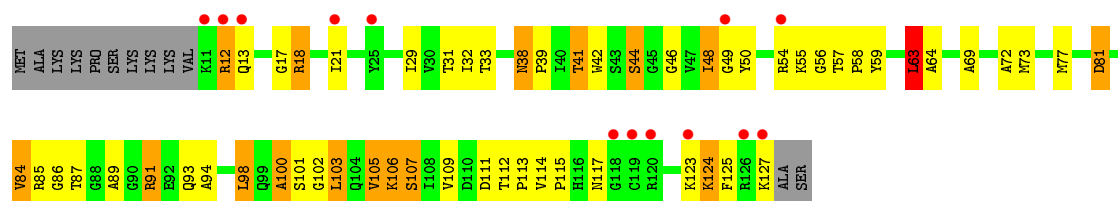
• Molecule 9: 30S ribosomal protein S9



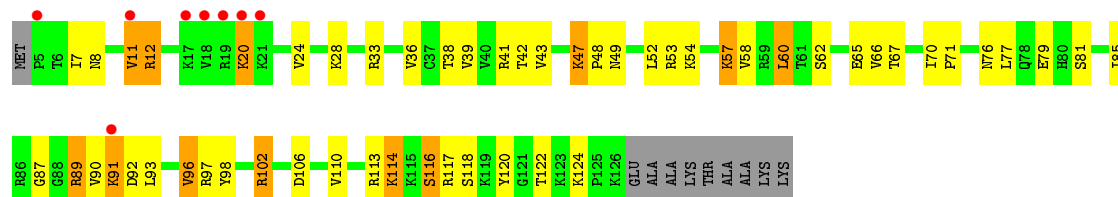




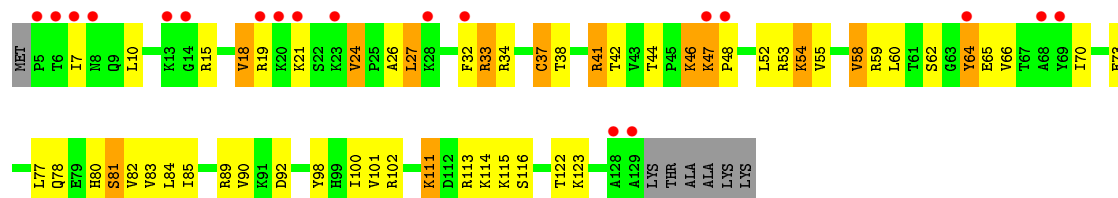




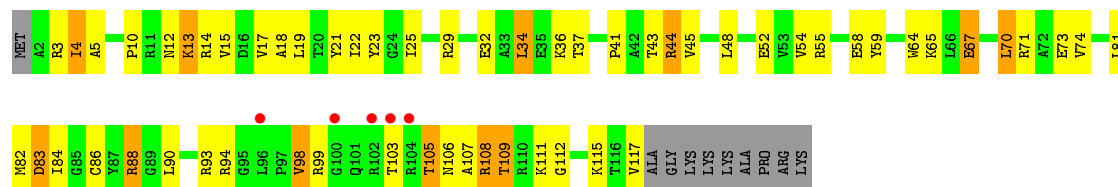
• Molecule 12: 30S ribosomal protein S12



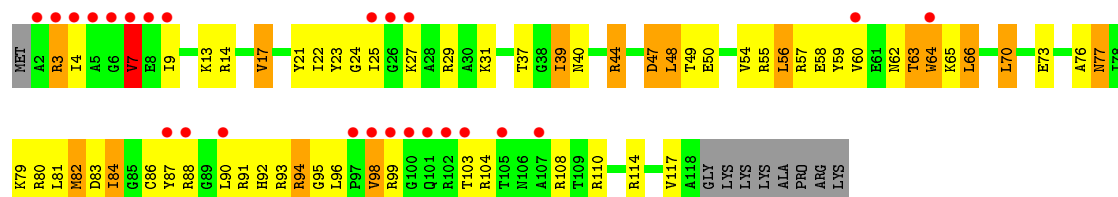
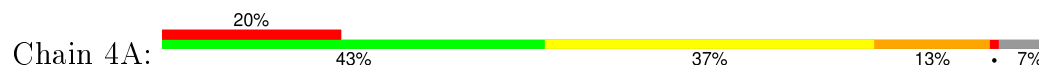
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

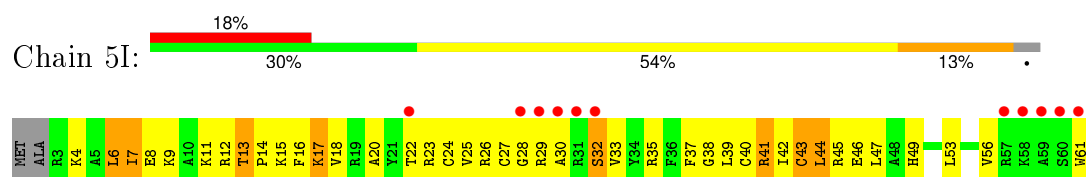


• Molecule 13: 30S ribosomal protein S13

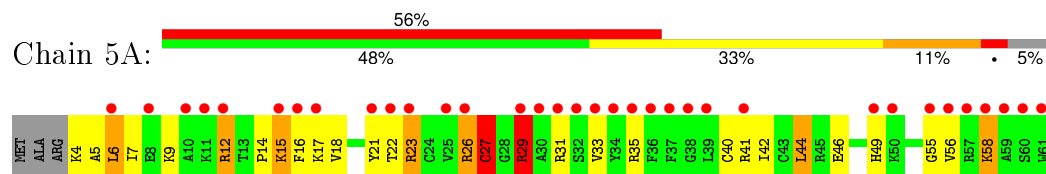


• Molecule 14: 30S ribosomal protein S14 type Z

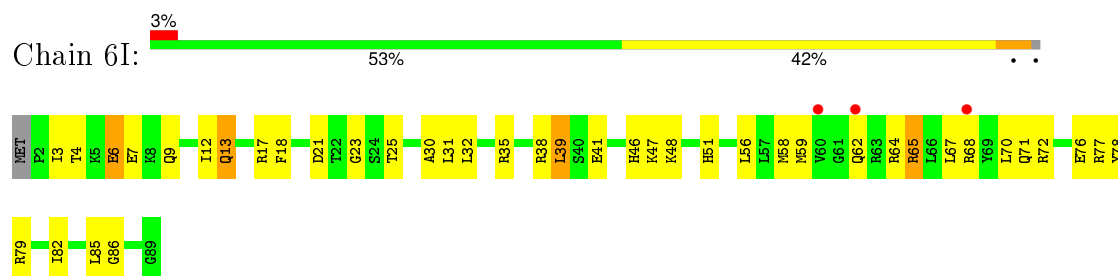




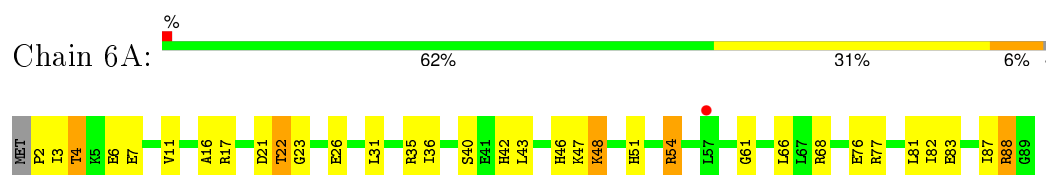
- Molecule 14: 30S ribosomal protein S14 type Z



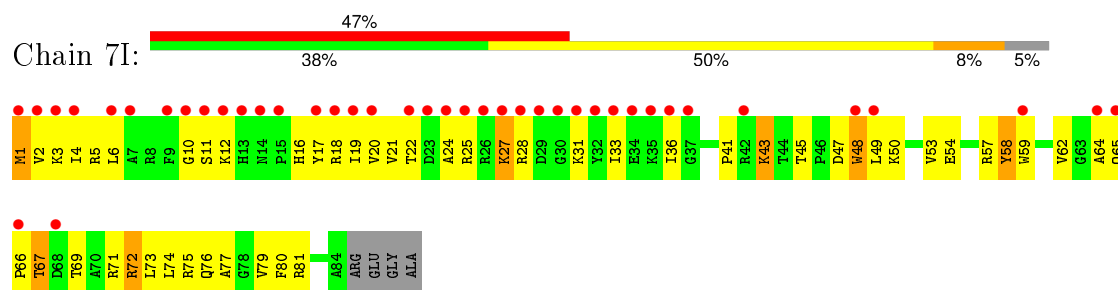
- Molecule 15: 30S ribosomal protein S15



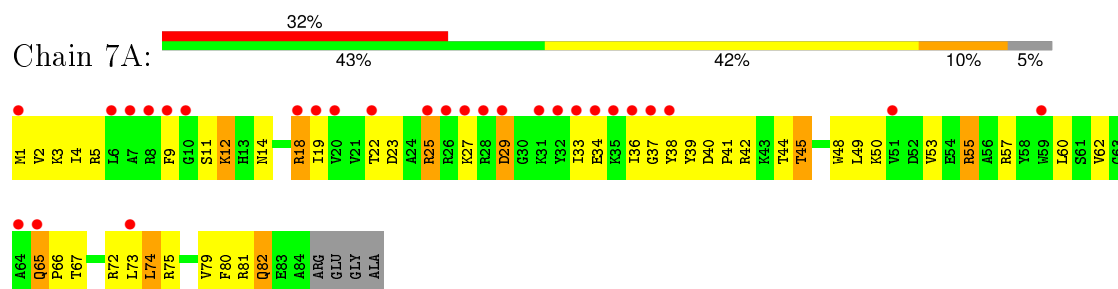
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

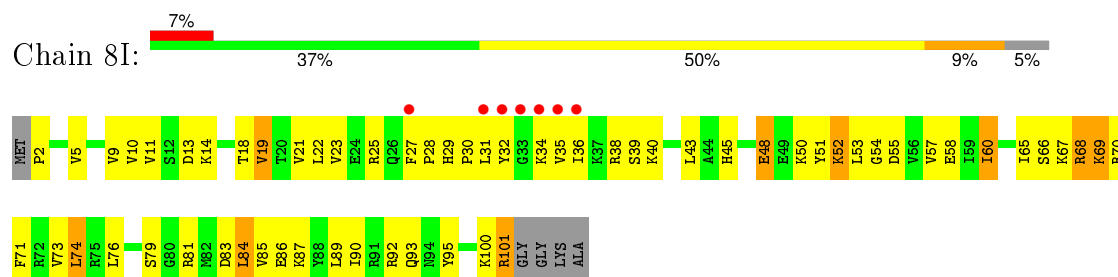


- Molecule 16: 30S ribosomal protein S16

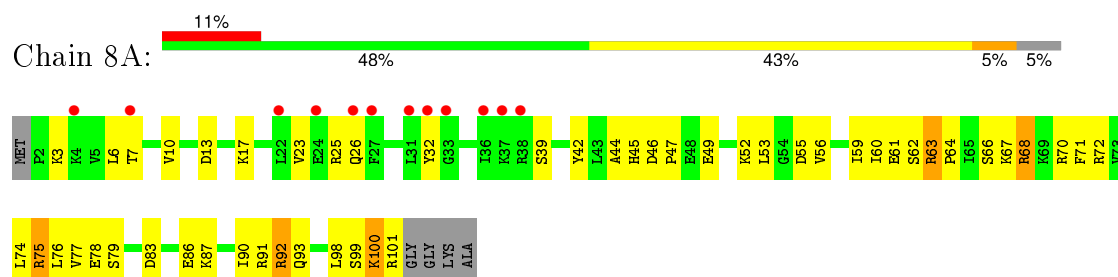




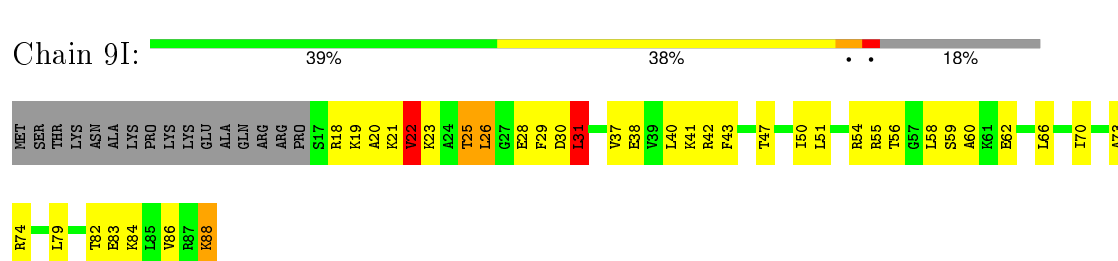
- Molecule 17: 30S ribosomal protein S17



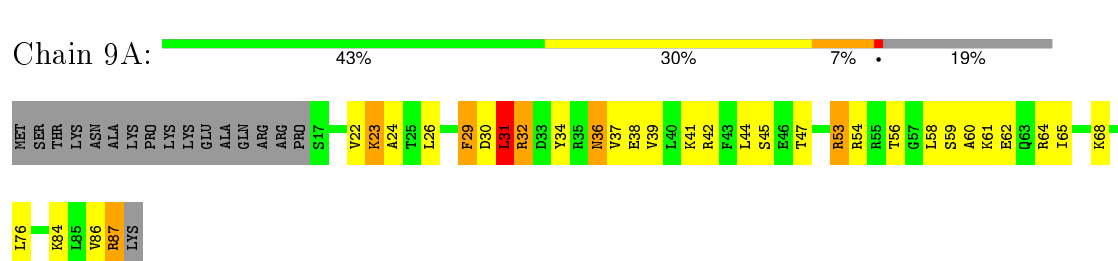
- Molecule 17: 30S ribosomal protein S17



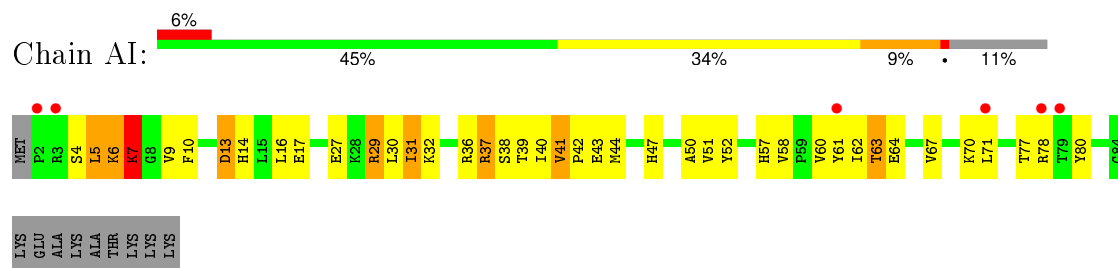
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

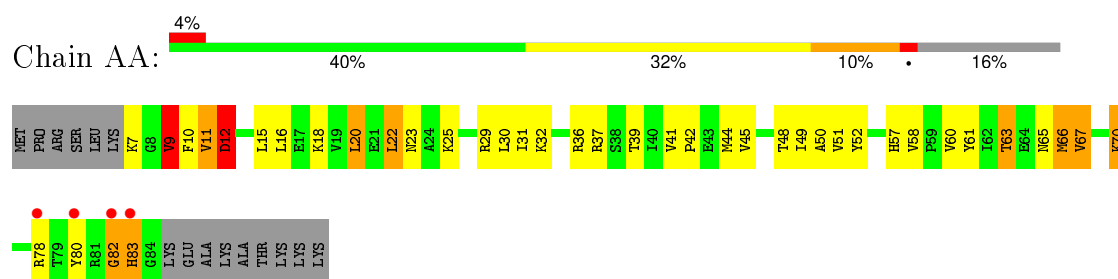


- Molecule 19: 30S ribosomal protein S19

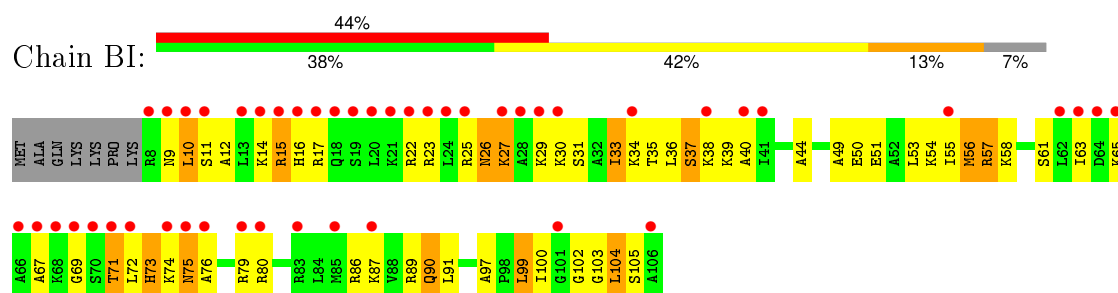


- Molecule 19: 30S ribosomal protein S19

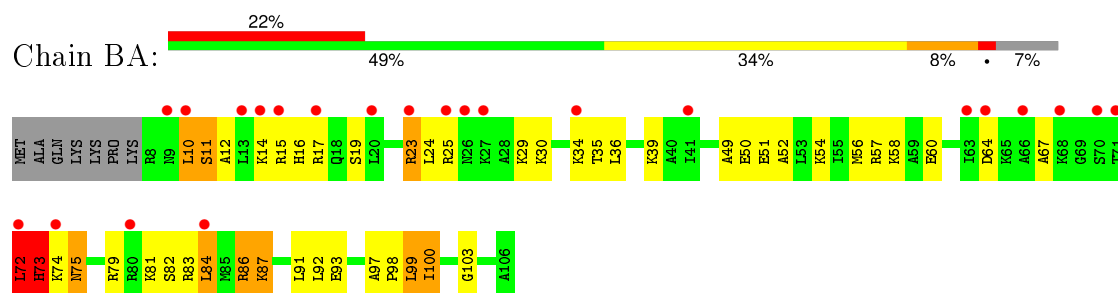




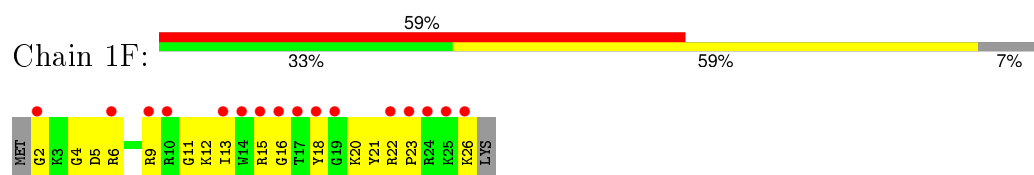
- Molecule 20: 30S ribosomal protein S20



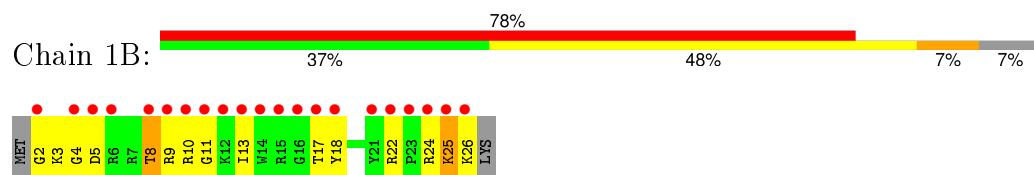
- Molecule 20: 30S ribosomal protein S20



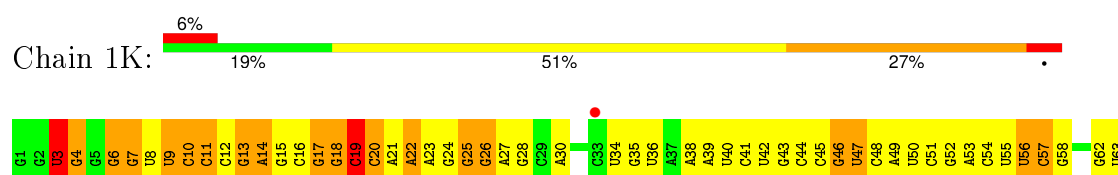
- Molecule 21: 30S ribosomal protein Thx



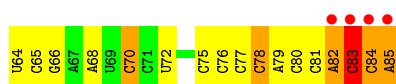
- Molecule 21: 30S ribosomal protein Thx



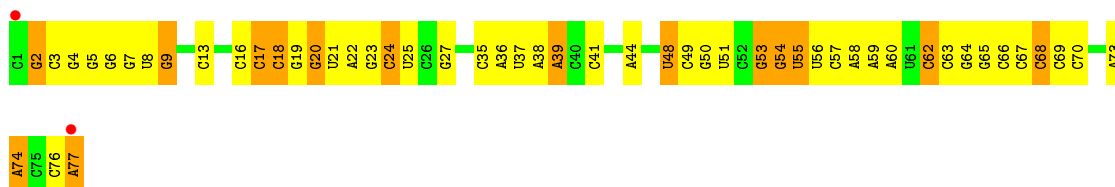
- Molecule 22: tRNA-Tyr







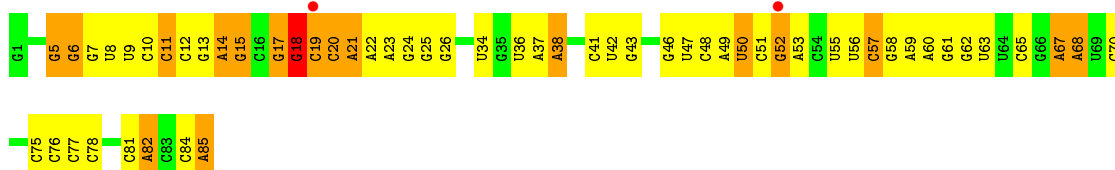
- Molecule 23: tRNA-fMet



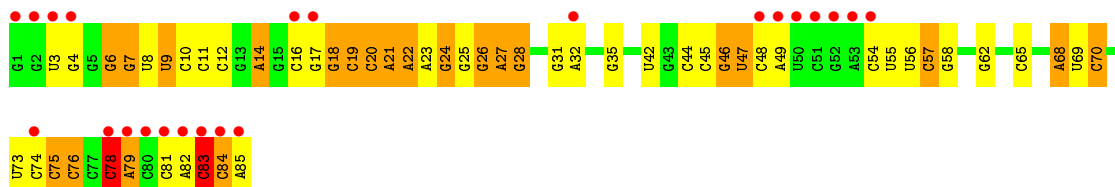
- Molecule 23: tRNA-fMet



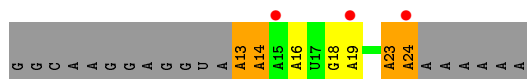
- Molecule 24: tRNA-Tyr



- Molecule 24: tRNA-Tyr



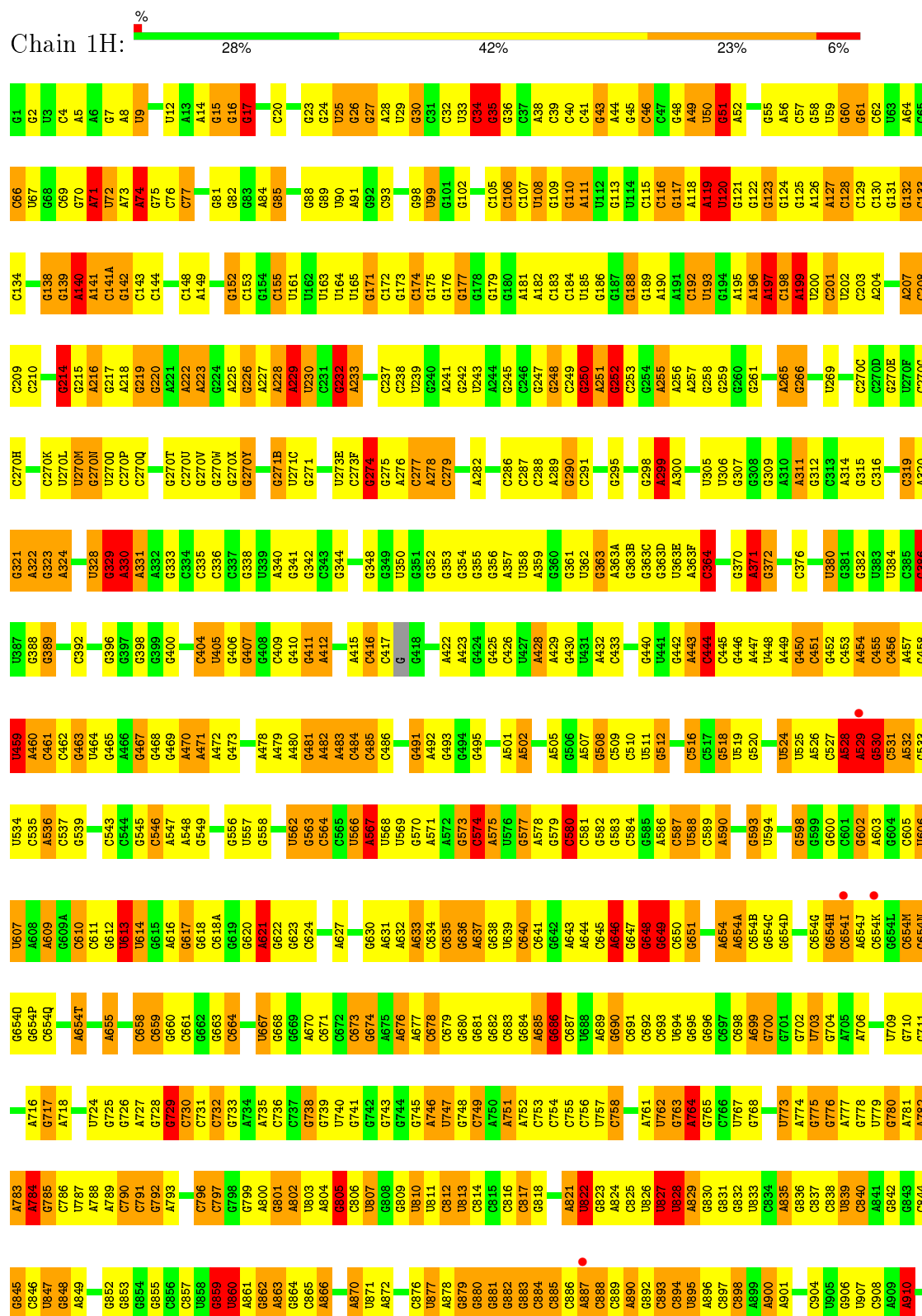
- Molecule 25: mRNA



- Molecule 25: mRNA



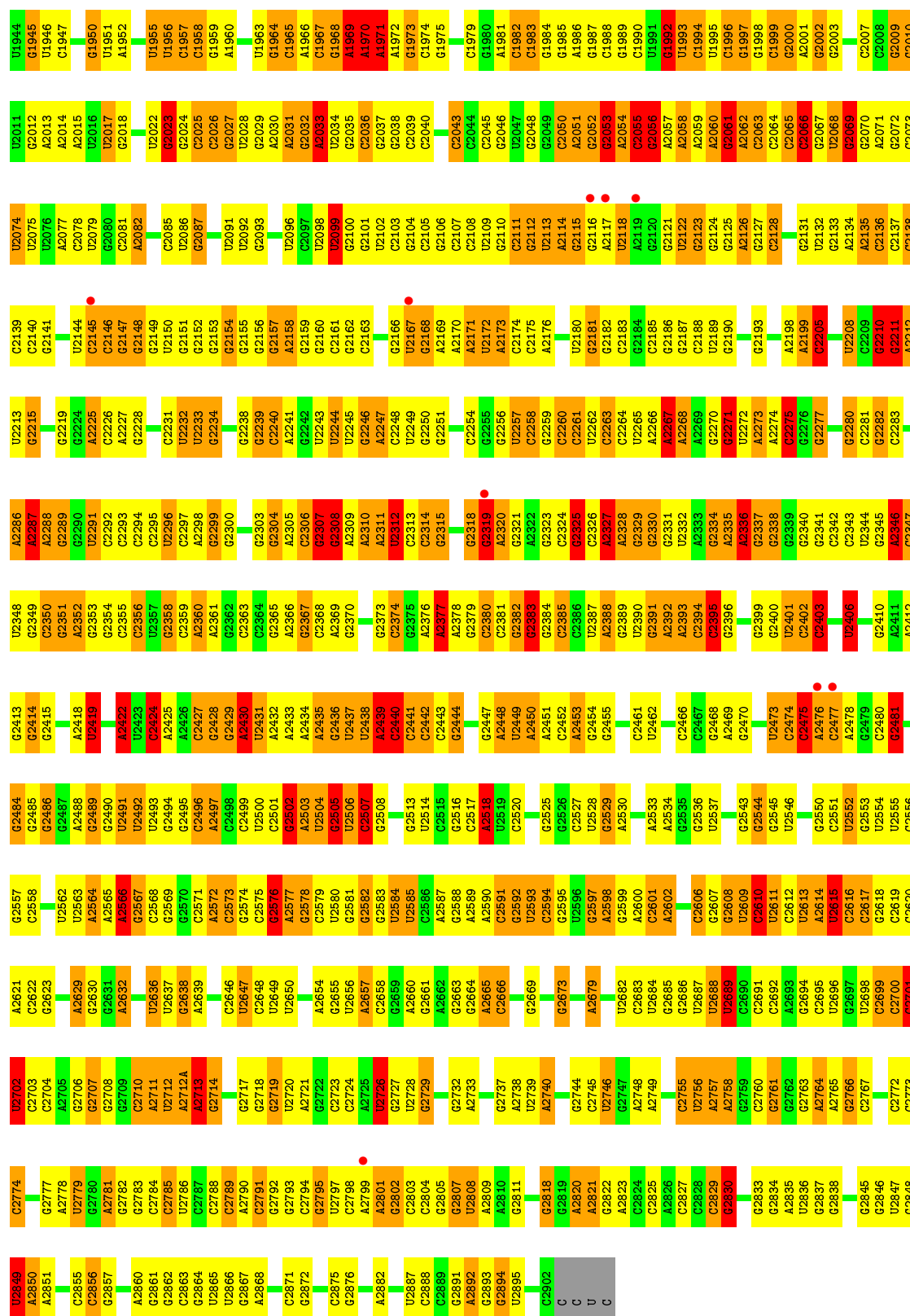












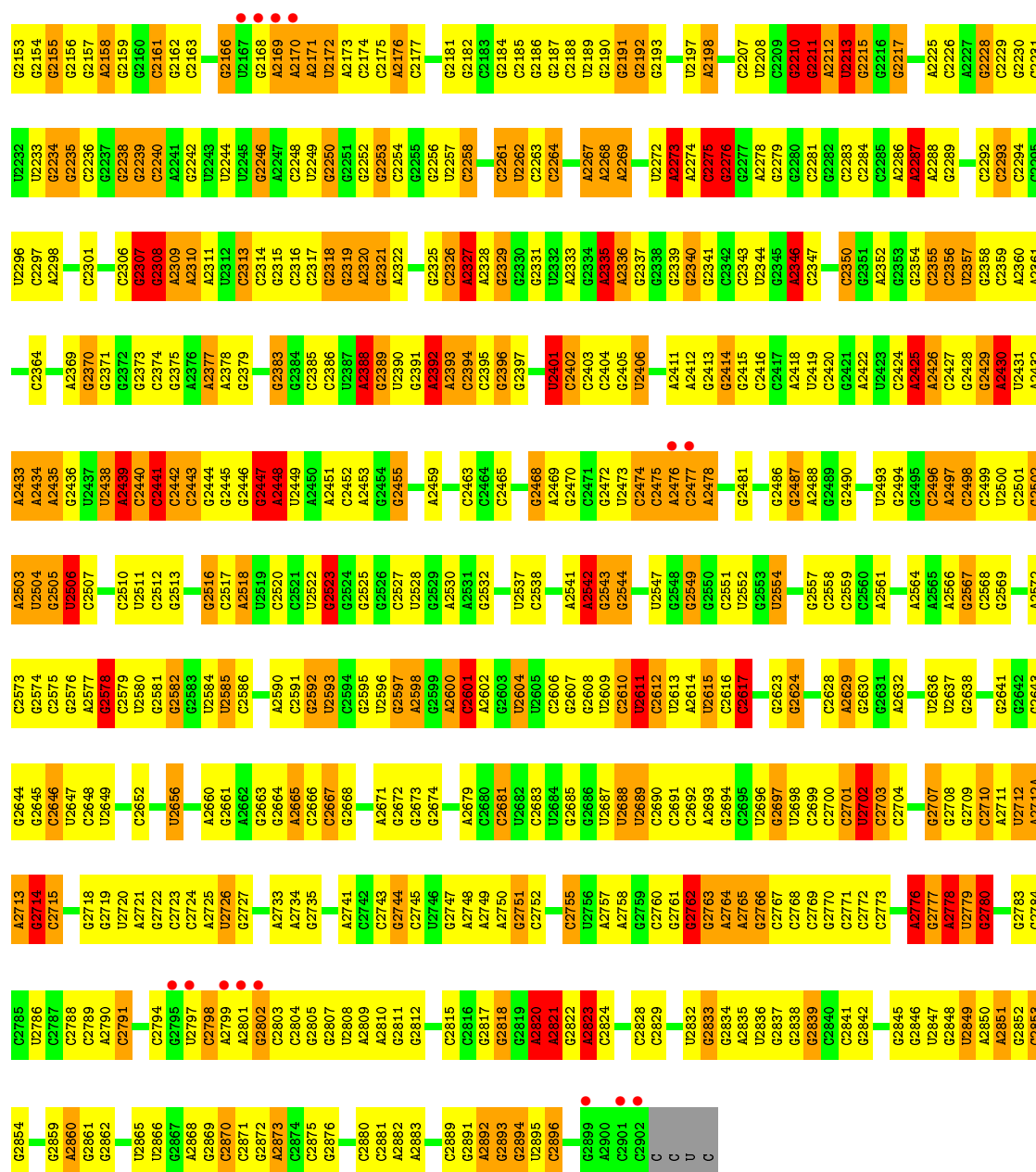


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A941	G942	U943	G944	A945	G946			G949	G950	G951	G952	A953		G956	A957	U958	A959	A960	G961	G962	U963	G964	G965	G966	G967	G968	U969	G970	G971	G972	G973	G974	G977			A980	A981	G982	A983	A984	G985	G986	G987	A988	G989	A990	G991	G992	G993		A996	G997	G998	G999	U1000	U1001	G1002	G1003	C1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U877	A878	G879	G880	G881	G882	G883	A884	G885	G886	A887	G888	A889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929		G932	A933	G934	G935		G938																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U811	C812	U813	C814		C817	C818	A819	A820	A821	U822	G823	A824	G825	U826	U827	U828	C829	G830	G831	G832	U833	C834	A835	G836	C837	G838	U839	C840		G843	C844	G845	U846	U847	C848	A849		G852	G853	A854	G855	C856	G857	U858	G859	U860	C861	G862	A863	G864	C865	A866	G867	U868	G869	A870	U871	A872	G873																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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U877	A878	G879	G880	G881	G882	G883	A884	G885	G886	A887	G888	A889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929		G932	A933	G934	G935		G938																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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G217	A218		A221	A222	A223	G224	A225		A229	G232	A233	C234	U235	C236		U239	G240	G241	A242	U243	A244		G247	G248	C249	G250	A251	G252		A255		G259	G260	C261	A262	C263	C264	A265		C268	U269	A270		G270E	U270F	C270G	C270H	C270I	G270J	C270K	U270L	U270M	G270N	U270O	C270P	C270Q	G270V																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G270Y	U270Z		G271A	G271B	G271C	G271D	G271E	G271F	G271G	G271H	G271I	G271J	G271K	G271L	G271M	G271N	G271O	G271P	G271Q	G271R	G271S	G271T	G271U	G271V	G271W	G271X	G271Y	G271Z		U2703	G2704	U2705	U2706	U2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C336		A340	G341		G352	G353	G354		A357	U358	U359	U360	G361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376		C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401		U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U99

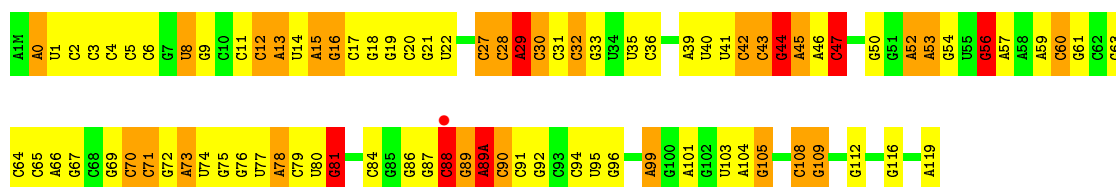




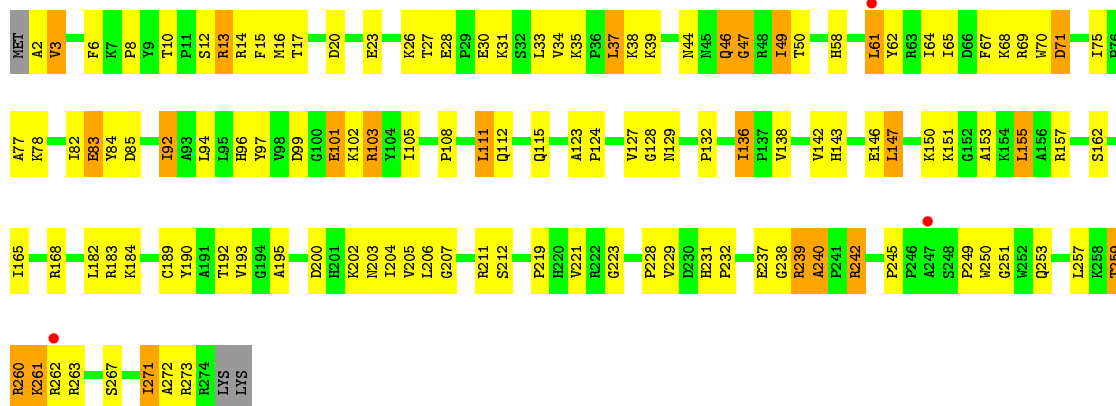




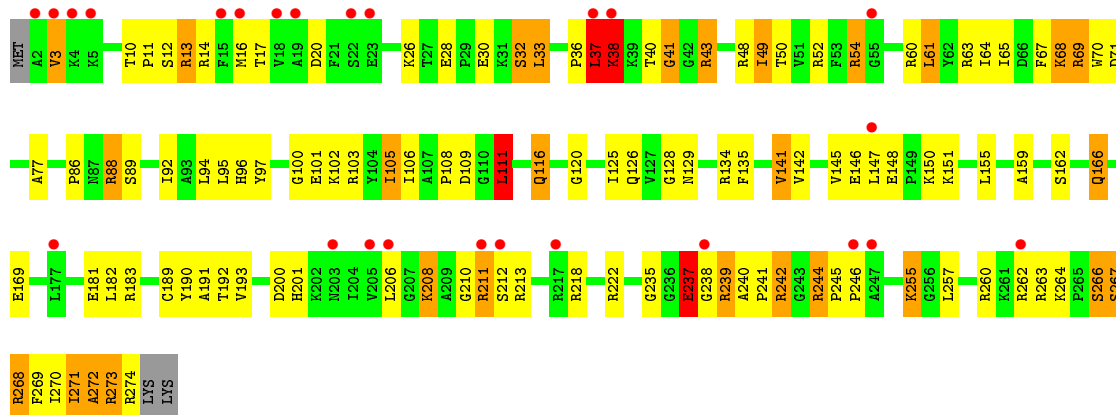




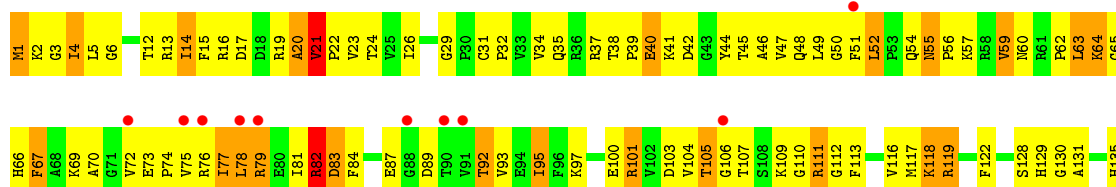
• Molecule 28: 50S ribosomal protein L2



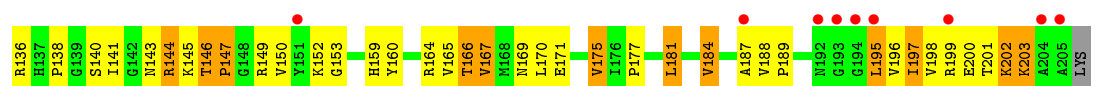
• Molecule 28: 50S ribosomal protein L2



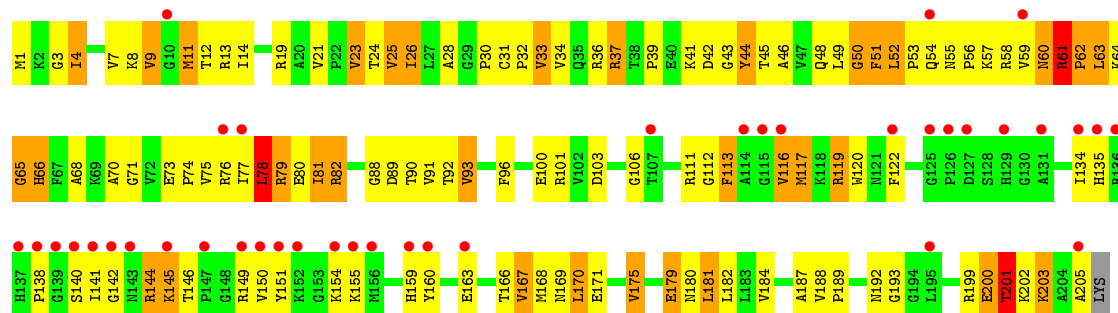
• Molecule 29: 50S ribosomal protein L3



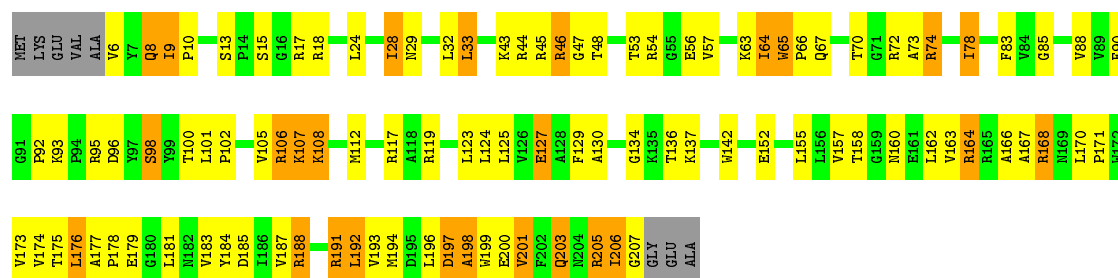




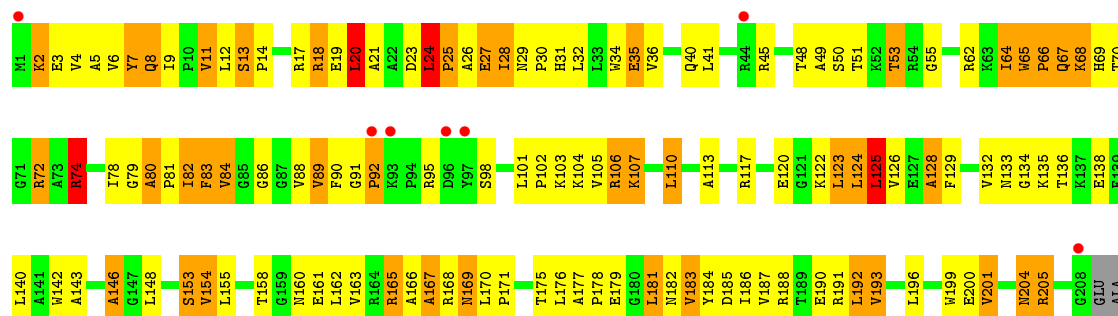
• Molecule 29: 50S ribosomal protein L3



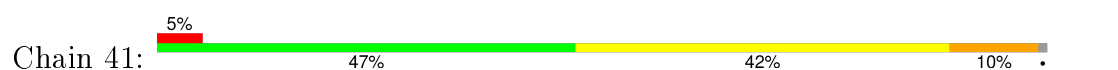
• Molecule 30: 50S ribosomal protein L4



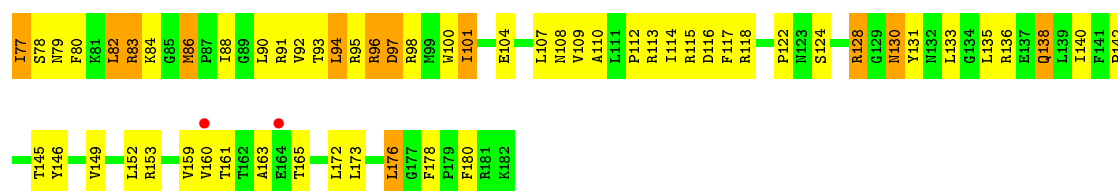
• Molecule 30: 50S ribosomal protein L4



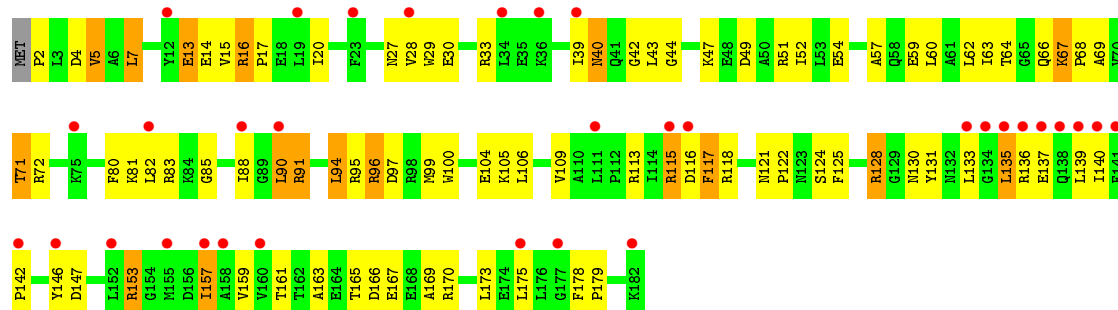
• Molecule 31: 50S ribosomal protein L5



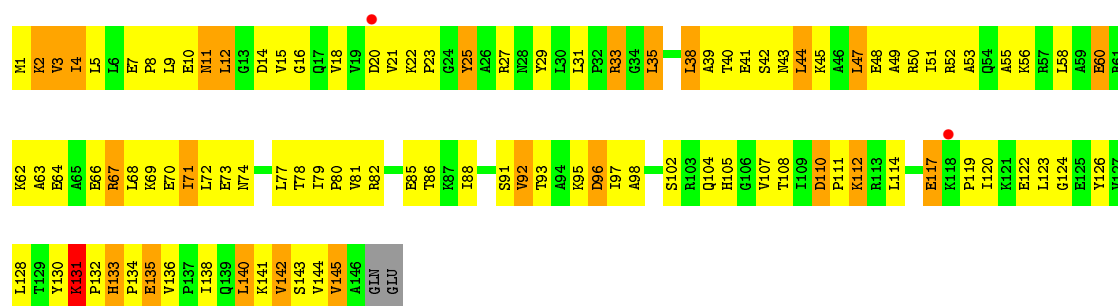




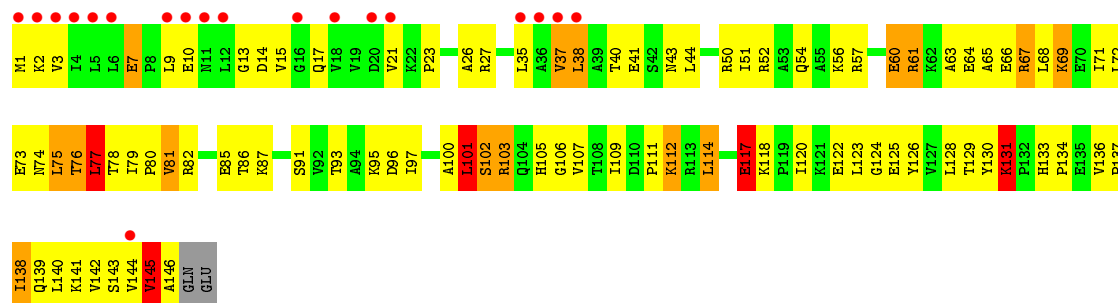
• Molecule 31: 50S ribosomal protein L5



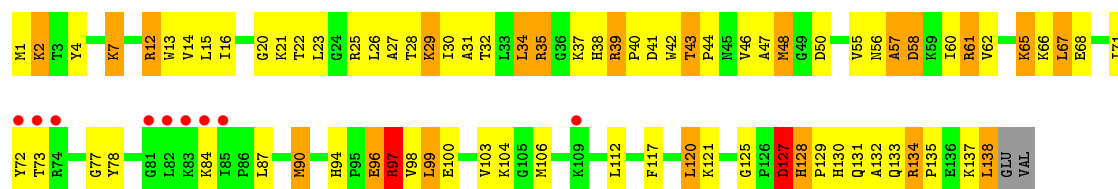




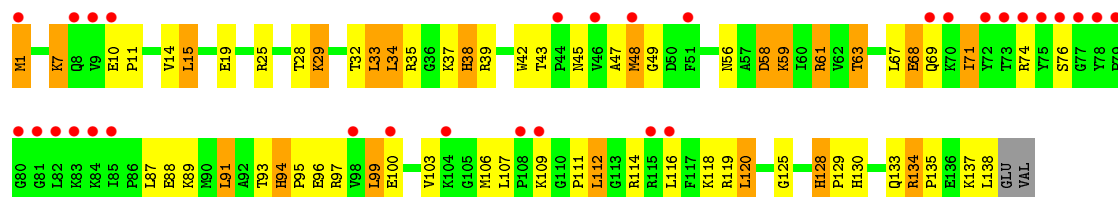
• Molecule 33: 50S ribosomal protein L9



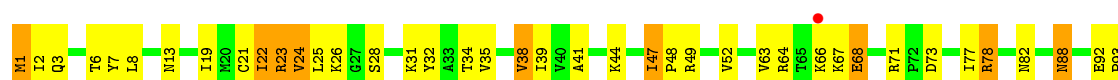
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13



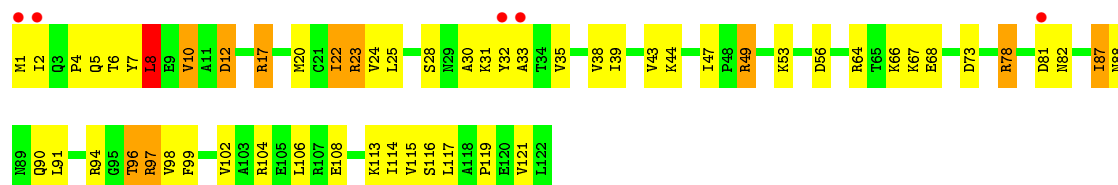
• Molecule 35: 50S ribosomal protein L14



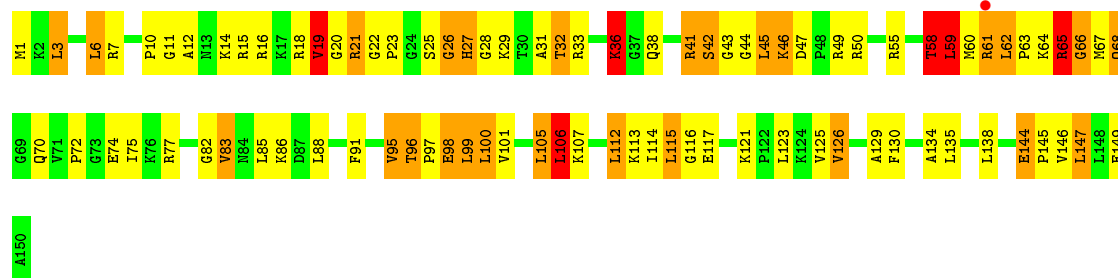




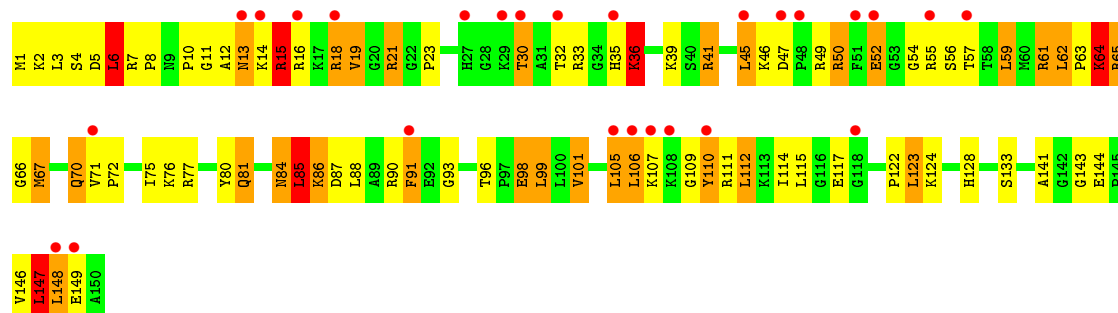
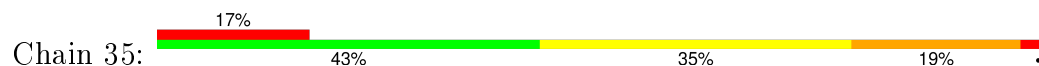
• Molecule 35: 50S ribosomal protein L14



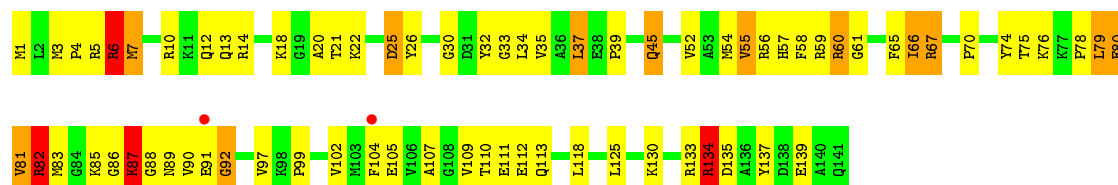
• Molecule 36: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16





Chain 45:

Amino Acid	Frequency (%)
R133	42%
R134	40%
D135	40%
A136	40%
X137	40%
D138	40%
E139	40%
ALA	40%
GLN	40%
R67	42%
I68	40%
F69	40%
P70	40%
D71	40%
K72	40%
P73	40%
Y74	40%
T75	40%
K76	40%
K77	40%
P78	40%
L79	40%
E80	40%
V81	40%
R82	40%
M83	40%
G84	40%
K85	40%
G86	40%
K87	40%
G88	40%
M89	40%
V90	40%
E91	40%
G92	40%
Y93	40%
V97	42%
K98	40%
P99	40%
G100	40%
V101	40%
R102	40%
M103	40%
F104	40%
E105	40%
V106	40%
A107	40%
T110	42%
E111	40%
E112	40%
Q113	40%
E116	42%
A117	40%
L118	40%
R119	40%
I120	40%
A121	40%
L125	42%
P126	40%
I127	40%
K128	40%
T129	40%
K130	40%
V131	40%
V132	40%
V133	40%
R134	40%
D135	40%
A136	40%
X137	40%
D138	40%
E139	40%
ALA	40%
GLN	40%

**Chain 98:**

Model	Success Rate (%)
M1	3%
R2	32%
H3	32%
L4	32%
K5	32%
S6	32%
G7	32%
R8	32%
K9	32%
L10	32%
N11	32%
H16	32%
A17	32%
L18	32%
Q24	32%
L28	32%
L29	32%
T30	32%
H31	32%
G32	32%
R33	32%
I34	32%
T35	32%
T36	32%
T37	32%
V38	32%
P39	32%
K40	32%
A41	32%
K42	32%
E43	32%
L44	32%
A45	32%
G46	32%
F47	32%
V48	32%
D49	32%
H50	32%
L51	32%
I52	32%
H53	32%
L54	32%
A55	32%
K56	32%
D59	32%
L60	32%
H61	32%
A62	32%
R63	32%
R64	32%
L65	32%
V66	32%
L67	32%
R68	32%
D69	32%
L70	32%
Q71	32%
D72	32%
V73	32%
K74	32%
L75	32%
V76	32%
R77	32%
K78	32%
R79	32%
F80	32%
D81	32%
E82	32%
I83	32%
A84	32%
P85	32%
R86	32%
Y87	32%
R90	32%
Q91	32%
G92	32%
G93	32%
Y94	32%
T95	32%
R96	32%
V97	32%
L98	32%
K99	32%
L100	32%
A101	32%
E102	32%
R103	32%
R104	32%
R105	32%
E106	32%
D107	32%
G108	32%
A109	32%
P110	32%
L113	32%
V114	32%
E115	32%
L116	32%
V117	32%
E118	32%

Chain 55:

7% 42% 44% 12%

••

MET R2 H3 L4 K5 S6 G7 R8 K9 L10 N11 R12 H16 R17 L18 Y21 Q24 L28 L29 T30 H31 G32 R33 I34 T35 V38 K42 E43 L44 R45 G46 F47 V48 L51 I52 H53 L54 A55 K56 R57 G58 D59 R63 R64 L65 V66 L67 R68 D69 L70 Q71 D72

Chain A8:

Amino Acid Type	Category	Percentage
MET	Grey	4%
ALA	Grey	4%
R3	Grey	4%
L4	Grey	4%
Y7	Grey	4%
E8	Grey	4%
R9	Grey	4%
R10	Green	41%
K11	Green	41%
F12	Green	41%
R13	Green	41%
V14	Green	41%
N16	Green	41%
R17	Green	41%
R20	Green	41%
L24	Yellow	44%
R25	Yellow	44%
L26	Yellow	44%
S27	Yellow	44%
V28	Yellow	44%
F29	Yellow	44%
R30	Yellow	44%
S31	Yellow	44%
L32	Yellow	44%
K33	Yellow	44%
H34	Yellow	44%
I35	Yellow	44%
Y36	Yellow	44%
A37	Yellow	44%
Q38	Yellow	44%
I39	Yellow	44%
L40	Yellow	44%
D41	Yellow	44%
D42	Yellow	44%
E43	Yellow	44%
K44	Yellow	44%
T47	Yellow	44%
L48	Yellow	44%
V49	Yellow	44%
S50	Yellow	44%
A51	Yellow	44%
L54	Yellow	44%
K57	Yellow	44%
L58	Yellow	44%
K59	Yellow	44%
G60	Yellow	44%
T63	Yellow	44%
R67	Yellow	44%
Q68	Yellow	44%
V69	Yellow	44%
L73	Green	41%
A74	Green	41%
L78	Green	41%
A79	Green	41%
L80	Green	41%
G81	Green	41%
I82	Green	41%
K83	Green	41%
F87	Green	41%
D88	Green	41%
R89	Green	41%
G90	Green	41%
P91	Green	41%
Y92	Green	41%
K93	Green	41%
Y94	Green	41%
H95	Green	41%
G96	Green	41%
R97	Green	41%
V98	Green	41%
L101	Yellow	44%
A102	Yellow	44%
E103	Yellow	44%
R106	Yellow	44%
E107	Yellow	44%
G108	Yellow	44%
G109	Yellow	44%
L110	Yellow	44%
E111	Yellow	44%
F112	Yellow	44%

Chain 65:

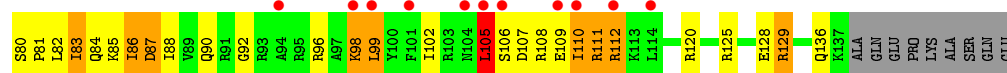
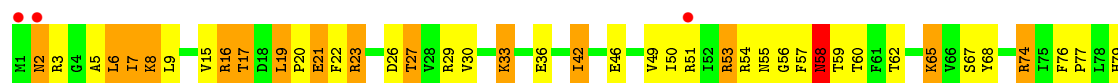
13% 35% 50% 13%

A1 A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26 A27 A28 A29 A30 A31 A32 A33 A34 A35 A36 A37 A38 A39 A40 A41 A42 A43 A44 A45 A46 A47 A48 A49 A50 A51 A52 A53 A54 A55 A56 A57 A58 A59 A60 A61 A62

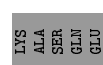




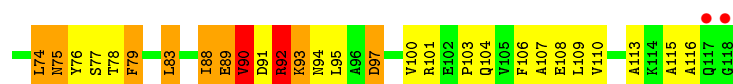
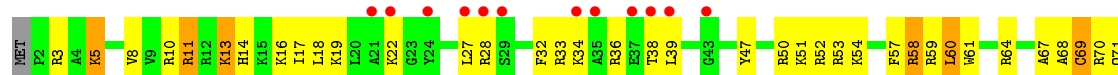
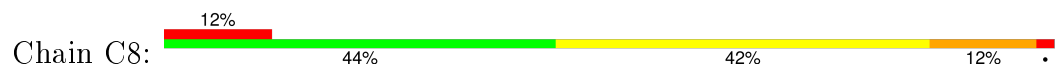
- Molecule 40: 50S ribosomal protein L19



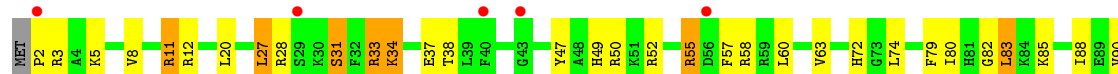
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



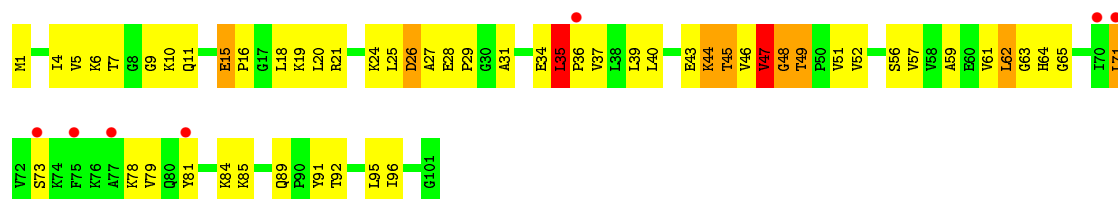
- Molecule 41: 50S ribosomal protein L20



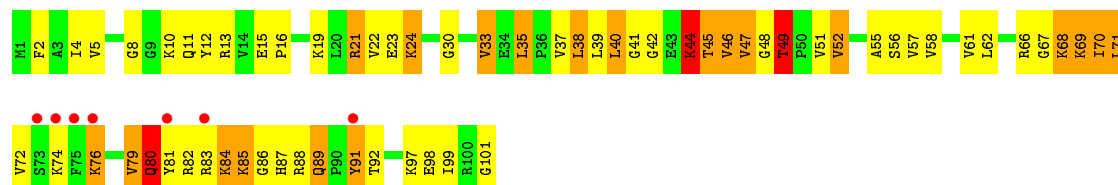
- Molecule 42: 50S ribosomal protein L21



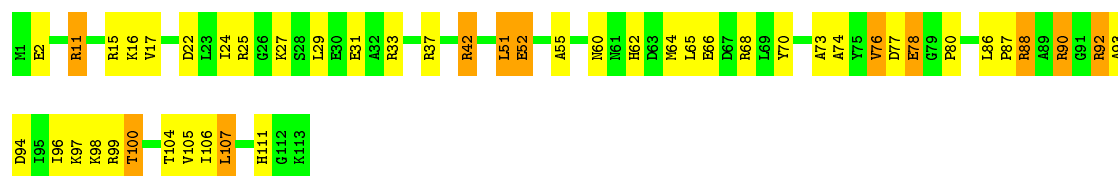




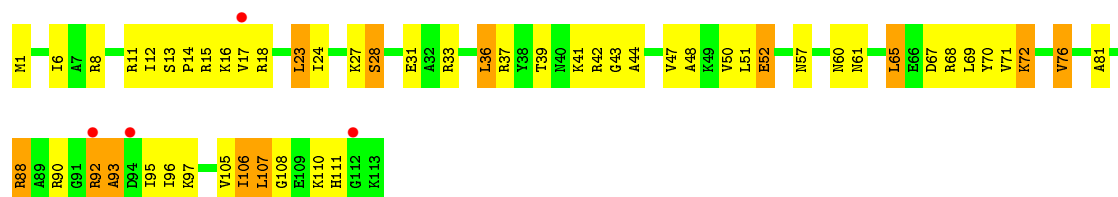
- Molecule 42: 50S ribosomal protein L21



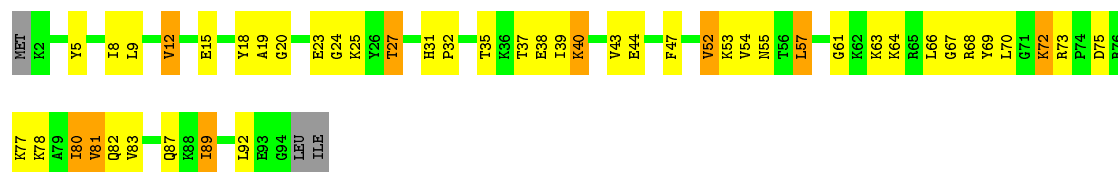
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23



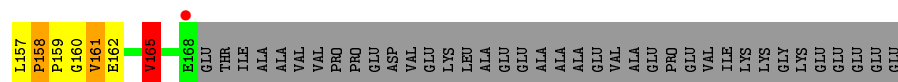
- Molecule 44: 50S ribosomal protein L23



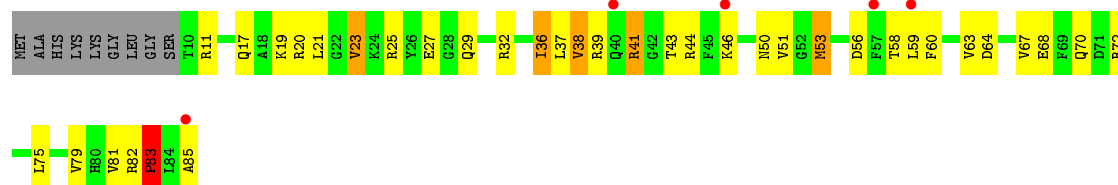




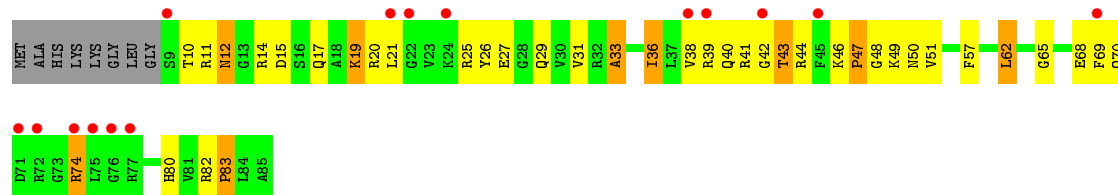




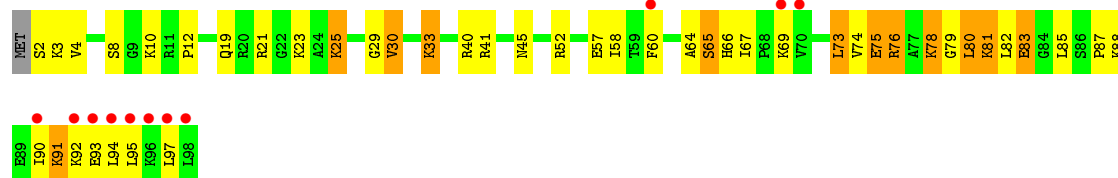
- Molecule 47: 50S ribosomal protein L27



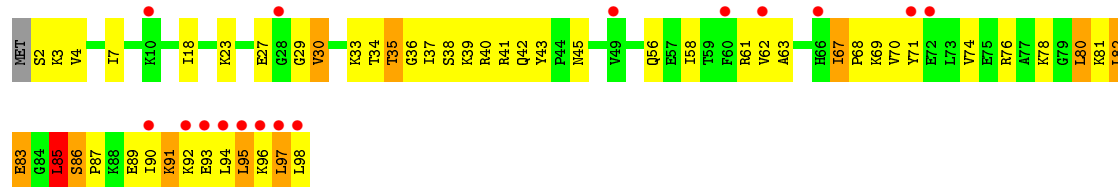
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



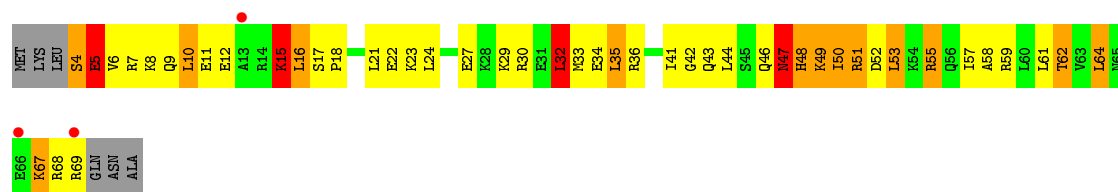
- Molecule 48: 50S ribosomal protein L28



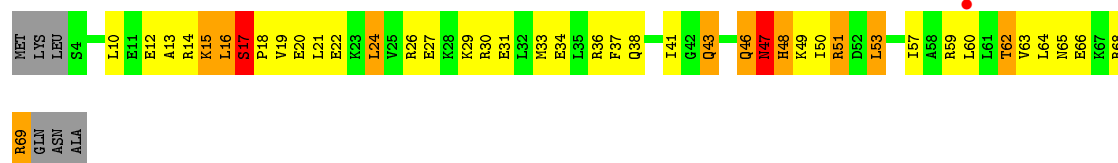
- Molecule 49: 50S ribosomal protein L29







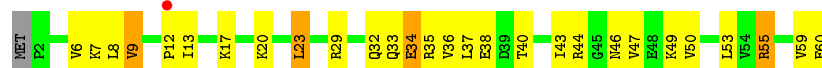
- Molecule 49: 50S ribosomal protein L29



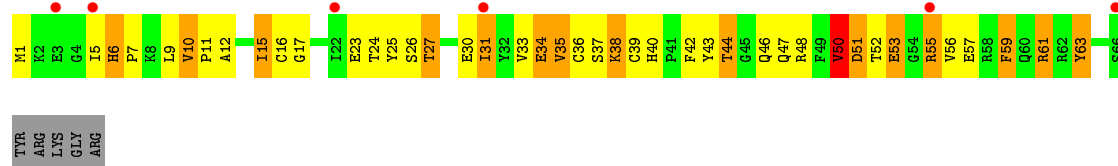
- Molecule 50: 50S ribosomal protein L30



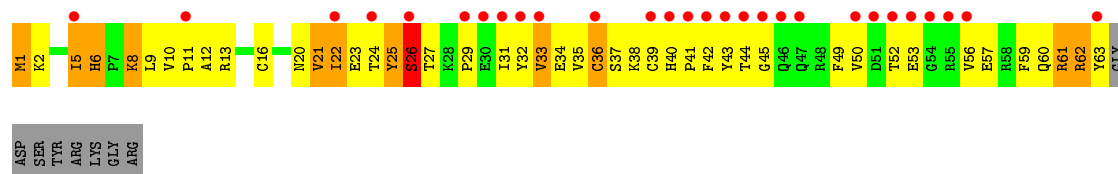
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31

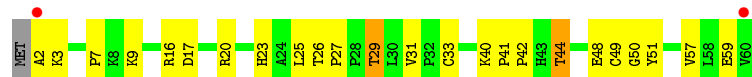




- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



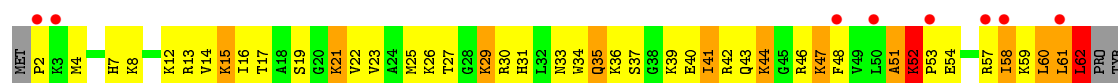
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34

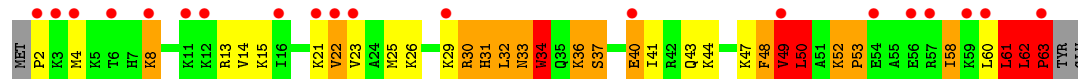
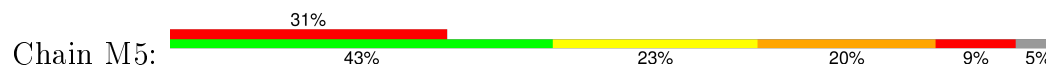


- Molecule 54: 50S ribosomal protein L35



GLU

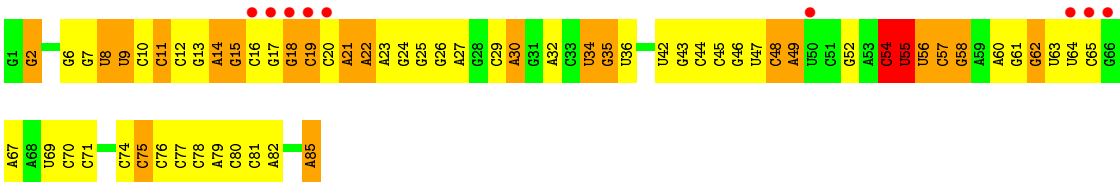
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: tRNA-Tyr









## 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 450.90Å 622.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.45 – 3.05 225.45 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (225.45-3.05) 92.8 (225.45-3.05)	Depositor EDS
$R_{merge}$	0.38	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.195 , 0.249 0.201 , 0.254	Depositor DCC
$R_{free}$ test set	1999 reflections (0.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 1108158 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	299607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

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

<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, PAR, MIA, MG, ZN, 4SU, QUO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	13	0.75	4/36215 (0.0%)	1.42	401/56524 (0.7%)
1	1G	0.66	1/36187 (0.0%)	1.30	253/56481 (0.4%)
2	12	0.38	0/1959	0.66	0/2642
2	1E	0.42	0/1959	0.70	1/2642 (0.0%)
3	22	0.42	0/1636	0.65	0/2205
3	2E	0.52	0/1629	0.72	0/2195
4	32	0.50	0/1732	0.76	2/2318 (0.1%)
4	3E	0.60	1/1732 (0.1%)	0.76	1/2318 (0.0%)
5	42	0.47	0/1171	0.70	0/1576
5	4E	0.54	0/1171	0.72	1/1576 (0.1%)
6	52	0.52	0/855	0.68	2/1154 (0.2%)
6	5E	0.54	0/855	0.70	0/1154
7	62	0.45	0/1275	0.64	0/1709
7	6E	0.45	0/1261	0.60	0/1689
8	72	0.44	0/1127	0.65	0/1517
8	7E	0.51	0/1135	0.74	1/1527 (0.1%)
9	82	0.40	0/988	0.66	0/1324
9	8E	0.44	0/1028	0.67	0/1379
10	1A	0.37	0/814	0.62	0/1095
10	1I	0.45	0/814	0.66	0/1095
11	2A	0.47	0/888	0.67	1/1198 (0.1%)
11	2I	0.51	0/879	0.74	1/1187 (0.1%)
12	3A	0.58	0/991	0.80	0/1327
12	3I	0.73	0/972	0.91	0/1301
13	4A	0.38	0/943	0.65	1/1265 (0.1%)
13	4I	0.49	0/938	0.71	0/1258
14	5A	0.44	0/484	0.74	0/643
14	5I	0.69	2/489 (0.4%)	0.86	1/650 (0.2%)
15	6A	0.47	0/744	0.65	0/992
15	6I	0.54	0/744	0.73	0/992
16	7A	0.53	0/721	0.71	0/970
16	7I	0.51	0/721	0.75	0/970



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.50	0/847	0.65	0/1131
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.50	0/586	0.72	1/779 (0.1%)
18	9I	0.49	0/595	0.79	1/790 (0.1%)
19	AA	0.44	0/638	0.72	1/860 (0.1%)
19	AI	0.53	0/680	0.81	0/915
20	BA	0.48	0/764	0.78	1/1007 (0.1%)
20	BI	0.41	0/764	0.68	0/1007
21	1B	0.52	0/221	0.66	0/288
21	1F	0.49	0/221	0.70	0/288
22	1K	0.49	0/1899	1.15	11/2952 (0.4%)
23	2K	0.81	0/1747	1.41	18/2723 (0.7%)
23	2L	0.69	0/1747	1.26	9/2723 (0.3%)
24	1L	0.47	1/1996 (0.1%)	1.08	5/3108 (0.2%)
24	3K	0.41	0/1996	1.01	1/3108 (0.0%)
25	4K	0.78	0/319	1.31	3/495 (0.6%)
25	4L	0.78	0/294	1.50	5/456 (1.1%)
26	14	0.89	62/70167 (0.1%)	1.58	1423/109541 (1.3%)
26	1H	1.03	114/70233 (0.2%)	1.76	2174/109643 (2.0%)
27	16	0.83	1/2928 (0.0%)	1.57	49/4568 (1.1%)
27	1J	0.70	0/2928	1.37	27/4568 (0.6%)
28	11	0.77	2/2170 (0.1%)	0.93	1/2926 (0.0%)
28	19	0.73	0/2170	0.94	6/2926 (0.2%)
29	21	0.70	0/1601	0.96	1/2160 (0.0%)
29	29	0.66	0/1601	0.98	3/2160 (0.1%)
30	31	0.72	0/1620	0.90	2/2194 (0.1%)
30	39	0.61	1/1662 (0.1%)	0.89	4/2249 (0.2%)
31	41	0.52	0/1498	0.75	1/2016 (0.0%)
31	49	0.42	0/1498	0.70	0/2016
32	51	0.65	0/1346	0.93	1/1821 (0.1%)
32	59	0.40	0/1332	0.74	3/1802 (0.2%)
33	61	0.52	0/1151	0.82	2/1558 (0.1%)
33	69	0.51	0/1151	0.77	3/1558 (0.2%)
34	15	0.49	0/1131	0.76	2/1525 (0.1%)
34	58	0.60	0/1131	0.83	0/1525
35	25	0.62	0/942	0.76	1/1269 (0.1%)
35	68	0.66	0/942	0.76	0/1269
36	35	0.67	0/1161	1.12	7/1544 (0.5%)
36	78	0.71	0/1161	1.13	7/1544 (0.5%)
37	45	0.70	2/1128 (0.2%)	0.98	3/1508 (0.2%)
37	88	0.82	1/1142 (0.1%)	1.11	4/1527 (0.3%)
38	55	0.65	0/973	0.84	1/1302 (0.1%)
38	98	0.57	0/981	0.79	1/1312 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	65	0.54	0/891	0.90	2/1187 (0.2%)
39	A8	0.62	0/886	0.89	2/1180 (0.2%)
40	75	0.58	0/1155	0.76	0/1542
40	B8	0.62	0/1155	0.83	1/1542 (0.1%)
41	85	0.59	0/981	0.78	1/1306 (0.1%)
41	C8	0.71	1/981 (0.1%)	0.89	2/1306 (0.2%)
42	95	0.66	0/789	0.88	1/1057 (0.1%)
42	D8	0.60	0/789	0.82	2/1057 (0.2%)
43	A5	0.72	0/910	0.86	1/1220 (0.1%)
43	E8	0.65	0/910	0.84	0/1220
44	B5	0.80	1/739 (0.1%)	0.88	0/993
44	F8	0.73	0/744	0.83	0/1000
45	C5	0.61	0/807	0.89	1/1076 (0.1%)
45	G8	0.65	0/804	0.94	3/1073 (0.3%)
46	D5	0.43	0/1165	0.72	0/1574
46	H8	0.50	0/1427	0.80	1/1935 (0.1%)
47	E5	0.63	0/620	0.85	0/827
47	I8	0.71	0/614	0.89	0/819
48	F5	0.64	0/769	0.96	2/1022 (0.2%)
48	J8	0.70	0/769	0.86	0/1022
49	G5	0.60	0/560	0.81	0/741
49	K8	0.78	1/560 (0.2%)	0.98	2/741 (0.3%)
50	H5	0.48	0/473	0.69	0/635
50	L8	0.61	0/473	0.78	1/635 (0.2%)
51	I5	0.52	0/527	0.84	0/709
51	M8	0.50	0/545	0.87	0/733
52	J5	0.59	0/472	0.84	0/639
52	N8	0.65	0/472	0.86	1/639 (0.2%)
53	L5	0.70	0/399	0.88	0/526
53	P8	0.88	1/404 (0.2%)	0.97	0/533
54	M5	0.88	0/502	1.22	6/661 (0.9%)
54	Q8	0.85	0/494	1.10	1/649 (0.2%)
55	3L	0.39	0/1970	1.00	4/3065 (0.1%)
All	All	0.80	196/322722 (0.1%)	1.40	4482/483529 (0.9%)

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

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

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

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

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	783	A	N3-C4	-11.75	1.27	1.34
26	1H	2430	A	N9-C4	-11.09	1.31	1.37
26	14	783	A	N9-C4	-10.86	1.31	1.37
26	1H	71	A	N9-C4	-10.78	1.31	1.37
26	1H	676	A	N9-C4	-10.74	1.31	1.37

The worst 5 of 4482 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-20.97	113.42	126.00
26	14	1899	G	N3-C4-N9	-17.93	115.24	126.00
26	1H	1899	G	N3-C2-N2	-17.01	107.99	119.90
26	1H	2430	A	O5'-P-OP2	-17.00	90.30	110.70
26	1H	676	A	C2-N3-C4	-16.89	102.15	110.60

All (2) chirality outliers are listed below:

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

5 of 128 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
4	3E	29	PRO	Peptide
12	3I	47	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32352	0	16325	789	1
1	1G	32327	0	16316	749	3
2	12	1924	0	1975	103	0
2	1E	1924	0	1975	102	0
3	22	1612	0	1677	70	0
3	2E	1605	0	1668	56	0
4	32	1702	0	1763	78	0
4	3E	1702	0	1761	94	0
5	42	1155	0	1213	55	0
5	4E	1155	0	1213	49	0
6	52	842	0	857	32	0
6	5E	842	0	857	37	0
7	62	1256	0	1296	49	0
7	6E	1243	0	1284	50	0
8	72	1107	0	1165	53	0
8	7E	1115	0	1177	59	0
9	82	971	0	1001	55	0
9	8E	1009	0	1037	68	0
10	1A	801	0	849	52	0
10	1I	801	0	849	46	0
11	2A	873	0	894	47	0
11	2I	864	0	881	41	0
12	3A	975	0	1062	40	0
12	3I	956	0	1046	41	0
13	4A	933	0	992	53	0
13	4I	928	0	987	42	0
14	5A	475	0	511	25	0
14	5I	480	0	513	36	0
15	6A	733	0	771	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	733	0	771	27	0
16	7A	705	0	725	37	0
16	7I	705	0	725	49	0
17	8A	834	0	904	39	0
17	8I	834	0	904	54	0
18	9A	581	0	649	33	0
18	9I	590	0	662	29	0
19	AA	624	0	636	31	0
19	AI	665	0	686	39	0
20	BA	762	0	861	30	0
20	BI	762	0	861	52	0
21	1B	217	0	234	13	0
21	1F	217	0	234	12	0
22	1K	1824	0	945	57	0
23	2K	1645	0	841	30	0
23	2L	1645	0	841	33	0
24	1L	1807	0	920	32	0
24	3K	1807	0	920	47	0
25	4K	283	0	143	9	0
25	4L	261	0	132	6	0
26	14	62647	0	31582	1375	1
26	1H	62707	0	31612	1450	1
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	80	0
28	11	2120	0	2197	92	0
28	19	2120	0	2197	89	0
29	21	1568	0	1634	111	0
29	29	1568	0	1634	113	0
30	31	1585	0	1632	87	0
30	39	1627	0	1680	110	0
31	41	1473	0	1535	72	0
31	49	1473	0	1535	63	0
32	51	1321	0	1388	82	0
32	59	1307	0	1382	64	1
33	61	1136	0	1223	65	1
33	69	1136	0	1223	50	0
34	15	1104	0	1180	57	0
34	58	1104	0	1180	81	0
35	25	932	0	996	42	0
35	68	932	0	996	40	0
36	35	1144	0	1228	92	0
36	78	1144	0	1228	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1107	0	1166	74	0
37	88	1121	0	1179	57	0
38	55	959	0	1021	47	0
38	98	967	0	1033	64	0
39	65	881	0	943	62	0
39	A8	876	0	938	47	0
40	75	1141	0	1202	71	0
40	B8	1141	0	1202	64	0
41	85	963	0	1022	44	0
41	C8	963	0	1022	66	0
42	95	778	0	852	69	0
42	D8	778	0	852	40	0
43	A5	899	0	964	27	0
43	E8	899	0	964	32	0
44	B5	725	0	778	36	0
44	F8	730	0	780	31	0
45	C5	794	0	884	54	0
45	G8	791	0	882	54	0
46	D5	1139	0	1163	53	0
46	H8	1397	0	1430	79	0
47	E5	612	0	633	31	0
47	I8	606	0	628	24	0
48	F5	762	0	848	36	0
48	J8	762	0	848	34	0
49	G5	558	0	610	30	0
49	K8	558	0	610	37	0
50	H5	468	0	518	13	0
50	L8	468	0	518	20	0
51	I5	515	0	514	54	0
51	M8	533	0	526	37	0
52	J5	458	0	480	21	0
52	N8	458	0	480	25	0
53	L5	391	0	432	9	0
53	P8	396	0	434	14	0
54	M5	495	0	567	62	0
54	Q8	488	0	560	55	0
55	3L	1814	0	932	51	0
56	11	2	0	0	0	0
56	13	146	0	0	0	0
56	14	391	0	0	0	0
56	16	12	0	0	0	0
56	1G	86	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	5	0	0	3	0
59	29	3	0	0	1	0
59	2K	6	0	0	0	0
59	31	5	0	0	0	0
59	39	5	0	0	0	0
59	3E	1	0	0	0	0
59	3I	2	0	0	0	0
59	4K	3	0	0	0	0
59	55	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	6A	1	0	0	0	0
59	75	1	0	0	0	0
59	78	4	0	0	2	0
59	85	1	0	0	1	0
59	A5	1	0	0	0	0
59	BA	1	0	0	0	0
59	F8	1	0	0	0	0
59	G8	2	0	0	0	0
59	J8	1	0	0	0	0
59	L8	2	0	0	1	0
59	M5	2	0	0	0	0
All	All	299607	0	199932	8541	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8541 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
4:32:26:CYS:HB3	4:32:31:CYS:SG	1.85	1.17
26:14:2701:C:H3'	26:14:2702:U:H5''	1.31	1.12
26:14:2711:A:OP2	59:14:3464:HOH:O	1.70	1.09
26:1H:229:A:H4'	26:1H:230:U:H5'	1.33	1.08

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:85:U:O2'	32:59:100:GLY:O[3_555]	1.97	0.23
1:1G:86:U:N3	26:14:275:G:OP2[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.19	0.01
33:61:91:SER:OG	1:1G:368:U:OP1[4_555]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	195 (83%)	35 (15%)	5 (2%)	9	35
2	1E	235/256 (92%)	200 (85%)	34 (14%)	1 (0%)	39	74
3	22	204/239 (85%)	184 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	180 (89%)	22 (11%)	1 (0%)	34	70
4	32	206/209 (99%)	181 (88%)	24 (12%)	1 (0%)	34	70
4	3E	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	4E	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	26	64
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
7	6E	148/156 (95%)	140 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	13	44
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	26	64
9	82	118/128 (92%)	105 (89%)	12 (10%)	1 (1%)	24	61
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	115/129 (89%)	104 (90%)	8 (7%)	3 (3%)	7	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	114/129 (88%)	101 (89%)	12 (10%)	1 (1%)	21	58
12	3A	123/132 (93%)	101 (82%)	19 (15%)	3 (2%)	7	31
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	24	61
13	4A	115/126 (91%)	95 (83%)	18 (16%)	2 (2%)	11	41
13	4I	114/126 (90%)	96 (84%)	16 (14%)	2 (2%)	11	39
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	11	39
14	5I	57/61 (93%)	46 (81%)	9 (16%)	2 (4%)	4	23
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	8A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
18	9A	69/88 (78%)	66 (96%)	3 (4%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	14	46
19	AA	76/93 (82%)	62 (82%)	11 (14%)	3 (4%)	4	20
19	AI	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	7	30
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	19	56
20	BI	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	19	56
21	1B	23/27 (85%)	21 (91%)	1 (4%)	1 (4%)	3	18
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276 (98%)	249 (92%)	18 (7%)	4 (2%)	13	44
28	19	271/276 (98%)	253 (93%)	13 (5%)	5 (2%)	11	39
29	21	203/206 (98%)	161 (79%)	33 (16%)	9 (4%)	3	17
29	29	203/206 (98%)	158 (78%)	36 (18%)	9 (4%)	3	17
30	31	200/210 (95%)	178 (89%)	21 (10%)	1 (0%)	34	70
30	39	206/210 (98%)	161 (78%)	38 (18%)	7 (3%)	5	23
31	41	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	11	41
31	49	179/182 (98%)	158 (88%)	20 (11%)	1 (1%)	30	66
32	51	171/180 (95%)	137 (80%)	21 (12%)	13 (8%)	1	6
32	59	168/180 (93%)	128 (76%)	31 (18%)	9 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	61	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	9	35
33	69	144/148 (97%)	113 (78%)	27 (19%)	4 (3%)	6	28
34	15	136/140 (97%)	121 (89%)	14 (10%)	1 (1%)	26	64
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	6	27
35	25	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	24	61
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	35	148/150 (99%)	113 (76%)	32 (22%)	3 (2%)	9	36
36	78	148/150 (99%)	110 (74%)	30 (20%)	8 (5%)	2	13
37	45	137/141 (97%)	110 (80%)	25 (18%)	2 (2%)	13	44
37	88	139/141 (99%)	107 (77%)	26 (19%)	6 (4%)	3	18
38	55	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	11	41
38	98	116/118 (98%)	106 (91%)	9 (8%)	1 (1%)	21	58
39	65	109/112 (97%)	85 (78%)	22 (20%)	2 (2%)	11	39
39	A8	108/112 (96%)	89 (82%)	18 (17%)	1 (1%)	21	58
40	75	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
40	B8	135/146 (92%)	123 (91%)	12 (9%)	0	100	100
41	85	115/118 (98%)	98 (85%)	17 (15%)	0	100	100
41	C8	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	4	23
42	95	99/101 (98%)	77 (78%)	18 (18%)	4 (4%)	4	19
42	D8	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	5	26
43	A5	111/113 (98%)	101 (91%)	7 (6%)	3 (3%)	6	28
43	E8	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
44	B5	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	8	34
44	F8	91/96 (95%)	83 (91%)	6 (7%)	2 (2%)	8	34
45	C5	102/110 (93%)	76 (74%)	24 (24%)	2 (2%)	9	36
45	G8	102/110 (93%)	83 (81%)	13 (13%)	6 (6%)	2	11
46	D5	132/206 (64%)	104 (79%)	24 (18%)	4 (3%)	5	26
46	H8	173/206 (84%)	133 (77%)	33 (19%)	7 (4%)	4	19
47	E5	75/85 (88%)	68 (91%)	5 (7%)	2 (3%)	6	28
47	I8	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	6	28
48	F5	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	17	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	9	35
49	G5	64/72 (89%)	60 (94%)	2 (3%)	2 (3%)	5	25
49	K8	64/72 (89%)	59 (92%)	2 (3%)	3 (5%)	3	16
50	H5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	I5	61/71 (86%)	36 (59%)	21 (34%)	4 (7%)	1	8
51	M8	64/71 (90%)	36 (56%)	25 (39%)	3 (5%)	3	16
52	J5	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	11	39
52	N8	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
53	L5	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
53	P8	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	M5	60/65 (92%)	46 (77%)	11 (18%)	3 (5%)	3	15
54	Q8	59/65 (91%)	52 (88%)	3 (5%)	4 (7%)	1	8
All	All	11183/11946 (94%)	9677 (86%)	1306 (12%)	200 (2%)	11	39

5 of 200 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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%)	161 (78%)	44 (22%)	1	5
2	1E	205/220 (93%)	159 (78%)	46 (22%)	1	4
3	22	160/188 (85%)	121 (76%)	39 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2E	159/188 (85%)	119 (75%)	40 (25%)	1	2
4	32	180/181 (99%)	139 (77%)	41 (23%)	1	4
4	3E	180/181 (99%)	138 (77%)	42 (23%)	1	3
5	42	116/123 (94%)	89 (77%)	27 (23%)	1	3
5	4E	116/123 (94%)	94 (81%)	22 (19%)	2	7
6	52	90/90 (100%)	71 (79%)	19 (21%)	1	5
6	5E	90/90 (100%)	71 (79%)	19 (21%)	1	5
7	62	126/127 (99%)	101 (80%)	25 (20%)	1	6
7	6E	126/127 (99%)	106 (84%)	20 (16%)	3	12
8	72	118/119 (99%)	96 (81%)	22 (19%)	2	8
8	7E	119/119 (100%)	92 (77%)	27 (23%)	1	4
9	82	95/99 (96%)	76 (80%)	19 (20%)	1	6
9	8E	98/99 (99%)	74 (76%)	24 (24%)	1	2
10	1A	89/92 (97%)	68 (76%)	21 (24%)	1	3
10	1I	89/92 (97%)	70 (79%)	19 (21%)	1	5
11	2A	89/99 (90%)	69 (78%)	20 (22%)	1	4
11	2I	88/99 (89%)	70 (80%)	18 (20%)	1	6
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	4
12	3I	103/109 (94%)	85 (82%)	18 (18%)	2	9
13	4A	94/101 (93%)	70 (74%)	24 (26%)	1	2
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	48/50 (96%)	34 (71%)	14 (29%)	0	1
14	5I	48/50 (96%)	35 (73%)	13 (27%)	0	1
15	6A	79/80 (99%)	68 (86%)	11 (14%)	4	18
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	7A	72/74 (97%)	58 (81%)	14 (19%)	2	7
16	7I	72/74 (97%)	60 (83%)	12 (17%)	3	10
17	8A	95/97 (98%)	80 (84%)	15 (16%)	3	12
17	8I	95/97 (98%)	78 (82%)	17 (18%)	2	9
18	9A	62/77 (80%)	46 (74%)	16 (26%)	0	2
18	9I	63/77 (82%)	53 (84%)	10 (16%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AA	67/80 (84%)	50 (75%)	17 (25%)	1	2
19	AI	72/80 (90%)	56 (78%)	16 (22%)	1	4
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	3
20	BI	76/82 (93%)	54 (71%)	22 (29%)	0	1
21	1B	20/22 (91%)	18 (90%)	2 (10%)	9	32
21	1F	20/22 (91%)	18 (90%)	2 (10%)	9	32
28	11	214/218 (98%)	172 (80%)	42 (20%)	1	7
28	19	214/218 (98%)	170 (79%)	44 (21%)	1	6
29	21	165/166 (99%)	121 (73%)	44 (27%)	0	1
29	29	165/166 (99%)	124 (75%)	41 (25%)	1	2
30	31	161/166 (97%)	125 (78%)	36 (22%)	1	4
30	39	165/166 (99%)	121 (73%)	44 (27%)	0	1
31	41	155/156 (99%)	124 (80%)	31 (20%)	1	6
31	49	155/156 (99%)	123 (79%)	32 (21%)	1	6
32	51	142/148 (96%)	108 (76%)	34 (24%)	1	3
32	59	142/148 (96%)	107 (75%)	35 (25%)	1	2
33	61	122/124 (98%)	90 (74%)	32 (26%)	0	1
33	69	122/124 (98%)	86 (70%)	36 (30%)	0	1
34	15	117/119 (98%)	90 (77%)	27 (23%)	1	4
34	58	117/119 (98%)	91 (78%)	26 (22%)	1	4
35	25	100/100 (100%)	77 (77%)	23 (23%)	1	4
35	68	100/100 (100%)	82 (82%)	18 (18%)	2	9
36	35	116/116 (100%)	76 (66%)	40 (34%)	0	0
36	78	116/116 (100%)	81 (70%)	35 (30%)	0	1
37	45	110/111 (99%)	81 (74%)	29 (26%)	0	1
37	88	111/111 (100%)	85 (77%)	26 (23%)	1	3
38	55	100/101 (99%)	72 (72%)	28 (28%)	0	1
38	98	101/101 (100%)	76 (75%)	25 (25%)	1	2
39	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
39	A8	87/88 (99%)	62 (71%)	25 (29%)	0	1
40	75	120/127 (94%)	86 (72%)	34 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	B8	120/127 (94%)	89 (74%)	31 (26%)	0	2
41	85	93/94 (99%)	69 (74%)	24 (26%)	0	2
41	C8	93/94 (99%)	75 (81%)	18 (19%)	2	7
42	95	82/82 (100%)	55 (67%)	27 (33%)	0	0
42	D8	82/82 (100%)	63 (77%)	19 (23%)	1	3
43	A5	92/92 (100%)	69 (75%)	23 (25%)	1	2
43	E8	92/92 (100%)	72 (78%)	20 (22%)	1	5
44	B5	74/78 (95%)	59 (80%)	15 (20%)	1	6
44	F8	74/78 (95%)	62 (84%)	12 (16%)	3	11
45	C5	85/91 (93%)	59 (69%)	26 (31%)	0	1
45	G8	85/91 (93%)	60 (71%)	25 (29%)	0	1
46	D5	127/179 (71%)	102 (80%)	25 (20%)	1	7
46	H8	154/179 (86%)	118 (77%)	36 (23%)	1	3
47	E5	62/67 (92%)	50 (81%)	12 (19%)	2	7
47	I8	61/67 (91%)	50 (82%)	11 (18%)	2	9
48	F5	82/83 (99%)	57 (70%)	25 (30%)	0	1
48	J8	82/83 (99%)	67 (82%)	15 (18%)	2	8
49	G5	62/67 (92%)	42 (68%)	20 (32%)	0	0
49	K8	62/67 (92%)	41 (66%)	21 (34%)	0	0
50	H5	51/52 (98%)	37 (72%)	14 (28%)	0	1
50	L8	51/52 (98%)	38 (74%)	13 (26%)	1	2
51	I5	57/63 (90%)	44 (77%)	13 (23%)	1	4
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	J5	51/52 (98%)	45 (88%)	6 (12%)	6	24
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	3
53	L5	38/42 (90%)	31 (82%)	7 (18%)	2	8
53	P8	38/42 (90%)	30 (79%)	8 (21%)	1	5
54	M5	52/55 (94%)	36 (69%)	16 (31%)	0	1
54	Q8	51/55 (93%)	38 (74%)	13 (26%)	1	2
All	All	9444/9894 (96%)	7253 (77%)	2191 (23%)	1	3

5 of 2191 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
49	K8	24	LEU
6	52	25	ILE
44	B5	78	LYS
51	M8	15	ILE
3	22	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
37	88	13	GLN
46	H8	30	ASN
28	19	96	HIS
35	68	88	ASN
29	29	60	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1504/1522 (98%)	381 (25%)	35 (2%)
1	1G	1503/1522 (98%)	361 (24%)	37 (2%)
22	1K	82/85 (96%)	37 (45%)	8 (9%)
23	2K	76/77 (98%)	21 (27%)	3 (3%)
23	2L	76/77 (98%)	17 (22%)	1 (1%)
24	1L	84/85 (98%)	35 (41%)	8 (9%)
24	3K	84/85 (98%)	27 (32%)	4 (4%)
25	4K	11/30 (36%)	3 (27%)	1 (9%)
25	4L	12/30 (40%)	6 (50%)	3 (25%)
26	14	2908/2918 (99%)	759 (26%)	56 (1%)
26	1H	2911/2918 (99%)	725 (24%)	60 (2%)
27	16	121/122 (99%)	20 (16%)	0
27	1J	121/122 (99%)	33 (27%)	3 (2%)
55	3L	83/85 (97%)	34 (40%)	4 (4%)
All	All	9576/9678 (98%)	2459 (25%)	223 (2%)

5 of 2459 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	13	13	U

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2172	U
1	1G	429	U
26	14	2335	A
26	1H	2428	G
1	1G	89	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	QUO	1K	35	25,22	27,35,36	5.75	9 (33%)	30,52,55	4.04	10 (33%)
22	MIA	1K	38	22	22,31,32	1.02	2 (9%)	26,44,47	2.42	2 (7%)
22	PSU	1K	40	22	15,21,22	0.91	1 (6%)	16,30,33	1.96	4 (25%)
22	5MU	1K	63	22	13,22,23	1.68	2 (15%)	16,32,35	1.53	1 (6%)
22	PSU	1K	64	22	15,21,22	1.00	1 (6%)	16,30,33	2.45	3 (18%)
24	PSU	1L	40	24	15,21,22	1.05	1 (6%)	16,30,33	1.82	4 (25%)
23	OMC	2K	33	23	15,22,23	2.17	4 (26%)	20,31,34	1.15	1 (5%)
23	5MU	2K	55	23	13,22,23	1.73	2 (15%)	16,32,35	1.51	1 (6%)
23	PSU	2K	56	23	15,21,22	1.04	1 (6%)	16,30,33	1.81	4 (25%)
23	4SU	2K	8	23	12,21,22	3.27	2 (16%)	15,30,33	0.90	1 (6%)
23	OMC	2L	33	23	15,22,23	2.30	4 (26%)	20,31,34	1.21	3 (15%)
23	5MU	2L	55	23	13,22,23	1.62	2 (15%)	16,32,35	1.32	1 (6%)
23	PSU	2L	56	23	15,21,22	0.96	1 (6%)	16,30,33	1.90	4 (25%)
23	4SU	2L	8	23	12,21,22	3.18	2 (16%)	15,30,33	0.73	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	3K	40	24	15,21,22	1.01	1 (6%)	16,30,33	1.98	3 (18%)
55	MIA	3L	38	55	22,31,32	1.22	1 (4%)	26,44,47	1.80	5 (19%)
55	PSU	3L	40	55	15,21,22	1.16	1 (6%)	16,30,33	2.13	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	QUO	1K	35	25,22	-	0/6/43/44	0/4/4/4
22	MIA	1K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	1K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
24	PSU	1L	40	24	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
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	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
24	PSU	3K	40	24	-	0/7/25/26	0/2/2/2
55	MIA	3L	38	55	-	0/11/33/34	0/3/3/3
55	PSU	3L	40	55	-	0/7/25/26	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	35	QUO	C8-N9	-10.66	1.22	1.38
22	1K	35	QUO	C6-N1	-9.54	1.15	1.33
22	1K	35	QUO	C6-C5	-5.96	1.31	1.41
23	2L	55	5MU	C4-N3	-3.03	1.27	1.33
22	1K	63	5MU	C4-N3	-2.99	1.27	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	35	QUO	C8-N9-C1'	-15.26	113.53	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	38	MIA	C11-S10-C2	-11.36	94.30	102.31
22	1K	35	QUO	C1'-N9-C4	-7.42	118.52	126.81
22	1K	35	QUO	N3-C2-N1	-7.18	117.78	127.56
22	1K	64	PSU	C5-C1'-C2'	-5.68	105.80	115.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	PAR	13	1745	-	45,45,45	0.82	2 (4%)	60,67,67	2.00	17 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	PAR	1G	1686	-	45,45,45	0.71	1 (2%)	60,67,67	1.76	11 (18%)

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
57	PAR	13	1745	-	-	0/18/94/94	0/4/4/4
57	PAR	1G	1686	-	-	0/18/94/94	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1686	PAR	C24-N24	-2.30	1.43	1.47
57	13	1745	PAR	C21-N21	-2.17	1.44	1.47
57	13	1745	PAR	C24-N24	-2.17	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1G	1686	PAR	C13-O52-C52	-6.18	101.57	118.00
57	13	1745	PAR	C22-C12-C62	-4.22	103.60	110.14
57	13	1745	PAR	C31-C21-N21	-3.47	104.49	110.72
57	13	1745	PAR	O11-C11-C21	-3.31	102.15	108.16
57	1G	1686	PAR	C62-C12-N12	-3.15	105.19	110.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	1505/1522 (98%)	0.12	30 (1%) 68 44	53, 96, 178, 280	0
1	1G	1504/1522 (98%)	0.10	34 (2%) 64 38	67, 108, 172, 272	0
2	12	237/256 (92%)	0.03	7 (2%) 54 27	122, 156, 179, 190	0
2	1E	237/256 (92%)	-0.04	5 (2%) 67 42	101, 137, 165, 175	0
3	22	206/239 (86%)	0.00	8 (3%) 43 20	114, 132, 162, 173	0
3	2E	205/239 (85%)	0.16	10 (4%) 33 14	81, 103, 132, 138	0
4	32	208/209 (99%)	0.28	5 (2%) 62 37	88, 109, 130, 142	0
4	3E	208/209 (99%)	0.67	21 (10%) 9 3	77, 98, 122, 131	0
5	42	151/162 (93%)	0.53	15 (9%) 9 3	99, 115, 136, 155	0
5	4E	151/162 (93%)	0.42	13 (8%) 13 4	72, 91, 112, 150	0
6	52	101/101 (100%)	-0.39	0 100 100	78, 94, 114, 144	0
6	5E	101/101 (100%)	-0.12	2 (1%) 68 44	75, 94, 115, 132	0
7	62	155/156 (99%)	0.49	21 (13%) 4 1	105, 120, 143, 157	0
7	6E	152/156 (97%)	0.27	11 (7%) 18 6	96, 114, 137, 148	0
8	72	137/138 (99%)	1.22	37 (27%) 1 0	98, 119, 131, 137	0
8	7E	138/138 (100%)	1.00	28 (20%) 1 0	81, 100, 114, 126	0
9	82	122/128 (95%)	2.18	60 (49%) 0 0	102, 149, 166, 170	0
9	8E	127/128 (99%)	1.38	42 (33%) 0 0	81, 135, 158, 168	0
10	1A	99/105 (94%)	0.93	25 (25%) 1 0	111, 148, 164, 171	0
10	1I	99/105 (94%)	1.34	29 (29%) 1 0	73, 128, 159, 161	0
11	2A	117/129 (90%)	0.72	13 (11%) 7 2	81, 103, 120, 147	0
11	2I	116/129 (89%)	0.27	7 (6%) 25 10	72, 98, 120, 150	0
12	3A	125/132 (94%)	0.71	19 (15%) 3 1	78, 96, 129, 157	0
12	3I	122/132 (92%)	0.32	8 (6%) 22 7	61, 71, 97, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	117/126 (92%)	0.93	25 (21%) 1 0	102, 137, 157, 170	0
13	4I	116/126 (92%)	0.09	5 (4%) 39 17	78, 117, 136, 144	0
14	5A	58/61 (95%)	2.78	34 (58%) 0 0	116, 131, 146, 154	0
14	5I	59/61 (96%)	1.26	11 (18%) 2 0	82, 92, 108, 118	0
15	6A	88/89 (98%)	0.15	1 (1%) 82 63	80, 105, 121, 127	0
15	6I	88/89 (98%)	0.31	3 (3%) 49 23	67, 93, 110, 123	0
16	7A	84/88 (95%)	1.62	28 (33%) 0 0	85, 98, 124, 154	0
16	7I	84/88 (95%)	1.88	41 (48%) 0 0	90, 104, 132, 160	0
17	8A	100/105 (95%)	0.50	12 (12%) 6 2	91, 106, 124, 128	0
17	8I	100/105 (95%)	0.10	7 (7%) 19 7	81, 99, 111, 121	0
18	9A	71/88 (80%)	-0.33	0 100 100	84, 107, 134, 164	0
18	9I	72/88 (81%)	-0.02	0 100 100	80, 98, 126, 161	0
19	AA	78/93 (83%)	0.35	4 (5%) 32 13	124, 142, 171, 180	0
19	AI	83/93 (89%)	0.22	6 (7%) 18 6	90, 116, 137, 145	0
20	BA	99/106 (93%)	0.99	23 (23%) 1 0	83, 105, 133, 143	0
20	BI	99/106 (93%)	1.75	47 (47%) 0 0	101, 115, 146, 151	0
21	1B	25/27 (92%)	3.82	21 (84%) 0 0	110, 126, 143, 163	0
21	1F	25/27 (92%)	2.87	16 (64%) 0 0	90, 102, 117, 142	0
22	1K	80/85 (94%)	0.12	5 (6%) 23 9	81, 190, 249, 257	0
23	2K	73/77 (94%)	-0.05	2 (2%) 58 32	68, 96, 122, 140	0
23	2L	73/77 (94%)	-0.29	1 (1%) 78 57	76, 105, 138, 160	0
24	1L	84/85 (98%)	1.37	23 (27%) 1 0	107, 214, 302, 318	0
24	3K	84/85 (98%)	-0.18	2 (2%) 62 37	68, 209, 252, 259	0
25	4K	12/30 (40%)	1.37	3 (25%) 1 0	64, 94, 132, 145	0
25	4L	12/30 (40%)	1.32	4 (33%) 0 0	85, 117, 155, 188	0
26	14	2909/2918 (99%)	0.11	39 (1%) 79 59	48, 80, 223, 333	0
26	1H	2912/2918 (99%)	0.14	22 (0%) 87 72	38, 71, 217, 270	0
27	16	122/122 (100%)	-0.20	0 100 100	65, 91, 113, 185	0
27	1J	122/122 (100%)	-0.33	1 (0%) 87 72	73, 107, 128, 182	0
28	11	273/276 (98%)	0.34	3 (1%) 82 63	39, 62, 80, 92	0
28	19	273/276 (98%)	0.76	25 (9%) 11 4	42, 70, 88, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	21	205/206 (99%)	0.79	19 (9%) 11 4	48, 85, 125, 137	0
29	29	205/206 (99%)	0.84	39 (19%) 2 0	56, 87, 129, 148	0
30	31	202/210 (96%)	0.02	0 100 100	38, 74, 110, 127	0
30	39	208/210 (99%)	0.20	7 (3%) 49 23	54, 95, 146, 178	0
31	41	181/182 (99%)	0.27	9 (4%) 32 13	79, 102, 133, 149	0
31	49	181/182 (99%)	1.01	33 (18%) 2 1	104, 125, 154, 169	0
32	51	173/180 (96%)	-0.03	2 (1%) 81 61	79, 102, 115, 151	0
32	59	170/180 (94%)	1.81	58 (34%) 0 0	134, 183, 210, 241	0
33	61	146/148 (98%)	-0.07	2 (1%) 78 57	74, 122, 140, 145	0
33	69	146/148 (98%)	0.47	19 (13%) 5 2	77, 118, 142, 146	0
34	15	138/140 (98%)	1.04	31 (22%) 1 0	75, 100, 129, 137	0
34	58	138/140 (98%)	0.47	9 (6%) 22 8	61, 88, 126, 143	0
35	25	122/122 (100%)	0.44	5 (4%) 41 18	61, 84, 102, 110	0
35	68	122/122 (100%)	0.50	2 (1%) 74 52	55, 74, 92, 101	0
36	35	150/150 (100%)	0.85	26 (17%) 2 1	54, 96, 133, 159	0
36	78	150/150 (100%)	0.24	1 (0%) 89 75	45, 81, 111, 152	0
37	45	139/141 (98%)	1.85	59 (42%) 0 0	69, 98, 116, 136	0
37	88	141/141 (100%)	0.36	2 (1%) 78 57	52, 77, 101, 129	0
38	55	117/118 (99%)	0.63	8 (6%) 20 7	56, 75, 92, 108	0
38	98	118/118 (100%)	0.50	4 (3%) 49 23	56, 80, 101, 107	0
39	65	111/112 (99%)	0.71	14 (12%) 5 2	75, 102, 120, 132	0
39	A8	110/112 (98%)	0.27	5 (4%) 37 17	70, 86, 110, 125	0
40	75	137/146 (93%)	0.35	11 (8%) 15 5	75, 91, 148, 185	0
40	B8	137/146 (93%)	0.50	14 (10%) 9 3	70, 89, 136, 159	0
41	85	117/118 (99%)	0.41	5 (4%) 39 17	62, 88, 122, 143	0
41	C8	117/118 (99%)	0.84	14 (11%) 6 2	50, 76, 107, 141	0
42	95	101/101 (100%)	0.28	7 (6%) 20 7	61, 116, 131, 136	0
42	D8	101/101 (100%)	0.29	7 (6%) 20 7	53, 100, 124, 139	0
43	A5	113/113 (100%)	0.40	4 (3%) 48 22	56, 71, 100, 159	0
43	E8	113/113 (100%)	0.16	0 100 100	52, 72, 105, 140	0
44	B5	92/96 (95%)	0.12	2 (2%) 65 40	64, 79, 106, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	F8	93/96 (96%)	-0.05	0 100 100	51, 67, 93, 102	0
45	C5	104/110 (94%)	0.99	18 (17%) 2 1	89, 119, 158, 166	0
45	G8	104/110 (94%)	0.45	3 (2%) 55 29	69, 96, 140, 148	0
46	D5	138/206 (66%)	0.40	10 (7%) 18 6	103, 134, 178, 186	0
46	H8	175/206 (84%)	-0.21	1 (0%) 90 78	84, 119, 190, 195	0
47	E5	77/85 (90%)	1.24	15 (19%) 1 0	64, 81, 99, 131	0
47	I8	76/85 (89%)	0.68	5 (6%) 22 7	52, 69, 85, 113	0
48	F5	97/98 (98%)	1.42	16 (16%) 2 1	57, 77, 122, 143	0
48	J8	97/98 (98%)	0.88	11 (11%) 7 2	48, 72, 124, 150	0
49	G5	66/72 (91%)	0.15	1 (1%) 76 55	74, 96, 114, 135	0
49	K8	66/72 (91%)	0.36	3 (4%) 37 17	59, 77, 90, 124	0
50	H5	59/60 (98%)	0.51	1 (1%) 73 49	74, 94, 132, 157	0
50	L8	59/60 (98%)	0.39	0 100 100	56, 78, 114, 137	0
51	I5	63/71 (88%)	2.18	28 (44%) 0 0	138, 171, 190, 192	0
51	M8	66/71 (92%)	0.50	6 (9%) 11 4	105, 154, 174, 184	0
52	J5	59/60 (98%)	0.49	2 (3%) 49 23	56, 80, 147, 187	0
52	N8	59/60 (98%)	0.66	6 (10%) 9 3	51, 86, 152, 158	0
53	L5	45/49 (91%)	0.45	1 (2%) 65 40	47, 56, 69, 84	0
53	P8	46/49 (93%)	0.10	0 100 100	40, 48, 66, 81	0
54	M5	62/65 (95%)	1.57	20 (32%) 1 0	65, 77, 93, 107	0
54	Q8	61/65 (93%)	1.02	8 (13%) 5 2	56, 66, 80, 98	0
55	3L	83/85 (97%)	0.32	9 (10%) 8 2	72, 217, 260, 269	0
All	All	20954/21624 (96%)	0.37	1446 (6%) 20 7	38, 95, 175, 333	0

The worst 5 of 1446 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	99	VAL	15.7
48	F5	98	LEU	14.8
48	F5	97	LEU	11.9
32	59	96	ALA	11.0
11	2A	11	LYS	10.2



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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
23	OMC	2K	33	21/22	0.98	0.26	-	70,74,82,85	0
22	PSU	1K	40	20/21	0.95	0.15	-	78,96,104,105	0
23	OMC	2L	33	21/22	0.91	0.22	-	86,95,99,102	0
23	5MU	2K	55	21/22	0.95	0.14	-	88,99,104,112	0
23	PSU	2K	56	20/21	0.95	0.12	-	93,98,101,113	0
23	4SU	2K	8	20/21	0.94	0.16	-	83,89,99,107	0
55	MIA	3L	38	29/30	0.93	0.26	-	102,116,135,141	0
22	5MU	1K	63	21/22	0.92	0.16	-	106,124,138,141	0
24	PSU	1L	40	20/21	0.92	0.26	-	99,116,121,124	0
23	PSU	2L	56	20/21	0.91	0.10	-	101,108,114,119	0
22	PSU	1K	64	20/21	0.92	0.14	-	106,129,138,140	0
55	PSU	3L	40	20/21	0.93	0.24	-	110,117,123,123	0
24	PSU	3K	40	20/21	0.95	0.12	-	106,113,117,119	0
22	QUO	1K	35	32/33	0.94	0.37	-	67,86,101,111	0
22	MIA	1K	38	29/30	0.95	0.29	-	67,84,98,112	0
23	4SU	2L	8	20/21	0.91	0.14	-	99,106,113,117	0
23	5MU	2L	55	21/22	0.95	0.11	-	101,110,116,118	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	1H	3357	1/1	0.97	0.29	33.94	62,62,62,62	0
56	MG	13	1611	1/1	0.94	0.30	24.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3299	1/1	0.74	0.37	18.86	82,82,82,82	0
56	MG	1H	3141	1/1	0.94	0.38	18.66	60,60,60,60	0
56	MG	14	3117	1/1	0.80	0.34	16.05	76,76,76,76	0
56	MG	14	3299	1/1	0.90	0.32	14.53	70,70,70,70	0
56	MG	1H	3265	1/1	0.92	0.84	14.49	54,54,54,54	0
56	MG	1G	1655	1/1	0.96	0.39	14.34	79,79,79,79	0
56	MG	16	205	1/1	0.84	0.30	13.81	77,77,77,77	0
56	MG	1H	3297	1/1	0.96	0.33	13.64	71,71,71,71	0
56	MG	1G	1610	1/1	0.89	0.37	11.73	77,77,77,77	0
56	MG	1H	3007	1/1	0.98	0.32	11.17	46,46,46,46	0
56	MG	1H	3367	1/1	0.97	0.30	11.00	66,66,66,66	0
56	MG	1H	3306	1/1	0.92	0.27	10.51	86,86,86,86	0
56	MG	1H	3084	1/1	0.98	0.28	10.28	48,48,48,48	0
56	MG	1H	3118	1/1	0.91	0.26	9.62	52,52,52,52	0
56	MG	1H	3075	1/1	0.96	0.39	9.35	70,70,70,70	0
56	MG	1H	3153	1/1	0.85	0.33	8.80	64,64,64,64	0
56	MG	14	3186	1/1	0.93	0.28	8.46	54,54,54,54	0
56	MG	1H	3205	1/1	0.76	0.36	8.41	62,62,62,62	0
56	MG	14	3136	1/1	0.85	0.28	8.08	73,73,73,73	0
56	MG	1H	3095	1/1	0.94	0.41	7.83	49,49,49,49	0
56	MG	1H	3366	1/1	0.76	0.39	7.53	74,74,74,74	0
56	MG	1H	3175	1/1	0.98	0.29	7.43	67,67,67,67	0
56	MG	13	1625	1/1	0.98	0.34	7.25	45,45,45,45	0
56	MG	1H	3028	1/1	0.92	0.27	6.81	67,67,67,67	0
56	MG	1H	3310	1/1	0.92	0.28	6.76	69,69,69,69	0
56	MG	13	1696	1/1	0.78	0.26	6.72	116,116,116,116	0
56	MG	1H	3177	1/1	0.85	0.30	6.71	55,55,55,55	0
56	MG	14	3092	1/1	0.93	0.28	6.62	41,41,41,41	0
56	MG	1H	3315	1/1	0.94	0.28	6.43	66,66,66,66	0
56	MG	14	3202	1/1	0.97	0.38	5.95	55,55,55,55	0
56	MG	13	1654	1/1	0.97	0.23	5.76	75,75,75,75	0
56	MG	1H	3094	1/1	0.94	0.28	5.55	41,41,41,41	0
56	MG	14	3235	1/1	0.95	0.26	5.51	72,72,72,72	0
56	MG	2K	102	1/1	0.72	0.23	5.34	83,83,83,83	0
56	MG	14	3281	1/1	0.93	0.22	5.33	73,73,73,73	0
56	MG	1H	3241	1/1	0.90	0.25	5.33	65,65,65,65	0
56	MG	14	3197	1/1	0.93	0.28	5.31	89,89,89,89	0
56	MG	14	3192	1/1	0.90	0.35	5.19	80,80,80,80	0
56	MG	1H	3128	1/1	0.85	0.28	5.02	57,57,57,57	0
56	MG	14	3045	1/1	0.94	0.32	4.98	57,57,57,57	0
56	MG	14	3224	1/1	0.92	0.49	4.87	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3122	1/1	0.87	0.24	4.73	49,49,49,49	0
56	MG	14	3305	1/1	0.77	0.17	4.71	79,79,79,79	0
56	MG	1H	3050	1/1	0.90	0.28	4.69	36,36,36,36	0
56	MG	1H	3193	1/1	0.96	0.29	4.68	69,69,69,69	0
56	MG	1H	3161	1/1	0.89	0.26	4.60	55,55,55,55	0
56	MG	1H	3148	1/1	0.88	0.29	4.54	82,82,82,82	0
56	MG	1G	1642	1/1	0.83	0.35	4.50	81,81,81,81	0
56	MG	14	3078	1/1	0.99	0.29	4.49	50,50,50,50	0
56	MG	14	3253	1/1	0.95	0.30	4.41	74,74,74,74	0
56	MG	14	3138	1/1	0.89	0.33	4.38	79,79,79,79	0
56	MG	1H	3046	1/1	0.96	0.34	4.32	67,67,67,67	0
56	MG	1G	1637	1/1	0.96	0.41	4.24	81,81,81,81	0
56	MG	13	1680	1/1	0.97	0.28	4.15	69,69,69,69	0
56	MG	1H	3149	1/1	0.97	0.34	4.02	65,65,65,65	0
56	MG	41	201	1/1	0.88	0.37	3.94	82,82,82,82	0
56	MG	1H	3144	1/1	0.71	0.27	3.75	66,66,66,66	0
56	MG	13	1649	1/1	0.79	0.21	3.35	85,85,85,85	0
56	MG	1H	3022	1/1	0.98	0.27	3.28	53,53,53,53	0
56	MG	1H	3081	1/1	0.90	0.22	3.28	61,61,61,61	0
56	MG	14	3126	1/1	0.97	0.31	3.20	66,66,66,66	0
56	MG	14	3031	1/1	0.96	0.27	3.14	60,60,60,60	0
56	MG	14	3301	1/1	0.92	0.27	2.80	86,86,86,86	0
56	MG	16	201	1/1	0.88	0.24	2.76	78,78,78,78	0
56	MG	13	1705	1/1	0.88	0.37	2.73	94,94,94,94	0
56	MG	14	3142	1/1	0.84	0.21	2.67	59,59,59,59	0
56	MG	1H	3014	1/1	0.97	0.27	2.67	43,43,43,43	0
56	MG	14	3159	1/1	0.84	0.22	2.67	73,73,73,73	0
58	ZN	32	301	1/1	0.98	0.36	2.66	96,96,96,96	0
56	MG	1H	3049	1/1	0.98	0.28	2.63	60,60,60,60	0
56	MG	1H	3221	1/1	0.84	0.24	2.61	80,80,80,80	0
56	MG	14	3291	1/1	0.90	0.26	2.48	55,55,55,55	0
56	MG	13	1613	1/1	0.93	0.27	2.35	71,71,71,71	0
56	MG	1H	3206	1/1	0.97	0.23	2.09	63,63,63,63	0
56	MG	1H	3089	1/1	0.92	0.26	2.09	45,45,45,45	0
58	ZN	3E	302	1/1	0.97	0.35	1.99	89,89,89,89	0
57	PAR	1G	1686	42/42	0.97	0.25	1.96	69,76,87,91	0
56	MG	13	1648	1/1	0.90	0.19	1.80	69,69,69,69	0
56	MG	1H	3079	1/1	0.98	0.26	1.78	45,45,45,45	0
56	MG	14	3391	1/1	0.93	0.71	1.75	58,58,58,58	0
56	MG	16	209	1/1	0.95	0.20	1.71	56,56,56,56	0
56	MG	1H	3068	1/1	0.80	0.29	1.63	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3114	1/1	0.98	0.23	1.59	48,48,48,48	0
56	MG	1H	3291	1/1	0.98	0.25	1.47	40,40,40,40	0
56	MG	1H	3064	1/1	0.95	0.26	1.27	56,56,56,56	0
57	PAR	13	1745	42/42	0.97	0.22	1.26	57,66,72,75	0
56	MG	1H	3047	1/1	0.93	0.21	1.21	70,70,70,70	0
56	MG	1H	3185	1/1	0.64	0.19	1.14	71,71,71,71	0
56	MG	1H	3151	1/1	0.91	0.20	1.12	66,66,66,66	0
56	MG	1H	3277	1/1	0.97	0.27	1.04	70,70,70,70	0
56	MG	1G	1659	1/1	0.84	0.20	1.03	93,93,93,93	0
56	MG	14	3097	1/1	0.90	0.21	1.01	59,59,59,59	0
56	MG	14	3147	1/1	0.93	0.18	0.93	78,78,78,78	0
56	MG	14	3103	1/1	0.95	0.21	0.93	67,67,67,67	0
56	MG	13	1601	1/1	0.99	0.23	0.92	46,46,46,46	0
56	MG	1H	3239	1/1	0.63	0.22	0.86	72,72,72,72	0
56	MG	1H	3330	1/1	0.71	0.22	0.75	67,67,67,67	0
56	MG	1H	3334	1/1	0.84	0.23	0.68	60,60,60,60	0
56	MG	16	204	1/1	0.88	0.19	0.68	86,86,86,86	0
56	MG	1G	1653	1/1	0.95	0.23	0.65	90,90,90,90	0
56	MG	13	1644	1/1	0.86	0.34	0.63	76,76,76,76	0
56	MG	1H	3201	1/1	0.71	0.20	0.61	59,59,59,59	0
56	MG	1H	3060	1/1	0.94	0.20	0.58	74,74,74,74	0
56	MG	14	3098	1/1	0.97	0.22	0.55	54,54,54,54	0
56	MG	21	302	1/1	0.93	0.32	0.43	66,66,66,66	0
56	MG	14	3028	1/1	0.94	0.18	0.43	73,73,73,73	0
56	MG	14	3225	1/1	0.94	0.20	0.41	78,78,78,78	0
56	MG	1G	1640	1/1	0.97	0.19	0.40	80,80,80,80	0
56	MG	14	3111	1/1	0.98	0.22	0.33	55,55,55,55	0
56	MG	13	1689	1/1	0.90	0.38	0.33	120,120,120,120	0
56	MG	1H	3165	1/1	0.89	0.23	0.33	61,61,61,61	0
56	MG	1H	3207	1/1	0.72	0.21	0.29	73,73,73,73	0
56	MG	14	3129	1/1	0.86	0.24	0.25	63,63,63,63	0
56	MG	13	1707	1/1	0.78	0.25	0.22	96,96,96,96	0
56	MG	14	3156	1/1	0.92	0.18	0.14	60,60,60,60	0
56	MG	13	1632	1/1	0.94	0.18	0.13	63,63,63,63	0
56	MG	14	3294	1/1	0.95	0.24	0.12	74,74,74,74	0
56	MG	14	3125	1/1	0.88	0.19	0.07	53,53,53,53	0
56	MG	16	203	1/1	0.72	0.17	0.04	68,68,68,68	0
56	MG	1G	1677	1/1	0.87	0.19	0.04	104,104,104,104	0
56	MG	1H	3052	1/1	0.97	0.22	0.01	46,46,46,46	0
56	MG	14	3258	1/1	0.86	0.14	-0.02	73,73,73,73	0
56	MG	1H	3247	1/1	0.93	0.24	-0.02	64,64,64,64	0
56	MG	13	1615	1/1	0.98	0.28	-0.04	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3132	1/1	0.95	0.21	-0.04	45,45,45,45	0
56	MG	85	201	1/1	0.86	0.22	-0.11	69,69,69,69	0
56	MG	14	3266	1/1	0.93	0.21	-0.16	68,68,68,68	0
56	MG	14	3053	1/1	0.99	0.22	-0.16	52,52,52,52	0
56	MG	13	1746	1/1	0.92	0.18	-0.17	72,72,72,72	0
56	MG	14	3061	1/1	0.99	0.22	-0.18	50,50,50,50	0
56	MG	1H	3111	1/1	0.99	0.20	-0.22	43,43,43,43	0
56	MG	14	3245	1/1	0.96	0.21	-0.27	70,70,70,70	0
56	MG	1H	3090	1/1	0.98	0.21	-0.29	44,44,44,44	0
56	MG	14	3183	1/1	0.97	0.26	-0.30	46,46,46,46	0
56	MG	14	3386	1/1	0.96	0.22	-0.31	60,60,60,60	0
56	MG	1G	1601	1/1	0.98	0.20	-0.37	65,65,65,65	0
56	MG	29	302	1/1	0.96	0.29	-0.38	65,65,65,65	0
56	MG	1G	1615	1/1	0.97	0.17	-0.38	87,87,87,87	0
56	MG	1G	1670	1/1	0.83	0.20	-0.38	77,77,77,77	0
56	MG	14	3209	1/1	0.94	0.16	-0.40	74,74,74,74	0
56	MG	1H	3224	1/1	0.89	0.22	-0.42	61,61,61,61	0
56	MG	88	201	1/1	0.92	0.20	-0.43	78,78,78,78	0
56	MG	14	3222	1/1	0.97	0.18	-0.43	83,83,83,83	0
56	MG	1H	3125	1/1	0.84	0.20	-0.46	49,49,49,49	0
56	MG	1H	3152	1/1	0.87	0.21	-0.59	75,75,75,75	0
56	MG	14	3076	1/1	0.92	0.29	-0.61	54,54,54,54	0
56	MG	29	303	1/1	0.99	0.20	-0.61	71,71,71,71	0
56	MG	1H	3233	1/1	0.79	0.21	-0.61	53,53,53,53	0
56	MG	1J	201	1/1	0.94	0.16	-0.62	87,87,87,87	0
56	MG	1H	3480	1/1	0.99	0.19	-0.69	56,56,56,56	0
56	MG	1H	3317	1/1	0.92	0.18	-0.69	61,61,61,61	0
56	MG	39	301	1/1	0.77	0.23	-0.69	71,71,71,71	0
56	MG	1H	3409	1/1	0.80	0.20	-0.70	53,53,53,53	0
56	MG	1H	3037	1/1	0.93	0.20	-0.72	62,62,62,62	0
56	MG	1H	3106	1/1	0.87	0.17	-0.75	58,58,58,58	0
56	MG	14	3191	1/1	0.97	0.20	-0.76	57,57,57,57	0
56	MG	2K	107	1/1	0.98	0.20	-0.78	59,59,59,59	0
56	MG	14	3011	1/1	0.93	0.18	-0.83	43,43,43,43	0
56	MG	1H	3427	1/1	0.95	0.23	-0.84	76,76,76,76	0
56	MG	14	3214	1/1	0.83	0.17	-0.85	65,65,65,65	0
56	MG	1G	1638	1/1	0.95	0.16	-0.86	75,75,75,75	0
56	MG	13	1638	1/1	0.97	0.19	-0.86	53,53,53,53	0
56	MG	14	3199	1/1	0.66	0.20	-0.87	69,69,69,69	0
56	MG	13	1606	1/1	0.97	0.20	-0.90	63,63,63,63	0
56	MG	1H	3259	1/1	0.83	0.20	-0.93	81,81,81,81	0
56	MG	14	3040	1/1	0.98	0.21	-0.95	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3320	1/1	0.98	0.23	-0.95	60,60,60,60	0
56	MG	13	1677	1/1	0.92	0.17	-0.96	71,71,71,71	0
56	MG	1H	3127	1/1	0.96	0.19	-0.96	52,52,52,52	0
56	MG	14	3218	1/1	0.79	0.19	-0.97	77,77,77,77	0
56	MG	1J	204	1/1	0.92	0.12	-0.98	95,95,95,95	0
58	ZN	G8	201	1/1	0.23	0.14	-0.98	178,178,178,178	0
56	MG	1G	1684	1/1	0.58	0.13	-0.98	122,122,122,122	0
56	MG	1H	3017	1/1	0.98	0.20	-0.99	41,41,41,41	0
56	MG	1H	3250	1/1	0.78	0.16	-1.02	68,68,68,68	0
58	ZN	5I	101	1/1	0.98	0.16	-1.07	88,88,88,88	0
56	MG	14	3276	1/1	0.87	0.15	-1.09	76,76,76,76	0
56	MG	14	3165	1/1	0.96	0.16	-1.09	58,58,58,58	0
58	ZN	C5	202	1/1	0.57	0.15	-1.13	192,192,192,192	0
56	MG	14	3121	1/1	0.83	0.17	-1.15	58,58,58,58	0
56	MG	1H	3016	1/1	0.92	0.22	-1.17	45,45,45,45	0
56	MG	14	3049	1/1	0.99	0.18	-1.17	54,54,54,54	0
56	MG	1G	1612	1/1	0.96	0.18	-1.19	63,63,63,63	0
56	MG	1H	3230	1/1	0.98	0.19	-1.19	37,37,37,37	0
56	MG	13	1605	1/1	0.98	0.18	-1.20	67,67,67,67	0
56	MG	14	3349	1/1	0.94	0.20	-1.20	63,63,63,63	0
58	ZN	5A	101	1/1	0.97	0.14	-1.22	121,121,121,121	0
56	MG	1H	3039	1/1	0.93	0.19	-1.23	47,47,47,47	0
56	MG	1G	1616	1/1	0.96	0.15	-1.25	86,86,86,86	0
56	MG	14	3013	1/1	0.96	0.18	-1.25	54,54,54,54	0
56	MG	13	1653	1/1	0.88	0.09	-1.27	75,75,75,75	0
56	MG	14	3122	1/1	0.81	0.14	-1.30	68,68,68,68	0
56	MG	1H	3033	1/1	0.90	0.15	-1.32	67,67,67,67	0
56	MG	14	3032	1/1	0.97	0.17	-1.32	65,65,65,65	0
56	MG	13	1747	1/1	0.89	0.21	-1.34	64,64,64,64	0
56	MG	1H	3013	1/1	0.96	0.19	-1.37	31,31,31,31	0
56	MG	14	3048	1/1	0.96	0.15	-1.42	67,67,67,67	0
56	MG	13	1629	1/1	0.98	0.18	-1.45	46,46,46,46	0
56	MG	14	3068	1/1	0.96	0.19	-1.47	69,69,69,69	0
56	MG	13	1729	1/1	0.94	0.06	-1.48	97,97,97,97	0
56	MG	1H	3428	1/1	0.98	0.15	-1.52	47,47,47,47	0
56	MG	1H	3058	1/1	0.89	0.17	-1.53	61,61,61,61	0
56	MG	11	302	1/1	0.87	0.19	-1.53	42,42,42,42	0
56	MG	14	3082	1/1	0.96	0.16	-1.54	67,67,67,67	0
56	MG	14	3084	1/1	0.98	0.18	-1.54	43,43,43,43	0
56	MG	3E	301	1/1	0.81	0.11	-1.57	112,112,112,112	0
56	MG	13	1722	1/1	0.93	0.11	-1.60	76,76,76,76	0
56	MG	1G	1680	1/1	0.91	0.27	-1.62	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	13	1683	1/1	0.96	0.14	-1.65	69,69,69,69	0
56	MG	14	3060	1/1	0.97	0.14	-1.67	48,48,48,48	0
56	MG	14	3038	1/1	0.98	0.15	-1.74	34,34,34,34	0
56	MG	14	3039	1/1	0.96	0.17	-1.75	38,38,38,38	0
56	MG	14	3357	1/1	0.97	0.15	-1.83	62,62,62,62	0
56	MG	1H	3031	1/1	0.95	0.17	-1.83	71,71,71,71	0
56	MG	14	3371	1/1	0.96	0.13	-1.83	56,56,56,56	0
56	MG	1H	3002	1/1	0.98	0.18	-1.86	40,40,40,40	0
56	MG	1H	3365	1/1	0.97	0.17	-1.86	64,64,64,64	0
56	MG	14	3211	1/1	0.96	0.15	-1.88	67,67,67,67	0
56	MG	1H	3369	1/1	0.95	0.12	-1.89	45,45,45,45	0
56	MG	1H	3113	1/1	0.89	0.13	-1.91	41,41,41,41	0
56	MG	14	3113	1/1	0.91	0.13	-1.94	42,42,42,42	0
56	MG	14	3131	1/1	0.93	0.17	-1.95	70,70,70,70	0
56	MG	1H	3191	1/1	0.95	0.18	-1.98	75,75,75,75	0
56	MG	1H	3413	1/1	0.98	0.17	-1.98	44,44,44,44	0
56	MG	14	3074	1/1	0.95	0.16	-2.01	66,66,66,66	0
56	MG	14	3188	1/1	0.96	0.17	-2.04	56,56,56,56	0
56	MG	14	3332	1/1	0.82	0.17	-2.05	73,73,73,73	0
56	MG	2L	101	1/1	0.97	0.15	-2.06	76,76,76,76	0
56	MG	1H	3103	1/1	0.91	0.16	-2.07	30,30,30,30	0
56	MG	78	201	1/1	0.92	0.18	-2.07	59,59,59,59	0
56	MG	1H	3212	1/1	0.93	0.15	-2.09	63,63,63,63	0
56	MG	1H	3100	1/1	0.97	0.17	-2.12	43,43,43,43	0
56	MG	13	1672	1/1	0.92	0.07	-2.17	91,91,91,91	0
56	MG	14	3022	1/1	0.94	0.14	-2.17	72,72,72,72	0
56	MG	1H	3038	1/1	0.94	0.13	-2.23	55,55,55,55	0
56	MG	14	3345	1/1	0.87	0.15	-2.26	81,81,81,81	0
56	MG	1G	1687	1/1	0.96	0.10	-2.30	81,81,81,81	0
56	MG	1H	3018	1/1	0.96	0.17	-2.31	52,52,52,52	0
56	MG	1G	1621	1/1	0.94	0.15	-2.43	81,81,81,81	0
56	MG	14	3189	1/1	0.83	0.16	-2.45	60,60,60,60	0
56	MG	14	3316	1/1	0.97	0.10	-2.45	49,49,49,49	0
56	MG	14	3016	1/1	0.96	0.12	-2.47	54,54,54,54	0
56	MG	13	1712	1/1	0.96	0.16	-2.47	77,77,77,77	0
56	MG	14	3102	1/1	0.88	0.15	-2.51	49,49,49,49	0
56	MG	1H	3035	1/1	0.98	0.15	-2.52	61,61,61,61	0
56	MG	14	3184	1/1	0.91	0.15	-2.53	53,53,53,53	0
56	MG	13	1635	1/1	0.95	0.12	-2.53	59,59,59,59	0
56	MG	14	3169	1/1	0.73	0.14	-2.53	77,77,77,77	0
56	MG	13	1737	1/1	0.95	0.07	-2.58	62,62,62,62	0
56	MG	13	1608	1/1	0.99	0.17	-2.61	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3309	1/1	0.96	0.11	-2.61	58,58,58,58	0
56	MG	13	1682	1/1	0.93	0.11	-2.62	86,86,86,86	0
56	MG	14	3024	1/1	0.95	0.14	-2.65	74,74,74,74	0
56	MG	14	3302	1/1	0.79	0.15	-2.65	72,72,72,72	0
56	MG	1H	3452	1/1	0.90	0.13	-2.68	49,49,49,49	0
56	MG	14	3046	1/1	0.99	0.09	-2.70	53,53,53,53	0
56	MG	14	3106	1/1	0.94	0.13	-2.73	50,50,50,50	0
56	MG	1H	3070	1/1	0.92	0.16	-2.78	46,46,46,46	0
56	MG	1H	3374	1/1	0.99	0.10	-2.79	50,50,50,50	0
56	MG	14	3308	1/1	0.94	0.12	-2.79	46,46,46,46	0
56	MG	14	3330	1/1	0.96	0.06	-2.82	48,48,48,48	0
56	MG	14	3376	1/1	0.94	0.13	-2.89	87,87,87,87	0
56	MG	13	1670	1/1	0.81	0.13	-2.90	78,78,78,78	0
56	MG	13	1639	1/1	0.96	0.12	-2.93	56,56,56,56	0
56	MG	1H	3071	1/1	0.97	0.16	-2.95	53,53,53,53	0
56	MG	1H	3415	1/1	0.97	0.17	-2.98	68,68,68,68	0
56	MG	13	1723	1/1	0.95	0.08	-3.05	86,86,86,86	0
56	MG	14	3333	1/1	0.98	0.12	-3.06	58,58,58,58	0
56	MG	1G	1607	1/1	0.98	0.16	-3.06	81,81,81,81	0
56	MG	13	1620	1/1	0.97	0.21	-3.07	51,51,51,51	0
56	MG	1H	3381	1/1	0.96	0.11	-3.14	40,40,40,40	0
56	MG	1G	1681	1/1	0.93	0.18	-3.16	110,110,110,110	0
56	MG	1H	3316	1/1	0.85	0.15	-3.20	74,74,74,74	0
56	MG	1H	3156	1/1	0.86	0.11	-3.20	54,54,54,54	0
56	MG	14	3006	1/1	0.97	0.16	-3.21	48,48,48,48	0
56	MG	13	1730	1/1	0.86	0.11	-3.26	86,86,86,86	0
56	MG	1H	3180	1/1	0.92	0.18	-3.28	59,59,59,59	0
56	MG	14	3360	1/1	0.98	0.13	-3.28	63,63,63,63	0
56	MG	1H	3261	1/1	0.88	0.15	-3.29	61,61,61,61	0
56	MG	1G	1676	1/1	0.97	0.07	-3.32	75,75,75,75	0
56	MG	14	3251	1/1	0.93	0.15	-3.35	48,48,48,48	0
56	MG	1H	3160	1/1	0.97	0.14	-3.36	56,56,56,56	0
56	MG	14	3341	1/1	0.89	0.11	-3.39	48,48,48,48	0
56	MG	13	1720	1/1	0.75	0.11	-3.42	62,62,62,62	0
56	MG	14	3373	1/1	0.92	0.11	-3.52	69,69,69,69	0
56	MG	1H	3371	1/1	0.97	0.16	-3.53	46,46,46,46	0
56	MG	14	3340	1/1	0.91	0.10	-3.54	59,59,59,59	0
56	MG	14	3109	1/1	0.96	0.09	-3.56	78,78,78,78	0
56	MG	14	3329	1/1	0.97	0.12	-3.58	45,45,45,45	0
56	MG	1H	3414	1/1	0.97	0.13	-3.67	53,53,53,53	0
56	MG	14	3351	1/1	0.99	0.13	-3.77	43,43,43,43	0
56	MG	13	1628	1/1	0.86	0.13	-3.79	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3412	1/1	0.97	0.15	-3.79	32,32,32,32	0
56	MG	1H	3104	1/1	0.98	0.15	-3.79	41,41,41,41	0
56	MG	1H	3389	1/1	0.98	0.14	-3.80	68,68,68,68	0
56	MG	1H	3010	1/1	0.98	0.18	-3.87	54,54,54,54	0
56	MG	1H	3444	1/1	0.88	0.13	-3.88	59,59,59,59	0
56	MG	1G	1613	1/1	0.97	0.08	-3.89	87,87,87,87	0
56	MG	14	3314	1/1	0.92	0.12	-3.97	55,55,55,55	0
56	MG	14	3364	1/1	0.97	0.08	-4.05	75,75,75,75	0
56	MG	1H	3235	1/1	0.95	0.14	-4.08	38,38,38,38	0
56	MG	1H	3384	1/1	0.88	0.07	-4.08	57,57,57,57	0
56	MG	14	3327	1/1	0.94	0.10	-4.09	58,58,58,58	0
56	MG	1H	3373	1/1	0.94	0.15	-4.11	45,45,45,45	0
56	MG	1G	1611	1/1	0.95	0.13	-4.16	72,72,72,72	0
56	MG	14	3036	1/1	0.96	0.16	-4.16	42,42,42,42	0
56	MG	14	3344	1/1	0.98	0.09	-4.17	51,51,51,51	0
56	MG	3I	201	1/1	0.86	0.07	-4.20	58,58,58,58	0
56	MG	14	3359	1/1	0.91	0.09	-4.22	87,87,87,87	0
56	MG	1H	3034	1/1	0.91	0.12	-4.23	51,51,51,51	0
56	MG	1H	3167	1/1	0.89	0.15	-4.25	67,67,67,67	0
56	MG	1G	1673	1/1	0.94	0.06	-4.29	74,74,74,74	0
56	MG	1H	3252	1/1	0.97	0.12	-4.31	49,49,49,49	0
56	MG	14	3346	1/1	0.94	0.12	-4.32	59,59,59,59	0
56	MG	1H	3451	1/1	0.66	0.13	-4.32	46,46,46,46	0
56	MG	1H	3251	1/1	0.95	0.10	-4.34	61,61,61,61	0
56	MG	14	3037	1/1	0.94	0.16	-4.36	61,61,61,61	0
56	MG	14	3204	1/1	0.94	0.19	-4.47	51,51,51,51	0
56	MG	1H	3040	1/1	0.96	0.14	-4.48	49,49,49,49	0
56	MG	14	3361	1/1	0.97	0.07	-4.50	60,60,60,60	0
56	MG	1H	3455	1/1	0.99	0.08	-4.51	57,57,57,57	0
56	MG	14	3027	1/1	0.97	0.12	-4.75	70,70,70,70	0
56	MG	14	3319	1/1	0.98	0.08	-4.80	62,62,62,62	0
56	MG	14	3206	1/1	0.95	0.15	-4.85	48,48,48,48	0
56	MG	1H	3134	1/1	0.92	0.12	-4.90	61,61,61,61	0
56	MG	14	3215	1/1	0.94	0.12	-4.97	50,50,50,50	0
56	MG	1H	3382	1/1	0.95	0.09	-5.14	45,45,45,45	0
56	MG	14	3193	1/1	0.93	0.14	-5.21	59,59,59,59	0
56	MG	1H	3442	1/1	0.98	0.11	-5.25	42,42,42,42	0
56	MG	13	1725	1/1	0.96	0.08	-5.26	62,62,62,62	0
56	MG	14	3315	1/1	0.94	0.13	-5.28	68,68,68,68	0
56	MG	1H	3155	1/1	0.92	0.15	-5.32	74,74,74,74	0
56	MG	1H	3465	1/1	0.92	0.10	-5.35	94,94,94,94	0
56	MG	1H	3445	1/1	0.98	0.10	-5.39	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3390	1/1	0.93	0.10	-5.45	66,66,66,66	0
56	MG	14	3219	1/1	0.95	0.14	-5.51	56,56,56,56	0
56	MG	13	1640	1/1	0.98	0.10	-5.51	75,75,75,75	0
56	MG	1G	1602	1/1	0.98	0.11	-5.52	64,64,64,64	0
56	MG	1H	3092	1/1	0.91	0.11	-5.55	50,50,50,50	0
56	MG	1H	3376	1/1	0.96	0.08	-5.55	36,36,36,36	0
56	MG	14	3056	1/1	0.95	0.18	-5.69	51,51,51,51	0
56	MG	1H	3232	1/1	0.97	0.13	-5.74	43,43,43,43	0
56	MG	1H	3181	1/1	0.94	0.14	-5.75	54,54,54,54	0
56	MG	14	3335	1/1	0.97	0.06	-5.81	55,55,55,55	0
56	MG	13	1666	1/1	0.89	0.12	-5.88	58,58,58,58	0
56	MG	1H	3418	1/1	0.98	0.06	-5.88	42,42,42,42	0
56	MG	14	3080	1/1	0.97	0.07	-5.95	69,69,69,69	0
56	MG	14	3135	1/1	0.81	0.10	-6.05	78,78,78,78	0
56	MG	14	3273	1/1	0.91	0.09	-6.21	73,73,73,73	0
56	MG	1H	3379	1/1	0.90	0.10	-6.22	46,46,46,46	0
56	MG	1H	3394	1/1	0.89	0.10	-6.23	57,57,57,57	0
56	MG	1H	3429	1/1	0.93	0.08	-6.23	40,40,40,40	0
56	MG	14	3323	1/1	0.90	0.06	-6.26	55,55,55,55	0
56	MG	1G	1674	1/1	0.94	0.11	-6.28	70,70,70,70	0
56	MG	1H	3061	1/1	0.99	0.12	-6.30	48,48,48,48	0
56	MG	1H	3408	1/1	0.98	0.11	-6.31	47,47,47,47	0
56	MG	14	3003	1/1	0.98	0.09	-6.64	54,54,54,54	0
56	MG	14	3348	1/1	0.91	0.09	-6.68	54,54,54,54	0
56	MG	1H	3120	1/1	0.95	0.13	-7.13	60,60,60,60	0
56	MG	1H	3143	1/1	0.95	0.13	-7.14	49,49,49,49	0
56	MG	1H	3478	1/1	0.91	0.11	-7.24	102,102,102,102	0
56	MG	14	3311	1/1	0.98	0.12	-7.38	51,51,51,51	0
56	MG	1H	3001	1/1	0.97	0.18	-7.51	49,49,49,49	0
56	MG	13	1675	1/1	0.98	0.10	-7.52	73,73,73,73	0
56	MG	14	3297	1/1	0.93	0.08	-7.56	74,74,74,74	0
56	MG	14	3347	1/1	0.99	0.07	-7.71	56,56,56,56	0
56	MG	1H	3395	1/1	0.98	0.09	-7.71	45,45,45,45	0
56	MG	13	1663	1/1	0.80	0.13	-7.72	88,88,88,88	0
56	MG	1H	3378	1/1	0.95	0.14	-8.25	55,55,55,55	0
56	MG	1H	3440	1/1	0.97	0.12	-8.51	61,61,61,61	0
56	MG	1H	3420	1/1	0.94	0.16	-8.58	48,48,48,48	0
56	MG	1H	3404	1/1	0.97	0.08	-8.64	45,45,45,45	0
56	MG	14	3378	1/1	0.82	0.10	-8.91	79,79,79,79	0
56	MG	14	3342	1/1	0.81	0.12	-9.04	74,74,74,74	0
56	MG	1H	3411	1/1	0.97	0.08	-9.29	53,53,53,53	0
56	MG	1H	3459	1/1	0.72	0.08	-9.47	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3466	1/1	0.96	0.07	-10.47	56,56,56,56	0
56	MG	1H	3093	1/1	0.98	0.09	-11.10	47,47,47,47	0
56	MG	1H	3425	1/1	0.90	0.07	-11.28	67,67,67,67	0
56	MG	1H	3450	1/1	0.91	0.05	-11.40	67,67,67,67	0
56	MG	1H	3380	1/1	0.98	0.12	-11.52	41,41,41,41	0
56	MG	14	3313	1/1	0.97	0.06	-12.10	50,50,50,50	0
56	MG	1H	3422	1/1	0.93	0.09	-12.90	54,54,54,54	0
56	MG	14	3384	1/1	0.95	0.09	-14.28	62,62,62,62	0
56	MG	1H	3375	1/1	0.95	0.10	-14.51	37,37,37,37	0
56	MG	14	3064	1/1	0.98	0.15	-	71,71,71,71	0
56	MG	1H	3278	1/1	0.92	0.25	-	76,76,76,76	0
56	MG	14	3288	1/1	0.90	0.16	-	74,74,74,74	0
56	MG	1H	3364	1/1	0.89	0.09	-	68,68,68,68	0
56	MG	1H	3454	1/1	0.89	0.12	-	98,98,98,98	0
56	MG	1H	3248	1/1	0.70	0.32	-	80,80,80,80	0
56	MG	1H	3268	1/1	0.96	0.23	-	46,46,46,46	0
56	MG	14	3328	1/1	0.96	0.10	-	62,62,62,62	0
56	MG	1H	3401	1/1	0.87	0.07	-	64,64,64,64	0
56	MG	14	3205	1/1	0.92	0.25	-	71,71,71,71	0
56	MG	13	1744	1/1	0.96	0.07	-	95,95,95,95	0
56	MG	13	1732	1/1	0.96	0.13	-	62,62,62,62	0
56	MG	14	3101	1/1	0.97	0.26	-	84,84,84,84	0
56	MG	14	3278	1/1	0.90	0.19	-	98,98,98,98	0
56	MG	14	3172	1/1	0.88	0.35	-	69,69,69,69	0
56	MG	1H	3163	1/1	0.76	0.34	-	87,87,87,87	0
56	MG	2K	104	1/1	0.95	0.29	-	98,98,98,98	0
56	MG	1H	3359	1/1	0.84	0.53	-	84,84,84,84	0
56	MG	1H	3456	1/1	0.96	0.12	-	92,92,92,92	0
56	MG	1G	1667	1/1	0.70	0.25	-	80,80,80,80	0
56	MG	2L	103	1/1	0.85	0.23	-	89,89,89,89	0
56	MG	14	3356	1/1	0.95	0.09	-	72,72,72,72	0
56	MG	14	3274	1/1	0.86	0.26	-	82,82,82,82	0
56	MG	13	1743	1/1	0.61	0.36	-	102,102,102,102	0
56	MG	13	1647	1/1	0.58	0.21	-	77,77,77,77	0
56	MG	14	3133	1/1	0.81	0.19	-	86,86,86,86	0
56	MG	14	3077	1/1	0.78	0.30	-	68,68,68,68	0
56	MG	1H	3351	1/1	0.93	0.25	-	70,70,70,70	0
56	MG	13	1719	1/1	0.89	0.24	-	89,89,89,89	0
56	MG	13	1697	1/1	0.77	0.15	-	82,82,82,82	0
56	MG	1J	203	1/1	0.88	0.29	-	81,81,81,81	0
56	MG	1G	1672	1/1	0.93	0.10	-	78,78,78,78	0
56	MG	1H	3443	1/1	0.88	0.06	-	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	14	3203	1/1	0.96	0.19	-	55,55,55,55	0
56	MG	1H	3309	1/1	0.95	0.48	-	98,98,98,98	0
56	MG	14	3139	1/1	0.69	0.20	-	81,81,81,81	0
56	MG	14	3094	1/1	0.74	0.18	-	69,69,69,69	0
56	MG	1H	3410	1/1	0.98	0.11	-	46,46,46,46	0
56	MG	14	3163	1/1	0.97	0.20	-	80,80,80,80	0
56	MG	14	3279	1/1	0.93	0.11	-	60,60,60,60	0
56	MG	13	1617	1/1	0.62	0.26	-	86,86,86,86	0
56	MG	14	3114	1/1	0.95	0.25	-	44,44,44,44	0
56	MG	1H	3423	1/1	0.99	0.07	-	44,44,44,44	0
56	MG	1H	3303	1/1	0.95	0.19	-	65,65,65,65	0
56	MG	13	1619	1/1	0.96	0.26	-	64,64,64,64	0
56	MG	1G	1635	1/1	0.95	0.34	-	98,98,98,98	0
56	MG	2K	103	1/1	0.95	0.18	-	81,81,81,81	0
56	MG	13	1710	1/1	0.81	0.12	-	128,128,128,128	0
56	MG	14	3071	1/1	0.99	0.19	-	61,61,61,61	0
56	MG	1H	3024	1/1	0.97	0.32	-	46,46,46,46	0
56	MG	13	1721	1/1	0.93	0.14	-	90,90,90,90	0
56	MG	14	3220	1/1	0.85	0.22	-	82,82,82,82	0
56	MG	1H	3166	1/1	0.97	0.26	-	72,72,72,72	0
56	MG	1G	1614	1/1	0.96	0.27	-	72,72,72,72	0
56	MG	1H	3168	1/1	0.83	0.44	-	79,79,79,79	0
56	MG	13	1668	1/1	0.87	0.22	-	76,76,76,76	0
56	MG	1H	3426	1/1	0.90	0.13	-	59,59,59,59	0
56	MG	1H	3386	1/1	0.75	0.12	-	53,53,53,53	0
56	MG	1H	3186	1/1	0.88	0.20	-	83,83,83,83	0
56	MG	14	3030	1/1	0.99	0.14	-	55,55,55,55	0
56	MG	1H	3055	1/1	0.94	0.11	-	61,61,61,61	0
56	MG	14	3372	1/1	0.86	0.22	-	84,84,84,84	0
56	MG	14	3174	1/1	0.94	0.18	-	66,66,66,66	0
56	MG	14	3025	1/1	0.98	0.22	-	84,84,84,84	0
56	MG	14	3151	1/1	0.64	0.23	-	72,72,72,72	0
56	MG	1H	3023	1/1	0.97	0.21	-	51,51,51,51	0
56	MG	14	3075	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	14	3146	1/1	0.94	0.29	-	69,69,69,69	0
56	MG	1H	3362	1/1	0.98	0.23	-	69,69,69,69	0
56	MG	1G	1664	1/1	0.84	0.42	-	102,102,102,102	0
56	MG	1H	3154	1/1	0.89	0.34	-	74,74,74,74	0
56	MG	13	1728	1/1	0.85	0.11	-	85,85,85,85	0
56	MG	13	1626	1/1	0.97	0.29	-	68,68,68,68	0
56	MG	13	1700	1/1	0.90	0.26	-	71,71,71,71	0
56	MG	1G	1620	1/1	0.74	0.34	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3247	1/1	0.90	0.11	-	67,67,67,67	0
56	MG	14	3167	1/1	0.73	0.14	-	59,59,59,59	0
56	MG	14	3104	1/1	0.84	0.28	-	84,84,84,84	0
56	MG	1H	3272	1/1	0.87	0.31	-	69,69,69,69	0
56	MG	1H	3174	1/1	0.88	0.27	-	63,63,63,63	0
56	MG	13	1643	1/1	0.86	0.34	-	80,80,80,80	0
56	MG	1H	3096	1/1	0.87	0.23	-	54,54,54,54	0
56	MG	14	3231	1/1	0.93	0.22	-	74,74,74,74	0
56	MG	14	3130	1/1	0.86	0.26	-	71,71,71,71	0
56	MG	1H	3446	1/1	0.89	0.15	-	78,78,78,78	0
56	MG	14	3365	1/1	0.78	0.07	-	85,85,85,85	0
56	MG	13	1731	1/1	0.96	0.10	-	94,94,94,94	0
56	MG	14	3312	1/1	0.96	0.07	-	67,67,67,67	0
56	MG	1J	205	1/1	0.90	0.10	-	82,82,82,82	0
56	MG	1H	3402	1/1	0.98	0.10	-	48,48,48,48	0
56	MG	14	3228	1/1	0.90	0.46	-	98,98,98,98	0
56	MG	1H	3280	1/1	0.84	0.20	-	59,59,59,59	0
56	MG	1H	3216	1/1	0.93	0.24	-	67,67,67,67	0
56	MG	14	3178	1/1	0.97	0.21	-	80,80,80,80	0
56	MG	14	3067	1/1	0.92	0.18	-	48,48,48,48	0
56	MG	13	1692	1/1	0.78	0.17	-	79,79,79,79	0
56	MG	25	201	1/1	0.43	0.38	-	107,107,107,107	0
56	MG	14	3260	1/1	0.70	0.27	-	85,85,85,85	0
56	MG	14	3306	1/1	0.89	0.15	-	69,69,69,69	0
56	MG	13	1661	1/1	0.95	0.29	-	54,54,54,54	0
56	MG	13	1733	1/1	0.86	0.06	-	73,73,73,73	0
56	MG	1G	1624	1/1	0.93	0.18	-	63,63,63,63	0
56	MG	13	1734	1/1	0.96	0.07	-	86,86,86,86	0
56	MG	1H	3219	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	1H	3347	1/1	0.92	0.55	-	85,85,85,85	0
56	MG	1H	3218	1/1	0.90	0.14	-	61,61,61,61	0
56	MG	1H	3321	1/1	0.82	0.42	-	86,86,86,86	0
56	MG	14	3154	1/1	0.85	0.12	-	82,82,82,82	0
56	MG	I8	101	1/1	0.94	0.39	-	53,53,53,53	0
56	MG	1H	3260	1/1	0.96	0.11	-	72,72,72,72	0
56	MG	1H	3069	1/1	0.94	0.09	-	44,44,44,44	0
56	MG	1G	1662	1/1	0.90	0.19	-	73,73,73,73	0
56	MG	1G	1609	1/1	0.85	0.36	-	81,81,81,81	0
56	MG	1H	3231	1/1	0.91	0.14	-	31,31,31,31	0
56	MG	14	3269	1/1	0.91	0.19	-	59,59,59,59	0
56	MG	1H	3295	1/1	0.69	0.17	-	76,76,76,76	0
56	MG	1H	3370	1/1	0.95	0.12	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3184	1/1	0.96	0.19	-	45,45,45,45	0
56	MG	14	3179	1/1	0.96	0.28	-	64,64,64,64	0
56	MG	1G	1606	1/1	0.95	0.25	-	79,79,79,79	0
56	MG	1H	3121	1/1	0.95	0.18	-	64,64,64,64	0
56	MG	14	3042	1/1	0.86	0.16	-	72,72,72,72	0
56	MG	1H	3308	1/1	0.91	0.22	-	65,65,65,65	0
56	MG	1H	3220	1/1	0.94	0.11	-	50,50,50,50	0
56	MG	13	1679	1/1	0.82	0.28	-	77,77,77,77	0
56	MG	14	3093	1/1	0.97	0.26	-	48,48,48,48	0
56	MG	1H	3293	1/1	0.76	0.46	-	90,90,90,90	0
56	MG	1H	3437	1/1	0.92	0.11	-	59,59,59,59	0
56	MG	1H	3273	1/1	0.70	0.41	-	87,87,87,87	0
56	MG	1H	3254	1/1	0.91	0.19	-	77,77,77,77	0
56	MG	13	1727	1/1	0.98	0.06	-	76,76,76,76	0
56	MG	14	3252	1/1	0.92	0.38	-	96,96,96,96	0
56	MG	14	3368	1/1	0.98	0.10	-	53,53,53,53	0
56	MG	13	1607	1/1	0.94	0.18	-	77,77,77,77	0
56	MG	1H	3109	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	14	3370	1/1	0.98	0.10	-	68,68,68,68	0
56	MG	14	3065	1/1	0.97	0.28	-	46,46,46,46	0
56	MG	1H	3243	1/1	0.74	0.23	-	69,69,69,69	0
56	MG	16	211	1/1	0.98	0.13	-	85,85,85,85	0
56	MG	14	3119	1/1	0.90	0.22	-	69,69,69,69	0
56	MG	13	1671	1/1	0.93	0.12	-	98,98,98,98	0
56	MG	1H	3056	1/1	0.98	0.33	-	70,70,70,70	0
56	MG	14	3271	1/1	0.87	0.14	-	87,87,87,87	0
56	MG	14	3001	1/1	0.97	0.23	-	53,53,53,53	0
56	MG	1G	1629	1/1	0.92	0.24	-	79,79,79,79	0
56	MG	1H	3008	1/1	0.96	0.33	-	42,42,42,42	0
56	MG	14	3160	1/1	0.91	0.12	-	73,73,73,73	0
56	MG	1H	3105	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	1H	3142	1/1	0.90	0.14	-	39,39,39,39	0
56	MG	1H	3264	1/1	0.77	0.22	-	58,58,58,58	0
56	MG	1H	3244	1/1	0.94	0.17	-	39,39,39,39	0
56	MG	1H	3097	1/1	0.93	0.15	-	67,67,67,67	0
56	MG	1G	1685	1/1	0.88	0.08	-	111,111,111,111	0
56	MG	1H	3392	1/1	0.96	0.12	-	64,64,64,64	0
56	MG	1H	3285	1/1	0.90	0.21	-	61,61,61,61	0
56	MG	13	1621	1/1	0.98	0.27	-	74,74,74,74	0
56	MG	1H	3116	1/1	0.96	0.37	-	62,62,62,62	0
56	MG	1H	3314	1/1	0.76	0.37	-	90,90,90,90	0
56	MG	1H	3204	1/1	0.92	0.25	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3158	1/1	0.90	0.15	-	70,70,70,70	0
56	MG	1H	3226	1/1	0.90	0.27	-	69,69,69,69	0
56	MG	14	3009	1/1	0.98	0.18	-	51,51,51,51	0
56	MG	1H	3457	1/1	0.94	0.06	-	92,92,92,92	0
56	MG	14	3379	1/1	0.89	0.12	-	72,72,72,72	0
56	MG	1H	3287	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	1H	3076	1/1	0.74	0.41	-	75,75,75,75	0
56	MG	1H	3356	1/1	0.91	0.14	-	79,79,79,79	0
56	MG	14	3230	1/1	0.99	0.30	-	73,73,73,73	0
56	MG	14	3085	1/1	0.97	0.13	-	50,50,50,50	0
56	MG	16	206	1/1	0.90	0.40	-	60,60,60,60	0
56	MG	14	3079	1/1	0.97	0.15	-	57,57,57,57	0
56	MG	1H	3217	1/1	0.74	0.46	-	93,93,93,93	0
56	MG	14	3241	1/1	0.88	0.26	-	91,91,91,91	0
56	MG	1H	3170	1/1	0.82	0.22	-	61,61,61,61	0
56	MG	14	3382	1/1	0.95	0.08	-	69,69,69,69	0
56	MG	1H	3032	1/1	0.93	0.30	-	78,78,78,78	0
56	MG	1H	3346	1/1	0.91	0.21	-	73,73,73,73	0
56	MG	14	3095	1/1	0.88	0.20	-	56,56,56,56	0
56	MG	1H	3417	1/1	0.98	0.15	-	61,61,61,61	0
56	MG	1H	3085	1/1	0.92	0.21	-	66,66,66,66	0
56	MG	1H	3361	1/1	0.93	0.21	-	53,53,53,53	0
56	MG	1H	3468	1/1	0.87	0.14	-	71,71,71,71	0
56	MG	1H	3453	1/1	0.77	0.12	-	76,76,76,76	0
56	MG	1H	3115	1/1	0.98	0.34	-	51,51,51,51	0
56	MG	1H	3101	1/1	0.77	0.43	-	62,62,62,62	0
56	MG	14	3283	1/1	0.79	0.12	-	102,102,102,102	0
56	MG	1H	3099	1/1	0.98	0.33	-	53,53,53,53	0
56	MG	14	3293	1/1	0.67	0.48	-	88,88,88,88	0
56	MG	13	1664	1/1	0.97	0.21	-	59,59,59,59	0
56	MG	14	3059	1/1	0.89	0.23	-	52,52,52,52	0
56	MG	14	3367	1/1	0.88	0.13	-	70,70,70,70	0
56	MG	1H	3213	1/1	0.87	0.32	-	77,77,77,77	0
56	MG	1H	3307	1/1	0.93	0.21	-	80,80,80,80	0
56	MG	2K	105	1/1	0.90	0.34	-	78,78,78,78	0
56	MG	14	3181	1/1	0.95	0.19	-	55,55,55,55	0
56	MG	1H	3107	1/1	0.99	0.28	-	65,65,65,65	0
56	MG	14	3390	1/1	0.94	0.15	-	90,90,90,90	0
56	MG	1H	3326	1/1	0.69	0.55	-	96,96,96,96	0
56	MG	14	3198	1/1	0.93	0.25	-	78,78,78,78	0
56	MG	14	3237	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	14	3317	1/1	0.96	0.10	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3017	1/1	0.93	0.17	-	49,49,49,49	0
56	MG	1H	3434	1/1	0.93	0.08	-	75,75,75,75	0
56	MG	13	1711	1/1	0.86	0.21	-	79,79,79,79	0
56	MG	14	3029	1/1	0.92	0.12	-	80,80,80,80	0
56	MG	13	1685	1/1	0.59	0.22	-	91,91,91,91	0
56	MG	1H	3192	1/1	0.89	0.19	-	72,72,72,72	0
56	MG	14	3141	1/1	0.93	0.11	-	76,76,76,76	0
56	MG	14	3262	1/1	0.98	0.13	-	66,66,66,66	0
56	MG	1G	1634	1/1	0.92	0.33	-	76,76,76,76	0
56	MG	1H	3067	1/1	0.82	0.25	-	49,49,49,49	0
56	MG	14	3145	1/1	0.85	0.16	-	81,81,81,81	0
56	MG	14	3100	1/1	0.96	0.17	-	63,63,63,63	0
56	MG	14	3350	1/1	0.91	0.11	-	83,83,83,83	0
56	MG	13	1657	1/1	0.94	0.27	-	69,69,69,69	0
56	MG	14	3118	1/1	0.63	0.42	-	86,86,86,86	0
56	MG	1H	3222	1/1	0.77	0.36	-	80,80,80,80	0
56	MG	13	1618	1/1	0.99	0.17	-	58,58,58,58	0
56	MG	1H	3449	1/1	0.96	0.06	-	72,72,72,72	0
56	MG	1H	3292	1/1	0.94	0.21	-	60,60,60,60	0
56	MG	1H	3048	1/1	0.94	0.24	-	48,48,48,48	0
56	MG	1H	3313	1/1	0.81	0.21	-	65,65,65,65	0
56	MG	1G	1645	1/1	0.96	0.12	-	73,73,73,73	0
56	MG	1H	3342	1/1	0.80	0.30	-	98,98,98,98	0
56	MG	1H	3019	1/1	0.97	0.22	-	38,38,38,38	0
56	MG	13	1624	1/1	0.95	0.28	-	48,48,48,48	0
56	MG	14	3054	1/1	0.92	0.35	-	74,74,74,74	0
56	MG	14	3124	1/1	0.92	0.22	-	63,63,63,63	0
56	MG	1H	3383	1/1	0.95	0.18	-	52,52,52,52	0
56	MG	1H	3240	1/1	0.81	0.18	-	73,73,73,73	0
56	MG	16	210	1/1	0.92	0.28	-	89,89,89,89	0
56	MG	14	3255	1/1	0.94	0.14	-	65,65,65,65	0
56	MG	1H	3183	1/1	0.92	0.38	-	66,66,66,66	0
56	MG	1H	3311	1/1	0.76	0.27	-	78,78,78,78	0
56	MG	1H	3073	1/1	0.95	0.28	-	63,63,63,63	0
56	MG	14	3091	1/1	0.82	0.22	-	84,84,84,84	0
56	MG	1H	3318	1/1	0.92	0.15	-	56,56,56,56	0
56	MG	14	3284	1/1	0.77	0.11	-	88,88,88,88	0
56	MG	1H	3190	1/1	0.94	0.14	-	67,67,67,67	0
56	MG	14	3190	1/1	0.77	0.26	-	85,85,85,85	0
56	MG	13	1684	1/1	0.87	0.30	-	62,62,62,62	0
56	MG	16	202	1/1	0.88	0.38	-	59,59,59,59	0
56	MG	1H	3349	1/1	0.73	0.35	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3355	1/1	0.98	0.09	-	47,47,47,47	0
56	MG	14	3264	1/1	0.73	0.28	-	67,67,67,67	0
56	MG	1H	3430	1/1	0.95	0.07	-	76,76,76,76	0
56	MG	14	3353	1/1	0.91	0.23	-	83,83,83,83	0
56	MG	1H	3333	1/1	0.91	0.46	-	93,93,93,93	0
56	MG	13	1687	1/1	0.76	0.21	-	70,70,70,70	0
56	MG	1G	1649	1/1	0.97	0.14	-	72,72,72,72	0
56	MG	L5	101	1/1	0.92	0.21	-	73,73,73,73	0
56	MG	14	3128	1/1	0.95	0.29	-	58,58,58,58	0
56	MG	1H	3479	1/1	0.92	0.15	-	90,90,90,90	0
56	MG	1H	3182	1/1	0.96	0.20	-	87,87,87,87	0
56	MG	13	1656	1/1	0.97	0.26	-	91,91,91,91	0
56	MG	13	1665	1/1	0.90	0.24	-	67,67,67,67	0
56	MG	1H	3331	1/1	0.83	0.23	-	76,76,76,76	0
56	MG	13	1735	1/1	0.97	0.06	-	71,71,71,71	0
56	MG	14	3023	1/1	0.92	0.17	-	40,40,40,40	0
56	MG	13	1641	1/1	0.88	0.16	-	59,59,59,59	0
56	MG	1J	202	1/1	0.89	0.34	-	73,73,73,73	0
56	MG	C5	201	1/1	0.81	0.27	-	104,104,104,104	0
56	MG	1H	3146	1/1	0.81	0.24	-	75,75,75,75	0
56	MG	1H	3138	1/1	0.83	0.35	-	66,66,66,66	0
56	MG	14	3073	1/1	0.97	0.16	-	80,80,80,80	0
56	MG	1H	3258	1/1	0.96	0.22	-	63,63,63,63	0
56	MG	1H	3215	1/1	0.91	0.22	-	85,85,85,85	0
56	MG	14	3140	1/1	0.91	0.31	-	92,92,92,92	0
56	MG	14	3137	1/1	0.81	0.34	-	69,69,69,69	0
56	MG	1H	3172	1/1	0.83	0.40	-	84,84,84,84	0
56	MG	14	3210	1/1	0.90	0.26	-	71,71,71,71	0
56	MG	1H	3065	1/1	0.93	0.20	-	54,54,54,54	0
56	MG	14	3208	1/1	0.87	0.15	-	68,68,68,68	0
56	MG	14	3055	1/1	0.96	0.15	-	64,64,64,64	0
56	MG	14	3217	1/1	0.77	0.28	-	68,68,68,68	0
56	MG	14	3015	1/1	0.94	0.18	-	71,71,71,71	0
56	MG	1H	3338	1/1	0.83	0.23	-	60,60,60,60	0
56	MG	13	1699	1/1	0.92	0.20	-	75,75,75,75	0
56	MG	1H	3396	1/1	0.95	0.18	-	57,57,57,57	0
56	MG	11	301	1/1	0.99	0.20	-	48,48,48,48	0
56	MG	14	3033	1/1	0.82	0.18	-	64,64,64,64	0
56	MG	1H	3283	1/1	0.94	0.31	-	74,74,74,74	0
56	MG	13	1724	1/1	0.97	0.18	-	78,78,78,78	0
56	MG	1H	3025	1/1	0.97	0.23	-	53,53,53,53	0
56	MG	1H	3460	1/1	0.94	0.13	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3388	1/1	0.88	0.06	-	88,88,88,88	0
56	MG	1H	3102	1/1	0.97	0.14	-	60,60,60,60	0
56	MG	1H	3246	1/1	0.91	0.26	-	79,79,79,79	0
56	MG	1H	3432	1/1	0.95	0.12	-	65,65,65,65	0
56	MG	14	3086	1/1	0.98	0.06	-	65,65,65,65	0
56	MG	13	1645	1/1	0.95	0.10	-	79,79,79,79	0
56	MG	1H	3372	1/1	0.89	0.08	-	37,37,37,37	0
56	MG	14	3161	1/1	0.83	0.24	-	86,86,86,86	0
56	MG	1H	3431	1/1	0.79	0.21	-	99,99,99,99	0
56	MG	1H	3086	1/1	0.93	0.29	-	66,66,66,66	0
56	MG	1H	3062	1/1	0.94	0.36	-	65,65,65,65	0
56	MG	1G	1671	1/1	0.90	0.09	-	73,73,73,73	0
56	MG	1H	3481	1/1	0.96	0.12	-	77,77,77,77	0
56	MG	1G	1665	1/1	0.78	0.13	-	94,94,94,94	0
56	MG	1H	3210	1/1	0.89	0.43	-	77,77,77,77	0
56	MG	L8	101	1/1	0.90	0.24	-	70,70,70,70	0
56	MG	1H	3178	1/1	0.67	0.27	-	63,63,63,63	0
56	MG	1H	3257	1/1	0.89	0.42	-	85,85,85,85	0
56	MG	13	1706	1/1	0.93	0.17	-	79,79,79,79	0
56	MG	14	3185	1/1	0.91	0.11	-	52,52,52,52	0
56	MG	13	1736	1/1	0.92	0.07	-	73,73,73,73	0
56	MG	1H	3195	1/1	0.95	0.27	-	65,65,65,65	0
56	MG	1H	3133	1/1	0.96	0.17	-	60,60,60,60	0
56	MG	1H	3262	1/1	0.95	0.39	-	56,56,56,56	0
56	MG	1G	1675	1/1	0.82	0.08	-	110,110,110,110	0
56	MG	13	1622	1/1	0.94	0.35	-	79,79,79,79	0
56	MG	14	3375	1/1	0.91	0.06	-	91,91,91,91	0
56	MG	1H	3467	1/1	0.67	0.09	-	75,75,75,75	0
56	MG	14	3270	1/1	0.91	0.12	-	56,56,56,56	0
56	MG	1H	3229	1/1	0.94	0.33	-	95,95,95,95	0
56	MG	14	3044	1/1	0.95	0.08	-	53,53,53,53	0
56	MG	14	3239	1/1	0.94	0.16	-	76,76,76,76	0
56	MG	1H	3080	1/1	0.97	0.29	-	53,53,53,53	0
56	MG	14	3020	1/1	0.81	0.15	-	68,68,68,68	0
56	MG	1H	3352	1/1	0.95	0.13	-	61,61,61,61	0
56	MG	14	3244	1/1	0.95	0.16	-	65,65,65,65	0
56	MG	16	207	1/1	0.83	0.28	-	71,71,71,71	0
56	MG	1K	101	1/1	0.93	0.19	-	75,75,75,75	0
56	MG	1H	3358	1/1	0.80	0.25	-	80,80,80,80	0
56	MG	1H	3290	1/1	0.82	0.41	-	84,84,84,84	0
56	MG	1H	3439	1/1	0.95	0.10	-	69,69,69,69	0
56	MG	1H	3036	1/1	0.97	0.33	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3057	1/1	0.84	0.35	-	57,57,57,57	0
56	MG	13	1742	1/1	0.92	0.10	-	115,115,115,115	0
56	MG	1H	3255	1/1	0.88	0.26	-	76,76,76,76	0
56	MG	14	3173	1/1	0.84	0.16	-	62,62,62,62	0
56	MG	14	3280	1/1	0.80	0.43	-	87,87,87,87	0
56	MG	14	3034	1/1	0.88	0.10	-	86,86,86,86	0
56	MG	1H	3242	1/1	0.98	0.29	-	58,58,58,58	0
56	MG	14	3304	1/1	0.94	0.10	-	68,68,68,68	0
56	MG	1H	3082	1/1	0.95	0.27	-	70,70,70,70	0
56	MG	14	3254	1/1	0.54	0.27	-	102,102,102,102	0
56	MG	1G	1626	1/1	0.91	0.27	-	79,79,79,79	0
56	MG	14	3052	1/1	0.97	0.24	-	62,62,62,62	0
56	MG	1H	3194	1/1	0.86	0.24	-	62,62,62,62	0
56	MG	1H	3043	1/1	0.94	0.45	-	84,84,84,84	0
56	MG	13	1690	1/1	0.90	0.25	-	113,113,113,113	0
56	MG	14	3249	1/1	0.66	0.19	-	77,77,77,77	0
56	MG	1H	3129	1/1	0.83	0.20	-	68,68,68,68	0
56	MG	1H	3011	1/1	0.96	0.20	-	48,48,48,48	0
56	MG	1H	3424	1/1	0.91	0.14	-	58,58,58,58	0
56	MG	21	301	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	13	1652	1/1	0.99	0.20	-	80,80,80,80	0
56	MG	1H	3322	1/1	0.79	0.36	-	80,80,80,80	0
56	MG	1H	3275	1/1	0.64	0.44	-	75,75,75,75	0
56	MG	13	1738	1/1	0.97	0.09	-	72,72,72,72	0
56	MG	14	3090	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	14	3263	1/1	0.89	0.32	-	71,71,71,71	0
56	MG	14	3153	1/1	0.80	0.17	-	94,94,94,94	0
56	MG	13	1709	1/1	0.94	0.22	-	89,89,89,89	0
56	MG	14	3236	1/1	0.98	0.23	-	75,75,75,75	0
56	MG	14	3110	1/1	0.86	0.19	-	64,64,64,64	0
56	MG	1G	1625	1/1	0.91	0.38	-	84,84,84,84	0
56	MG	1H	3063	1/1	0.95	0.44	-	65,65,65,65	0
56	MG	1G	1647	1/1	0.93	0.16	-	102,102,102,102	0
56	MG	14	3096	1/1	0.80	0.19	-	78,78,78,78	0
56	MG	14	3162	1/1	0.95	0.38	-	56,56,56,56	0
56	MG	1H	3458	1/1	0.87	0.15	-	84,84,84,84	0
56	MG	14	3201	1/1	0.93	0.25	-	72,72,72,72	0
56	MG	14	3089	1/1	0.87	0.38	-	79,79,79,79	0
56	MG	1H	3091	1/1	0.89	0.21	-	55,55,55,55	0
56	MG	1H	3123	1/1	0.96	0.23	-	52,52,52,52	0
56	MG	13	1701	1/1	0.81	0.12	-	80,80,80,80	0
56	MG	1H	3198	1/1	0.92	0.43	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3355	1/1	0.94	0.22	-	60,60,60,60	0
56	MG	1H	3298	1/1	0.77	0.29	-	79,79,79,79	0
56	MG	1H	3004	1/1	0.95	0.41	-	47,47,47,47	0
56	MG	1H	3054	1/1	0.88	0.33	-	59,59,59,59	0
56	MG	1H	3464	1/1	0.87	0.08	-	92,92,92,92	0
56	MG	14	3105	1/1	0.98	0.19	-	47,47,47,47	0
56	MG	1H	3472	1/1	0.99	0.14	-	56,56,56,56	0
56	MG	14	3050	1/1	0.99	0.20	-	63,63,63,63	0
56	MG	1H	3462	1/1	0.80	0.06	-	92,92,92,92	0
56	MG	1H	3345	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1H	3237	1/1	0.92	0.15	-	57,57,57,57	0
56	MG	1G	1639	1/1	0.97	0.09	-	85,85,85,85	0
56	MG	1H	3286	1/1	0.95	0.21	-	70,70,70,70	0
56	MG	14	3200	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	14	3158	1/1	0.74	0.41	-	67,67,67,67	0
56	MG	1G	1660	1/1	0.95	0.10	-	74,74,74,74	0
56	MG	14	3387	1/1	0.90	0.09	-	97,97,97,97	0
56	MG	1H	3009	1/1	0.98	0.27	-	43,43,43,43	0
56	MG	1H	3136	1/1	0.99	0.27	-	41,41,41,41	0
56	MG	1H	3470	1/1	0.89	0.12	-	106,106,106,106	0
56	MG	1H	3469	1/1	0.91	0.10	-	90,90,90,90	0
56	MG	1H	3350	1/1	0.93	0.08	-	67,67,67,67	0
56	MG	14	3322	1/1	0.94	0.10	-	77,77,77,77	0
56	MG	14	3259	1/1	0.90	0.23	-	82,82,82,82	0
56	MG	13	1703	1/1	0.82	0.20	-	89,89,89,89	0
56	MG	1H	3340	1/1	0.94	0.14	-	74,74,74,74	0
56	MG	1H	3471	1/1	0.94	0.09	-	68,68,68,68	0
56	MG	14	3318	1/1	0.99	0.10	-	57,57,57,57	0
56	MG	1G	1631	1/1	0.93	0.21	-	86,86,86,86	0
56	MG	14	3257	1/1	0.92	0.17	-	79,79,79,79	0
56	MG	1H	3179	1/1	0.94	0.25	-	55,55,55,55	0
56	MG	13	1662	1/1	0.81	0.30	-	73,73,73,73	0
56	MG	1H	3302	1/1	0.97	0.12	-	59,59,59,59	0
56	MG	2K	106	1/1	0.94	0.06	-	84,84,84,84	0
56	MG	13	1614	1/1	0.96	0.19	-	79,79,79,79	0
56	MG	1H	3200	1/1	0.97	0.19	-	59,59,59,59	0
56	MG	13	1655	1/1	0.94	0.13	-	73,73,73,73	0
56	MG	13	1609	1/1	0.89	0.35	-	86,86,86,86	0
56	MG	1H	3020	1/1	0.99	0.20	-	47,47,47,47	0
56	MG	1G	1632	1/1	0.94	0.20	-	70,70,70,70	0
56	MG	14	3285	1/1	0.85	0.40	-	74,74,74,74	0
56	MG	14	3150	1/1	0.98	0.18	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3286	1/1	0.73	0.23	-	78,78,78,78	0
56	MG	1H	3407	1/1	0.98	0.07	-	57,57,57,57	0
56	MG	14	3002	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	1G	1628	1/1	0.90	0.22	-	77,77,77,77	0
56	MG	1H	3475	1/1	0.87	0.10	-	79,79,79,79	0
56	MG	16	212	1/1	0.92	0.14	-	73,73,73,73	0
56	MG	14	3374	1/1	0.97	0.17	-	76,76,76,76	0
56	MG	13	1688	1/1	0.68	0.26	-	77,77,77,77	0
56	MG	13	1716	1/1	0.86	0.14	-	92,92,92,92	0
56	MG	1H	3223	1/1	0.51	0.58	-	102,102,102,102	0
56	MG	13	1713	1/1	0.93	0.16	-	70,70,70,70	0
56	MG	1H	3208	1/1	0.96	0.25	-	78,78,78,78	0
56	MG	1H	3202	1/1	0.83	0.17	-	66,66,66,66	0
56	MG	1H	3353	1/1	0.88	0.24	-	73,73,73,73	0
56	MG	1G	1648	1/1	0.79	0.43	-	121,121,121,121	0
56	MG	13	1740	1/1	0.90	0.12	-	88,88,88,88	0
56	MG	1H	3270	1/1	0.92	0.30	-	94,94,94,94	0
56	MG	1H	3323	1/1	0.80	0.50	-	82,82,82,82	0
56	MG	14	3083	1/1	0.97	0.15	-	60,60,60,60	0
56	MG	1H	3328	1/1	0.77	0.47	-	91,91,91,91	0
56	MG	14	3120	1/1	0.93	0.28	-	75,75,75,75	0
56	MG	13	1659	1/1	0.90	0.21	-	66,66,66,66	0
56	MG	1H	3284	1/1	0.91	0.18	-	62,62,62,62	0
56	MG	14	3187	1/1	0.98	0.21	-	53,53,53,53	0
56	MG	14	3303	1/1	0.82	0.15	-	101,101,101,101	0
56	MG	14	3326	1/1	0.95	0.14	-	65,65,65,65	0
56	MG	1H	3281	1/1	0.82	0.38	-	74,74,74,74	0
56	MG	14	3057	1/1	0.95	0.16	-	68,68,68,68	0
56	MG	1G	1651	1/1	0.96	0.17	-	84,84,84,84	0
56	MG	13	1708	1/1	0.81	0.22	-	85,85,85,85	0
56	MG	1G	1605	1/1	0.97	0.13	-	74,74,74,74	0
56	MG	1H	3406	1/1	0.89	0.10	-	45,45,45,45	0
56	MG	1H	3332	1/1	0.78	0.47	-	88,88,88,88	0
56	MG	1H	3164	1/1	0.96	0.18	-	52,52,52,52	0
56	MG	1H	3343	1/1	0.90	0.43	-	75,75,75,75	0
56	MG	31	301	1/1	0.75	0.10	-	56,56,56,56	0
56	MG	1G	1630	1/1	0.98	0.24	-	75,75,75,75	0
56	MG	14	3149	1/1	0.75	0.33	-	84,84,84,84	0
56	MG	14	3195	1/1	0.84	0.25	-	65,65,65,65	0
56	MG	14	3334	1/1	0.96	0.08	-	79,79,79,79	0
56	MG	1H	3461	1/1	0.79	0.09	-	108,108,108,108	0
56	MG	14	3107	1/1	0.94	0.24	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	45	201	1/1	0.97	0.11	-	50,50,50,50	0
56	MG	1H	3300	1/1	0.64	0.31	-	77,77,77,77	0
56	MG	1G	1661	1/1	0.95	0.21	-	73,73,73,73	0
56	MG	1H	3021	1/1	0.97	0.22	-	45,45,45,45	0
56	MG	1H	3117	1/1	0.85	0.31	-	80,80,80,80	0
56	MG	13	1667	1/1	0.97	0.19	-	92,92,92,92	0
56	MG	14	3261	1/1	0.44	0.38	-	93,93,93,93	0
56	MG	1G	1623	1/1	0.81	0.22	-	73,73,73,73	0
56	MG	14	3338	1/1	0.94	0.13	-	53,53,53,53	0
56	MG	1G	1603	1/1	0.96	0.12	-	76,76,76,76	0
56	MG	14	3087	1/1	0.93	0.33	-	62,62,62,62	0
56	MG	1H	3053	1/1	0.83	0.36	-	72,72,72,72	0
56	MG	1G	1656	1/1	0.83	0.28	-	72,72,72,72	0
56	MG	14	3207	1/1	0.87	0.59	-	81,81,81,81	0
56	MG	1H	3130	1/1	0.94	0.24	-	54,54,54,54	0
56	MG	1H	3199	1/1	0.86	0.31	-	57,57,57,57	0
56	MG	14	3265	1/1	0.66	0.34	-	121,121,121,121	0
56	MG	13	1660	1/1	0.88	0.13	-	91,91,91,91	0
56	MG	14	3008	1/1	0.94	0.21	-	54,54,54,54	0
56	MG	14	3289	1/1	0.53	0.27	-	79,79,79,79	0
56	MG	1H	3473	1/1	0.97	0.17	-	73,73,73,73	0
56	MG	1J	206	1/1	0.93	0.13	-	73,73,73,73	0
56	MG	13	1693	1/1	0.89	0.15	-	65,65,65,65	0
56	MG	5E	201	1/1	0.95	0.18	-	70,70,70,70	0
56	MG	14	3007	1/1	0.95	0.13	-	48,48,48,48	0
56	MG	14	3166	1/1	0.93	0.22	-	70,70,70,70	0
56	MG	1H	3433	1/1	0.96	0.09	-	83,83,83,83	0
56	MG	14	3298	1/1	0.77	0.40	-	103,103,103,103	0
56	MG	1H	3387	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	1H	3169	1/1	0.90	0.35	-	62,62,62,62	0
56	MG	14	3127	1/1	0.81	0.17	-	64,64,64,64	0
56	MG	13	1698	1/1	0.88	0.15	-	74,74,74,74	0
56	MG	14	3296	1/1	0.91	0.15	-	74,74,74,74	0
56	MG	1H	3124	1/1	0.99	0.19	-	52,52,52,52	0
56	MG	14	3268	1/1	0.85	0.19	-	57,57,57,57	0
56	MG	1H	3041	1/1	0.93	0.28	-	87,87,87,87	0
56	MG	14	3212	1/1	0.96	0.12	-	65,65,65,65	0
56	MG	1H	3400	1/1	0.97	0.13	-	47,47,47,47	0
56	MG	1H	3296	1/1	0.96	0.26	-	90,90,90,90	0
56	MG	1H	3397	1/1	0.94	0.11	-	66,66,66,66	0
56	MG	1H	3438	1/1	0.86	0.12	-	54,54,54,54	0
56	MG	1H	3015	1/1	0.96	0.22	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3175	1/1	0.88	0.15	-	56,56,56,56	0
56	MG	13	1669	1/1	0.92	0.19	-	76,76,76,76	0
56	MG	1H	3325	1/1	0.90	0.38	-	96,96,96,96	0
56	MG	1H	3341	1/1	0.79	0.33	-	67,67,67,67	0
56	MG	13	1634	1/1	0.90	0.25	-	74,74,74,74	0
56	MG	1G	1636	1/1	0.84	0.16	-	84,84,84,84	0
56	MG	1H	3274	1/1	0.65	0.47	-	80,80,80,80	0
56	MG	13	1627	1/1	0.97	0.22	-	62,62,62,62	0
56	MG	14	3354	1/1	0.94	0.10	-	71,71,71,71	0
56	MG	14	3014	1/1	0.97	0.22	-	58,58,58,58	0
56	MG	14	3115	1/1	0.85	0.36	-	88,88,88,88	0
56	MG	1H	3301	1/1	0.87	0.29	-	79,79,79,79	0
56	MG	1H	3312	1/1	0.85	0.47	-	78,78,78,78	0
56	MG	14	3363	1/1	0.93	0.07	-	74,74,74,74	0
56	MG	14	3005	1/1	0.99	0.21	-	53,53,53,53	0
56	MG	13	1646	1/1	0.90	0.18	-	95,95,95,95	0
56	MG	14	3307	1/1	0.92	0.17	-	60,60,60,60	0
56	MG	1G	1682	1/1	0.96	0.08	-	74,74,74,74	0
56	MG	14	3277	1/1	0.96	0.17	-	66,66,66,66	0
56	MG	1H	3188	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	1H	3276	1/1	0.86	0.34	-	55,55,55,55	0
56	MG	14	3123	1/1	0.97	0.13	-	60,60,60,60	0
56	MG	14	3070	1/1	0.97	0.20	-	39,39,39,39	0
56	MG	1H	3140	1/1	0.91	0.45	-	63,63,63,63	0
56	MG	14	3047	1/1	0.95	0.11	-	60,60,60,60	0
56	MG	14	3272	1/1	0.82	0.35	-	82,82,82,82	0
56	MG	2K	101	1/1	0.94	0.34	-	79,79,79,79	0
56	MG	14	3238	1/1	0.91	0.23	-	85,85,85,85	0
56	MG	14	3019	1/1	0.98	0.12	-	74,74,74,74	0
56	MG	1H	3003	1/1	0.96	0.26	-	35,35,35,35	0
56	MG	14	3275	1/1	0.77	0.27	-	60,60,60,60	0
56	MG	14	3170	1/1	0.80	0.31	-	79,79,79,79	0
56	MG	1H	3388	1/1	0.93	0.14	-	64,64,64,64	0
56	MG	35	201	1/1	0.93	0.19	-	60,60,60,60	0
56	MG	1H	3150	1/1	0.87	0.20	-	59,59,59,59	0
56	MG	14	3088	1/1	0.90	0.43	-	71,71,71,71	0
56	MG	13	1691	1/1	0.93	0.12	-	64,64,64,64	0
56	MG	14	3352	1/1	0.93	0.07	-	84,84,84,84	0
56	MG	13	1651	1/1	0.90	0.20	-	87,87,87,87	0
56	MG	13	1631	1/1	0.89	0.28	-	73,73,73,73	0
56	MG	16	208	1/1	0.86	0.33	-	66,66,66,66	0
56	MG	1H	3269	1/1	0.86	0.37	-	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	1H	3059	1/1	0.96	0.13	-	68,68,68,68	0
56	MG	14	3144	1/1	0.65	0.39	-	79,79,79,79	0
56	MG	1H	3236	1/1	0.92	0.18	-	68,68,68,68	0
56	MG	1H	3112	1/1	0.92	0.24	-	66,66,66,66	0
56	MG	13	1604	1/1	0.98	0.10	-	68,68,68,68	0
56	MG	13	1623	1/1	0.68	0.44	-	94,94,94,94	0
56	MG	13	1702	1/1	0.97	0.27	-	62,62,62,62	0
56	MG	14	3267	1/1	0.78	0.22	-	81,81,81,81	0
56	MG	1H	3391	1/1	0.96	0.09	-	71,71,71,71	0
56	MG	14	3227	1/1	0.98	0.13	-	88,88,88,88	0
56	MG	1H	3405	1/1	0.96	0.20	-	61,61,61,61	0
56	MG	14	3143	1/1	0.98	0.20	-	67,67,67,67	0
56	MG	14	3242	1/1	0.97	0.17	-	74,74,74,74	0
56	MG	13	1741	1/1	0.74	0.09	-	110,110,110,110	0
56	MG	14	3213	1/1	0.90	0.27	-	85,85,85,85	0
56	MG	1G	1652	1/1	0.83	0.30	-	74,74,74,74	0
56	MG	13	1658	1/1	0.74	0.24	-	70,70,70,70	0
56	MG	1H	3147	1/1	0.90	0.47	-	68,68,68,68	0
56	MG	14	3157	1/1	0.94	0.12	-	88,88,88,88	0
56	MG	13	1673	1/1	0.70	0.23	-	73,73,73,73	0
56	MG	1H	3187	1/1	0.94	0.30	-	56,56,56,56	0
56	MG	1H	3363	1/1	0.96	0.23	-	68,68,68,68	0
56	MG	1G	1679	1/1	0.94	0.10	-	90,90,90,90	0
56	MG	13	1678	1/1	0.95	0.21	-	74,74,74,74	0
56	MG	13	1715	1/1	0.65	0.14	-	83,83,83,83	0
56	MG	1H	3393	1/1	0.79	0.10	-	65,65,65,65	0
56	MG	13	1726	1/1	0.95	0.13	-	77,77,77,77	0
56	MG	13	1739	1/1	0.96	0.21	-	73,73,73,73	0
56	MG	1H	3354	1/1	0.92	0.29	-	89,89,89,89	0
56	MG	1H	3304	1/1	0.92	0.29	-	69,69,69,69	0
56	MG	14	3240	1/1	0.92	0.10	-	77,77,77,77	0
56	MG	14	3012	1/1	0.97	0.26	-	77,77,77,77	0
56	MG	1H	3385	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	13	1637	1/1	0.81	0.24	-	61,61,61,61	0
56	MG	1H	3159	1/1	0.89	0.12	-	71,71,71,71	0
56	MG	14	3010	1/1	0.98	0.22	-	58,58,58,58	0
56	MG	14	3108	1/1	0.96	0.21	-	76,76,76,76	0
56	MG	1H	3463	1/1	0.87	0.18	-	101,101,101,101	0
56	MG	1G	1618	1/1	0.98	0.13	-	88,88,88,88	0
56	MG	1G	1604	1/1	0.96	0.12	-	77,77,77,77	0
56	MG	1H	3279	1/1	0.92	0.16	-	73,73,73,73	0
56	MG	1H	3006	1/1	0.97	0.17	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3203	1/1	0.80	0.40	-	80,80,80,80	0
56	MG	14	3369	1/1	0.81	0.12	-	97,97,97,97	0
56	MG	1G	1627	1/1	0.93	0.18	-	57,57,57,57	0
56	MG	13	1695	1/1	0.96	0.21	-	79,79,79,79	0
56	MG	1H	3227	1/1	0.88	0.49	-	74,74,74,74	0
56	MG	14	3336	1/1	0.96	0.09	-	52,52,52,52	0
56	MG	2L	104	1/1	0.89	0.14	-	65,65,65,65	0
56	MG	1G	1644	1/1	0.92	0.18	-	70,70,70,70	0
56	MG	14	3325	1/1	0.96	0.12	-	63,63,63,63	0
56	MG	1H	3416	1/1	0.62	0.12	-	77,77,77,77	0
56	MG	14	3233	1/1	0.90	0.11	-	61,61,61,61	0
56	MG	1H	3078	1/1	0.87	0.14	-	63,63,63,63	0
56	MG	14	3381	1/1	0.88	0.09	-	62,62,62,62	0
56	MG	1H	3139	1/1	0.81	0.17	-	66,66,66,66	0
56	MG	2L	102	1/1	0.54	0.22	-	79,79,79,79	0
56	MG	1H	3267	1/1	0.98	0.24	-	60,60,60,60	0
56	MG	1H	3288	1/1	0.82	0.13	-	54,54,54,54	0
56	MG	14	3324	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	1H	3108	1/1	0.98	0.20	-	34,34,34,34	0
56	MG	14	3248	1/1	0.96	0.16	-	76,76,76,76	0
56	MG	1G	1657	1/1	0.93	0.17	-	126,126,126,126	0
56	MG	13	1616	1/1	0.76	0.37	-	93,93,93,93	0
56	MG	1H	3339	1/1	0.72	0.30	-	88,88,88,88	0
56	MG	1H	3030	1/1	0.69	0.34	-	81,81,81,81	0
56	MG	14	3155	1/1	0.88	0.24	-	75,75,75,75	0
56	MG	14	3300	1/1	0.88	0.27	-	109,109,109,109	0
56	MG	14	3134	1/1	0.95	0.17	-	64,64,64,64	0
56	MG	1H	3335	1/1	0.91	0.26	-	87,87,87,87	0
56	MG	1H	3368	1/1	0.79	0.27	-	74,74,74,74	0
56	MG	14	3171	1/1	0.81	0.24	-	80,80,80,80	0
56	MG	1H	3051	1/1	0.92	0.15	-	65,65,65,65	0
56	MG	14	3229	1/1	0.93	0.14	-	65,65,65,65	0
56	MG	1H	3189	1/1	0.88	0.34	-	63,63,63,63	0
56	MG	13	1642	1/1	0.89	0.29	-	72,72,72,72	0
56	MG	1G	1683	1/1	0.92	0.10	-	104,104,104,104	0
56	MG	13	1610	1/1	0.92	0.29	-	72,72,72,72	0
56	MG	1H	3337	1/1	0.92	0.19	-	94,94,94,94	0
56	MG	1G	1650	1/1	0.81	0.40	-	87,87,87,87	0
56	MG	1H	3348	1/1	0.93	0.53	-	80,80,80,80	0
56	MG	1H	3329	1/1	0.94	0.39	-	73,73,73,73	0
56	MG	14	3116	1/1	0.87	0.25	-	56,56,56,56	0
56	MG	1H	3135	1/1	0.92	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3035	1/1	0.95	0.14	-	54,54,54,54	0
56	MG	13	1718	1/1	0.94	0.20	-	90,90,90,90	0
56	MG	1H	3403	1/1	0.99	0.16	-	43,43,43,43	0
56	MG	13	1612	1/1	0.94	0.16	-	63,63,63,63	0
56	MG	1G	1668	1/1	0.86	0.26	-	82,82,82,82	0
56	MG	14	3343	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	14	3226	1/1	0.74	0.18	-	82,82,82,82	0
56	MG	1H	3119	1/1	0.95	0.29	-	52,52,52,52	0
56	MG	14	3287	1/1	0.80	0.20	-	79,79,79,79	0
56	MG	14	3216	1/1	0.81	0.17	-	83,83,83,83	0
56	MG	1H	3110	1/1	0.88	0.38	-	57,57,57,57	0
56	MG	13	1650	1/1	0.96	0.16	-	68,68,68,68	0
56	MG	1H	3228	1/1	0.71	0.42	-	74,74,74,74	0
56	MG	14	3058	1/1	0.93	0.19	-	61,61,61,61	0
56	MG	14	3099	1/1	0.99	0.19	-	46,46,46,46	0
56	MG	14	3112	1/1	0.96	0.11	-	65,65,65,65	0
56	MG	14	3234	1/1	0.92	0.21	-	68,68,68,68	0
56	MG	13	1704	1/1	0.83	0.20	-	80,80,80,80	0
56	MG	1H	3294	1/1	0.95	0.19	-	47,47,47,47	0
56	MG	1G	1654	1/1	0.84	0.42	-	101,101,101,101	0
56	MG	14	3383	1/1	0.94	0.10	-	86,86,86,86	0
56	MG	14	3194	1/1	0.95	0.16	-	52,52,52,52	0
56	MG	1H	3474	1/1	0.92	0.11	-	64,64,64,64	0
56	MG	1G	1658	1/1	0.94	0.16	-	79,79,79,79	0
56	MG	1G	1663	1/1	0.90	0.20	-	75,75,75,75	0
56	MG	14	3282	1/1	0.72	0.32	-	86,86,86,86	0
56	MG	1H	3098	1/1	0.70	0.20	-	87,87,87,87	0
56	MG	14	3062	1/1	0.99	0.18	-	56,56,56,56	0
56	MG	1G	1622	1/1	0.80	0.16	-	72,72,72,72	0
56	MG	14	3066	1/1	0.95	0.14	-	49,49,49,49	0
56	MG	13	1674	1/1	0.92	0.19	-	94,94,94,94	0
56	MG	14	3021	1/1	0.98	0.19	-	55,55,55,55	0
56	MG	14	3358	1/1	0.96	0.22	-	77,77,77,77	0
56	MG	1H	3266	1/1	0.99	0.07	-	64,64,64,64	0
56	MG	14	3069	1/1	0.85	0.27	-	78,78,78,78	0
56	MG	1H	3271	1/1	0.84	0.30	-	65,65,65,65	0
56	MG	1H	3209	1/1	0.85	0.32	-	77,77,77,77	0
56	MG	1G	1619	1/1	0.94	0.19	-	84,84,84,84	0
56	MG	14	3295	1/1	0.96	0.23	-	64,64,64,64	0
56	MG	13	1630	1/1	0.98	0.18	-	43,43,43,43	0
56	MG	14	3182	1/1	0.48	0.24	-	72,72,72,72	0
56	MG	1H	3282	1/1	0.71	0.40	-	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	1G	1633	1/1	0.89	0.25	-	76,76,76,76	0
56	MG	1H	3263	1/1	0.86	0.32	-	76,76,76,76	0
56	MG	14	3362	1/1	0.96	0.08	-	69,69,69,69	0
56	MG	14	3389	1/1	0.86	0.18	-	97,97,97,97	0
56	MG	14	3072	1/1	0.93	0.15	-	45,45,45,45	0
56	MG	1H	3027	1/1	0.96	0.22	-	32,32,32,32	0
56	MG	14	3232	1/1	0.96	0.29	-	62,62,62,62	0
56	MG	1G	1643	1/1	0.86	0.37	-	88,88,88,88	0
56	MG	1G	1669	1/1	0.87	0.20	-	88,88,88,88	0
56	MG	1H	3162	1/1	0.95	0.25	-	68,68,68,68	0
56	MG	1H	3029	1/1	0.87	0.29	-	73,73,73,73	0
56	MG	1H	3176	1/1	0.96	0.16	-	60,60,60,60	0
56	MG	1H	3214	1/1	0.95	0.34	-	68,68,68,68	0
56	MG	1H	3305	1/1	0.77	0.29	-	75,75,75,75	0
56	MG	29	301	1/1	0.99	0.18	-	44,44,44,44	0
56	MG	14	3152	1/1	0.97	0.11	-	67,67,67,67	0
56	MG	14	3148	1/1	0.62	0.22	-	82,82,82,82	0
56	MG	1H	3074	1/1	0.96	0.28	-	70,70,70,70	0
56	MG	1H	3476	1/1	0.97	0.07	-	79,79,79,79	0
56	MG	14	3081	1/1	0.96	0.25	-	52,52,52,52	0
56	MG	13	1694	1/1	0.90	0.20	-	82,82,82,82	0
56	MG	1H	3421	1/1	0.80	0.07	-	57,57,57,57	0
56	MG	1H	3435	1/1	0.85	0.05	-	90,90,90,90	0
56	MG	1H	3211	1/1	0.79	0.43	-	64,64,64,64	0
56	MG	14	3339	1/1	0.90	0.17	-	94,94,94,94	0
56	MG	1H	3327	1/1	0.93	0.47	-	79,79,79,79	0
56	MG	1H	3088	1/1	0.92	0.33	-	73,73,73,73	0
56	MG	1G	1666	1/1	0.92	0.16	-	74,74,74,74	0
56	MG	14	3256	1/1	0.88	0.29	-	66,66,66,66	0
56	MG	1H	3477	1/1	0.79	0.06	-	106,106,106,106	0
56	MG	14	3168	1/1	0.92	0.24	-	71,71,71,71	0
56	MG	1H	3377	1/1	0.94	0.07	-	44,44,44,44	0
56	MG	1H	3044	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	1G	1641	1/1	0.49	0.26	-	73,73,73,73	0
56	MG	14	3018	1/1	0.90	0.13	-	68,68,68,68	0
56	MG	1H	3131	1/1	0.93	0.28	-	67,67,67,67	0
56	MG	13	1633	1/1	0.87	0.38	-	77,77,77,77	0
56	MG	1H	3448	1/1	0.97	0.06	-	88,88,88,88	0
56	MG	1H	3253	1/1	0.95	0.15	-	78,78,78,78	0
56	MG	14	3063	1/1	0.99	0.29	-	66,66,66,66	0
56	MG	1H	3225	1/1	0.97	0.32	-	57,57,57,57	0
56	MG	1G	1617	1/1	0.94	0.16	-	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	14	3051	1/1	0.92	0.14	-	78,78,78,78	0
56	MG	1H	3398	1/1	0.96	0.11	-	55,55,55,55	0
56	MG	14	3177	1/1	0.89	0.19	-	72,72,72,72	0
56	MG	14	3176	1/1	0.93	0.35	-	81,81,81,81	0
56	MG	1H	3145	1/1	0.91	0.25	-	49,49,49,49	0
56	MG	14	3331	1/1	0.97	0.12	-	70,70,70,70	0
56	MG	1H	3126	1/1	0.98	0.34	-	60,60,60,60	0
56	MG	14	3004	1/1	0.96	0.17	-	46,46,46,46	0
56	MG	1G	1608	1/1	0.88	0.26	-	88,88,88,88	0
56	MG	1H	3324	1/1	0.94	0.26	-	87,87,87,87	0
56	MG	13	1603	1/1	0.96	0.15	-	58,58,58,58	0
56	MG	14	3246	1/1	0.92	0.13	-	66,66,66,66	0
56	MG	1H	3005	1/1	0.96	0.22	-	53,53,53,53	0
56	MG	14	3026	1/1	0.93	0.13	-	65,65,65,65	0
56	MG	14	3180	1/1	0.66	0.18	-	71,71,71,71	0
56	MG	13	1686	1/1	0.86	0.18	-	69,69,69,69	0
56	MG	1H	3419	1/1	0.99	0.10	-	37,37,37,37	0
56	MG	13	1602	1/1	0.87	0.14	-	66,66,66,66	0
56	MG	14	3164	1/1	0.90	0.16	-	64,64,64,64	0
56	MG	14	3250	1/1	0.76	0.22	-	74,74,74,74	0
56	MG	1H	3066	1/1	0.92	0.17	-	67,67,67,67	0
56	MG	14	3221	1/1	0.97	0.29	-	58,58,58,58	0
56	MG	1H	3083	1/1	0.92	0.12	-	69,69,69,69	0
56	MG	1H	3320	1/1	0.92	0.18	-	91,91,91,91	0
56	MG	14	3132	1/1	0.71	0.30	-	86,86,86,86	0
56	MG	1H	3360	1/1	0.93	0.32	-	73,73,73,73	0
56	MG	1H	3173	1/1	0.87	0.32	-	52,52,52,52	0
56	MG	14	3243	1/1	0.89	0.22	-	72,72,72,72	0
56	MG	1G	1678	1/1	0.98	0.16	-	98,98,98,98	0
56	MG	13	1681	1/1	0.94	0.23	-	81,81,81,81	0
56	MG	14	3041	1/1	0.97	0.21	-	39,39,39,39	0
56	MG	1H	3344	1/1	0.88	0.52	-	87,87,87,87	0
56	MG	14	3290	1/1	0.75	0.23	-	82,82,82,82	0
56	MG	14	3385	1/1	0.92	0.20	-	72,72,72,72	0
56	MG	1H	3399	1/1	0.94	0.08	-	47,47,47,47	0
56	MG	14	3366	1/1	0.95	0.13	-	66,66,66,66	0
56	MG	14	3292	1/1	0.86	0.24	-	82,82,82,82	0
56	MG	13	1717	1/1	0.88	0.23	-	74,74,74,74	0
56	MG	1H	3171	1/1	0.73	0.14	-	79,79,79,79	0
56	MG	14	3321	1/1	0.96	0.08	-	62,62,62,62	0
56	MG	1H	3289	1/1	0.92	0.31	-	62,62,62,62	0
56	MG	1H	3249	1/1	0.83	0.26	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	P8	101	1/1	0.81	0.29	-	68,68,68,68	0
56	MG	1H	3336	1/1	0.89	0.26	-	79,79,79,79	0
56	MG	1H	3042	1/1	0.88	0.30	-	74,74,74,74	0
56	MG	1H	3087	1/1	0.99	0.37	-	43,43,43,43	0
56	MG	1H	3137	1/1	0.89	0.20	-	49,49,49,49	0
56	MG	1H	3436	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	1H	3256	1/1	0.95	0.20	-	57,57,57,57	0
56	MG	1H	3157	1/1	0.93	0.37	-	72,72,72,72	0
56	MG	1H	3238	1/1	0.80	0.21	-	54,54,54,54	0
56	MG	1H	3319	1/1	0.68	0.56	-	92,92,92,92	0
56	MG	1H	3245	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	1H	3045	1/1	0.91	0.35	-	66,66,66,66	0
56	MG	1H	3077	1/1	0.85	0.23	-	73,73,73,73	0
56	MG	1H	3447	1/1	0.98	0.11	-	76,76,76,76	0
56	MG	1H	3441	1/1	0.96	0.10	-	86,86,86,86	0
56	MG	14	3377	1/1	0.71	0.12	-	96,96,96,96	0
56	MG	1H	3197	1/1	0.84	0.29	-	66,66,66,66	0
56	MG	1H	3072	1/1	0.98	0.19	-	43,43,43,43	0
56	MG	14	3337	1/1	0.95	0.06	-	55,55,55,55	0
56	MG	1H	3196	1/1	0.95	0.08	-	68,68,68,68	0
56	MG	14	3310	1/1	0.94	0.09	-	50,50,50,50	0
56	MG	14	3380	1/1	0.94	0.10	-	93,93,93,93	0
56	MG	14	3043	1/1	0.96	0.15	-	67,67,67,67	0
56	MG	1H	3234	1/1	0.89	0.22	-	75,75,75,75	0
56	MG	13	1676	1/1	0.97	0.16	-	62,62,62,62	0
56	MG	1H	3012	1/1	0.96	0.34	-	45,45,45,45	0
56	MG	14	3196	1/1	0.91	0.20	-	90,90,90,90	0
56	MG	1G	1646	1/1	0.64	0.23	-	79,79,79,79	0
56	MG	13	1636	1/1	0.93	0.18	-	66,66,66,66	0
56	MG	13	1714	1/1	0.94	0.34	-	99,99,99,99	0
56	MG	14	3223	1/1	0.85	0.23	-	62,62,62,62	0
56	MG	1H	3026	1/1	0.97	0.23	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.