



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 02:07 AM GMT

PDB ID : 4WU1  
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with G-U mismatch in the second position in the P-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-30  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

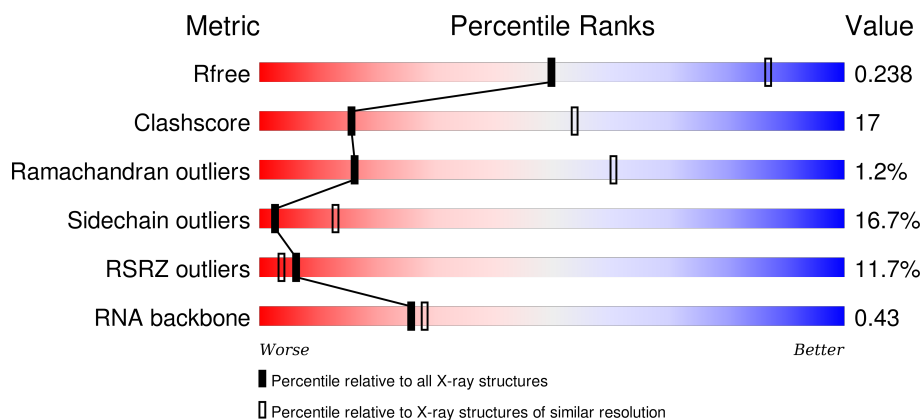
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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% 46% 17% ..</div> </div>
2	12	256	<div> <div>12%</div> <div>42% 42% 8% 7%</div> </div>
2	1E	256	<div> <div>15%</div> <div>43% 38% 12% 7%</div> </div>
3	22	239	<div> <div>12%</div> <div>49% 29% 8% 14%</div> </div>

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

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Mol	Chain	Length	Quality of chain
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	27	
23	4L	27	
24	14	2917	
24	1H	2917	
25	16	122	
25	1J	122	
26	71	229	
26	79	229	
27	11	276	

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	11	302	-	-	-	X
55	MG	13	1616	-	-	-	X
55	MG	13	1619	-	-	-	X
55	MG	13	1629	-	-	-	X
55	MG	13	1662	-	-	-	X
55	MG	13	1681	-	-	-	X
55	MG	13	1692	-	-	-	X
55	MG	14	3021	-	-	-	X
55	MG	14	3024	-	-	-	X
55	MG	14	3047	-	-	-	X
55	MG	14	3110	-	-	-	X
55	MG	14	3141	-	-	-	X
55	MG	14	3146	-	-	-	X
55	MG	14	3154	-	-	-	X
55	MG	14	3174	-	-	-	X
55	MG	14	3201	-	-	-	X
55	MG	14	3223	-	-	-	X
55	MG	14	3236	-	-	-	X
55	MG	14	3243	-	-	-	X
55	MG	14	3256	-	-	-	X
55	MG	14	3265	-	-	-	X
55	MG	14	3266	-	-	-	X
55	MG	14	3280	-	-	-	X
55	MG	14	3283	-	-	-	X
55	MG	14	3284	-	-	-	X
55	MG	14	3312	-	-	-	X
55	MG	14	3479	-	-	-	X
55	MG	15	201	-	-	-	X
55	MG	1G	1616	-	-	-	X
55	MG	1G	1642	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1G	1653	-	-	-	X
55	MG	1G	1685	-	-	-	X
55	MG	1G	1687	-	-	-	X
55	MG	1G	1700	-	-	-	X
55	MG	1G	1701	-	-	-	X
55	MG	1G	1712	-	-	-	X
55	MG	1G	1719	-	-	-	X
55	MG	1H	3001	-	-	-	X
55	MG	1H	3027	-	-	-	X
55	MG	1H	3031	-	-	-	X
55	MG	1H	3041	-	-	-	X
55	MG	1H	3047	-	-	-	X
55	MG	1H	3051	-	-	-	X
55	MG	1H	3059	-	-	-	X
55	MG	1H	3063	-	-	-	X
55	MG	1H	3073	-	-	-	X
55	MG	1H	3106	-	-	-	X
55	MG	1H	3108	-	-	-	X
55	MG	1H	3116	-	-	-	X
55	MG	1H	3119	-	-	-	X
55	MG	1H	3130	-	-	-	X
55	MG	1H	3131	-	-	-	X
55	MG	1H	3154	-	-	-	X
55	MG	1H	3155	-	-	-	X
55	MG	1H	3228	-	-	-	X
55	MG	1H	3235	-	-	-	X
55	MG	1H	3332	-	-	-	X
55	MG	1H	3334	-	-	-	X
55	MG	1H	3337	-	-	-	X
55	MG	1H	3342	-	-	-	X
55	MG	1H	3358	-	-	-	X
55	MG	1H	3361	-	-	-	X
55	MG	1H	3368	-	-	-	X
55	MG	1H	3395	-	-	-	X
55	MG	1J	206	-	-	-	X
55	MG	29	302	-	-	-	X
55	MG	29	303	-	-	-	X
55	MG	29	305	-	-	-	X
55	MG	42	201	-	-	-	X
55	MG	55	203	-	-	-	X



## 2 Entry composition

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called mRNA.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	45	1	Total	Mg	0	0
			1	1		
55	55	3	Total	Mg	0	0
			3	3		
55	32	1	Total	Mg	0	0
			1	1		
55	C5	1	Total	Mg	0	0
			1	1		
55	13	129	Total	Mg	0	0
			129	129		
55	1J	11	Total	Mg	0	0
			11	11		
55	16	12	Total	Mg	0	0
			12	12		
55	42	1	Total	Mg	0	0
			1	1		
55	25	1	Total	Mg	0	0
			1	1		
55	M5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	21	1	Total 1	Mg 1	0	0
55	2K	4	Total 4	Mg 4	0	0
55	Q8	1	Total 1	Mg 1	0	0
55	15	1	Total 1	Mg 1	0	0
55	3I	1	Total 1	Mg 1	0	0
55	I8	3	Total 3	Mg 3	0	0
55	5E	2	Total 2	Mg 2	0	0
55	29	5	Total 5	Mg 5	0	0
55	78	2	Total 2	Mg 2	0	0
55	J8	1	Total 1	Mg 1	0	0
55	39	1	Total 1	Mg 1	0	0
55	1G	147	Total 147	Mg 147	0	0
55	11	2	Total 2	Mg 2	0	0
55	1H	548	Total 548	Mg 548	0	0
55	F5	1	Total 1	Mg 1	0	0
55	E5	2	Total 2	Mg 2	0	0
55	88	2	Total 2	Mg 2	0	0
55	49	1	Total 1	Mg 1	0	0
55	14	489	Total 489	Mg 489	0	0
55	19	1	Total 1	Mg 1	0	0
55	3L	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2L	3	Total 3	Mg 3	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	5	Total O 5 5	0	0
57	14	6	Total O 6 6	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0
57	14	4	Total O 4 4	0	0
57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
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57	14	6	Total O 6 6	0	0
57	14	6	Total O 6 6	0	0
57	1J	6	Total O 6 6	0	0
57	1J	6	Total O 6 6	0	0
57	1J	6	Total O 6 6	0	0
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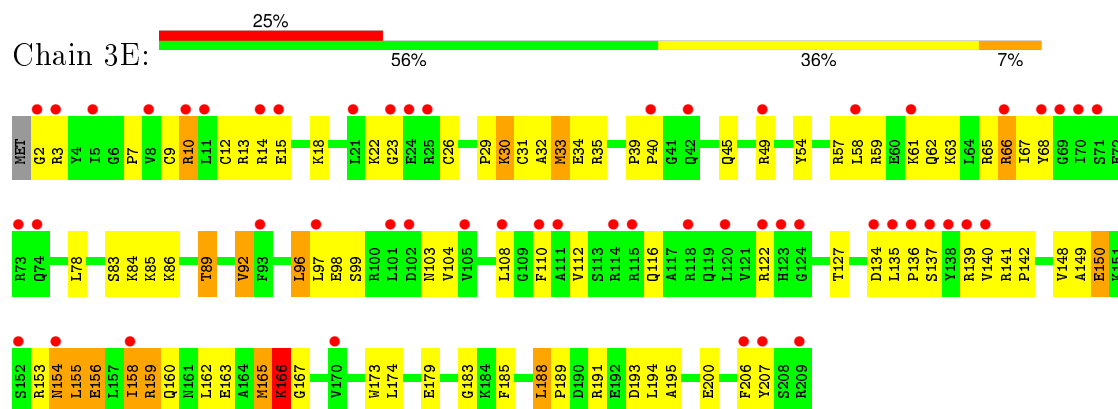




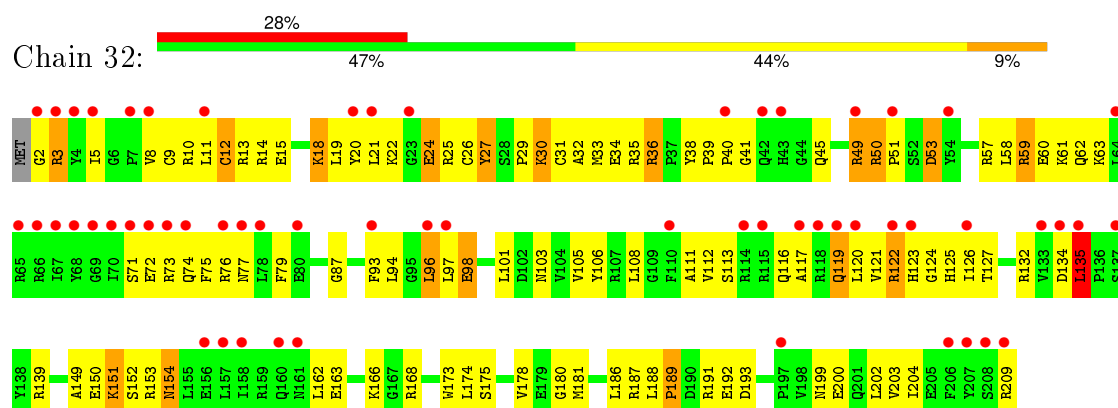


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VAL  
LYS  
GLU  
GLU

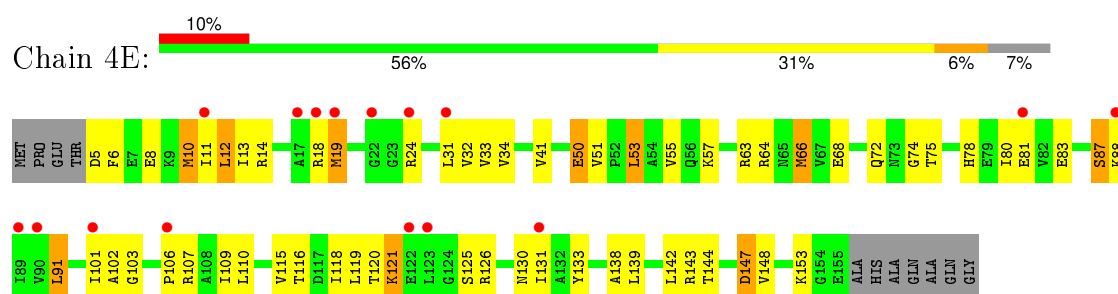
• Molecule 4: 30S ribosomal protein S4



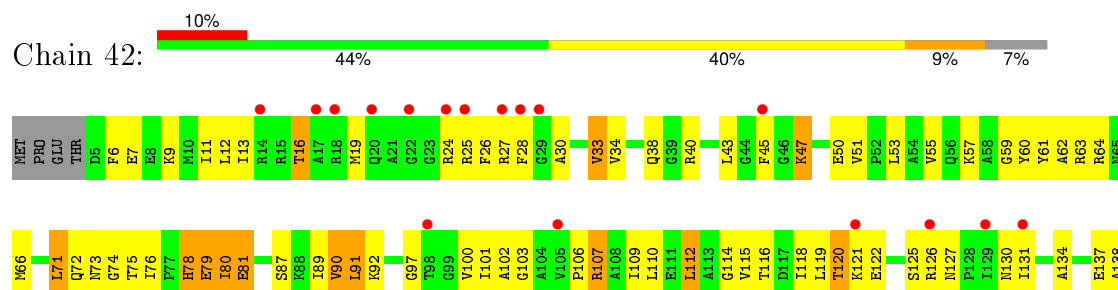
• Molecule 4: 30S ribosomal protein S4

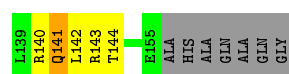


• Molecule 5: 30S ribosomal protein S5

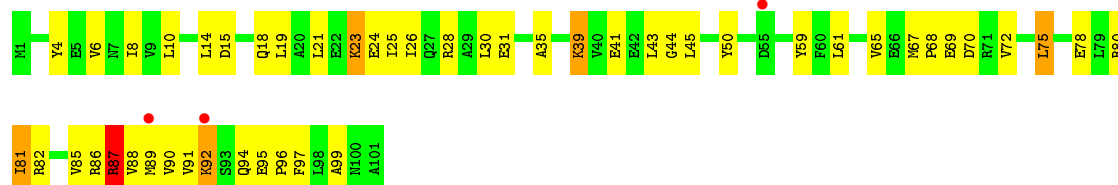


• Molecule 5: 30S ribosomal protein S5





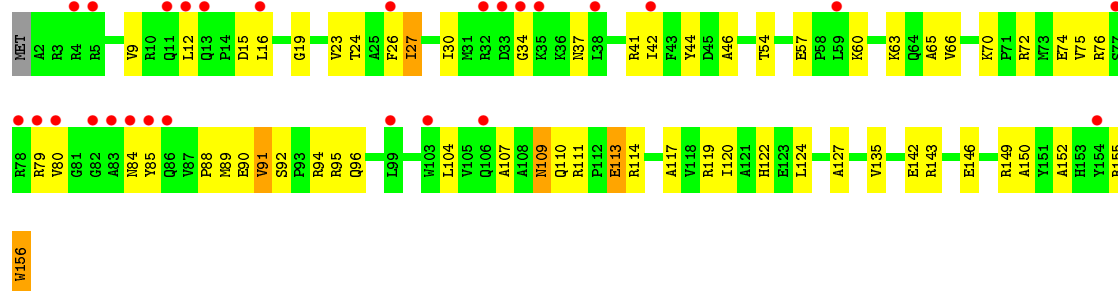
• Molecule 6: 30S ribosomal protein S6



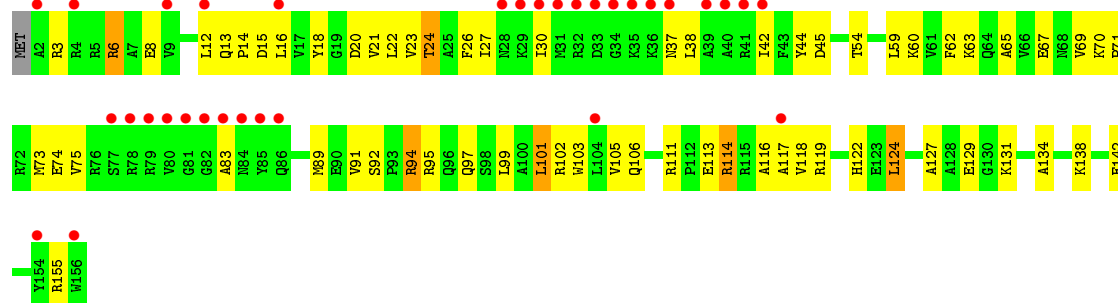
• Molecule 6: 30S ribosomal protein S6



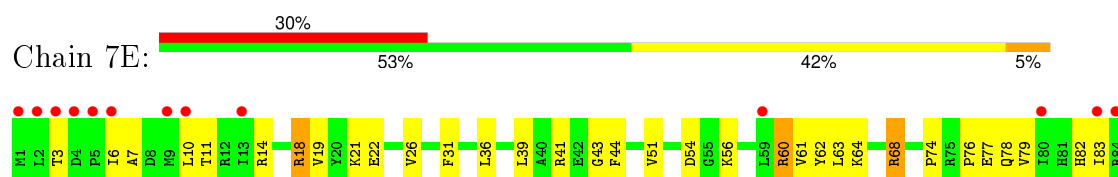
• Molecule 7: 30S ribosomal protein S7



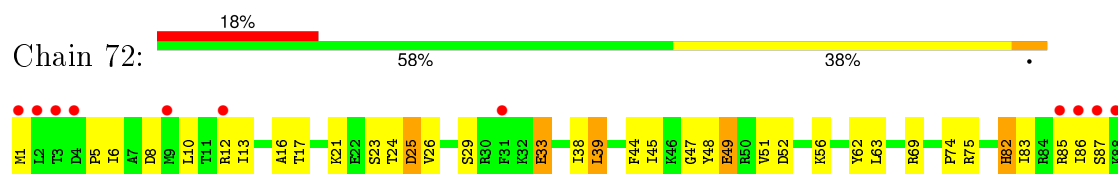
• Molecule 7: 30S ribosomal protein S7



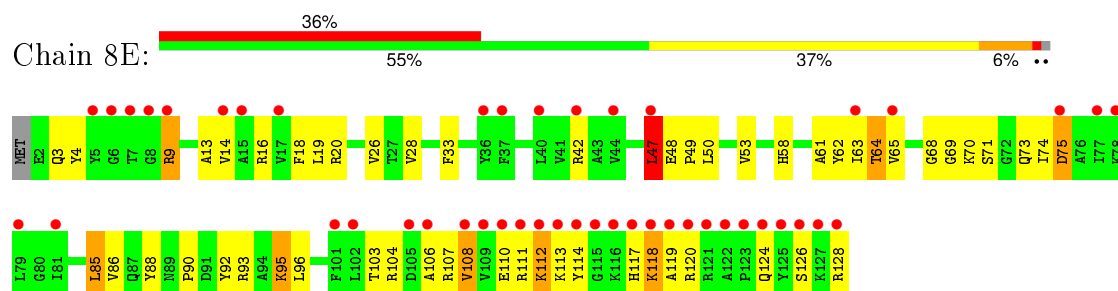
• Molecule 8: 30S ribosomal protein S8



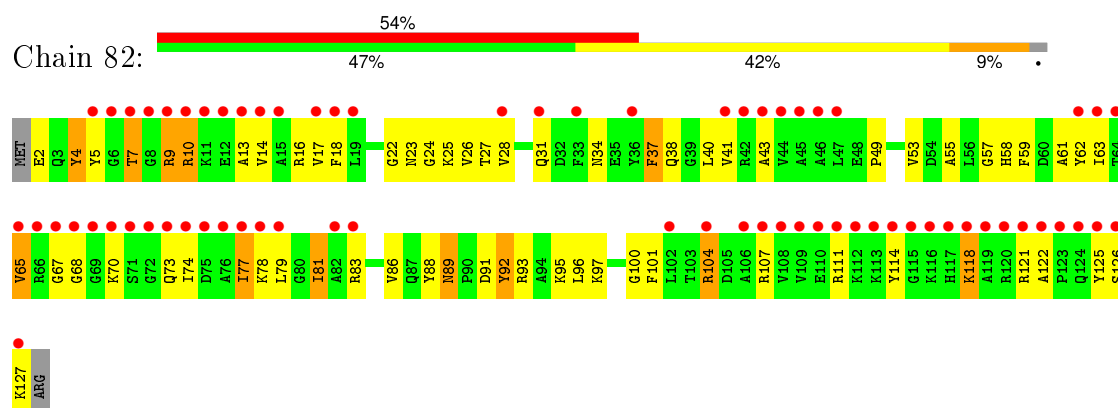
• Molecule 8: 30S ribosomal protein S8



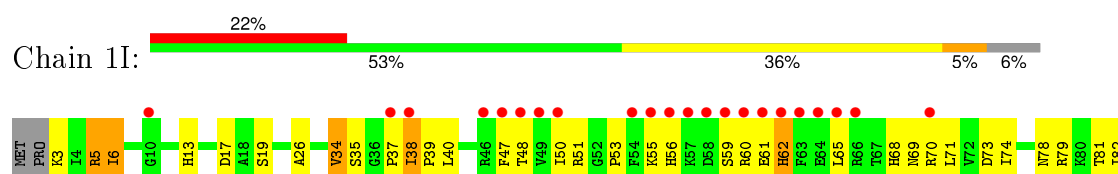
• Molecule 9: 30S ribosomal protein S9

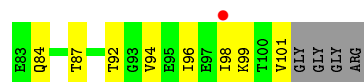


• Molecule 9: 30S ribosomal protein S9

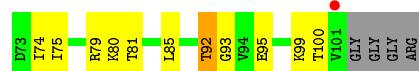
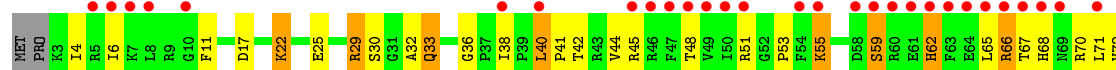


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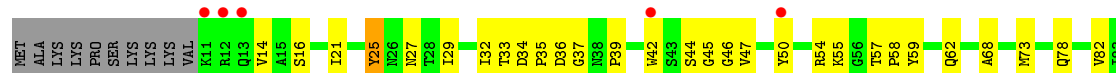




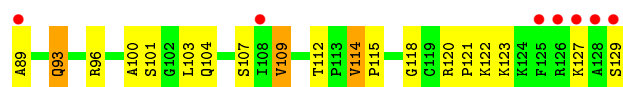
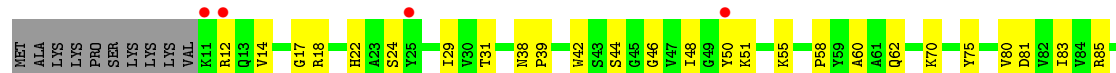
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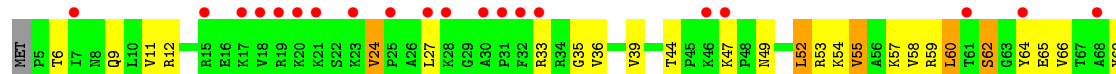
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

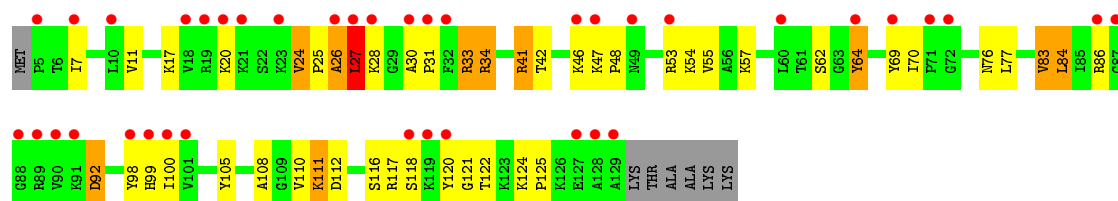


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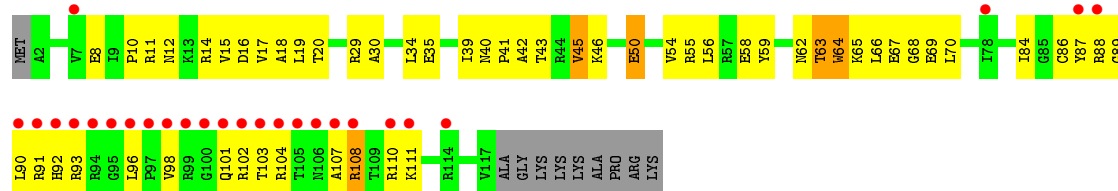


- Molecule 12: 30S ribosomal protein S12

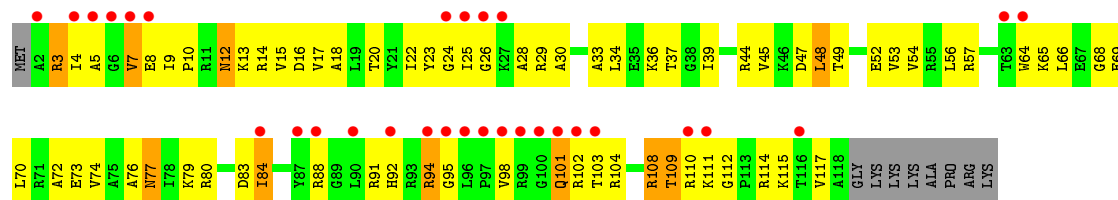




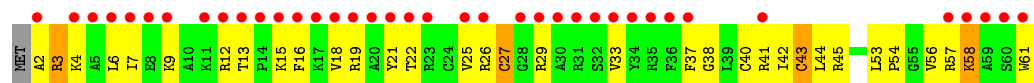
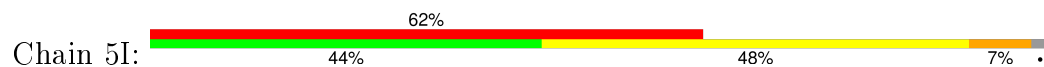
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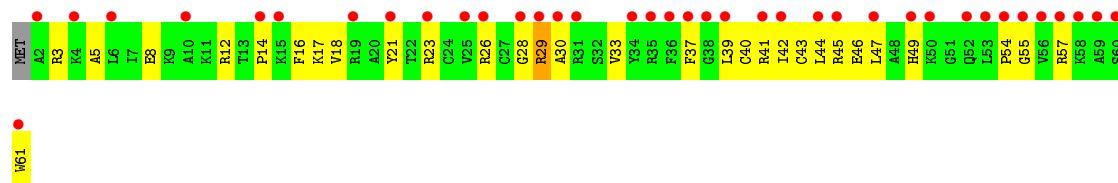
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z

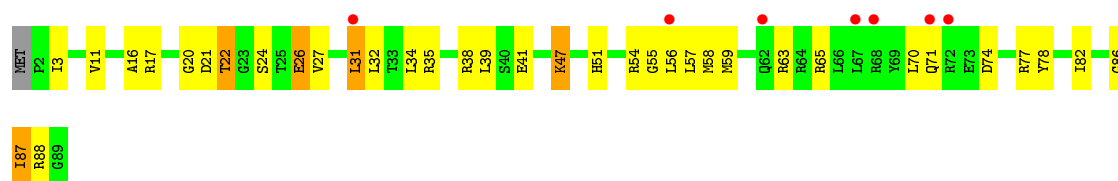


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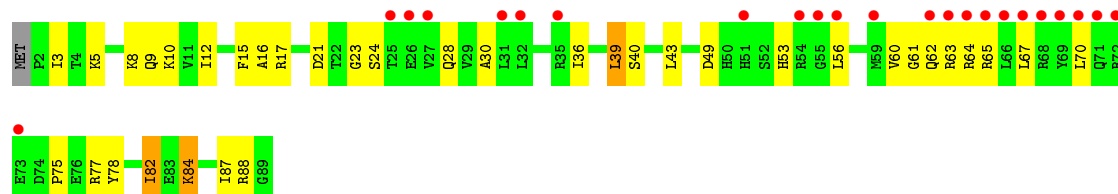


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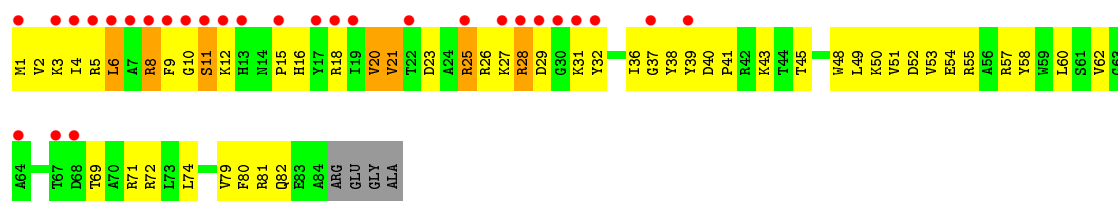




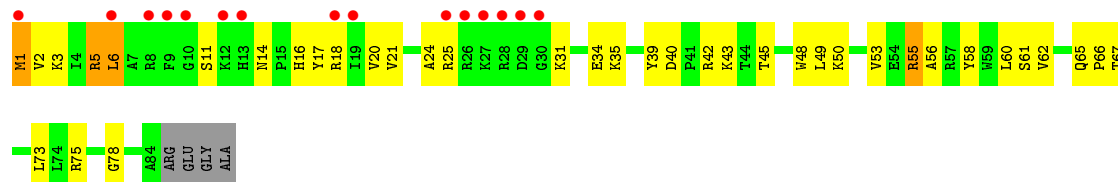
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- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



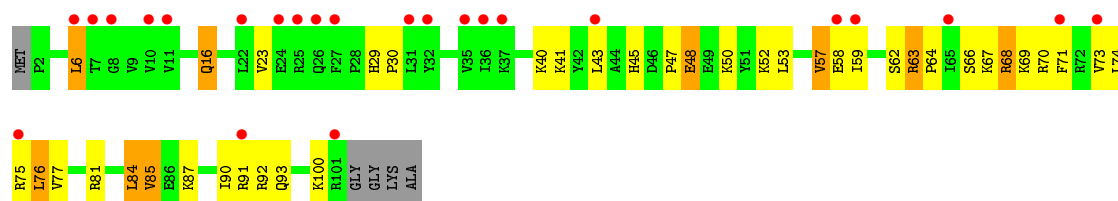
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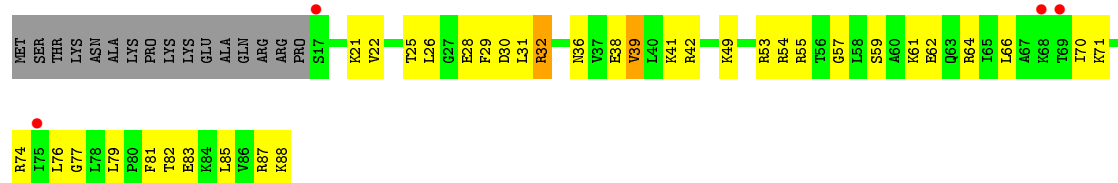
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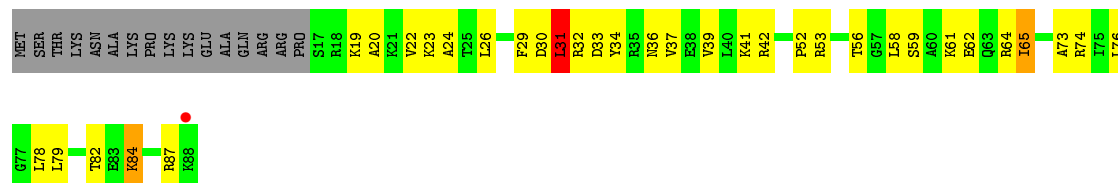
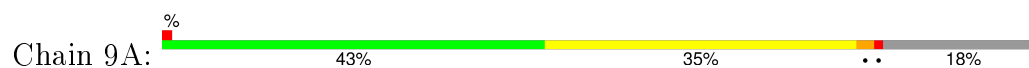




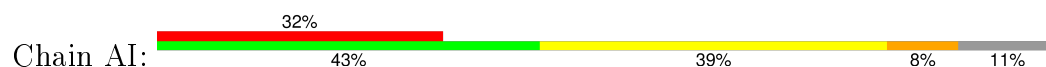
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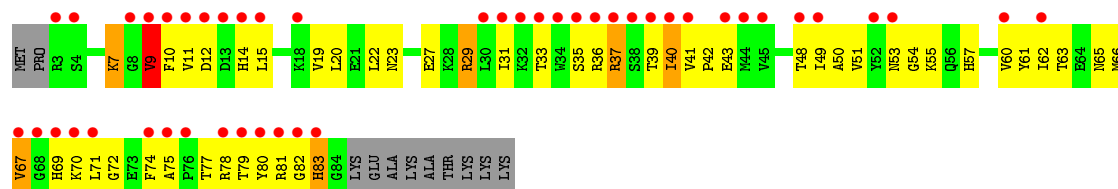
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• Molecule 19: 30S ribosomal protein S19

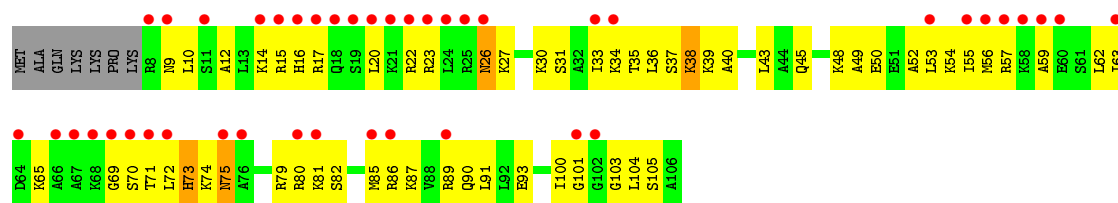


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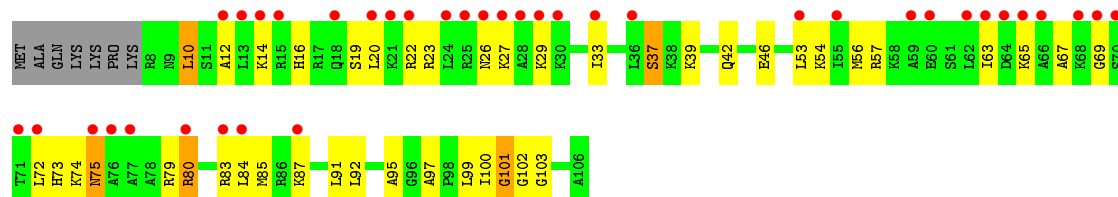


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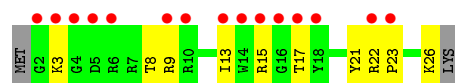




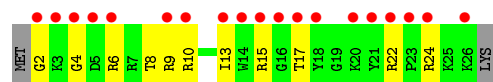
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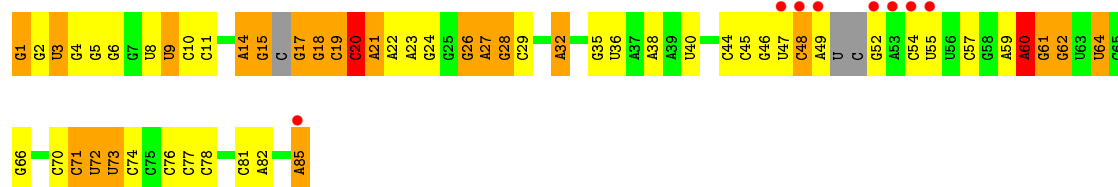
• Molecule 21: 30S ribosomal protein Thx



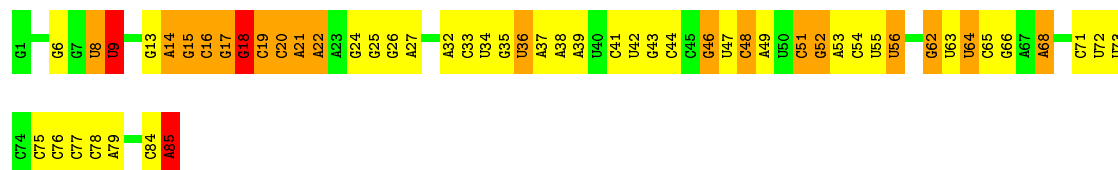
• Molecule 21: 30S ribosomal protein Thx



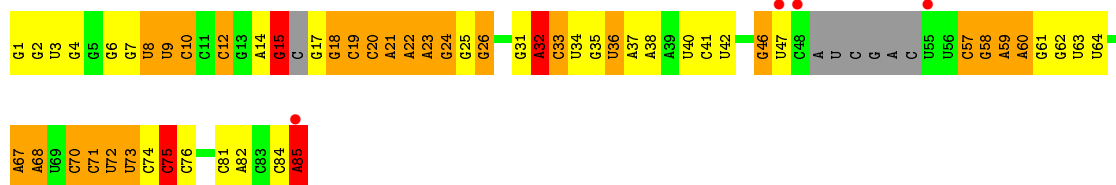
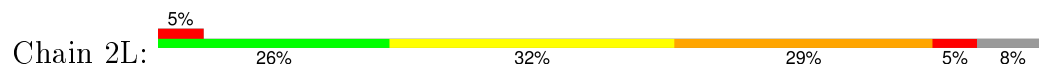
• Molecule 22: tRNA-Tyr



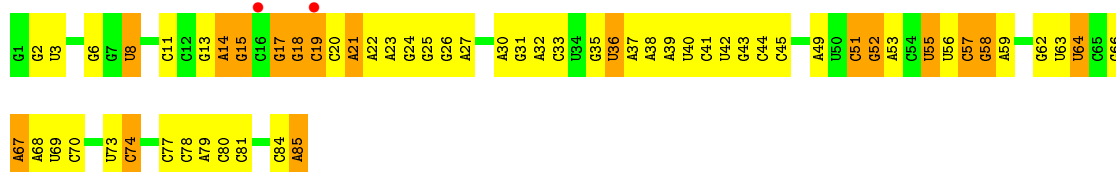
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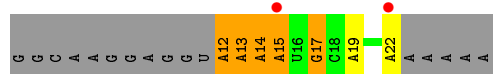
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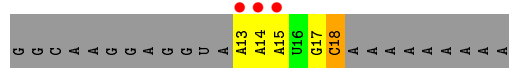
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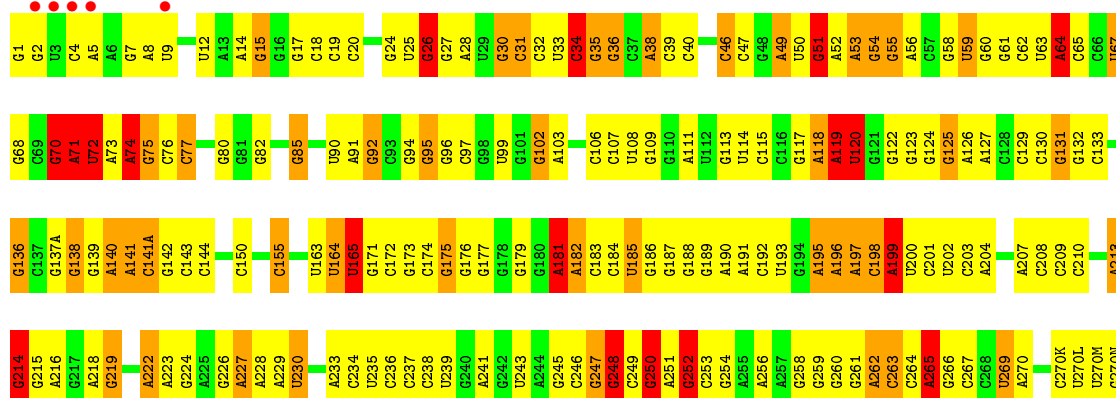
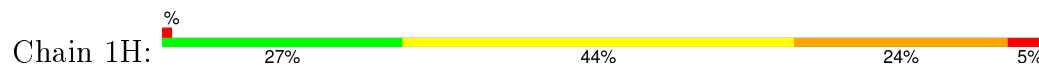
- Molecule 23: mRNA



- Molecule 23: mRNA

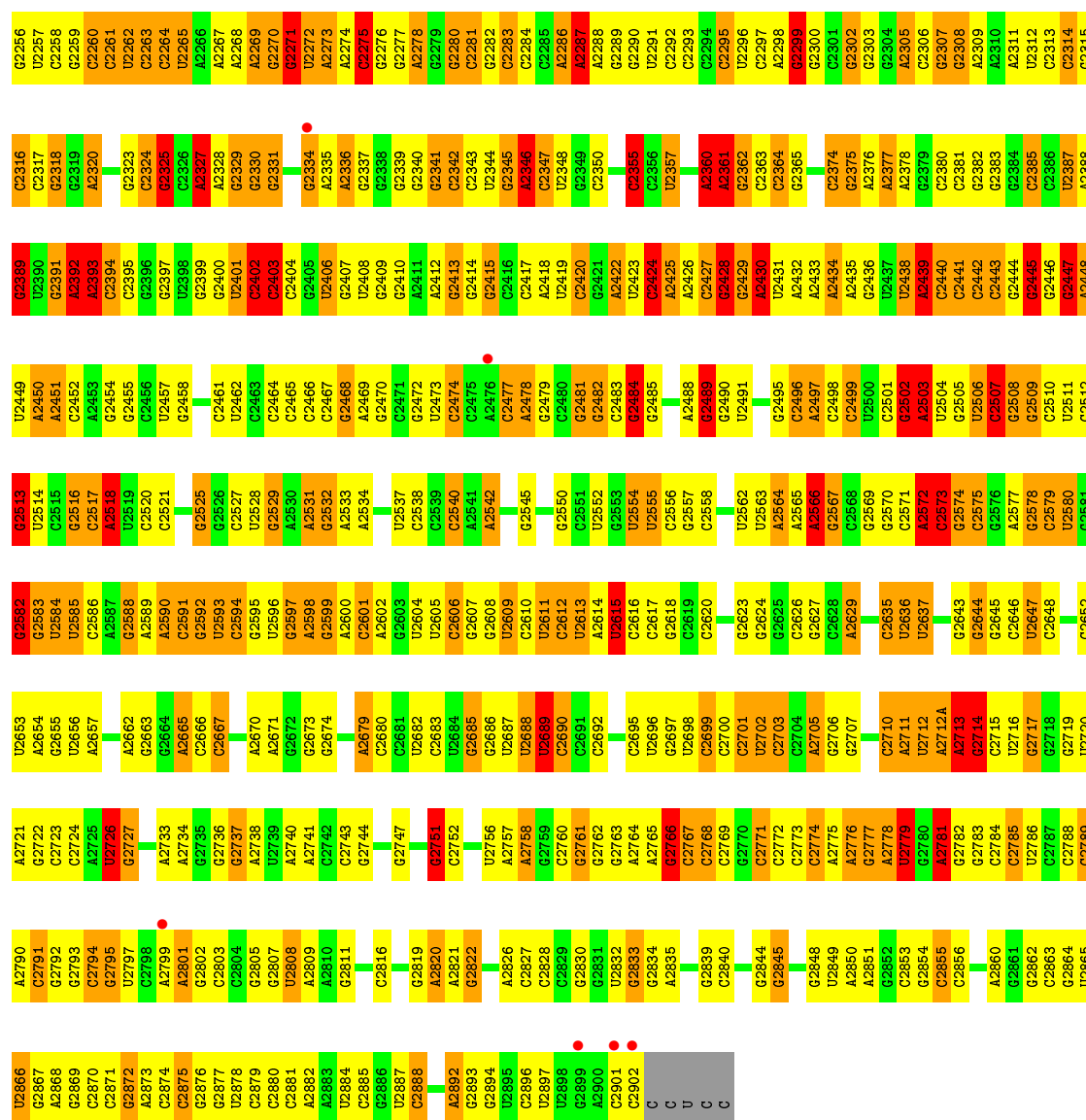


- Molecule 24: 23S ribosomal RNA

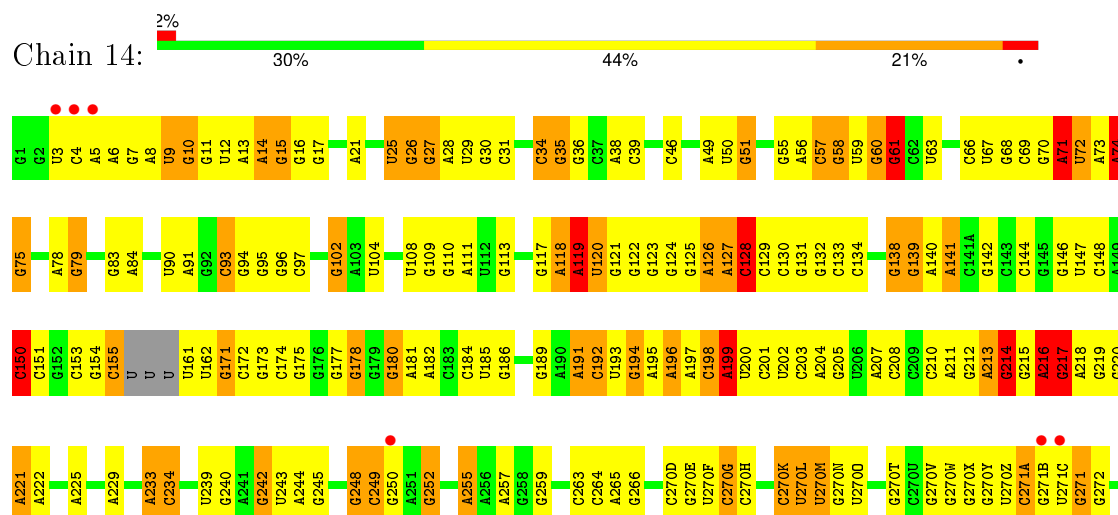


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C2183	C2184	C2185	C2186	C2187	C2190	C2191	C2192	C2193	C2194	C2195	A1298	A1299	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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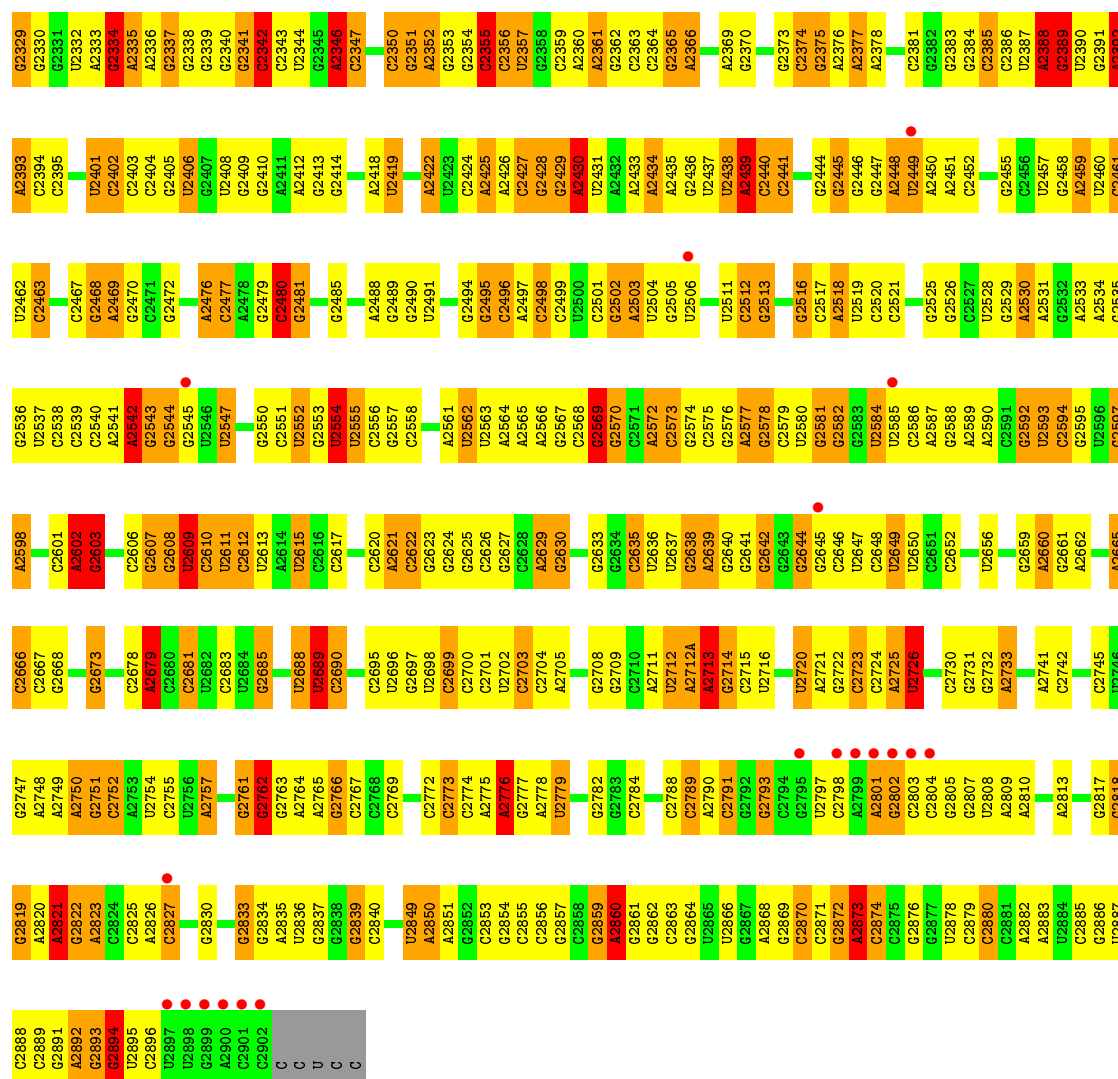
• Molecule 24: 23S ribosomal RNA



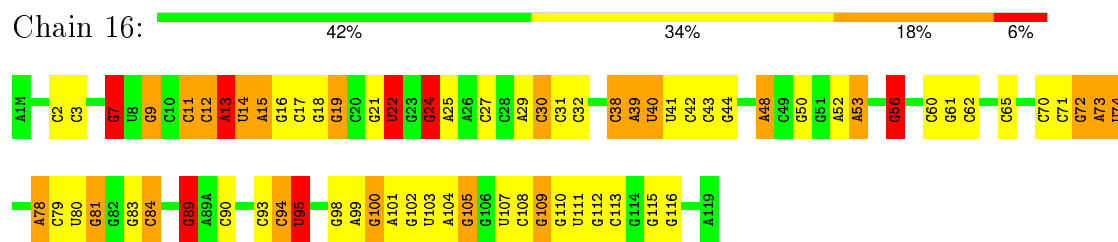
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	G1151	G1079	G1011	A945	G880	G681	G636	G570	G494	G430	G351	C273F
	C1152	C1079	U1012	G946	G881	G682	A637	A571	G495	G430	G352	G274
	C1153		U1013		G882	G683	G638	A572			G353	
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	U1159	G1087	U1019	G954	C888	G690	G647	G579	G506		G361	C287
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	G1162	U1090	G1022	A957	G892	A768	G649	C581	C510	A444	G363A	G290
U1234	G1163	U1091	U1023	U958	C893	G769	G650	G582	C511	C445	G363B	C291
	G1164	G1092	G1024	A959	C894	G770	G651	G583	U511	C446	G363C	C292
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G2281	G2211	G2138	U1931	G1845	U1778	G1686	G1625	G1560	G1492	G1429	A1360	C1297
G2282	A2212	C2142	G1932	G1846	U1779	U1688	G1626	A1561	A1493	C1430	G1361	C1298
C2283	G2213	A2143	G1933	A1847	U1780	A1689	G1627		C1494	C1431		G1299
A2284	G2215	U2144	A2001	G1848	C1781	A1690	U1629	G1564	A1495	U1433	G1364	A1301
C2285	G2216	G2145	A1936	G1849	G1782	C1691	G1630	A1566	A1496	A1434	A1366	A1302
A2286		C2146	A1937	G1850	A1783	G1694	G1631	A1567	U1497	G1435	A1367	G1303
A2287	G2224	G2147	A1938	A1853	A1784	G1695	A1631		G1500	G1436	G1368	A1307
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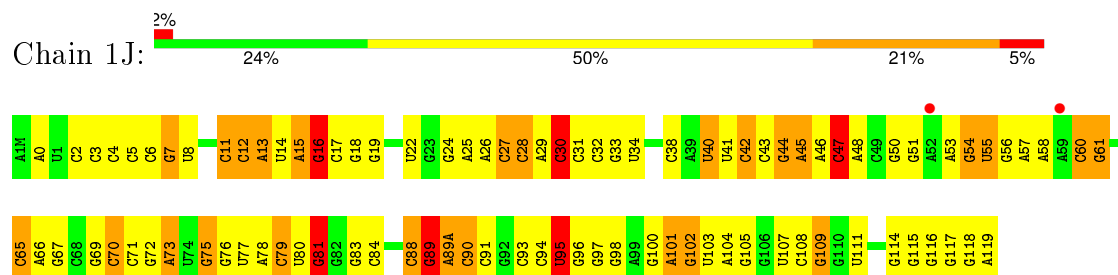




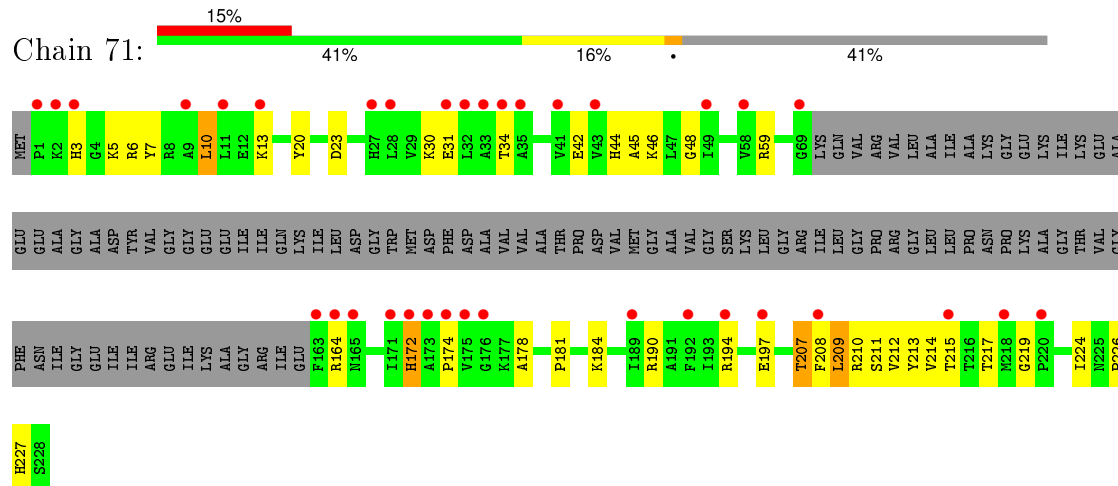
• Molecule 25: 5S ribosomal RNA



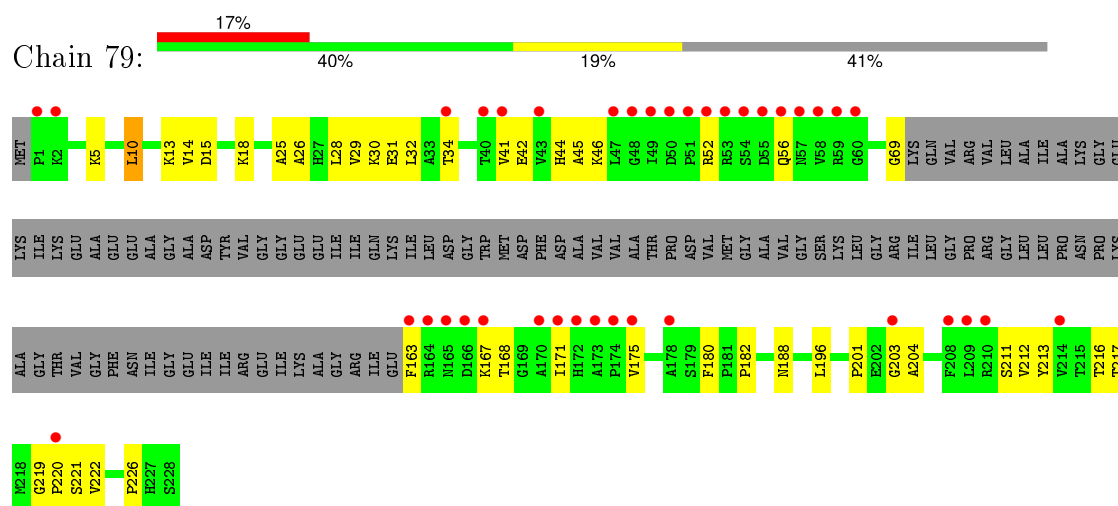
• Molecule 25: 5S ribosomal RNA

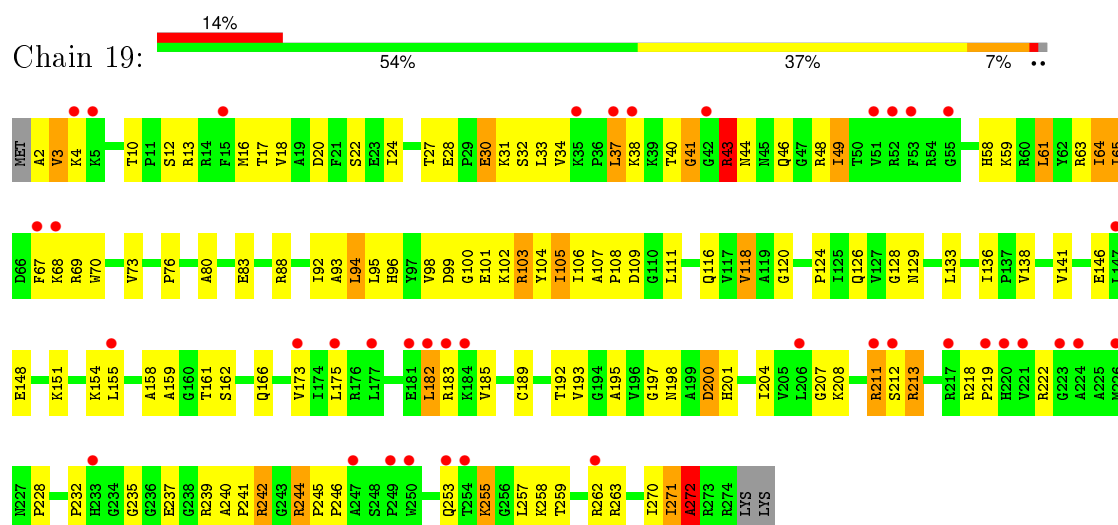


- Molecule 26: 50S ribosomal protein L1

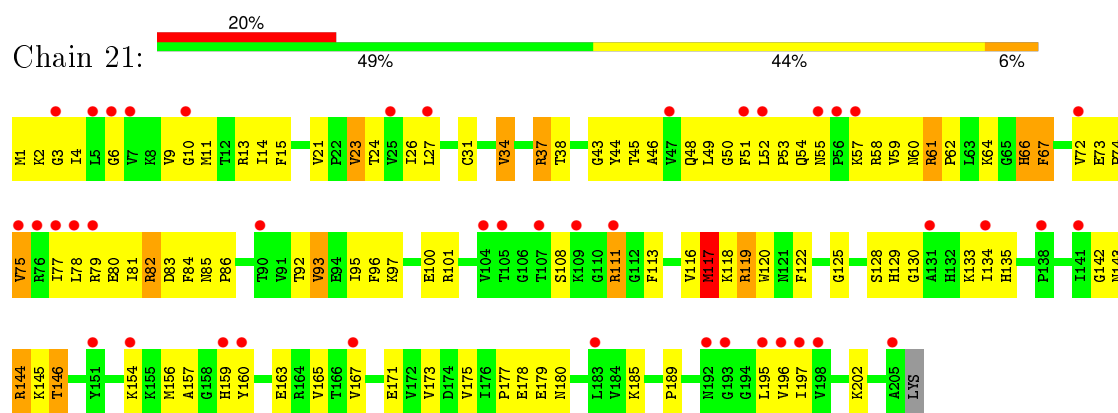


- Molecule 26: 50S ribosomal protein L1

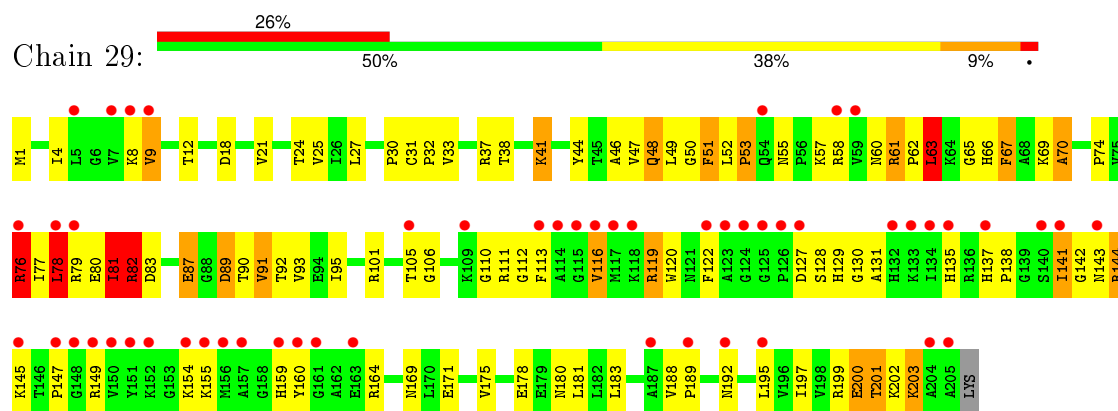




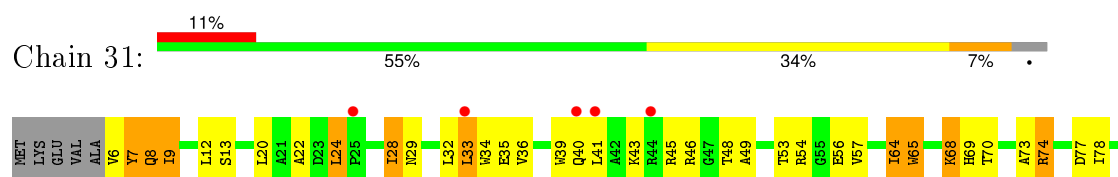
• Molecule 28: 50S ribosomal protein L3

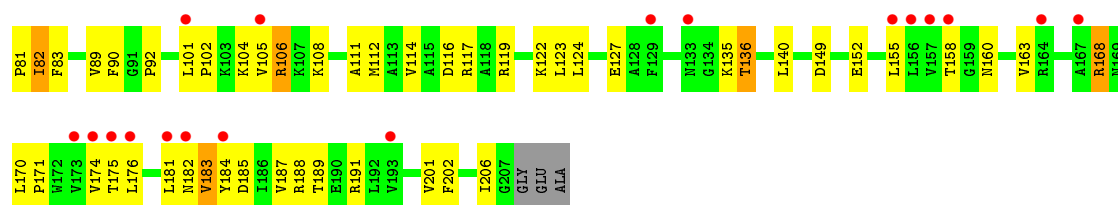


• Molecule 28: 50S ribosomal protein L3

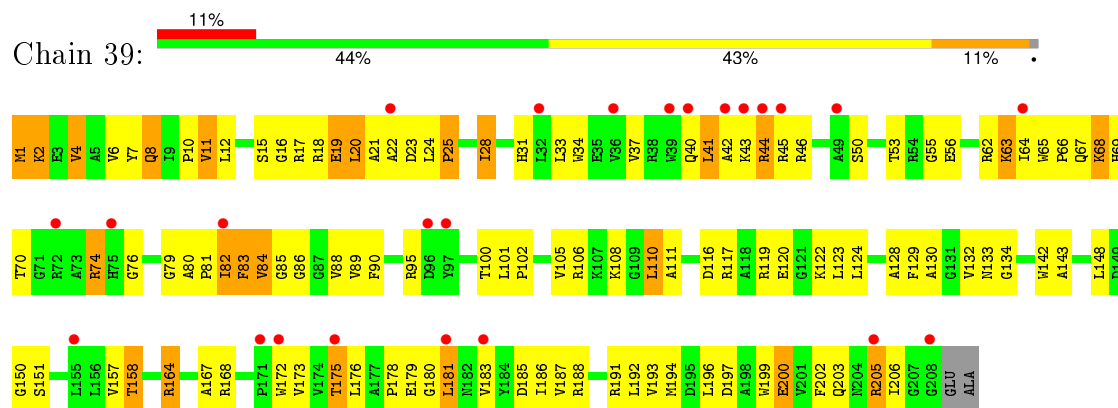


• Molecule 29: 50S ribosomal protein L4

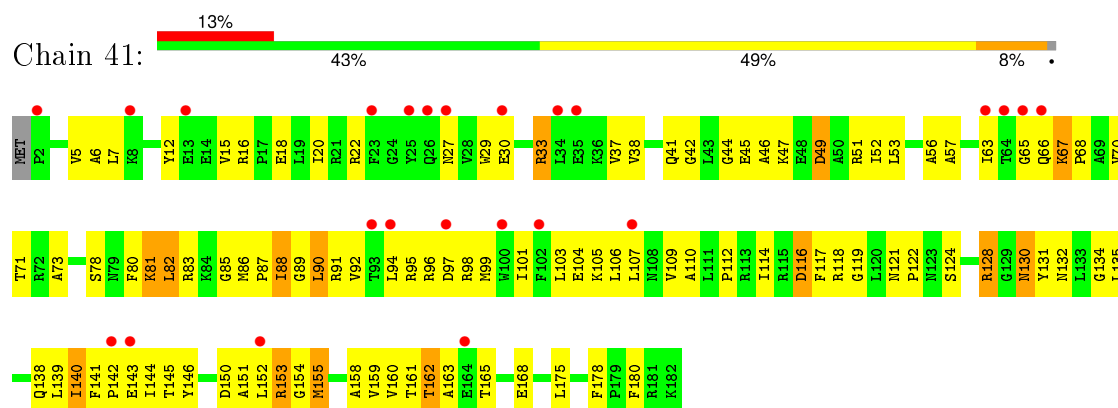




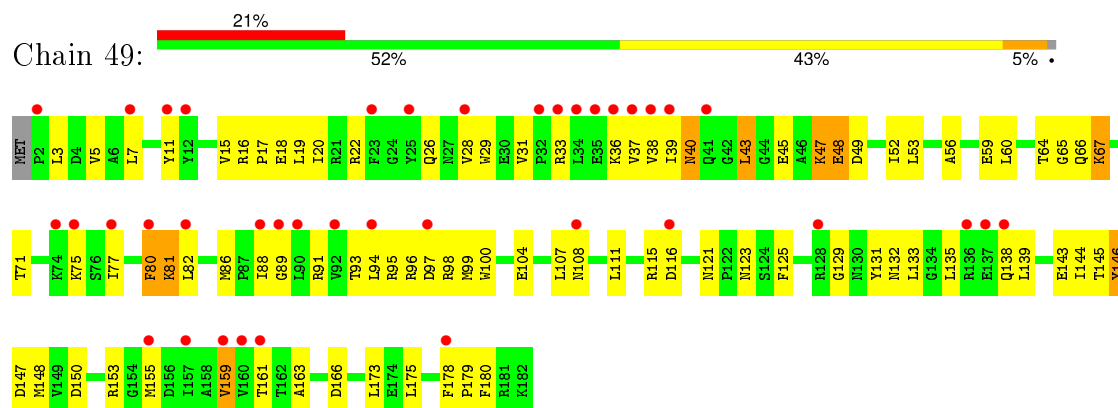
• Molecule 29: 50S ribosomal protein L4



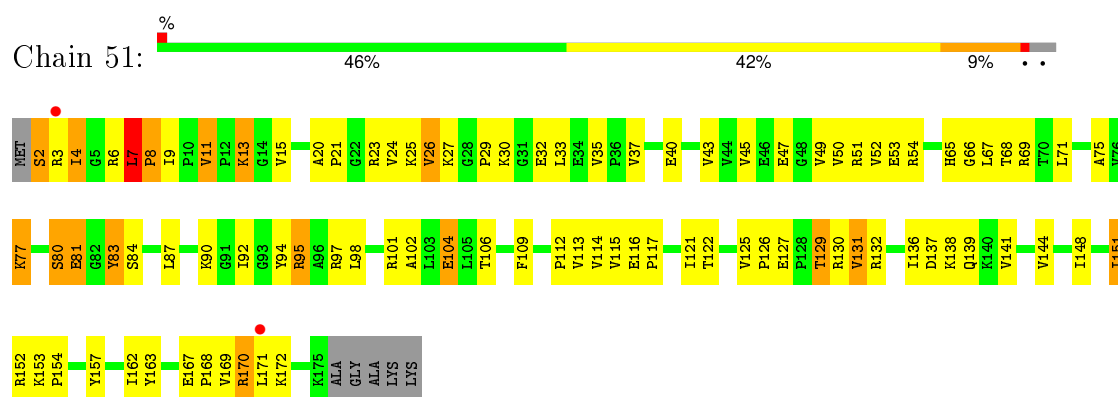
• Molecule 30: 50S ribosomal protein L5



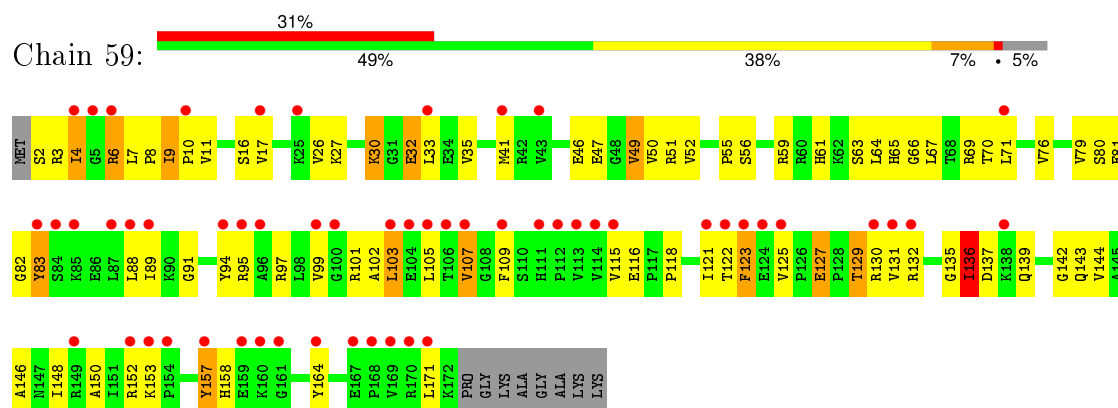
• Molecule 30: 50S ribosomal protein L5



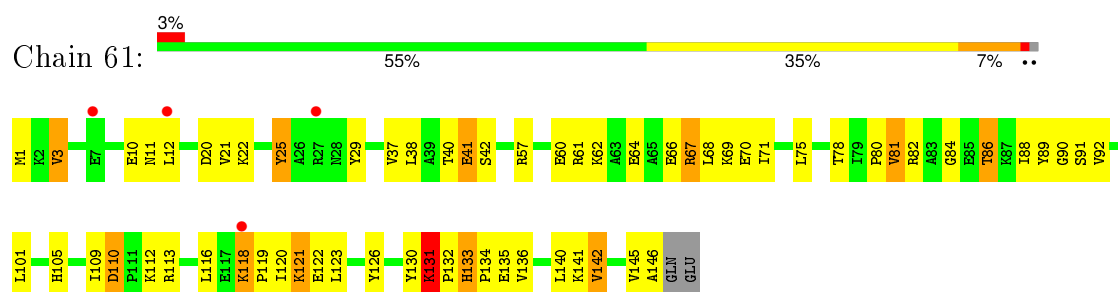
• Molecule 31: 50S ribosomal protein L6



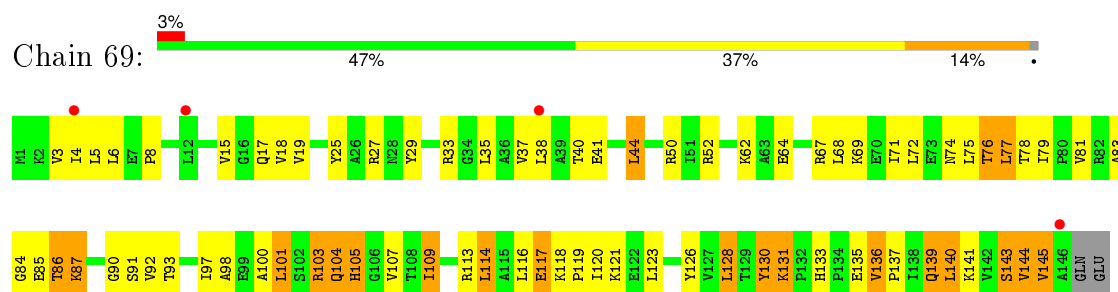
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

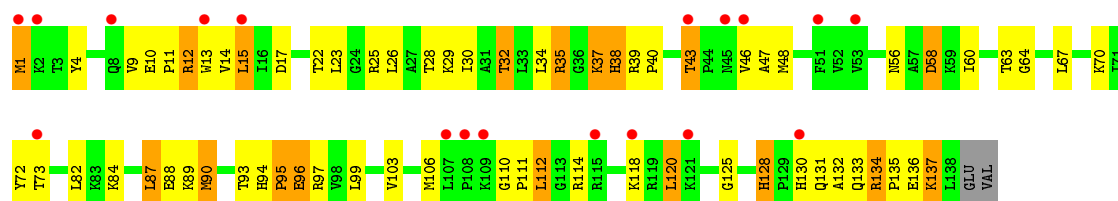


• Molecule 32: 50S ribosomal protein L9

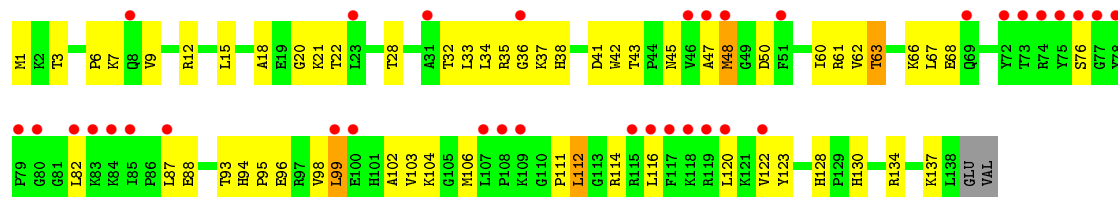


• Molecule 33: 50S ribosomal protein L13

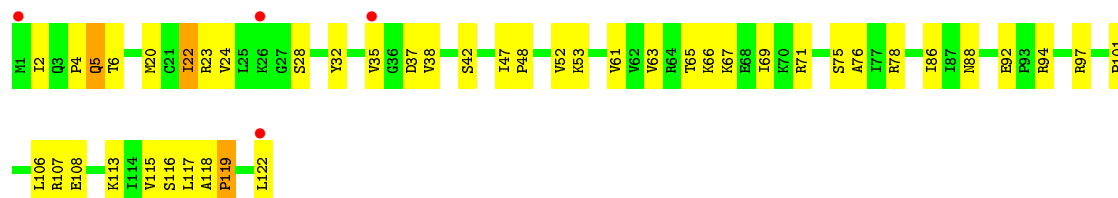




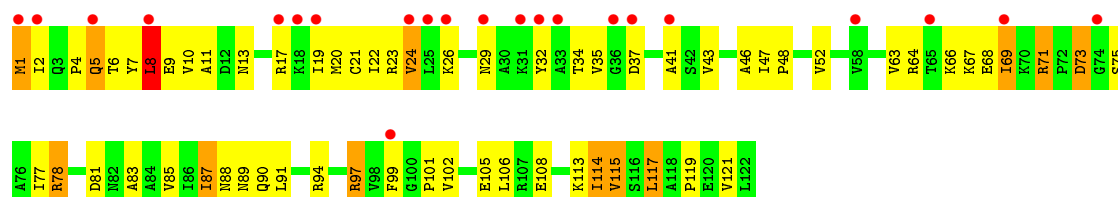
• Molecule 33: 50S ribosomal protein L13



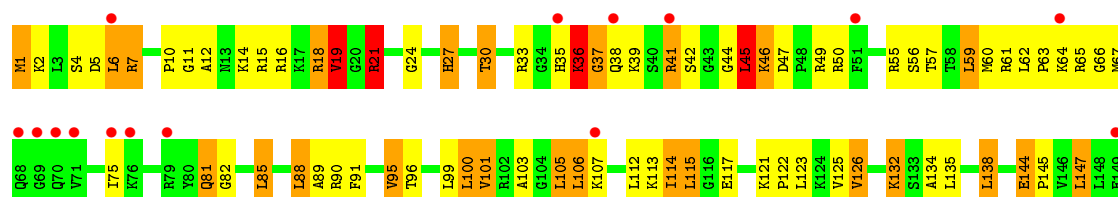
• Molecule 34: 50S ribosomal protein L14



• Molecule 34: 50S ribosomal protein L14

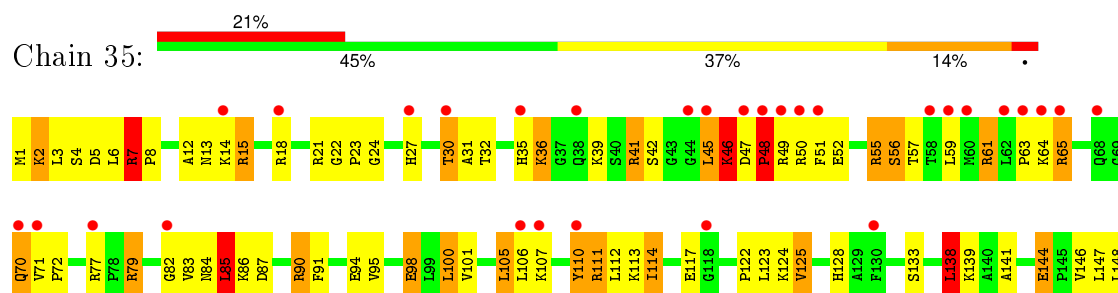


• Molecule 35: 50S ribosomal protein L15

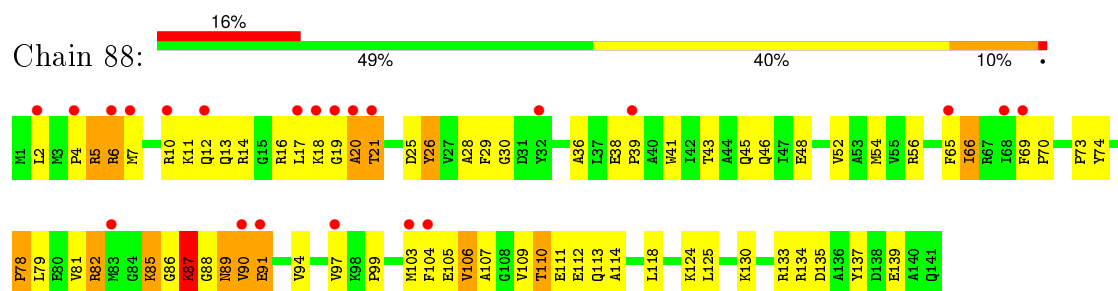




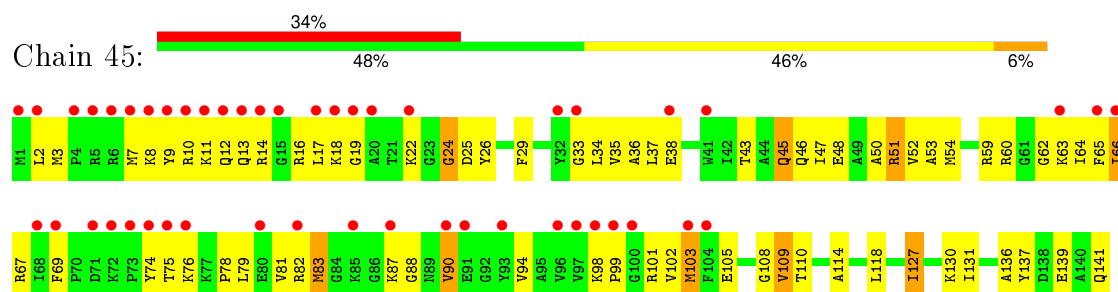
• Molecule 35: 50S ribosomal protein L15



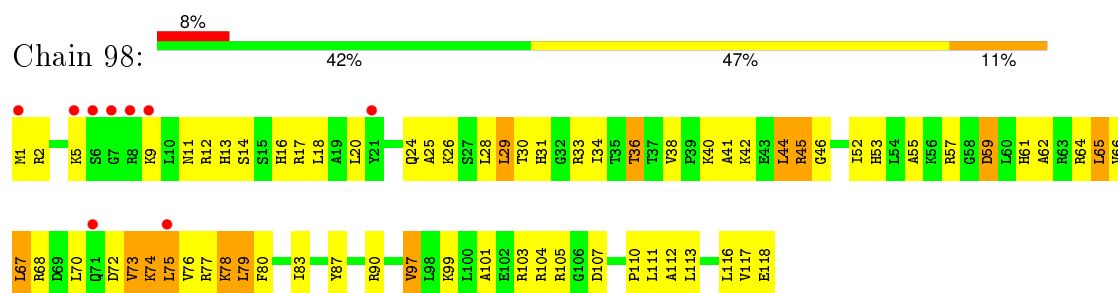
• Molecule 36: 50S ribosomal protein L16



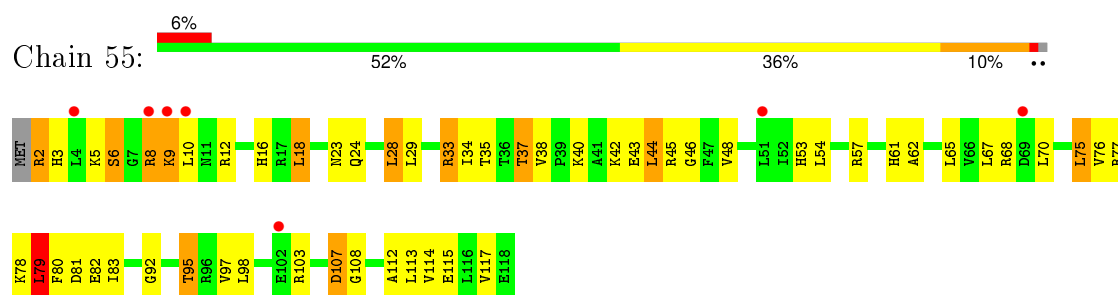
• Molecule 36: 50S ribosomal protein L16



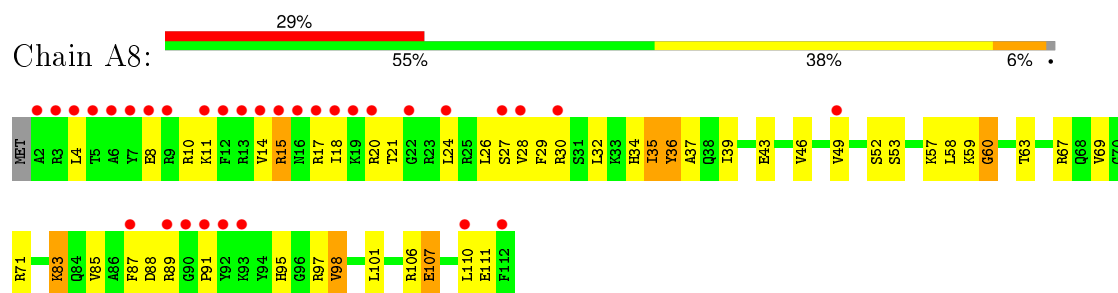
• Molecule 37: 50S ribosomal protein L17



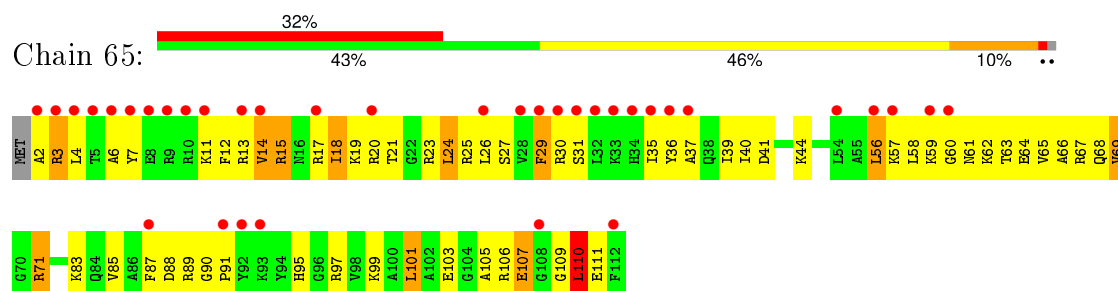
• Molecule 37: 50S ribosomal protein L17



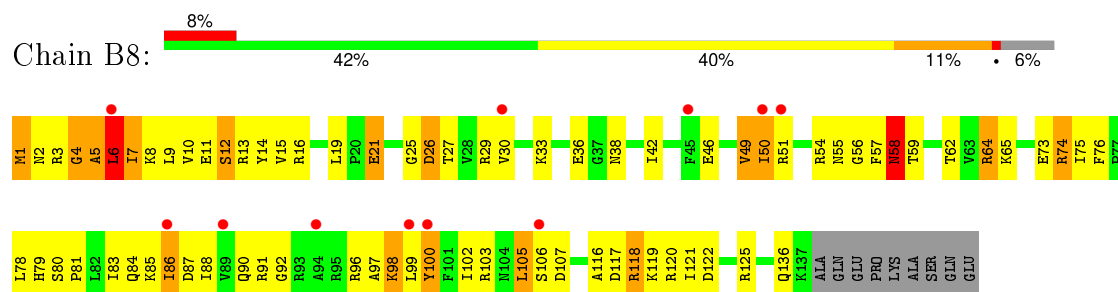
- Molecule 38: 50S ribosomal protein L18



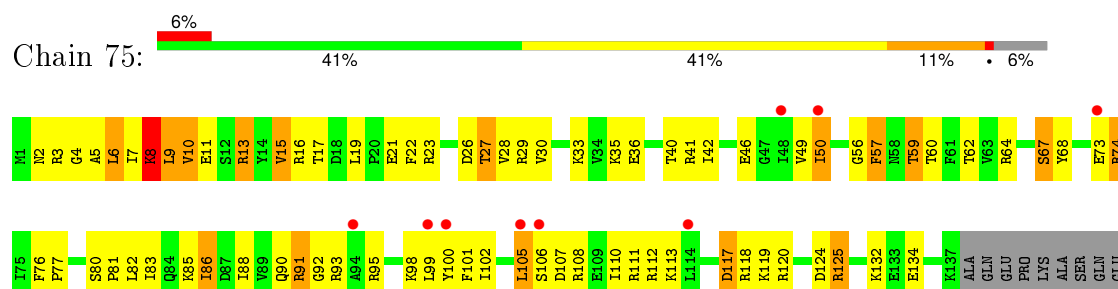
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

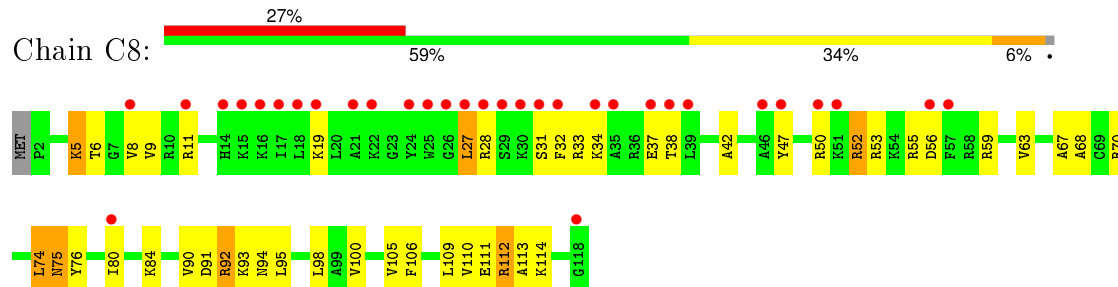


- Molecule 39: 50S ribosomal protein L19

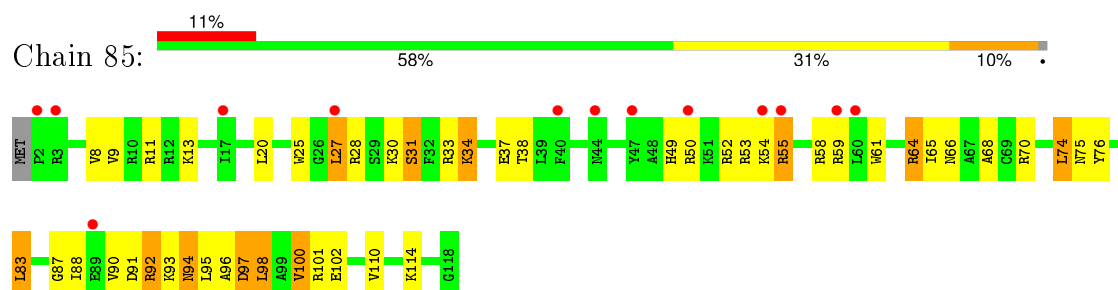




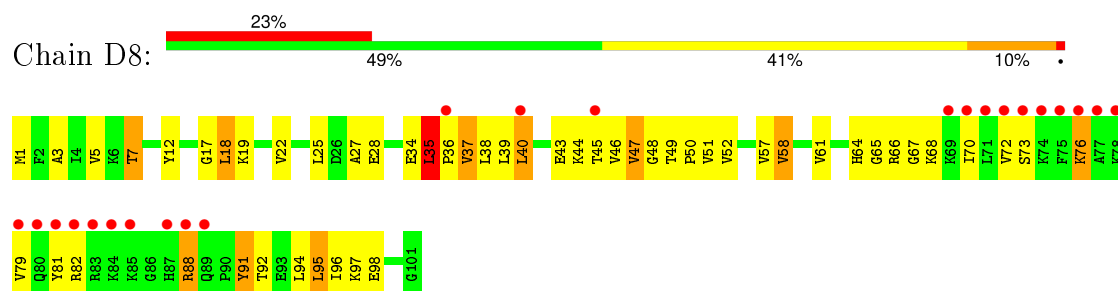
- Molecule 40: 50S ribosomal protein L20



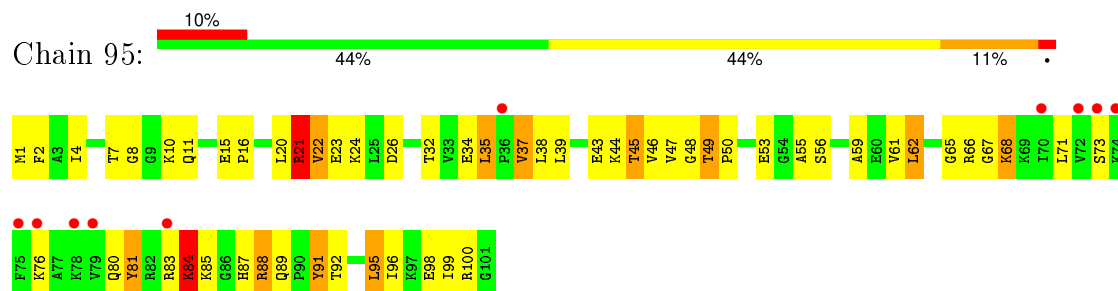
- Molecule 40: 50S ribosomal protein L20



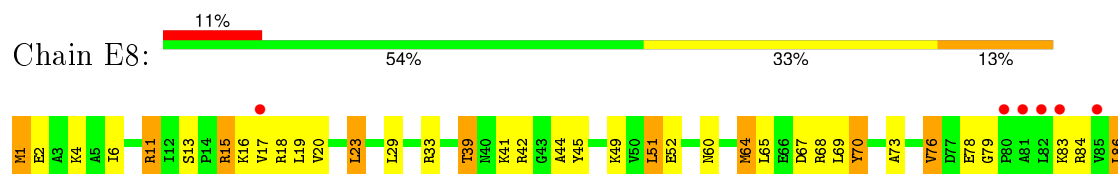
- Molecule 41: 50S ribosomal protein L21

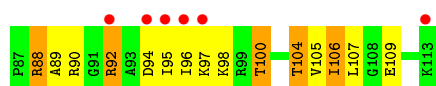


- Molecule 41: 50S ribosomal protein L21

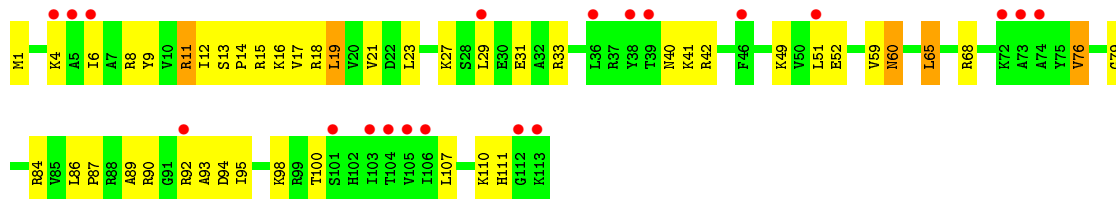


- Molecule 42: 50S ribosomal protein L22

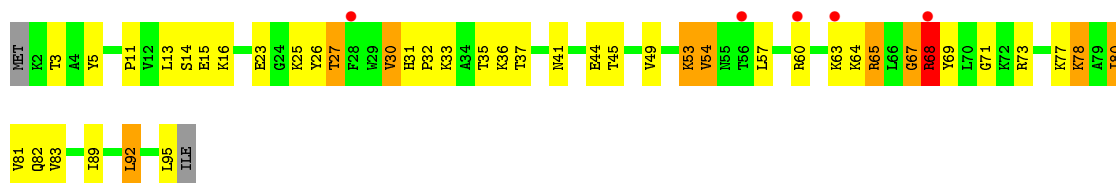




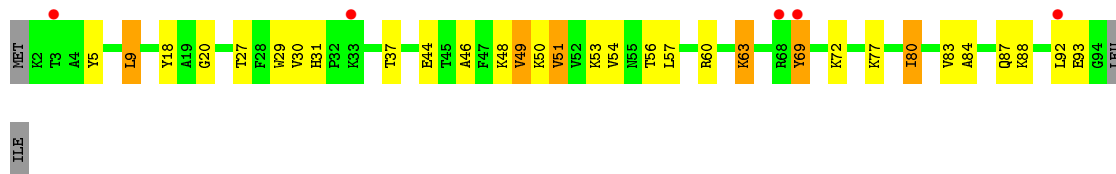
- Molecule 42: 50S ribosomal protein L22



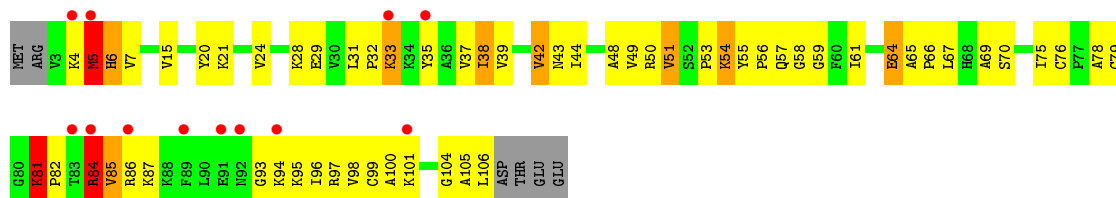
- Molecule 43: 50S ribosomal protein L23



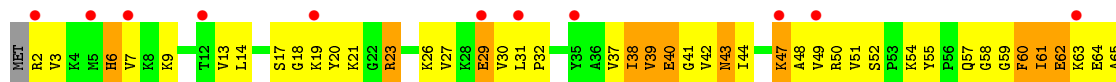
- Molecule 43: 50S ribosomal protein L23

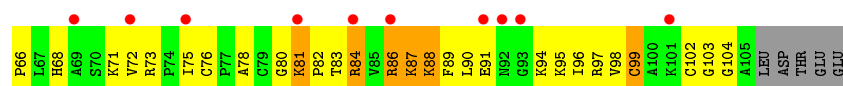


- Molecule 44: 50S ribosomal protein L24

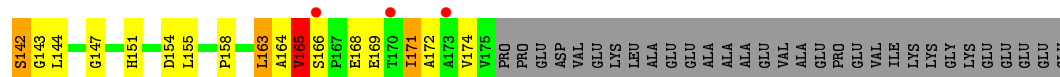
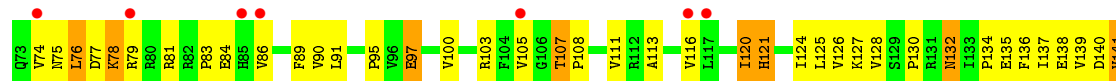
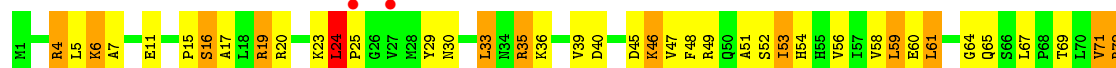
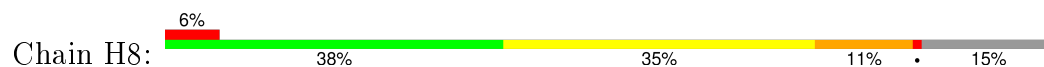


- Molecule 44: 50S ribosomal protein L24

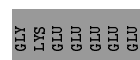
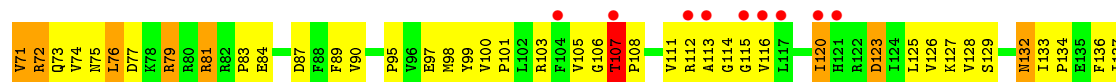




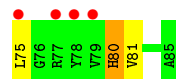
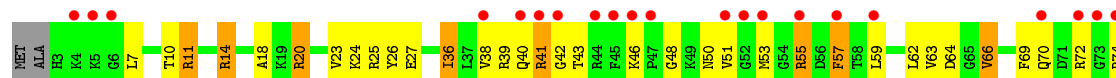
• Molecule 45: 50S ribosomal protein L25



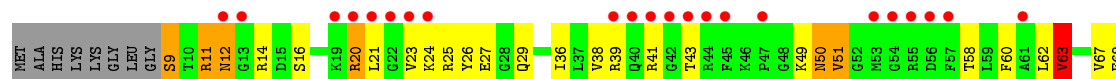
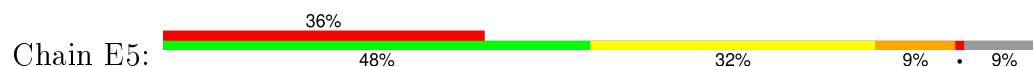
• Molecule 45: 50S ribosomal protein L25

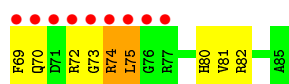


• Molecule 46: 50S ribosomal protein L27

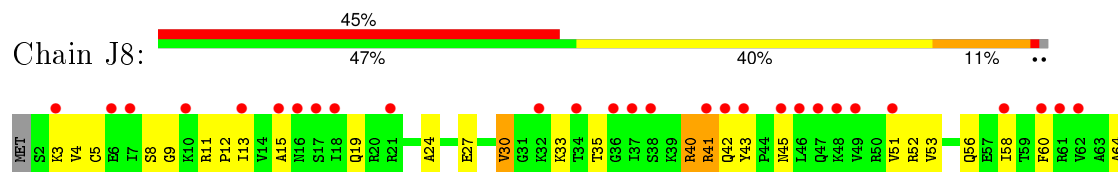


• Molecule 46: 50S ribosomal protein L27

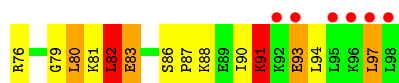
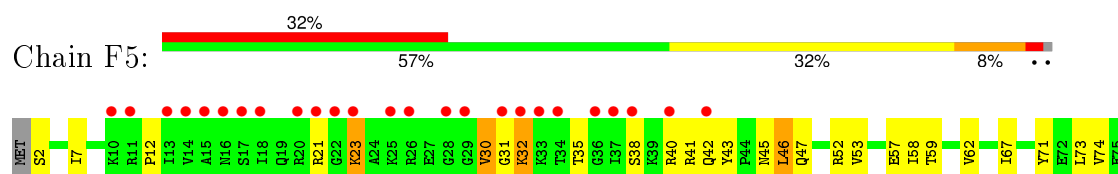




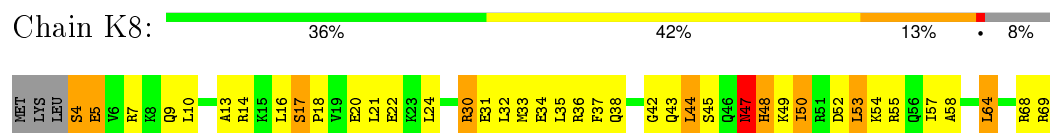
- Molecule 47: 50S ribosomal protein L28



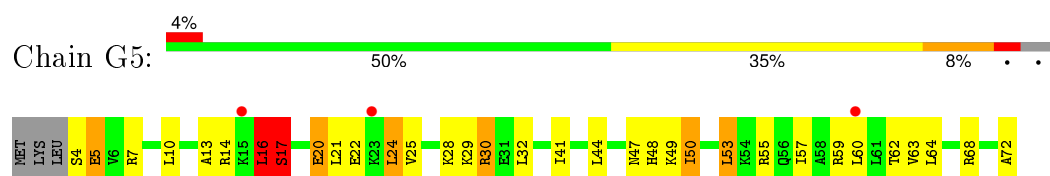
- Molecule 47: 50S ribosomal protein L28



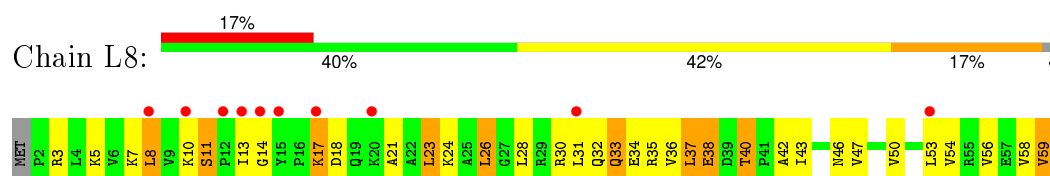
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

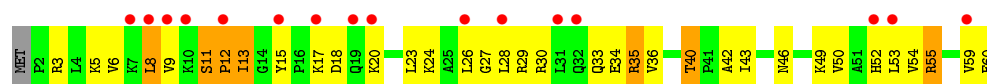


- Molecule 49: 50S ribosomal protein L30

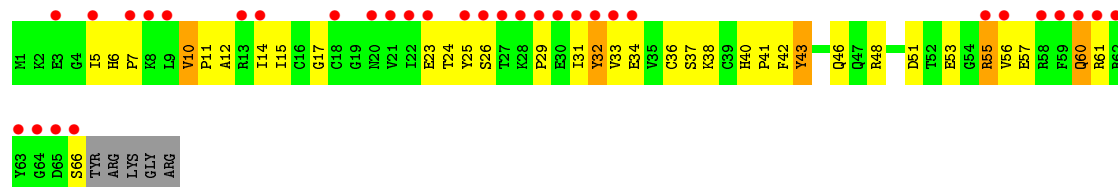


- Molecule 49: 50S ribosomal protein L30

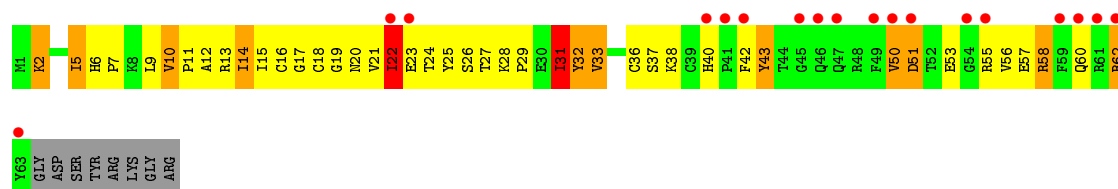




- Molecule 50: 50S ribosomal protein L31



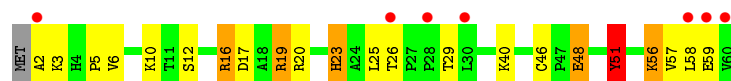
- Molecule 50: 50S ribosomal protein L31



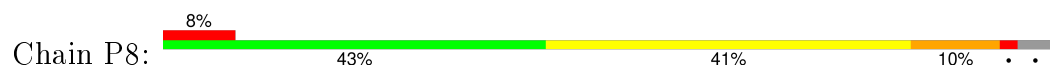
- Molecule 51: 50S ribosomal protein L32



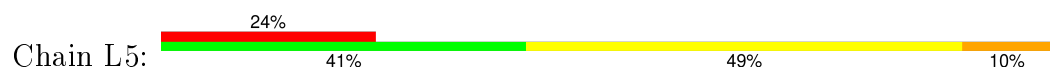
- Molecule 51: 50S ribosomal protein L32

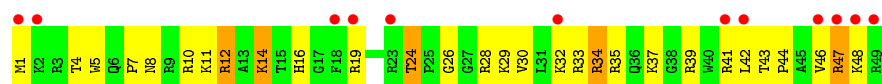


- Molecule 52: 50S ribosomal protein L34

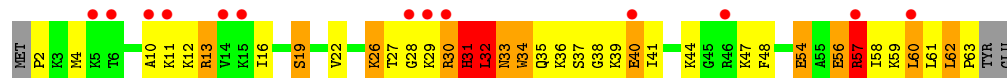


- Molecule 52: 50S ribosomal protein L34

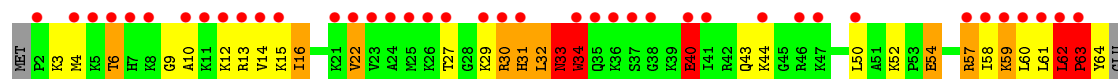




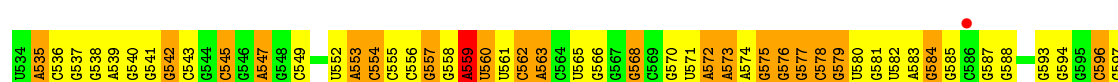
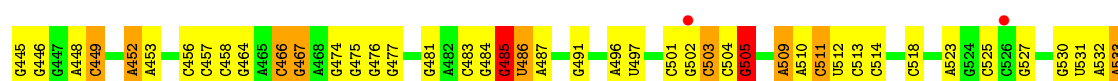
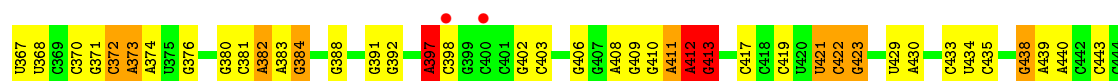
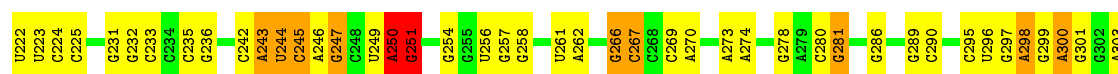
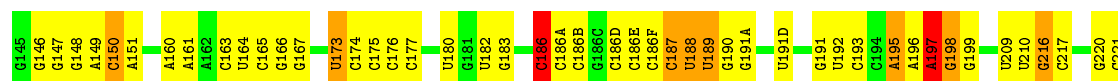
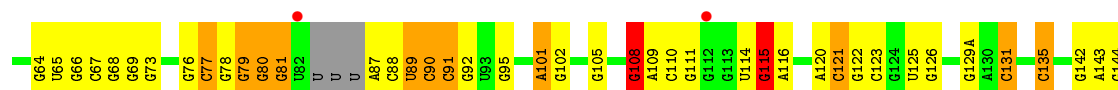
- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



- Molecule 54: 16S ribosomal RNA



A1483	U1393	C1321	C1246	A1183	G1048	A986	G924	G837	G756	C679
A1394	A1396	C1322	U1247	G1184	U1052	C989	G925	G838	U757	G684
G1487	A1397	G1323	A1250	G1185	G1053	C990	G926	U841	G758	A684
	C1397	A1324	A1251	G1187	C1054	U991	G927	U842	A759	G685
A1490	A1398	C1325	A1255	A1188	A1055	U992	G928	U843	U686	A687
G1491	C1399	C1326	G1255	C1189	U1056	C993	G929	C849	G764	G688
A1492	C1400	C1327	A1256	G1190	G1057	A994	C932	G853	G765	G689
A1493	G1401	C1328	U1257	A1123	G1058	C995	G933	G854	A766	G690
G1494	C1402	A1329	G1258	A1124	C1059	A996	G934	G855	A767	G691
	C1403	U1330	G1259	U1125	C1060	U997	G935	A768	A768	U692
G1497	G1404	G1331	C1260	U1126	C1061	C998	G936	G856	G769	G693
U1498	A1332	U1194	C1127	C1128	G1061	C998A	G937	C857	U772	
A1499	A1333	C1195	C1128	C1129	G106#	U999	G938	G858	G773	C699
A1500	G1334	U1196	U1197	A1130	U1065	C999	G939	A859	G774	A702
C1501	C1335	G1197	G1198	G1131	C1066	A1000	G940	A860	G775	G703
G1410	C1336	G1198	G1199	C1132	A1067	G1002	G941	G861	A777	
C1411	A1340	C1200	A1201	G1133	C1069	A1004	G942	C862		A706
C1412	U1341	G1202	G1203	U1136	U1070	C1008	G943	A865	G783	C707
A1413	C1342	G1203	U1204	C1137	C1071	G1009	G945	C866	G784	C708
U1414	G1343	A1205	U1205	G1138	U1072	G1010	G946	G867	G785	
G1415	U1344	G1206	G1207	G1139	U1073	G1011	G947	G868	U788	G711
G1419	C1345	A1206	C1208	C1141	G1074	U1012	U950	G869	U789	A716
C1420	A1346	G1207	C1209	G1142	C1076	G1013	G951	A872	A790	
G1421	G1347	U1281	C1282	G1143	G1077	A1014	G952	A873	G791	C719
	U1348	A1286	A1287	G1144	U1078	G953	U953	G874	A792	
G1432	A1349	A1288	A1289	C1145	G1079	A1016	G954	U793	A794	A722
G1435	C1351	U1211	C1212	C1146	A1080	G1017	U955	G878	U798	U728
U1436	G1352	U1212	G1215	C1147	G1081	C1018	U956	C879	G799	G724
G1437	G1353	A1287	C1214	U1148	G1082	G1022	U957	C883	G799	G725
G1440	C1354	A1288	G1215	C1149	U1083	G1023	A958	U884	G800	A728
G1441	A1357	G1290	C1216	U1150	G1084	G1024	U960	G885	U801	
G1442	U1358	G1291	C1217	A1151	U1085	U1025	U961	G886	A802	A729
G1443	G1359	U1292	C1218	A1152	U1086	G1026	G962	C886	G803	G730
A1446	U1360	G1293	G1221	C1153	G1087	G1027	G963	C897	U804	G731
G1447	A1361	C1297	G1222	G1154	G1088	C1028	A964	C898	C805	C732
G1448	C1362	C1298	C1223	A1157	G1089	C1028A	A965	C899	C811	A733
C1449	C1362A	A1299	G1224	C1158	A1093	G1028B	G966	G901	A815	G735
U1450	A1363	G1300	A1225	U1159	G1094	G1029	C967	A901	A816	C736
G1529	U1364	U1301	C1226	G1160	U1095	C1030	A968	G902	C817	A737
G1530	G1365	U1302	A1227	C1161	C1096	A1032	G970	G903		C738
A1531	C1366	C1303	C1228	G1162	G1098	G1032A	G971	C904		C739
G1455	C1367	G1304	C1229	A1169	G1099	G1032B	C972	U905	G821	
C1533	G1368	A1305	C1230	G1170	G1100	G1033	G973	G906	C822	G741
A	G1370	U1307	U1232	A1171	A1101	G1034	A974	A813	G823	G742
C	A1374	G1311	G1233	C1172	A1102	A1035	A975	A914	G824	U743
C	A1375	G1312	C1234	G1173	C1103	G1036	G976	A915	G825	C744
C	G1379	U1313	U1235	U1174	G1104	C1037	A977	A916	C826	C745
U		G1314	A1238	G1175	A1105	G1038	A978	G917	U827	A746
U	G1386	C1314	U1239	A1176	G1106	C1039	C979	G918	A828	C747
G	G1387	U1315	U1240	G1177	G1107	G1043	C980	A918	G829	C748
C	C1388	G1316	U1241	U1178	C1108	A1044	U981	A919	U833	C749
U	G1475	C1317	C1243	A1179	C1109	A1045	U982	U920	U834	G750
		A1318	C1244	A1180	A1110	A1046	A983	U921	U835	C754
		G1319	A1245	G1181	C1112	G1047	C984	G922	U836	G755
		C1320		G1182			C985	A923		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.00Å 451.50Å 616.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	198.79 – 3.20 254.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (198.79-3.20) 92.9 (254.63-3.20)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.188 , 0.238 0.191 , 0.238	Depositor DCC
$R_{free}$ test set	2000 reflections (0.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 83.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 953301 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	299678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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, ZN, OMG, MIA, MG, 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	0.73	3/36195 (0.0%)	1.37	334/56491 (0.6%)
2	12	0.38	0/1959	0.63	1/2642 (0.0%)
2	1E	0.42	0/1959	0.65	2/2642 (0.1%)
3	22	0.43	0/1636	0.62	0/2205
3	2E	0.45	0/1629	0.62	0/2195
4	32	0.52	0/1732	0.74	1/2318 (0.0%)
4	3E	0.58	1/1732 (0.1%)	0.74	1/2318 (0.0%)
5	42	0.53	0/1171	0.72	0/1576
5	4E	0.52	0/1171	0.71	0/1576
6	52	0.54	0/855	0.74	2/1154 (0.2%)
6	5E	0.56	0/855	0.70	1/1154 (0.1%)
7	62	0.45	0/1275	0.59	0/1709
7	6E	0.44	0/1275	0.60	0/1709
8	72	0.48	0/1135	0.68	0/1527
8	7E	0.49	0/1135	0.71	0/1527
9	82	0.45	0/1017	0.62	0/1365
9	8E	0.43	0/1028	0.61	1/1379 (0.1%)
10	1A	0.39	0/814	0.60	0/1095
10	1I	0.41	0/814	0.60	0/1095
11	2A	0.50	0/899	0.66	0/1213
11	2I	0.54	0/879	0.69	0/1187
12	3A	0.60	0/991	0.81	0/1327
12	3I	0.63	0/991	0.83	0/1327
13	4A	0.35	0/943	0.60	0/1265
13	4I	0.38	0/938	0.62	0/1258
14	5A	0.47	0/500	0.65	0/664
14	5I	0.62	2/500 (0.4%)	0.67	0/664
15	6A	0.53	0/744	0.64	0/992
15	6I	0.53	0/744	0.74	0/992
16	7A	0.54	0/721	0.73	0/970
16	7I	0.47	0/721	0.71	0/970
17	8A	0.54	0/847	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8I	0.53	0/847	0.66	0/1131
18	9A	0.50	0/595	0.68	1/790 (0.1%)
18	9I	0.51	0/595	0.68	0/790
19	AA	0.39	0/658	0.70	0/888
19	AI	0.38	0/680	0.67	0/915
20	BA	0.52	0/764	0.76	1/1007 (0.1%)
20	BI	0.42	0/764	0.70	0/1007
21	1B	0.41	0/221	0.56	0/288
21	1F	0.41	0/221	0.59	0/288
22	2K	0.72	0/1784	1.40	18/2771 (0.6%)
22	2L	0.68	0/1686	1.32	12/2618 (0.5%)
22	3K	0.46	0/1851	1.01	3/2877 (0.1%)
22	3L	0.47	0/1851	1.07	5/2877 (0.2%)
23	4K	0.92	1/269 (0.4%)	1.43	8/417 (1.9%)
23	4L	0.81	0/144	1.51	4/222 (1.8%)
24	14	0.99	89/70192 (0.1%)	1.66	1744/109580 (1.6%)
24	1H	1.08	133/70258 (0.2%)	1.78	2275/109682 (2.1%)
25	16	0.81	0/2928	1.50	41/4568 (0.9%)
25	1J	0.77	0/2928	1.47	35/4568 (0.8%)
26	71	0.29	0/1072	0.48	0/1447
26	79	0.29	0/1072	0.48	0/1447
27	11	0.83	0/2165	1.01	6/2919 (0.2%)
27	19	0.79	2/2170 (0.1%)	0.94	4/2926 (0.1%)
28	21	0.71	0/1601	0.89	1/2160 (0.0%)
28	29	0.69	0/1601	0.93	3/2160 (0.1%)
29	31	0.78	1/1620 (0.1%)	0.91	1/2194 (0.0%)
29	39	0.67	0/1662	0.87	0/2249
30	41	0.44	0/1498	0.65	1/2016 (0.0%)
30	49	0.40	0/1498	0.63	0/2016
31	51	0.60	0/1362	0.86	2/1841 (0.1%)
31	59	0.39	0/1337	0.68	0/1809
32	61	0.53	0/1151	0.78	3/1558 (0.2%)
32	69	0.51	0/1151	0.72	1/1558 (0.1%)
33	15	0.55	0/1131	0.73	0/1525
33	58	0.63	0/1131	0.82	1/1525 (0.1%)
34	25	0.74	0/942	0.82	1/1269 (0.1%)
34	68	0.70	0/942	0.79	0/1269
35	35	0.61	0/1161	0.92	2/1544 (0.1%)
35	78	0.73	0/1161	1.07	3/1544 (0.2%)
36	45	0.63	0/1142	0.88	1/1527 (0.1%)
36	88	0.78	2/1142 (0.2%)	0.97	3/1527 (0.2%)
37	55	0.73	0/973	0.99	2/1302 (0.2%)
37	98	0.61	0/981	0.82	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	65	0.57	0/891	0.85	1/1187 (0.1%)
38	A8	0.64	0/891	0.87	1/1187 (0.1%)
39	75	0.64	0/1145	0.82	0/1531
39	B8	0.65	0/1155	0.89	0/1542
40	85	0.64	1/981 (0.1%)	0.77	1/1306 (0.1%)
40	C8	0.70	0/981	0.79	0/1306
41	95	4.11	8/789 (1.0%)	1.36	6/1057 (0.6%)
41	D8	0.69	0/789	0.88	3/1057 (0.3%)
42	A5	0.70	0/910	0.85	1/1220 (0.1%)
42	E8	0.74	0/910	1.02	4/1220 (0.3%)
43	B5	0.76	0/744	0.80	0/1000
43	F8	0.83	0/752	0.94	1/1011 (0.1%)
44	C5	0.67	0/807	0.86	0/1076
44	G8	0.74	0/804	0.98	2/1073 (0.2%)
45	D5	0.43	0/1460	0.66	0/1982
45	H8	0.45	0/1427	0.71	3/1935 (0.2%)
46	E5	0.69	0/620	0.86	0/827
46	I8	0.73	0/647	0.89	0/864
47	F5	0.69	0/769	0.87	3/1022 (0.3%)
47	J8	0.73	0/769	0.93	0/1022
48	G5	0.60	0/582	0.78	0/771
48	K8	0.85	2/560 (0.4%)	0.95	0/741
49	H5	0.51	0/473	0.70	0/635
49	L8	0.61	0/473	0.79	0/635
50	I5	0.43	0/527	0.64	0/709
50	M8	0.36	0/545	0.56	0/733
51	J5	0.68	0/472	0.83	1/639 (0.2%)
51	N8	0.67	0/472	0.88	0/639
52	L5	0.75	0/437	0.95	2/575 (0.3%)
52	P8	0.89	0/417	1.17	1/550 (0.2%)
53	M5	0.99	1/515 (0.2%)	1.11	2/679 (0.3%)
53	Q8	0.90	1/502 (0.2%)	1.12	5/661 (0.8%)
54	1G	0.72	1/36189 (0.0%)	1.34	311/56482 (0.6%)
All	All	0.87	248/321112 (0.1%)	1.42	4873/480439 (1.0%)

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

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

*Continued on next page...*

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

The worst 5 of 248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	95	91	TYR	CD1-CE1	60.61	2.30	1.39
41	95	91	TYR	CD2-CE2	59.53	2.28	1.39
41	95	91	TYR	CE1-CZ	39.54	1.90	1.38
41	95	91	TYR	CE2-CZ	38.39	1.88	1.38
41	95	91	TYR	CG-CD1	31.53	1.80	1.39

The worst 5 of 4873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	95	21	ARG	CD-NE-CZ	22.50	155.09	123.60
41	95	21	ARG	NE-CZ-NH1	22.20	131.40	120.30
24	1H	676	A	C2-N3-C4	-19.76	100.72	110.60
24	1H	783	A	C2-N3-C4	-18.90	101.15	110.60
24	1H	1332	G	C2-N3-C4	-18.73	102.53	111.90

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32334	0	16320	769	0
2	12	1924	0	1975	86	0
2	1E	1924	0	1975	110	0
3	22	1612	0	1677	65	0
3	2E	1605	0	1668	66	0
4	32	1702	0	1763	97	1
4	3E	1702	0	1762	58	0
5	42	1155	0	1213	59	0
5	4E	1155	0	1213	42	0
6	52	842	0	857	26	0
6	5E	842	0	857	46	1
7	62	1256	0	1296	41	0
7	6E	1256	0	1296	44	0
8	72	1115	0	1177	32	0
8	7E	1115	0	1177	43	0
9	82	998	0	1024	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	8E	1009	0	1037	50	0
10	1A	801	0	849	36	0
10	1I	801	0	849	31	0
11	2A	884	0	904	28	0
11	2I	864	0	881	35	0
12	3A	975	0	1062	37	0
12	3I	975	0	1062	40	0
13	4A	933	0	992	56	0
13	4I	928	0	987	44	0
14	5A	491	0	529	30	0
14	5I	491	0	529	31	0
15	6A	733	0	771	26	0
15	6I	733	0	771	29	0
16	7A	705	0	725	27	0
16	7I	705	0	725	48	0
17	8A	834	0	904	32	0
17	8I	834	0	904	36	0
18	9A	590	0	662	24	0
18	9I	590	0	662	27	0
19	AA	644	0	644	48	0
19	AI	665	0	686	34	0
20	BA	762	0	861	35	0
20	BI	762	0	861	48	0
21	1B	217	0	234	13	0
21	1F	217	0	234	10	0
22	2K	1765	0	916	56	0
22	2L	1678	0	872	69	0
22	3K	1825	0	946	61	0
22	3L	1825	0	946	51	0
23	4K	239	0	121	12	0
23	4L	129	0	66	3	0
24	14	62669	0	31591	1357	0
24	1H	62729	0	31622	1439	1
25	16	2617	0	1328	59	0
25	1J	2617	0	1328	90	0
26	71	1049	0	1071	32	0
26	79	1049	0	1071	32	0
27	11	2115	0	2195	103	0
27	19	2120	0	2197	103	0
28	21	1568	0	1634	90	0
28	29	1568	0	1634	87	0
29	31	1585	0	1632	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	39	1627	0	1680	89	0
30	41	1473	0	1535	76	0
30	49	1473	0	1535	72	0
31	51	1336	0	1418	72	0
31	59	1312	0	1384	57	0
32	61	1136	0	1223	41	0
32	69	1136	0	1223	67	0
33	15	1104	0	1180	35	0
33	58	1104	0	1180	54	0
34	25	932	0	996	46	0
34	68	932	0	996	29	0
35	35	1144	0	1228	76	0
35	78	1144	0	1228	83	0
36	45	1121	0	1179	59	0
36	88	1121	0	1179	59	0
37	55	959	0	1021	44	0
37	98	967	0	1033	58	0
38	65	881	0	943	62	0
38	A8	881	0	943	34	0
39	75	1131	0	1180	69	0
39	B8	1141	0	1202	75	0
40	85	963	0	1022	48	0
40	C8	963	0	1022	36	0
41	95	778	0	852	85	0
41	D8	778	0	852	29	0
42	A5	899	0	964	34	0
42	E8	899	0	964	30	0
43	B5	730	0	780	23	0
43	F8	738	0	791	41	0
44	C5	794	0	884	70	0
44	G8	791	0	881	44	0
45	D5	1428	0	1454	96	0
45	H8	1397	0	1430	58	0
46	E5	612	0	633	38	0
46	I8	639	0	644	41	0
47	F5	762	0	848	26	0
47	J8	762	0	848	43	0
48	G5	580	0	629	28	1
48	K8	558	0	610	29	0
49	H5	468	0	518	27	0
49	L8	468	0	518	20	0
50	I5	515	0	514	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	M8	533	0	526	29	0
51	J5	458	0	480	25	0
51	N8	458	0	480	32	0
52	L5	429	0	480	30	0
52	P8	409	0	454	20	0
53	M5	507	0	576	35	0
53	Q8	495	0	567	47	0
54	1G	32329	0	16319	734	0
55	11	2	0	0	0	0
55	13	129	0	0	0	0
55	14	489	0	0	0	0
55	15	1	0	0	0	0
55	16	12	0	0	0	0
55	19	1	0	0	0	0
55	1G	147	0	0	0	0
55	1H	548	0	0	0	0
55	1J	11	0	0	0	0
55	21	1	0	0	0	0
55	25	1	0	0	0	0
55	29	5	0	0	0	0
55	2K	4	0	0	0	0
55	2L	3	0	0	0	0
55	32	1	0	0	0	0
55	39	1	0	0	0	0
55	3I	1	0	0	0	0
55	3L	2	0	0	0	0
55	42	1	0	0	0	0
55	45	1	0	0	0	0
55	49	1	0	0	0	0
55	55	3	0	0	0	0
55	5E	2	0	0	0	0
55	78	2	0	0	0	0
55	88	2	0	0	0	0
55	C5	1	0	0	0	0
55	E5	2	0	0	0	0
55	F5	1	0	0	0	0
55	I8	3	0	0	0	0
55	J8	1	0	0	0	0
55	M5	1	0	0	0	0
55	Q8	1	0	0	0	0
56	32	1	0	0	0	0
56	3E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	5A	1	0	0	0	0
56	5I	1	0	0	0	0
56	C5	1	0	0	0	0
56	G8	1	0	0	0	0
57	13	188	0	0	32	0
57	14	821	0	0	195	0
57	16	12	0	0	2	0
57	1G	156	0	0	26	0
57	1H	1038	0	0	252	0
57	1J	24	0	0	3	0
57	25	6	0	0	0	0
57	2K	6	0	0	0	0
57	2L	6	0	0	0	0
57	E5	6	0	0	0	0
57	J8	6	0	0	0	0
All	All	299678	0	200771	8223	2

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

The worst 5 of 8223 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:95:91:TYR:CD2	41:95:91:TYR:CG	1.79	1.66
41:95:91:TYR:CD1	41:95:91:TYR:CG	1.80	1.63
41:95:91:TYR:CZ	41:95:91:TYR:CE1	1.90	1.59
41:95:91:TYR:CZ	41:95:91:TYR:CE2	1.88	1.58
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.71	1.53

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

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	201 (86%)	32 (14%)	2 (1%)	21	67
2	1E	235/256 (92%)	198 (84%)	32 (14%)	5 (2%)	9	46
3	22	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	34	78
4	3E	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	19	65
5	42	149/162 (92%)	144 (97%)	5 (3%)	0	100	100
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	26	72
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	72	136/138 (99%)	129 (95%)	5 (4%)	2 (2%)	13	55
8	7E	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	82	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
9	8E	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	1A	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	1I	97/105 (92%)	83 (86%)	14 (14%)	0	100	100
11	2A	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	2I	114/129 (88%)	104 (91%)	9 (8%)	1 (1%)	21	67
12	3A	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	12	54
12	3I	123/132 (93%)	114 (93%)	9 (7%)	0	100	100
13	4A	115/126 (91%)	100 (87%)	11 (10%)	4 (4%)	4	31
13	4I	114/126 (90%)	100 (88%)	14 (12%)	0	100	100
14	5A	58/61 (95%)	50 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	6A	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	8A	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	70/88 (80%)	66 (94%)	4 (6%)	0	100	100
18	9I	70/88 (80%)	66 (94%)	3 (4%)	1 (1%)	14	57
19	AA	80/93 (86%)	59 (74%)	18 (22%)	3 (4%)	4	28
19	AI	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	16	60
20	BA	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	BI	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	1B	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	7I	131/229 (57%)	130 (99%)	1 (1%)	0	100	100
26	79	131/229 (57%)	129 (98%)	2 (2%)	0	100	100
27	11	270/276 (98%)	246 (91%)	19 (7%)	5 (2%)	10	50
27	19	271/276 (98%)	252 (93%)	16 (6%)	3 (1%)	17	62
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	34	78
28	29	203/206 (98%)	158 (78%)	38 (19%)	7 (3%)	5	31
29	31	200/210 (95%)	187 (94%)	13 (6%)	0	100	100
29	39	206/210 (98%)	176 (85%)	25 (12%)	5 (2%)	7	43
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	30	75
30	49	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	30	75
31	51	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	11	52
31	59	169/180 (94%)	133 (79%)	34 (20%)	2 (1%)	16	60
32	61	144/148 (97%)	123 (85%)	18 (12%)	3 (2%)	9	46
32	69	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	14	57
33	15	136/140 (97%)	126 (93%)	9 (7%)	1 (1%)	26	72
33	58	136/140 (97%)	115 (85%)	15 (11%)	6 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	35	148/150 (99%)	119 (80%)	24 (16%)	5 (3%)	5	31
35	78	148/150 (99%)	114 (77%)	30 (20%)	4 (3%)	6	39
36	45	139/141 (99%)	113 (81%)	23 (16%)	3 (2%)	8	45
36	88	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	6	36
37	55	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	21	67
37	98	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
38	65	109/112 (97%)	95 (87%)	12 (11%)	2 (2%)	11	51
38	A8	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	21	67
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	8	45
39	B8	135/146 (92%)	115 (85%)	20 (15%)	0	100	100
40	85	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
40	C8	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
41	95	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	5	35
41	D8	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
42	A5	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	E8	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
43	B5	91/96 (95%)	86 (94%)	4 (4%)	1 (1%)	17	62
43	F8	92/96 (96%)	85 (92%)	6 (6%)	1 (1%)	17	62
44	C5	102/110 (93%)	70 (69%)	29 (28%)	3 (3%)	6	36
44	G8	102/110 (93%)	80 (78%)	19 (19%)	3 (3%)	6	36
45	D5	177/206 (86%)	141 (80%)	31 (18%)	5 (3%)	6	37
45	H8	173/206 (84%)	141 (82%)	25 (14%)	7 (4%)	4	27
46	E5	75/85 (88%)	69 (92%)	5 (7%)	1 (1%)	15	59
46	I8	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	16	60
47	F5	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	17	62
47	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	9	46
48	G5	67/72 (93%)	57 (85%)	10 (15%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	1 (2%)	2 (3%)	5	34
49	H5	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	11	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	I5	61/71 (86%)	35 (57%)	22 (36%)	4 (7%)	1	12
50	M8	64/71 (90%)	44 (69%)	19 (30%)	1 (2%)	12	54
51	J5	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	4	31
51	N8	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	11	51
52	L5	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
52	P8	45/49 (92%)	41 (91%)	2 (4%)	2 (4%)	3	24
53	M5	61/65 (94%)	54 (88%)	4 (7%)	3 (5%)	3	22
53	Q8	60/65 (92%)	49 (82%)	7 (12%)	4 (7%)	1	12
All	All	11538/12404 (93%)	10164 (88%)	1238 (11%)	136 (1%)	16	60

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
27	11	122	ASP
33	58	22	THR
33	58	95	PRO
33	58	96	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	170 (83%)	35 (17%)	2	12
2	1E	205/220 (93%)	168 (82%)	37 (18%)	2	11
3	22	160/188 (85%)	131 (82%)	29 (18%)	2	11
3	2E	159/188 (85%)	136 (86%)	23 (14%)	4	19
4	32	180/181 (99%)	152 (84%)	28 (16%)	3	15
4	3E	180/181 (99%)	155 (86%)	25 (14%)	4	20
5	42	116/123 (94%)	96 (83%)	20 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4E	116/123 (94%)	92 (79%)	24 (21%)	1	7
6	52	90/90 (100%)	81 (90%)	9 (10%)	9	37
6	5E	90/90 (100%)	79 (88%)	11 (12%)	6	27
7	62	126/127 (99%)	110 (87%)	16 (13%)	5	25
7	6E	126/127 (99%)	111 (88%)	15 (12%)	6	28
8	72	119/119 (100%)	103 (87%)	16 (13%)	5	22
8	7E	119/119 (100%)	108 (91%)	11 (9%)	11	41
9	82	97/99 (98%)	81 (84%)	16 (16%)	3	13
9	8E	98/99 (99%)	85 (87%)	13 (13%)	5	23
10	1A	89/92 (97%)	79 (89%)	10 (11%)	7	32
10	1I	89/92 (97%)	78 (88%)	11 (12%)	6	27
11	2A	90/99 (91%)	79 (88%)	11 (12%)	6	27
11	2I	88/99 (89%)	79 (90%)	9 (10%)	9	36
12	3A	104/109 (95%)	90 (86%)	14 (14%)	5	22
12	3I	104/109 (95%)	93 (89%)	11 (11%)	8	34
13	4A	94/101 (93%)	79 (84%)	15 (16%)	3	14
13	4I	94/101 (93%)	85 (90%)	9 (10%)	10	39
14	5A	49/50 (98%)	43 (88%)	6 (12%)	6	27
14	5I	49/50 (98%)	41 (84%)	8 (16%)	3	14
15	6A	79/80 (99%)	72 (91%)	7 (9%)	12	44
15	6I	79/80 (99%)	72 (91%)	7 (9%)	12	44
16	7A	72/74 (97%)	61 (85%)	11 (15%)	3	17
16	7I	72/74 (97%)	58 (81%)	14 (19%)	2	9
17	8A	95/97 (98%)	84 (88%)	11 (12%)	7	30
17	8I	95/97 (98%)	82 (86%)	13 (14%)	4	21
18	9A	63/77 (82%)	56 (89%)	7 (11%)	8	32
18	9I	63/77 (82%)	56 (89%)	7 (11%)	8	32
19	AA	67/80 (84%)	61 (91%)	6 (9%)	12	43
19	AI	72/80 (90%)	63 (88%)	9 (12%)	6	26
20	BA	76/82 (93%)	67 (88%)	9 (12%)	6	29
20	BI	76/82 (93%)	66 (87%)	10 (13%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1B	20/22 (91%)	19 (95%)	1 (5%)	30	71
21	1F	20/22 (91%)	19 (95%)	1 (5%)	30	71
26	71	111/181 (61%)	106 (96%)	5 (4%)	34	74
26	79	111/181 (61%)	109 (98%)	2 (2%)	66	89
27	11	214/218 (98%)	174 (81%)	40 (19%)	2	10
27	19	214/218 (98%)	176 (82%)	38 (18%)	2	11
28	21	165/166 (99%)	140 (85%)	25 (15%)	3	17
28	29	165/166 (99%)	141 (86%)	24 (14%)	4	19
29	31	161/166 (97%)	133 (83%)	28 (17%)	2	12
29	39	165/166 (99%)	132 (80%)	33 (20%)	1	8
30	41	155/156 (99%)	132 (85%)	23 (15%)	4	18
30	49	155/156 (99%)	135 (87%)	20 (13%)	5	24
31	51	145/148 (98%)	117 (81%)	28 (19%)	2	9
31	59	142/148 (96%)	118 (83%)	24 (17%)	2	13
32	61	122/124 (98%)	105 (86%)	17 (14%)	4	20
32	69	122/124 (98%)	91 (75%)	31 (25%)	1	2
33	15	117/119 (98%)	96 (82%)	21 (18%)	2	11
33	58	117/119 (98%)	94 (80%)	23 (20%)	1	8
34	25	100/100 (100%)	79 (79%)	21 (21%)	1	7
34	68	100/100 (100%)	87 (87%)	13 (13%)	5	24
35	35	116/116 (100%)	85 (73%)	31 (27%)	0	2
35	78	116/116 (100%)	80 (69%)	36 (31%)	0	1
36	45	111/111 (100%)	96 (86%)	15 (14%)	5	22
36	88	111/111 (100%)	93 (84%)	18 (16%)	3	14
37	55	100/101 (99%)	80 (80%)	20 (20%)	1	8
37	98	101/101 (100%)	85 (84%)	16 (16%)	3	15
38	65	87/88 (99%)	68 (78%)	19 (22%)	1	6
38	A8	87/88 (99%)	65 (75%)	22 (25%)	1	2
39	75	117/127 (92%)	93 (80%)	24 (20%)	1	7
39	B8	120/127 (94%)	92 (77%)	28 (23%)	1	4
40	85	93/94 (99%)	78 (84%)	15 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	C8	93/94 (99%)	80 (86%)	13 (14%)	4	20
41	95	82/82 (100%)	63 (77%)	19 (23%)	1	4
41	D8	82/82 (100%)	58 (71%)	24 (29%)	0	1
42	A5	92/92 (100%)	78 (85%)	14 (15%)	3	17
42	E8	92/92 (100%)	71 (77%)	21 (23%)	1	5
43	B5	74/78 (95%)	63 (85%)	11 (15%)	4	17
43	F8	75/78 (96%)	61 (81%)	14 (19%)	2	10
44	C5	85/91 (93%)	62 (73%)	23 (27%)	0	2
44	G8	85/91 (93%)	65 (76%)	20 (24%)	1	4
45	D5	158/179 (88%)	133 (84%)	25 (16%)	3	15
45	H8	154/179 (86%)	118 (77%)	36 (23%)	1	4
46	E5	62/67 (92%)	50 (81%)	12 (19%)	2	9
46	I8	61/67 (91%)	50 (82%)	11 (18%)	2	11
47	F5	82/83 (99%)	66 (80%)	16 (20%)	2	9
47	J8	82/83 (99%)	65 (79%)	17 (21%)	1	7
48	G5	64/67 (96%)	53 (83%)	11 (17%)	2	12
48	K8	62/67 (92%)	46 (74%)	16 (26%)	0	2
49	H5	51/52 (98%)	39 (76%)	12 (24%)	1	4
49	L8	51/52 (98%)	35 (69%)	16 (31%)	0	1
50	I5	57/63 (90%)	42 (74%)	15 (26%)	0	2
50	M8	59/63 (94%)	49 (83%)	10 (17%)	2	13
51	J5	51/52 (98%)	41 (80%)	10 (20%)	1	9
51	N8	51/52 (98%)	38 (74%)	13 (26%)	1	2
52	L5	42/42 (100%)	34 (81%)	8 (19%)	2	10
52	P8	40/42 (95%)	34 (85%)	6 (15%)	3	17
53	M5	53/55 (96%)	41 (77%)	12 (23%)	1	5
53	Q8	52/55 (94%)	39 (75%)	13 (25%)	1	2
All	All	9717/10256 (95%)	8094 (83%)	1623 (17%)	3	13

5 of 1623 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	J8	76	ARG

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Mol	Chain	Res	Type
4	32	191	ARG
44	C5	98	VAL
48	K8	44	LEU
2	12	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
39	B8	79	HIS
45	H8	54	HIS
48	G5	38	GLN
45	H8	32	HIS
48	K8	47	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	326 (21%)	24 (1%)
22	2K	78/85 (91%)	28 (35%)	5 (6%)
22	2L	73/85 (85%)	25 (34%)	7 (9%)
22	3K	82/85 (96%)	22 (26%)	3 (3%)
22	3L	82/85 (96%)	22 (26%)	3 (3%)
23	4K	11/27 (40%)	3 (27%)	1 (9%)
23	4L	5/27 (18%)	2 (40%)	0
24	14	2907/2917 (99%)	652 (22%)	38 (1%)
24	1H	2910/2917 (99%)	677 (23%)	45 (1%)
25	16	121/122 (99%)	26 (21%)	0
25	1J	121/122 (99%)	29 (23%)	1 (0%)
54	1G	1503/1522 (98%)	322 (21%)	33 (2%)
All	All	9389/9516 (98%)	2134 (22%)	160 (1%)

5 of 2134 RNA backbone outliers are listed below:

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

5 of 160 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	1H	2439	A
54	1G	429	U
24	14	1912	A
24	1H	2481	G
54	1G	89	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	OMG	2K	17	22	18,26,27	5.64	6 (33%)	21,38,41	6.11	7 (33%)
22	QUO	2K	35	22,23	27,35,36	5.78	9 (33%)	30,52,55	4.03	9 (30%)
22	MIA	2K	38	22	22,31,32	1.55	2 (9%)	26,44,47	3.85	3 (11%)
22	PSU	2K	40	22	15,21,22	3.54	5 (33%)	16,30,33	2.00	2 (12%)
22	5MU	2K	63	22	13,22,23	1.58	2 (15%)	16,32,35	1.24	1 (6%)
22	PSU	2K	64	22	15,21,22	3.80	5 (33%)	16,30,33	2.00	4 (25%)
22	4SU	2K	8	22	12,21,22	3.18	2 (16%)	15,30,33	0.88	1 (6%)
22	OMG	2L	17	22	18,26,27	5.59	6 (33%)	21,38,41	6.18	6 (28%)
22	QUO	2L	35	22,23	27,35,36	5.88	9 (33%)	30,52,55	4.32	10 (33%)
22	MIA	2L	38	22	22,31,32	1.23	1 (4%)	26,44,47	3.02	5 (19%)
22	PSU	2L	40	22	15,21,22	3.55	4 (26%)	16,30,33	2.09	3 (18%)
22	5MU	2L	63	22	13,22,23	1.71	2 (15%)	16,32,35	1.20	1 (6%)
22	PSU	2L	64	22	15,21,22	4.07	5 (33%)	16,30,33	2.12	4 (25%)
22	4SU	2L	8	22	12,21,22	3.17	2 (16%)	15,30,33	1.23	1 (6%)
22	OMG	3K	17	22	18,26,27	5.56	6 (33%)	21,38,41	5.84	7 (33%)
22	QUO	3K	35	22	27,35,36	5.82	9 (33%)	30,52,55	3.98	11 (36%)
22	MIA	3K	38	22	22,31,32	1.56	2 (9%)	26,44,47	2.36	5 (19%)
22	PSU	3K	40	22	15,21,22	3.71	4 (26%)	16,30,33	2.02	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	5MU	3K	63	22	13,22,23	1.69	2 (15%)	16,32,35	1.57	1 (6%)
22	PSU	3K	64	22	15,21,22	3.92	5 (33%)	16,30,33	2.01	5 (31%)
22	4SU	3K	8	22	12,21,22	3.06	2 (16%)	15,30,33	0.63	0
22	OMG	3L	17	22	18,26,27	5.71	6 (33%)	21,38,41	6.07	9 (42%)
22	QUO	3L	35	22	27,35,36	5.89	9 (33%)	30,52,55	3.92	9 (30%)
22	MIA	3L	38	22	22,31,32	1.25	1 (4%)	26,44,47	2.82	5 (19%)
22	PSU	3L	40	22	15,21,22	3.80	5 (33%)	16,30,33	2.07	2 (12%)
22	5MU	3L	63	22	13,22,23	1.66	2 (15%)	16,32,35	1.59	1 (6%)
22	PSU	3L	64	22	15,21,22	3.97	5 (33%)	16,30,33	2.46	4 (25%)
22	4SU	3L	8	55,22	12,21,22	3.35	2 (16%)	15,30,33	1.12	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	2K	17	22	-	0/5/27/28	0/3/3/3
22	QUO	2K	35	22,23	-	0/6/43/44	0/4/4/4
22	MIA	2K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	2K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	2K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	2K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	2K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	2L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	2L	35	22,23	-	0/6/43/44	0/4/4/4
22	MIA	2L	38	22	-	0/11/33/34	0/3/3/3
22	PSU	2L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	2L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	2L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	2L	8	22	-	0/3/25/26	0/2/2/2
22	OMG	3K	17	22	-	0/5/27/28	0/3/3/3
22	QUO	3K	35	22	-	0/6/43/44	0/4/4/4
22	MIA	3K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	3L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	3L	35	22	-	0/6/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	3L	38	22	-	0/11/33/34	0/3/3/3
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3L	8	55,22	-	0/3/25/26	0/2/2/2

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2L	17	OMG	C8-N7	-13.62	1.08	1.34
22	2K	17	OMG	C8-N7	-13.44	1.08	1.34
22	3L	17	OMG	C8-N7	-13.40	1.08	1.34
22	3K	17	OMG	C8-N7	-13.23	1.09	1.34
22	2L	64	PSU	C5-C1'	-13.09	1.40	1.52

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2L	35	QUO	C8-N9-C1'	-14.88	113.83	125.45
22	2K	35	QUO	C8-N9-C1'	-13.98	114.53	125.45
22	3K	35	QUO	C1'-N9-C4	-13.78	111.42	126.81
22	3K	17	OMG	C6-C5-C4	-12.45	106.64	120.86
22	2L	17	OMG	C6-C5-C4	-12.08	107.06	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 58 short contacts:

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

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	1501/1522 (98%)	0.17	32 (2%) 67 52	77, 129, 208, 407	0
2	12	237/256 (92%)	0.43	31 (13%) 5 3	137, 175, 213, 240	0
2	1E	237/256 (92%)	0.70	39 (16%) 2 1	131, 168, 201, 234	0
3	22	206/239 (86%)	0.52	28 (13%) 4 2	135, 156, 189, 209	0
3	2E	205/239 (85%)	0.50	22 (10%) 8 4	122, 142, 197, 207	0
4	32	208/209 (99%)	1.30	58 (27%) 1 0	108, 130, 156, 169	0
4	3E	208/209 (99%)	1.37	53 (25%) 1 0	104, 129, 155, 182	0
5	42	151/162 (93%)	0.43	17 (11%) 7 4	107, 128, 153, 194	0
5	4E	151/162 (93%)	0.57	16 (10%) 8 4	102, 125, 153, 204	0
6	52	101/101 (100%)	0.01	1 (0%) 84 75	101, 120, 138, 153	0
6	5E	101/101 (100%)	0.25	3 (2%) 54 39	105, 129, 146, 163	0
7	62	155/156 (99%)	1.14	33 (21%) 1 1	128, 144, 162, 171	0
7	6E	155/156 (99%)	0.74	27 (17%) 2 1	123, 149, 172, 184	0
8	72	138/138 (100%)	0.75	25 (18%) 2 1	111, 132, 143, 170	0
8	7E	138/138 (100%)	1.26	41 (29%) 1 0	115, 134, 145, 157	0
9	82	126/128 (98%)	2.64	69 (54%) 0 0	124, 170, 197, 213	0
9	8E	127/128 (99%)	1.37	46 (36%) 0 0	119, 163, 179, 191	0
10	1A	99/105 (94%)	1.47	30 (30%) 1 0	135, 170, 191, 206	0
10	1I	99/105 (94%)	0.97	23 (23%) 1 1	121, 166, 195, 209	0
11	2A	119/129 (92%)	0.96	11 (9%) 11 6	105, 125, 157, 256	0
11	2I	116/129 (89%)	0.42	8 (6%) 20 11	93, 126, 153, 203	0
12	3A	125/132 (94%)	1.35	39 (31%) 1 0	96, 114, 144, 188	0
12	3I	125/132 (94%)	1.08	29 (23%) 1 1	91, 104, 136, 239	0
13	4A	117/126 (92%)	1.18	30 (25%) 1 0	138, 174, 197, 229	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4I	116/126 (92%)	0.92	26 (22%) 1 1	127, 173, 195, 208	0
14	5A	60/61 (98%)	3.07	38 (63%) 0 0	145, 163, 185, 186	0
14	5I	60/61 (98%)	2.60	38 (63%) 0 0	127, 137, 167, 186	0
15	6A	88/89 (98%)	1.00	23 (26%) 1 0	100, 128, 146, 152	0
15	6I	88/89 (98%)	0.45	7 (7%) 15 8	103, 127, 147, 154	0
16	7A	84/88 (95%)	0.75	15 (17%) 2 1	108, 121, 141, 189	0
16	7I	84/88 (95%)	1.38	29 (34%) 0 0	119, 136, 162, 196	0
17	8A	100/105 (95%)	1.22	24 (24%) 1 1	104, 121, 140, 197	0
17	8I	100/105 (95%)	0.83	14 (14%) 4 2	112, 132, 146, 150	0
18	9A	72/88 (81%)	0.33	1 (1%) 78 65	107, 127, 185, 223	0
18	9I	72/88 (81%)	0.22	4 (5%) 28 16	111, 130, 164, 208	0
19	AA	82/93 (88%)	2.45	46 (56%) 0 0	152, 196, 219, 232	0
19	AI	83/93 (89%)	1.63	30 (36%) 0 0	150, 176, 207, 222	0
20	BA	99/106 (93%)	1.54	38 (38%) 0 0	96, 125, 161, 175	0
20	BI	99/106 (93%)	1.92	43 (43%) 0 0	127, 147, 191, 205	0
21	1B	25/27 (92%)	3.48	19 (76%) 0 0	135, 158, 187, 196	0
21	1F	25/27 (92%)	3.04	15 (60%) 0 0	139, 156, 182, 190	0
22	2K	75/85 (88%)	0.28	8 (10%) 8 4	95, 145, 276, 308	0
22	2L	71/85 (83%)	-0.03	4 (5%) 28 16	95, 146, 228, 250	0
22	3K	78/85 (91%)	-0.40	0 100 100	95, 199, 288, 312	0
22	3L	78/85 (91%)	-0.39	2 (2%) 59 45	93, 213, 284, 309	0
23	4K	11/27 (40%)	0.97	2 (18%) 2 1	105, 139, 160, 164	0
23	4L	6/27 (22%)	1.90	3 (50%) 0 0	116, 126, 146, 163	0
24	14	2909/2917 (99%)	0.27	59 (2%) 68 54	65, 99, 266, 424	0
24	1H	2912/2917 (99%)	0.29	36 (1%) 81 69	57, 92, 251, 431	0
25	16	122/122 (100%)	-0.19	0 100 100	96, 125, 153, 258	0
25	1J	122/122 (100%)	-0.07	2 (1%) 74 62	102, 138, 160, 226	0
26	71	135/229 (58%)	1.45	35 (25%) 1 0	152, 213, 248, 256	0
26	79	135/229 (58%)	1.19	38 (28%) 1 0	159, 237, 261, 265	0
27	11	272/276 (98%)	0.64	16 (5%) 26 14	60, 82, 103, 122	0
27	19	273/276 (98%)	0.86	39 (14%) 4 2	64, 87, 104, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	21	205/206 (99%)	1.06	42 (20%) 1 1	68, 105, 159, 229	0
28	29	205/206 (99%)	1.20	53 (25%) 1 0	71, 102, 169, 251	0
29	31	202/210 (96%)	0.82	23 (11%) 7 4	61, 95, 137, 152	0
29	39	208/210 (99%)	0.80	24 (11%) 6 4	71, 113, 184, 198	0
30	41	181/182 (99%)	0.60	24 (13%) 4 2	127, 159, 197, 218	0
30	49	181/182 (99%)	1.01	39 (21%) 1 1	142, 165, 197, 213	0
31	51	174/180 (96%)	0.05	2 (1%) 82 72	98, 122, 145, 174	0
31	59	171/180 (95%)	1.35	55 (32%) 1 0	148, 205, 246, 335	0
32	61	146/148 (98%)	0.01	4 (2%) 58 44	99, 136, 162, 176	0
32	69	146/148 (98%)	0.01	4 (2%) 58 44	100, 143, 171, 191	0
33	15	138/140 (98%)	1.15	35 (25%) 1 0	86, 115, 153, 196	0
33	58	138/140 (98%)	0.88	18 (13%) 5 3	86, 108, 153, 174	0
34	25	122/122 (100%)	0.96	22 (18%) 2 1	77, 98, 113, 122	0
34	68	122/122 (100%)	0.48	4 (3%) 50 35	73, 96, 115, 134	0
35	35	150/150 (100%)	1.00	31 (20%) 1 1	74, 119, 159, 213	0
35	78	150/150 (100%)	0.72	16 (10%) 8 4	65, 101, 126, 244	0
36	45	141/141 (100%)	1.47	48 (34%) 0 0	88, 117, 144, 179	0
36	88	141/141 (100%)	0.92	22 (15%) 3 2	78, 107, 139, 170	0
37	55	117/118 (99%)	0.66	7 (5%) 25 14	74, 94, 109, 130	0
37	98	118/118 (100%)	0.59	9 (7%) 17 9	79, 100, 119, 136	0
38	65	111/112 (99%)	1.37	36 (32%) 1 0	109, 130, 159, 180	0
38	A8	111/112 (99%)	1.19	32 (28%) 1 0	102, 123, 157, 203	0
39	75	137/146 (93%)	0.46	9 (6%) 22 12	88, 105, 157, 218	0
39	B8	137/146 (93%)	0.58	11 (8%) 15 8	92, 113, 171, 204	0
40	85	117/118 (99%)	0.78	13 (11%) 7 4	77, 109, 146, 183	0
40	C8	117/118 (99%)	1.27	32 (27%) 1 0	66, 97, 138, 182	0
41	95	101/101 (100%)	0.40	10 (9%) 9 5	80, 136, 158, 200	0
41	D8	101/101 (100%)	1.03	23 (22%) 1 1	71, 118, 159, 234	0
42	A5	113/113 (100%)	1.28	20 (17%) 2 1	74, 89, 125, 209	0
42	E8	113/113 (100%)	0.74	12 (10%) 8 4	74, 89, 121, 227	0
43	B5	93/96 (96%)	0.48	5 (5%) 29 17	86, 97, 119, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	F8	94/96 (97%)	0.45	5 (5%) 30 17	68, 87, 111, 124	0
44	C5	104/110 (94%)	1.06	21 (20%) 1 1	102, 136, 209, 232	0
44	G8	104/110 (94%)	0.65	12 (11%) 6 4	85, 108, 158, 205	0
45	D5	179/206 (86%)	0.92	34 (18%) 2 1	121, 163, 275, 332	0
45	H8	175/206 (84%)	0.23	12 (6%) 20 11	111, 157, 273, 304	0
46	E5	77/85 (90%)	1.67	31 (40%) 0 0	86, 102, 123, 174	0
46	I8	83/85 (97%)	1.31	25 (30%) 1 0	83, 99, 122, 165	0
47	F5	97/98 (98%)	1.54	31 (31%) 1 0	76, 96, 155, 197	0
47	J8	97/98 (98%)	2.26	44 (45%) 0 0	70, 93, 171, 227	0
48	G5	69/72 (95%)	0.52	3 (4%) 39 25	99, 124, 152, 184	0
48	K8	66/72 (91%)	0.19	0 100 100	74, 95, 120, 165	0
49	H5	59/60 (98%)	1.38	16 (27%) 1 0	91, 112, 169, 182	0
49	L8	59/60 (98%)	0.87	10 (16%) 2 1	87, 103, 149, 177	0
50	I5	63/71 (88%)	1.61	18 (28%) 1 0	165, 225, 254, 292	0
50	M8	66/71 (92%)	2.51	33 (50%) 0 0	156, 231, 273, 282	0
51	J5	59/60 (98%)	0.82	7 (11%) 6 3	71, 96, 206, 229	0
51	N8	59/60 (98%)	0.92	6 (10%) 9 5	64, 101, 224, 243	0
52	L5	49/49 (100%)	1.50	12 (24%) 1 1	69, 74, 108, 147	0
52	P8	47/49 (95%)	0.97	4 (8%) 13 7	60, 66, 88, 140	0
53	M5	63/65 (96%)	2.24	40 (63%) 0 0	82, 96, 122, 134	0
53	Q8	62/65 (95%)	1.29	13 (20%) 1 1	77, 92, 120, 133	0
54	1G	1504/1522 (98%)	0.21	47 (3%) 52 38	83, 130, 201, 419	0
All	All	21123/21920 (96%)	0.64	2474 (11%) 6 4	57, 120, 217, 431	0

The worst 5 of 2474 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2A	129	SER	31.4
50	M8	66	SER	24.1
11	2A	128	ALA	21.5
26	71	1	PRO	20.6
19	AI	2	PRO	19.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	PSU	3K	64	20/21	0.81	0.12	-	175,186,200,205	0
22	PSU	2K	64	20/21	0.90	0.11	-	139,143,148,152	0
22	5MU	2L	63	21/22	0.90	0.16	-	144,157,165,169	0
22	OMG	2K	17	24/25	0.87	0.23	-	150,155,165,169	0
22	MIA	2L	38	29/30	0.96	0.30	-	112,124,132,146	0
22	MIA	3L	38	29/30	0.94	0.30	-	131,140,149,159	0
22	4SU	3L	8	20/21	0.77	0.19	-	193,208,220,222	0
22	OMG	3L	17	24/25	0.82	0.29	-	201,218,239,245	0
22	4SU	2L	8	20/21	0.90	0.12	-	142,153,161,169	0
22	QUO	2K	35	32/33	0.96	0.29	-	103,113,118,124	9
22	PSU	3L	40	20/21	0.93	0.18	-	132,140,144,144	0
22	PSU	3K	40	20/21	0.93	0.16	-	132,136,141,143	0
22	PSU	2L	40	20/21	0.95	0.29	-	108,120,128,130	0
22	4SU	3K	8	20/21	0.84	0.13	-	182,197,218,229	0
22	OMG	2L	17	24/25	0.81	0.17	-	161,167,175,176	0
22	5MU	3K	63	21/22	0.91	0.09	-	168,182,188,191	0
22	4SU	2K	8	20/21	0.91	0.15	-	139,144,148,151	0
22	PSU	3L	64	20/21	0.77	0.24	-	167,198,215,220	0
22	PSU	2K	40	20/21	0.95	0.20	-	96,112,117,120	0
22	QUO	3K	35	32/33	0.90	0.32	-	131,138,151,152	0
22	QUO	2L	35	32/33	0.94	0.47	-	111,120,135,136	8
22	PSU	2L	64	20/21	0.85	0.19	-	147,156,162,165	0
22	5MU	2K	63	21/22	0.93	0.13	-	136,142,148,150	0
22	MIA	2K	38	29/30	0.95	0.27	-	101,114,121,126	0
22	OMG	3K	17	24/25	0.86	0.17	-	201,213,227,235	0
22	MIA	3K	38	29/30	0.93	0.21	-	128,138,144,146	0
22	5MU	3L	63	21/22	0.84	0.20	-	164,182,191,194	0
22	QUO	3L	35	32/33	0.91	0.35	-	131,137,152,158	0

## 6.3 Carbohydrates [i](#)

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
55	MG	1H	3031	1/1	0.86	0.62	22.51	73,73,73,73	0
55	MG	1H	3059	1/1	0.97	0.48	19.89	90,90,90,90	0
55	MG	14	3174	1/1	0.92	0.60	14.75	85,85,85,85	0
55	MG	14	3141	1/1	0.96	0.50	14.13	64,64,64,64	0
55	MG	14	3280	1/1	0.95	0.59	13.65	79,79,79,79	0
55	MG	1H	3154	1/1	0.91	0.35	12.44	88,88,88,88	0
55	MG	1H	3108	1/1	0.95	0.36	12.34	79,79,79,79	0
55	MG	14	3256	1/1	0.88	0.41	12.21	96,96,96,96	0
55	MG	1H	3116	1/1	0.95	0.41	12.21	92,92,92,92	0
55	MG	1H	3063	1/1	0.97	0.41	11.64	76,76,76,76	0
55	MG	1H	3342	1/1	0.70	0.68	10.61	87,87,87,87	0
55	MG	14	3154	1/1	0.96	0.42	10.21	102,102,102,102	0
55	MG	13	1662	1/1	0.93	0.33	9.09	85,85,85,85	0
55	MG	1H	3047	1/1	0.98	0.38	8.89	84,84,84,84	0
55	MG	1H	3131	1/1	0.54	0.50	8.70	96,96,96,96	0
55	MG	14	3243	1/1	0.98	0.33	8.60	89,89,89,89	0
55	MG	13	1681	1/1	0.80	0.81	8.22	117,117,117,117	0
55	MG	1G	1719	1/1	0.72	0.36	8.00	118,118,118,118	0
55	MG	1H	3106	1/1	0.91	0.45	7.97	81,81,81,81	0
55	MG	1G	1700	1/1	0.76	0.22	7.39	99,99,99,99	0
55	MG	1H	3130	1/1	0.95	0.36	7.33	91,91,91,91	0
55	MG	1H	3235	1/1	0.89	0.26	7.20	107,107,107,107	0
55	MG	13	1692	1/1	0.81	0.39	7.11	101,101,101,101	0
55	MG	1G	1616	1/1	0.95	0.25	6.04	85,85,85,85	0
55	MG	14	3265	1/1	0.74	0.37	5.94	85,85,85,85	0
55	MG	1H	3073	1/1	0.84	0.42	5.45	71,71,71,71	0
55	MG	14	3201	1/1	0.59	0.34	5.42	84,84,84,84	0
55	MG	42	201	1/1	0.78	0.34	5.37	103,103,103,103	0
55	MG	29	305	1/1	0.83	0.99	5.11	86,86,86,86	0
55	MG	13	1616	1/1	0.63	0.27	5.08	133,133,133,133	0
55	MG	14	3283	1/1	0.94	0.40	4.94	81,81,81,81	0
55	MG	1G	1642	1/1	0.97	0.28	4.69	117,117,117,117	0
55	MG	1H	3332	1/1	0.77	0.70	4.64	101,101,101,101	0
55	MG	1H	3027	1/1	0.93	0.24	4.47	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3155	1/1	0.70	0.36	4.36	92,92,92,92	0
55	MG	14	3024	1/1	0.97	0.23	4.24	81,81,81,81	0
55	MG	1G	1685	1/1	0.97	0.21	4.20	83,83,83,83	0
55	MG	14	3266	1/1	0.86	0.20	4.11	101,101,101,101	0
55	MG	14	3021	1/1	0.93	0.42	4.08	87,87,87,87	0
55	MG	13	1629	1/1	0.99	0.27	4.03	88,88,88,88	0
55	MG	1H	3334	1/1	0.79	0.32	4.00	88,88,88,88	0
55	MG	14	3146	1/1	0.73	0.40	3.86	81,81,81,81	0
55	MG	1J	206	1/1	0.78	0.35	3.85	129,129,129,129	0
55	MG	1G	1701	1/1	0.84	0.41	3.80	106,106,106,106	0
55	MG	1H	3119	1/1	0.92	0.24	3.60	92,92,92,92	0
55	MG	1H	3337	1/1	0.94	0.40	3.52	87,87,87,87	0
55	MG	14	3223	1/1	0.80	0.23	3.31	97,97,97,97	0
55	MG	14	3047	1/1	0.97	0.26	3.04	78,78,78,78	0
55	MG	1H	3368	1/1	0.94	0.28	2.96	64,64,64,64	0
55	MG	1G	1687	1/1	0.97	0.23	2.92	120,120,120,120	0
55	MG	1H	3051	1/1	0.72	0.42	2.90	76,76,76,76	0
55	MG	14	3236	1/1	0.88	0.21	2.88	113,113,113,113	0
55	MG	14	3110	1/1	0.97	0.22	2.82	95,95,95,95	0
55	MG	15	201	1/1	0.97	0.47	2.78	110,110,110,110	0
55	MG	1H	3361	1/1	0.82	0.35	2.71	103,103,103,103	0
55	MG	14	3479	1/1	0.84	0.32	2.67	108,108,108,108	0
55	MG	13	1619	1/1	0.52	0.21	2.63	81,81,81,81	0
55	MG	1H	3395	1/1	0.94	0.40	2.59	107,107,107,107	0
55	MG	29	303	1/1	0.63	0.74	2.51	77,77,77,77	0
55	MG	14	3284	1/1	0.83	0.39	2.47	83,83,83,83	0
55	MG	1H	3041	1/1	0.95	0.24	2.30	68,68,68,68	0
55	MG	1G	1653	1/1	0.70	0.23	2.29	90,90,90,90	0
55	MG	1G	1712	1/1	0.90	0.28	2.28	122,122,122,122	0
55	MG	1H	3228	1/1	0.86	0.23	2.18	90,90,90,90	0
55	MG	1H	3358	1/1	0.74	0.42	2.08	115,115,115,115	0
55	MG	1H	3001	1/1	0.99	0.30	2.07	47,47,47,47	0
55	MG	14	3312	1/1	0.86	0.19	2.02	98,98,98,98	0
55	MG	1H	3210	1/1	0.76	0.22	1.96	97,97,97,97	0
55	MG	13	1620	1/1	0.96	0.28	1.92	67,67,67,67	0
55	MG	1H	3259	1/1	0.83	0.38	1.90	165,165,165,165	0
55	MG	29	302	1/1	0.93	0.58	1.85	81,81,81,81	0
55	MG	14	3220	1/1	0.74	0.18	1.79	89,89,89,89	0
55	MG	1J	207	1/1	0.80	0.21	1.79	97,97,97,97	0
55	MG	14	3086	1/1	0.91	0.22	1.77	68,68,68,68	0
55	MG	14	3334	1/1	0.69	0.24	1.76	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3252	1/1	0.93	0.24	1.74	79,79,79,79	0
55	MG	1H	3143	1/1	0.89	0.23	1.66	90,90,90,90	0
55	MG	14	3077	1/1	0.98	0.24	1.64	80,80,80,80	0
55	MG	1H	3084	1/1	0.81	0.29	1.63	83,83,83,83	0
55	MG	14	3031	1/1	0.61	0.23	1.63	95,95,95,95	0
55	MG	13	1630	1/1	0.97	0.22	1.62	92,92,92,92	0
55	MG	1G	1645	1/1	0.77	0.28	1.58	104,104,104,104	0
55	MG	16	201	1/1	0.94	0.18	1.56	112,112,112,112	0
55	MG	14	3199	1/1	0.91	0.24	1.54	94,94,94,94	0
55	MG	13	1606	1/1	0.96	0.27	1.48	100,100,100,100	0
55	MG	1H	3513	1/1	0.91	0.29	1.40	103,103,103,103	0
55	MG	14	3013	1/1	0.98	0.24	1.35	75,75,75,75	0
55	MG	11	302	1/1	0.87	0.55	1.32	63,63,63,63	0
55	MG	55	203	1/1	0.90	0.45	1.22	88,88,88,88	0
55	MG	14	3158	1/1	0.90	0.27	1.21	70,70,70,70	0
55	MG	1H	3268	1/1	0.07	0.22	1.20	85,85,85,85	0
55	MG	1H	3040	1/1	0.98	0.28	1.20	80,80,80,80	0
55	MG	1H	3117	1/1	0.94	0.26	1.14	83,83,83,83	0
55	MG	1H	3085	1/1	0.97	0.32	1.06	78,78,78,78	0
56	ZN	32	302	1/1	0.99	0.37	1.05	114,114,114,114	0
55	MG	14	3049	1/1	0.98	0.25	0.96	65,65,65,65	0
55	MG	1G	1697	1/1	0.97	0.23	0.94	83,83,83,83	0
55	MG	1H	3043	1/1	0.97	0.25	0.93	89,89,89,89	0
55	MG	18	101	1/1	0.59	0.34	0.91	93,93,93,93	0
55	MG	16	205	1/1	0.81	0.18	0.90	109,109,109,109	0
55	MG	14	3315	1/1	0.91	0.38	0.86	121,121,121,121	0
55	MG	14	3078	1/1	0.98	0.23	0.76	70,70,70,70	0
55	MG	14	3209	1/1	0.83	0.34	0.73	89,89,89,89	0
55	MG	1H	3077	1/1	0.98	0.26	0.73	59,59,59,59	0
55	MG	14	3194	1/1	0.98	0.33	0.72	92,92,92,92	0
55	MG	1H	3193	1/1	0.84	0.19	0.71	79,79,79,79	0
55	MG	1H	3016	1/1	0.94	0.24	0.63	75,75,75,75	0
55	MG	1H	3250	1/1	0.87	0.23	0.49	80,80,80,80	0
55	MG	1H	3359	1/1	0.87	0.27	0.49	70,70,70,70	0
55	MG	1G	1713	1/1	0.91	0.15	0.46	106,106,106,106	0
55	MG	13	1678	1/1	0.84	0.22	0.41	124,124,124,124	0
56	ZN	3E	301	1/1	0.99	0.36	0.39	109,109,109,109	0
55	MG	14	3005	1/1	0.98	0.24	0.37	72,72,72,72	0
55	MG	14	3473	1/1	0.87	0.24	0.31	108,108,108,108	0
55	MG	1H	3547	1/1	0.95	0.36	0.29	85,85,85,85	0
55	MG	1H	3134	1/1	0.89	0.27	0.28	78,78,78,78	0
55	MG	1G	1607	1/1	0.96	0.21	0.25	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
55	MG	14	3406	1/1	1.00	0.19	0.25	76,76,76,76	0
55	MG	1H	3236	1/1	0.87	0.24	0.24	77,77,77,77	0
55	MG	1H	3151	1/1	0.94	0.18	0.21	80,80,80,80	0
55	MG	1G	1650	1/1	0.90	0.18	0.21	99,99,99,99	0
55	MG	1G	1620	1/1	0.95	0.19	0.16	97,97,97,97	0
55	MG	1H	3465	1/1	0.98	0.24	0.15	73,73,73,73	0
55	MG	1H	3258	1/1	0.97	0.31	0.13	94,94,94,94	0
55	MG	1G	1738	1/1	0.94	0.28	0.07	108,108,108,108	0
55	MG	1H	3070	1/1	0.99	0.21	0.04	72,72,72,72	0
55	MG	1H	3241	1/1	0.97	0.23	-0.01	99,99,99,99	0
55	MG	1H	3254	1/1	0.76	0.17	-0.02	104,104,104,104	0
55	MG	13	1615	1/1	0.95	0.31	-0.08	146,146,146,146	0
55	MG	1G	1658	1/1	0.72	0.31	-0.11	106,106,106,106	0
55	MG	14	3027	1/1	0.95	0.22	-0.16	80,80,80,80	0
55	MG	14	3301	1/1	0.88	0.19	-0.18	91,91,91,91	0
55	MG	1H	3472	1/1	0.99	0.21	-0.18	94,94,94,94	0
55	MG	1G	1648	1/1	0.91	0.28	-0.30	109,109,109,109	0
55	MG	13	1608	1/1	0.98	0.21	-0.30	91,91,91,91	0
55	MG	14	3017	1/1	0.93	0.20	-0.33	79,79,79,79	0
55	MG	14	3089	1/1	0.83	0.21	-0.34	78,78,78,78	0
55	MG	1H	3066	1/1	0.96	0.26	-0.38	81,81,81,81	0
55	MG	1G	1694	1/1	0.96	0.18	-0.40	103,103,103,103	0
55	MG	14	3048	1/1	0.96	0.20	-0.40	69,69,69,69	0
55	MG	13	1655	1/1	0.86	0.24	-0.42	107,107,107,107	0
55	MG	1H	3083	1/1	0.99	0.18	-0.43	85,85,85,85	0
55	MG	14	3294	1/1	0.97	0.27	-0.43	82,82,82,82	0
55	MG	1H	3140	1/1	0.98	0.20	-0.44	87,87,87,87	0
55	MG	1H	3056	1/1	0.96	0.26	-0.52	67,67,67,67	0
55	MG	13	1632	1/1	0.92	0.25	-0.55	87,87,87,87	0
55	MG	14	3296	1/1	0.66	0.27	-0.55	87,87,87,87	0
55	MG	1H	3173	1/1	0.88	0.26	-0.55	88,88,88,88	0
55	MG	14	3462	1/1	0.85	0.21	-0.57	100,100,100,100	0
55	MG	1H	3126	1/1	0.78	0.24	-0.62	87,87,87,87	0
55	MG	1H	3221	1/1	0.98	0.21	-0.63	67,67,67,67	0
55	MG	1H	3025	1/1	0.68	0.15	-0.63	95,95,95,95	0
55	MG	14	3085	1/1	0.95	0.19	-0.66	67,67,67,67	0
55	MG	1H	3331	1/1	0.95	0.24	-0.66	62,62,62,62	0
55	MG	14	3168	1/1	0.94	0.18	-0.67	86,86,86,86	0
55	MG	1G	1640	1/1	0.97	0.17	-0.70	95,95,95,95	0
55	MG	14	3175	1/1	0.97	0.27	-0.70	95,95,95,95	0
55	MG	1H	3200	1/1	0.86	0.24	-0.72	109,109,109,109	0
55	MG	88	202	1/1	0.88	0.19	-0.74	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3487	1/1	0.89	0.17	-0.76	123,123,123,123	0
55	MG	1G	1695	1/1	0.94	0.14	-0.77	108,108,108,108	0
55	MG	1H	3079	1/1	0.95	0.21	-0.84	50,50,50,50	0
55	MG	13	1612	1/1	0.91	0.21	-0.88	117,117,117,117	0
55	MG	1G	1736	1/1	0.90	0.10	-0.88	151,151,151,151	0
55	MG	16	204	1/1	0.94	0.14	-0.89	121,121,121,121	0
55	MG	1H	3548	1/1	0.98	0.21	-0.90	76,76,76,76	0
55	MG	1H	3053	1/1	0.98	0.26	-0.90	74,74,74,74	0
55	MG	1G	1610	1/1	0.93	0.13	-0.90	156,156,156,156	0
55	MG	1H	3088	1/1	0.84	0.18	-0.90	55,55,55,55	0
55	MG	1H	3072	1/1	0.97	0.23	-0.96	65,65,65,65	0
55	MG	13	1605	1/1	0.94	0.11	-0.96	103,103,103,103	0
55	MG	16	203	1/1	0.78	0.14	-0.97	105,105,105,105	0
56	ZN	G8	201	1/1	0.57	0.12	-0.99	201,201,201,201	0
55	MG	14	3044	1/1	0.98	0.19	-1.02	78,78,78,78	0
55	MG	1H	3101	1/1	0.97	0.20	-1.02	64,64,64,64	0
55	MG	49	201	1/1	0.87	0.22	-1.04	134,134,134,134	0
55	MG	14	3488	1/1	0.98	0.21	-1.06	81,81,81,81	0
55	MG	14	3020	1/1	0.99	0.18	-1.07	71,71,71,71	0
55	MG	1J	201	1/1	0.97	0.16	-1.08	125,125,125,125	0
56	ZN	5I	101	1/1	0.96	0.14	-1.08	138,138,138,138	0
56	ZN	5A	101	1/1	0.81	0.14	-1.09	155,155,155,155	0
55	MG	F5	101	1/1	0.96	0.18	-1.10	90,90,90,90	0
55	MG	1G	1606	1/1	0.94	0.14	-1.11	108,108,108,108	0
55	MG	21	301	1/1	0.88	0.21	-1.17	69,69,69,69	0
55	MG	1H	3232	1/1	0.92	0.18	-1.18	82,82,82,82	0
55	MG	1H	3121	1/1	0.86	0.20	-1.19	82,82,82,82	0
55	MG	14	3088	1/1	0.93	0.13	-1.19	99,99,99,99	0
55	MG	13	1659	1/1	0.69	0.14	-1.22	108,108,108,108	0
55	MG	13	1604	1/1	0.93	0.13	-1.25	96,96,96,96	0
55	MG	14	3487	1/1	0.94	0.16	-1.30	73,73,73,73	0
56	ZN	C5	202	1/1	0.70	0.11	-1.35	206,206,206,206	0
55	MG	1H	3384	1/1	0.92	0.12	-1.36	72,72,72,72	0
55	MG	1G	1627	1/1	0.96	0.21	-1.37	89,89,89,89	0
55	MG	14	3394	1/1	0.97	0.10	-1.38	100,100,100,100	0
55	MG	14	3062	1/1	0.79	0.20	-1.39	79,79,79,79	0
55	MG	14	3217	1/1	0.85	0.14	-1.39	88,88,88,88	0
55	MG	1G	1618	1/1	0.89	0.14	-1.40	110,110,110,110	0
55	MG	14	3124	1/1	0.87	0.15	-1.41	92,92,92,92	0
55	MG	1H	3010	1/1	0.97	0.22	-1.42	57,57,57,57	0
55	MG	13	1709	1/1	0.97	0.08	-1.42	126,126,126,126	0
55	MG	13	1603	1/1	0.96	0.15	-1.43	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3400	1/1	0.93	0.18	-1.43	61,61,61,61	0
55	MG	14	3349	1/1	0.99	0.15	-1.44	66,66,66,66	0
55	MG	13	1626	1/1	0.86	0.21	-1.45	69,69,69,69	0
55	MG	13	1702	1/1	0.91	0.12	-1.45	140,140,140,140	0
55	MG	1G	1716	1/1	0.93	0.13	-1.46	98,98,98,98	0
55	MG	1H	3471	1/1	0.95	0.10	-1.46	89,89,89,89	0
55	MG	14	3218	1/1	0.92	0.14	-1.48	77,77,77,77	0
55	MG	14	3011	1/1	0.98	0.20	-1.48	54,54,54,54	0
55	MG	1H	3182	1/1	0.79	0.23	-1.51	68,68,68,68	0
55	MG	14	3359	1/1	0.95	0.11	-1.56	87,87,87,87	0
55	MG	1G	1601	1/1	0.91	0.21	-1.57	89,89,89,89	0
55	MG	14	3372	1/1	0.96	0.13	-1.58	65,65,65,65	0
55	MG	13	1651	1/1	0.98	0.16	-1.62	91,91,91,91	0
55	MG	J8	101	1/1	0.93	0.19	-1.64	83,83,83,83	0
55	MG	14	3160	1/1	0.83	0.21	-1.69	82,82,82,82	0
55	MG	14	3355	1/1	0.95	0.16	-1.69	97,97,97,97	0
55	MG	14	3259	1/1	0.90	0.14	-1.76	86,86,86,86	0
55	MG	1H	3413	1/1	0.94	0.11	-1.78	83,83,83,83	0
55	MG	2L	101	1/1	0.98	0.16	-1.79	92,92,92,92	0
55	MG	1G	1617	1/1	0.93	0.15	-1.80	74,74,74,74	0
55	MG	14	3037	1/1	0.97	0.11	-1.81	48,48,48,48	0
55	MG	2K	101	1/1	0.95	0.18	-1.81	84,84,84,84	0
55	MG	1H	3388	1/1	0.97	0.10	-1.82	77,77,77,77	0
55	MG	14	3287	1/1	0.91	0.14	-1.83	111,111,111,111	0
55	MG	14	3059	1/1	0.95	0.14	-1.85	64,64,64,64	0
55	MG	1G	1614	1/1	0.94	0.17	-1.87	89,89,89,89	0
55	MG	1H	3390	1/1	0.93	0.10	-1.89	67,67,67,67	0
55	MG	1G	1746	1/1	0.96	0.10	-1.89	162,162,162,162	0
55	MG	14	3091	1/1	0.96	0.17	-1.91	73,73,73,73	0
55	MG	14	3396	1/1	0.92	0.19	-1.93	94,94,94,94	0
55	MG	14	3028	1/1	0.98	0.17	-1.94	76,76,76,76	0
55	MG	1H	3030	1/1	0.94	0.12	-1.95	66,66,66,66	0
55	MG	14	3054	1/1	0.99	0.17	-1.98	65,65,65,65	0
55	MG	1H	3005	1/1	0.96	0.17	-2.00	64,64,64,64	0
55	MG	14	3169	1/1	0.90	0.20	-2.02	69,69,69,69	0
55	MG	1H	3087	1/1	0.98	0.22	-2.05	81,81,81,81	0
55	MG	1H	3032	1/1	0.92	0.19	-2.07	76,76,76,76	0
55	MG	14	3375	1/1	0.93	0.11	-2.09	75,75,75,75	0
55	MG	19	301	1/1	0.95	0.23	-2.11	76,76,76,76	0
55	MG	14	3285	1/1	0.96	0.08	-2.14	107,107,107,107	0
55	MG	14	3362	1/1	0.97	0.17	-2.16	79,79,79,79	0
55	MG	13	1673	1/1	0.98	0.14	-2.20	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3100	1/1	0.86	0.13	-2.21	81,81,81,81	0
55	MG	13	1657	1/1	0.95	0.16	-2.22	109,109,109,109	0
55	MG	1H	3376	1/1	0.98	0.10	-2.23	78,78,78,78	0
55	MG	14	3198	1/1	0.98	0.13	-2.26	88,88,88,88	0
55	MG	14	3172	1/1	0.96	0.15	-2.27	74,74,74,74	0
55	MG	14	3202	1/1	0.85	0.18	-2.28	90,90,90,90	0
55	MG	1H	3421	1/1	0.95	0.18	-2.29	63,63,63,63	0
55	MG	14	3402	1/1	0.98	0.09	-2.31	76,76,76,76	0
55	MG	14	3427	1/1	0.98	0.09	-2.32	72,72,72,72	0
55	MG	1H	3371	1/1	0.89	0.11	-2.32	72,72,72,72	0
55	MG	13	1717	1/1	0.97	0.11	-2.34	91,91,91,91	0
55	MG	14	3060	1/1	0.99	0.24	-2.34	56,56,56,56	0
55	MG	14	3163	1/1	0.83	0.10	-2.37	86,86,86,86	0
55	MG	14	3242	1/1	0.93	0.13	-2.40	100,100,100,100	0
55	MG	14	3356	1/1	0.96	0.10	-2.40	64,64,64,64	0
55	MG	1H	3401	1/1	0.97	0.17	-2.41	82,82,82,82	0
55	MG	14	3019	1/1	0.98	0.15	-2.45	73,73,73,73	0
55	MG	14	3093	1/1	0.96	0.13	-2.46	66,66,66,66	0
55	MG	1G	1667	1/1	0.94	0.12	-2.48	92,92,92,92	0
55	MG	1H	3286	1/1	0.99	0.17	-2.49	69,69,69,69	0
55	MG	14	3411	1/1	0.97	0.10	-2.49	60,60,60,60	0
55	MG	14	3403	1/1	0.90	0.14	-2.51	88,88,88,88	0
55	MG	14	3038	1/1	0.98	0.17	-2.51	58,58,58,58	0
55	MG	14	3055	1/1	0.98	0.17	-2.52	72,72,72,72	0
55	MG	1H	3185	1/1	0.82	0.19	-2.53	73,73,73,73	0
55	MG	13	1710	1/1	0.98	0.15	-2.53	119,119,119,119	0
55	MG	13	1697	1/1	0.92	0.14	-2.54	100,100,100,100	0
55	MG	14	3358	1/1	0.91	0.10	-2.57	102,102,102,102	0
55	MG	14	3390	1/1	0.98	0.14	-2.59	70,70,70,70	0
55	MG	14	3472	1/1	0.75	0.06	-2.59	121,121,121,121	0
55	MG	13	1661	1/1	0.91	0.21	-2.64	127,127,127,127	0
55	MG	14	3465	1/1	0.92	0.14	-2.65	92,92,92,92	0
55	MG	1H	3544	1/1	0.97	0.08	-2.67	59,59,59,59	0
55	MG	1H	3195	1/1	0.90	0.15	-2.67	78,78,78,78	0
55	MG	14	3486	1/1	0.96	0.07	-2.68	64,64,64,64	0
55	MG	1G	1671	1/1	0.88	0.14	-2.72	102,102,102,102	0
55	MG	13	1698	1/1	0.95	0.14	-2.73	77,77,77,77	0
55	MG	14	3084	1/1	0.97	0.17	-2.74	78,78,78,78	0
55	MG	1J	202	1/1	0.97	0.11	-2.83	107,107,107,107	0
55	MG	1H	3161	1/1	0.99	0.15	-2.85	73,73,73,73	0
55	MG	14	3210	1/1	0.93	0.17	-2.86	89,89,89,89	0
55	MG	1H	3475	1/1	0.91	0.12	-2.89	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3036	1/1	0.95	0.20	-2.91	84,84,84,84	0
55	MG	13	1687	1/1	0.67	0.11	-2.95	111,111,111,111	0
55	MG	1H	3381	1/1	0.96	0.17	-2.98	78,78,78,78	0
55	MG	14	3041	1/1	0.89	0.13	-2.98	76,76,76,76	0
55	MG	14	3410	1/1	0.79	0.11	-3.03	109,109,109,109	0
55	MG	14	3200	1/1	0.88	0.15	-3.03	89,89,89,89	0
55	MG	1H	3539	1/1	0.94	0.09	-3.04	123,123,123,123	0
55	MG	1H	3048	1/1	0.99	0.17	-3.04	67,67,67,67	0
55	MG	1H	3081	1/1	0.95	0.15	-3.04	66,66,66,66	0
55	MG	16	209	1/1	0.72	0.12	-3.05	101,101,101,101	0
55	MG	14	3107	1/1	0.91	0.15	-3.05	78,78,78,78	0
55	MG	14	3034	1/1	0.98	0.20	-3.06	67,67,67,67	0
55	MG	1G	1690	1/1	0.98	0.12	-3.06	122,122,122,122	0
55	MG	1H	3183	1/1	0.97	0.26	-3.08	55,55,55,55	0
55	MG	1G	1660	1/1	0.97	0.11	-3.13	112,112,112,112	0
55	MG	1H	3026	1/1	0.97	0.16	-3.14	68,68,68,68	0
55	MG	1G	1724	1/1	0.95	0.10	-3.14	95,95,95,95	0
55	MG	88	201	1/1	0.96	0.18	-3.17	93,93,93,93	0
55	MG	1H	3385	1/1	0.98	0.10	-3.18	58,58,58,58	0
55	MG	1H	3246	1/1	0.97	0.16	-3.20	86,86,86,86	0
55	MG	13	1705	1/1	0.97	0.15	-3.22	85,85,85,85	0
55	MG	1H	3423	1/1	0.95	0.15	-3.23	64,64,64,64	0
55	MG	14	3482	1/1	0.85	0.12	-3.24	118,118,118,118	0
55	MG	1G	1602	1/1	0.97	0.18	-3.24	84,84,84,84	0
55	MG	1H	3386	1/1	0.98	0.14	-3.24	72,72,72,72	0
55	MG	1G	1639	1/1	0.97	0.14	-3.24	102,102,102,102	0
55	MG	14	3426	1/1	0.95	0.10	-3.27	96,96,96,96	0
55	MG	1H	3506	1/1	0.96	0.17	-3.31	102,102,102,102	0
55	MG	39	301	1/1	0.83	0.13	-3.34	108,108,108,108	0
55	MG	14	3382	1/1	0.97	0.11	-3.39	93,93,93,93	0
55	MG	1H	3383	1/1	0.97	0.12	-3.43	74,74,74,74	0
55	MG	14	3025	1/1	0.78	0.09	-3.45	85,85,85,85	0
55	MG	1H	3354	1/1	0.98	0.16	-3.53	82,82,82,82	0
55	MG	14	3152	1/1	0.94	0.16	-3.55	80,80,80,80	0
55	MG	1H	3107	1/1	0.97	0.20	-3.55	84,84,84,84	0
55	MG	1H	3360	1/1	0.97	0.08	-3.59	96,96,96,96	0
55	MG	1G	1643	1/1	0.95	0.12	-3.62	128,128,128,128	0
55	MG	1H	3089	1/1	0.94	0.13	-3.62	62,62,62,62	0
55	MG	14	3035	1/1	0.89	0.19	-3.64	74,74,74,74	0
55	MG	13	1703	1/1	0.98	0.09	-3.64	108,108,108,108	0
55	MG	1H	3382	1/1	0.99	0.16	-3.65	61,61,61,61	0
55	MG	1H	3439	1/1	1.00	0.11	-3.66	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1672	1/1	0.88	0.16	-3.66	105,105,105,105	0
55	MG	14	3353	1/1	0.92	0.08	-3.68	74,74,74,74	0
55	MG	1H	3226	1/1	0.84	0.15	-3.76	89,89,89,89	0
55	MG	14	3056	1/1	0.95	0.16	-3.77	74,74,74,74	0
55	MG	14	3351	1/1	0.97	0.10	-3.78	82,82,82,82	0
55	MG	14	3467	1/1	0.98	0.21	-3.83	95,95,95,95	0
55	MG	1H	3397	1/1	0.78	0.09	-3.84	90,90,90,90	0
55	MG	13	1633	1/1	0.95	0.09	-3.84	107,107,107,107	0
55	MG	1H	3374	1/1	0.93	0.15	-3.85	64,64,64,64	0
55	MG	14	3449	1/1	0.86	0.08	-3.88	135,135,135,135	0
55	MG	1H	3496	1/1	0.94	0.12	-3.92	91,91,91,91	0
55	MG	14	3231	1/1	0.92	0.07	-3.96	112,112,112,112	0
55	MG	14	3079	1/1	0.90	0.20	-3.97	75,75,75,75	0
55	MG	1G	1604	1/1	0.92	0.09	-4.00	106,106,106,106	0
55	MG	1H	3118	1/1	0.91	0.15	-4.00	56,56,56,56	0
55	MG	1H	3181	1/1	0.93	0.19	-4.03	69,69,69,69	0
55	MG	14	3129	1/1	0.96	0.19	-4.10	77,77,77,77	0
55	MG	14	3170	1/1	0.93	0.13	-4.10	77,77,77,77	0
55	MG	14	3413	1/1	0.98	0.15	-4.16	74,74,74,74	0
55	MG	1G	1725	1/1	0.81	0.10	-4.18	124,124,124,124	0
55	MG	1H	3103	1/1	0.92	0.13	-4.18	74,74,74,74	0
55	MG	1G	1720	1/1	0.87	0.12	-4.19	97,97,97,97	0
55	MG	14	3453	1/1	0.98	0.11	-4.22	73,73,73,73	0
55	MG	14	3354	1/1	0.94	0.15	-4.23	92,92,92,92	0
55	MG	14	3371	1/1	0.96	0.09	-4.26	66,66,66,66	0
55	MG	14	3205	1/1	0.92	0.12	-4.30	82,82,82,82	0
55	MG	14	3075	1/1	0.97	0.19	-4.32	65,65,65,65	0
55	MG	1H	3180	1/1	0.91	0.16	-4.41	53,53,53,53	0
55	MG	14	3436	1/1	0.95	0.12	-4.42	99,99,99,99	0
55	MG	1H	3454	1/1	0.75	0.11	-4.46	89,89,89,89	0
55	MG	14	3385	1/1	0.97	0.13	-4.48	96,96,96,96	0
55	MG	1H	3477	1/1	0.93	0.09	-4.50	80,80,80,80	0
55	MG	1H	3392	1/1	0.96	0.16	-4.52	70,70,70,70	0
55	MG	14	3103	1/1	0.87	0.13	-4.52	74,74,74,74	0
55	MG	1H	3445	1/1	0.96	0.10	-4.53	76,76,76,76	0
55	MG	14	3142	1/1	0.91	0.10	-4.57	67,67,67,67	0
55	MG	1H	3349	1/1	0.94	0.15	-4.60	95,95,95,95	0
55	MG	1H	3428	1/1	0.98	0.15	-4.65	60,60,60,60	0
55	MG	1H	3113	1/1	0.89	0.10	-4.77	98,98,98,98	0
55	MG	1H	3096	1/1	0.51	0.15	-4.90	74,74,74,74	0
55	MG	1H	3425	1/1	0.98	0.12	-4.93	63,63,63,63	0
55	MG	14	3429	1/1	0.97	0.09	-4.98	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3323	1/1	0.87	0.12	-4.98	84,84,84,84	0
55	MG	14	3275	1/1	0.88	0.10	-4.99	84,84,84,84	0
55	MG	14	3395	1/1	0.99	0.09	-4.99	73,73,73,73	0
55	MG	14	3448	1/1	0.72	0.09	-5.03	123,123,123,123	0
55	MG	14	3308	1/1	0.97	0.19	-5.05	74,74,74,74	0
55	MG	1H	3417	1/1	0.97	0.13	-5.08	70,70,70,70	0
55	MG	1H	3110	1/1	0.81	0.14	-5.10	65,65,65,65	0
55	MG	1H	3538	1/1	0.90	0.11	-5.13	67,67,67,67	0
55	MG	1H	3054	1/1	0.98	0.18	-5.22	66,66,66,66	0
55	MG	1H	3403	1/1	0.90	0.13	-5.22	78,78,78,78	0
55	MG	1G	1722	1/1	0.98	0.10	-5.24	83,83,83,83	0
55	MG	14	3439	1/1	0.93	0.06	-5.30	109,109,109,109	0
55	MG	1H	3435	1/1	0.99	0.10	-5.30	60,60,60,60	0
55	MG	14	3115	1/1	0.92	0.09	-5.32	94,94,94,94	0
55	MG	1H	3422	1/1	0.99	0.12	-5.32	70,70,70,70	0
55	MG	1H	3322	1/1	0.97	0.12	-5.33	103,103,103,103	0
55	MG	1H	3540	1/1	0.97	0.09	-5.36	54,54,54,54	0
55	MG	14	3456	1/1	0.93	0.06	-5.38	125,125,125,125	0
55	MG	1G	1727	1/1	0.96	0.08	-5.51	126,126,126,126	0
55	MG	1H	3378	1/1	0.92	0.12	-5.66	59,59,59,59	0
55	MG	1H	3372	1/1	0.94	0.10	-5.72	68,68,68,68	0
55	MG	1H	3463	1/1	0.99	0.10	-5.74	64,64,64,64	0
55	MG	1H	3012	1/1	0.98	0.15	-5.80	67,67,67,67	0
55	MG	14	3150	1/1	0.95	0.14	-5.90	64,64,64,64	0
55	MG	1H	3231	1/1	0.92	0.11	-6.16	81,81,81,81	0
55	MG	1H	3486	1/1	0.87	0.08	-6.33	104,104,104,104	0
55	MG	14	3365	1/1	0.95	0.09	-6.40	72,72,72,72	0
55	MG	1H	3529	1/1	0.91	0.08	-6.91	106,106,106,106	0
55	MG	1H	3461	1/1	0.98	0.12	-7.01	77,77,77,77	0
55	MG	1H	3415	1/1	0.89	0.09	-7.03	91,91,91,91	0
55	MG	14	3064	1/1	0.98	0.11	-7.04	84,84,84,84	0
55	MG	14	3401	1/1	0.97	0.13	-7.06	69,69,69,69	0
55	MG	14	3376	1/1	0.94	0.11	-7.17	84,84,84,84	0
55	MG	14	3083	1/1	0.91	0.09	-7.19	64,64,64,64	0
55	MG	1H	3427	1/1	0.98	0.12	-7.25	71,71,71,71	0
55	MG	1H	3404	1/1	0.81	0.11	-7.27	71,71,71,71	0
55	MG	14	3370	1/1	0.96	0.13	-7.29	76,76,76,76	0
55	MG	1H	3418	1/1	0.99	0.13	-7.31	60,60,60,60	0
55	MG	14	3381	1/1	0.91	0.09	-7.36	69,69,69,69	0
55	MG	1H	3429	1/1	0.95	0.12	-7.36	65,65,65,65	0
55	MG	1H	3485	1/1	0.92	0.09	-7.41	97,97,97,97	0
55	MG	1H	3447	1/1	0.94	0.12	-7.62	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
55	MG	1H	3379	1/1	0.96	0.14	-7.79	71,71,71,71	0
55	MG	1H	3097	1/1	0.92	0.09	-7.83	75,75,75,75	0
55	MG	1H	3375	1/1	0.94	0.12	-7.91	65,65,65,65	0
55	MG	1H	3426	1/1	0.96	0.10	-8.04	68,68,68,68	0
55	MG	14	3404	1/1	0.98	0.11	-8.11	54,54,54,54	0
55	MG	1H	3488	1/1	0.85	0.09	-8.24	117,117,117,117	0
55	MG	1H	3473	1/1	0.93	0.05	-8.24	95,95,95,95	0
55	MG	14	3368	1/1	0.96	0.13	-9.10	75,75,75,75	0
55	MG	1H	3498	1/1	0.97	0.08	-9.31	71,71,71,71	0
55	MG	14	3384	1/1	0.96	0.05	-9.35	75,75,75,75	0
55	MG	14	3452	1/1	0.88	0.09	-9.44	96,96,96,96	0
55	MG	14	3399	1/1	0.97	0.13	-9.71	63,63,63,63	0
55	MG	14	3350	1/1	0.98	0.13	-10.06	73,73,73,73	0
55	MG	14	3397	1/1	0.96	0.07	-11.45	79,79,79,79	0
55	MG	1H	3534	1/1	0.84	0.10	-16.83	115,115,115,115	0
55	MG	1G	1692	1/1	0.64	0.56	-	141,141,141,141	0
55	MG	14	3481	1/1	0.93	0.34	-	112,112,112,112	0
55	MG	14	3030	1/1	0.92	0.22	-	92,92,92,92	0
55	MG	1H	3325	1/1	0.77	0.35	-	78,78,78,78	0
55	MG	14	3246	1/1	0.61	0.26	-	101,101,101,101	0
55	MG	13	1631	1/1	0.89	0.22	-	101,101,101,101	0
55	MG	1H	3090	1/1	0.97	0.25	-	80,80,80,80	0
55	MG	13	1706	1/1	0.70	0.09	-	117,117,117,117	0
55	MG	14	3357	1/1	0.93	0.13	-	83,83,83,83	0
55	MG	1H	3067	1/1	0.96	0.22	-	79,79,79,79	0
55	MG	1H	3419	1/1	0.90	0.17	-	90,90,90,90	0
55	MG	1H	3112	1/1	0.92	0.29	-	64,64,64,64	0
55	MG	14	3143	1/1	0.95	0.12	-	58,58,58,58	0
55	MG	1H	3011	1/1	0.98	0.26	-	65,65,65,65	0
55	MG	1G	1679	1/1	0.85	0.14	-	106,106,106,106	0
55	MG	1H	3156	1/1	0.96	0.25	-	76,76,76,76	0
55	MG	14	3230	1/1	0.92	0.24	-	81,81,81,81	0
55	MG	1G	1654	1/1	0.91	0.11	-	88,88,88,88	0
55	MG	14	3214	1/1	0.16	0.21	-	122,122,122,122	0
55	MG	1H	3186	1/1	0.94	0.24	-	74,74,74,74	0
55	MG	1H	3459	1/1	0.97	0.16	-	86,86,86,86	0
55	MG	14	3414	1/1	0.96	0.13	-	99,99,99,99	0
55	MG	1H	3299	1/1	0.78	0.34	-	80,80,80,80	0
55	MG	1H	3526	1/1	0.95	0.08	-	106,106,106,106	0
55	MG	1H	3430	1/1	0.88	0.16	-	99,99,99,99	0
55	MG	1H	3133	1/1	0.72	0.17	-	92,92,92,92	0
55	MG	14	3121	1/1	0.94	0.21	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1718	1/1	0.58	0.33	-	94,94,94,94	0
55	MG	14	3070	1/1	0.97	0.30	-	72,72,72,72	0
55	MG	1H	3300	1/1	0.85	0.16	-	54,54,54,54	0
55	MG	1H	3391	1/1	0.97	0.06	-	84,84,84,84	0
55	MG	14	3081	1/1	0.60	0.28	-	80,80,80,80	0
55	MG	14	3307	1/1	0.79	0.12	-	90,90,90,90	0
55	MG	1H	3480	1/1	0.92	0.08	-	100,100,100,100	0
55	MG	1H	3004	1/1	0.96	0.21	-	74,74,74,74	0
55	MG	2K	103	1/1	0.49	0.36	-	140,140,140,140	0
55	MG	1H	3449	1/1	0.90	0.08	-	90,90,90,90	0
55	MG	13	1660	1/1	0.65	0.28	-	108,108,108,108	0
55	MG	1H	3309	1/1	0.83	0.26	-	96,96,96,96	0
55	MG	13	1611	1/1	0.97	0.17	-	103,103,103,103	0
55	MG	13	1701	1/1	0.96	0.05	-	89,89,89,89	0
55	MG	1H	3080	1/1	0.97	0.33	-	67,67,67,67	0
55	MG	1H	3013	1/1	0.99	0.15	-	57,57,57,57	0
55	MG	1H	3436	1/1	0.98	0.13	-	55,55,55,55	0
55	MG	14	3373	1/1	0.90	0.17	-	101,101,101,101	0
55	MG	14	3319	1/1	-0.08	0.34	-	110,110,110,110	0
55	MG	14	3096	1/1	0.96	0.20	-	78,78,78,78	0
55	MG	1H	3248	1/1	0.85	0.22	-	89,89,89,89	0
55	MG	14	3440	1/1	0.85	0.16	-	131,131,131,131	0
55	MG	13	1656	1/1	0.86	0.41	-	89,89,89,89	0
55	MG	1H	3493	1/1	0.61	0.10	-	133,133,133,133	0
55	MG	14	3241	1/1	0.95	0.10	-	117,117,117,117	0
55	MG	1H	3531	1/1	0.85	0.10	-	116,116,116,116	0
55	MG	14	3171	1/1	0.61	0.35	-	82,82,82,82	0
55	MG	14	3068	1/1	0.87	0.17	-	71,71,71,71	0
55	MG	13	1674	1/1	0.71	0.18	-	142,142,142,142	0
55	MG	14	3348	1/1	0.92	0.16	-	96,96,96,96	0
55	MG	1H	3293	1/1	0.95	0.45	-	89,89,89,89	0
55	MG	14	3185	1/1	0.85	0.16	-	92,92,92,92	0
55	MG	14	3050	1/1	0.96	0.27	-	75,75,75,75	0
55	MG	13	1624	1/1	0.90	0.28	-	77,77,77,77	0
55	MG	14	3477	1/1	0.91	0.28	-	117,117,117,117	0
55	MG	14	3111	1/1	0.79	0.22	-	85,85,85,85	0
55	MG	1H	3166	1/1	0.79	0.30	-	86,86,86,86	0
55	MG	1G	1688	1/1	0.95	0.18	-	115,115,115,115	0
55	MG	1H	3387	1/1	0.97	0.09	-	83,83,83,83	0
55	MG	32	301	1/1	0.83	0.19	-	109,109,109,109	0
55	MG	1H	3017	1/1	0.99	0.17	-	66,66,66,66	0
55	MG	1G	1644	1/1	0.85	0.12	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1685	1/1	0.47	0.26	-	119,119,119,119	0
55	MG	13	1643	1/1	0.97	0.24	-	111,111,111,111	0
55	MG	1H	3483	1/1	0.88	0.10	-	117,117,117,117	0
55	MG	14	3155	1/1	0.97	0.20	-	99,99,99,99	0
55	MG	14	3416	1/1	0.96	0.06	-	87,87,87,87	0
55	MG	1G	1702	1/1	0.92	0.34	-	173,173,173,173	0
55	MG	1H	3396	1/1	0.96	0.09	-	84,84,84,84	0
55	MG	1G	1684	1/1	0.95	0.21	-	108,108,108,108	0
55	MG	13	1718	1/1	0.89	0.17	-	125,125,125,125	0
55	MG	1H	3034	1/1	0.51	0.35	-	93,93,93,93	0
55	MG	1H	3518	1/1	0.89	0.18	-	99,99,99,99	0
55	MG	1G	1661	1/1	0.98	0.12	-	82,82,82,82	0
55	MG	1H	3208	1/1	0.76	0.60	-	110,110,110,110	0
55	MG	1H	3201	1/1	0.94	0.12	-	98,98,98,98	0
55	MG	1H	3279	1/1	0.82	0.42	-	101,101,101,101	0
55	MG	1H	3290	1/1	0.72	0.21	-	88,88,88,88	0
55	MG	1H	3115	1/1	0.86	0.39	-	89,89,89,89	0
55	MG	1G	1657	1/1	0.93	0.27	-	93,93,93,93	0
55	MG	1H	3479	1/1	0.93	0.05	-	97,97,97,97	0
55	MG	1G	1641	1/1	0.97	0.19	-	102,102,102,102	0
55	MG	14	3016	1/1	0.90	0.28	-	86,86,86,86	0
55	MG	14	3313	1/1	0.86	0.45	-	91,91,91,91	0
55	MG	14	3116	1/1	0.96	0.48	-	89,89,89,89	0
55	MG	1G	1632	1/1	0.84	0.31	-	88,88,88,88	0
55	MG	14	3235	1/1	0.72	0.36	-	109,109,109,109	0
55	MG	14	3445	1/1	0.87	0.11	-	104,104,104,104	0
55	MG	1H	3253	1/1	0.79	0.40	-	92,92,92,92	0
55	MG	1H	3369	1/1	0.98	0.75	-	77,77,77,77	0
55	MG	1H	3204	1/1	0.91	0.31	-	84,84,84,84	0
55	MG	1H	3160	1/1	0.86	0.63	-	91,91,91,91	0
55	MG	1G	1649	1/1	0.93	0.19	-	125,125,125,125	0
55	MG	14	3227	1/1	0.84	0.28	-	112,112,112,112	0
55	MG	1H	3521	1/1	0.86	0.10	-	125,125,125,125	0
55	MG	1H	3507	1/1	0.97	0.11	-	82,82,82,82	0
55	MG	14	3383	1/1	0.97	0.07	-	93,93,93,93	0
55	MG	14	3302	1/1	0.84	0.72	-	82,82,82,82	0
55	MG	13	1648	1/1	0.86	0.27	-	94,94,94,94	0
55	MG	14	3101	1/1	0.66	0.34	-	100,100,100,100	0
55	MG	14	3286	1/1	0.89	0.32	-	78,78,78,78	0
55	MG	1H	3405	1/1	0.96	0.11	-	94,94,94,94	0
55	MG	14	3118	1/1	0.91	0.16	-	96,96,96,96	0
55	MG	14	3475	1/1	0.96	0.35	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3216	1/1	0.69	0.16	-	104,104,104,104	0
55	MG	1G	1608	1/1	0.88	0.23	-	110,110,110,110	0
55	MG	13	1607	1/1	0.97	0.21	-	97,97,97,97	0
55	MG	14	3108	1/1	0.90	0.14	-	87,87,87,87	0
55	MG	1H	3123	1/1	0.91	0.30	-	93,93,93,93	0
55	MG	1H	3256	1/1	0.77	0.64	-	82,82,82,82	0
55	MG	1H	3433	1/1	0.90	0.12	-	92,92,92,92	0
55	MG	1G	1634	1/1	0.68	0.35	-	107,107,107,107	0
55	MG	1H	3302	1/1	0.89	0.31	-	90,90,90,90	0
55	MG	1H	3450	1/1	0.97	0.10	-	100,100,100,100	0
55	MG	1H	3111	1/1	0.84	0.34	-	111,111,111,111	0
55	MG	1H	3137	1/1	0.97	0.20	-	93,93,93,93	0
55	MG	1H	3457	1/1	0.98	0.11	-	79,79,79,79	0
55	MG	14	3133	1/1	0.88	0.18	-	85,85,85,85	0
55	MG	14	3126	1/1	0.93	0.27	-	110,110,110,110	0
55	MG	13	1683	1/1	0.84	0.17	-	111,111,111,111	0
55	MG	1H	3474	1/1	0.96	0.24	-	88,88,88,88	0
55	MG	1G	1703	1/1	0.68	0.23	-	113,113,113,113	0
55	MG	1H	3363	1/1	0.72	0.21	-	93,93,93,93	0
55	MG	13	1726	1/1	0.95	0.05	-	134,134,134,134	0
55	MG	1G	1735	1/1	0.94	0.06	-	128,128,128,128	0
55	MG	13	1708	1/1	0.89	0.13	-	103,103,103,103	0
55	MG	1H	3157	1/1	0.54	0.40	-	98,98,98,98	0
55	MG	1G	1740	1/1	0.70	0.52	-	135,135,135,135	0
55	MG	1H	3393	1/1	0.94	0.09	-	99,99,99,99	0
55	MG	1J	209	1/1	0.88	0.06	-	110,110,110,110	0
55	MG	14	3153	1/1	0.97	0.28	-	91,91,91,91	0
55	MG	1G	1622	1/1	0.95	0.27	-	124,124,124,124	0
55	MG	14	3178	1/1	0.94	0.51	-	87,87,87,87	0
55	MG	1H	3492	1/1	0.72	0.09	-	117,117,117,117	0
55	MG	1H	3287	1/1	0.95	0.17	-	67,67,67,67	0
55	MG	14	3112	1/1	0.94	0.32	-	81,81,81,81	0
55	MG	1G	1662	1/1	0.96	0.20	-	96,96,96,96	0
55	MG	1H	3350	1/1	0.97	0.21	-	72,72,72,72	0
55	MG	14	3279	1/1	0.63	0.31	-	103,103,103,103	0
55	MG	14	3420	1/1	0.86	0.05	-	125,125,125,125	0
55	MG	1H	3357	1/1	0.95	0.09	-	87,87,87,87	0
55	MG	13	1668	1/1	0.76	0.28	-	94,94,94,94	0
55	MG	1H	3455	1/1	0.97	0.07	-	97,97,97,97	0
55	MG	1H	3327	1/1	0.92	0.25	-	88,88,88,88	0
55	MG	14	3408	1/1	0.91	0.13	-	103,103,103,103	0
55	MG	1H	3339	1/1	0.66	0.37	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3520	1/1	0.93	0.07	-	104,104,104,104	0
55	MG	14	3392	1/1	0.97	0.20	-	65,65,65,65	0
55	MG	13	1650	1/1	0.84	0.17	-	116,116,116,116	0
55	MG	14	3260	1/1	0.94	0.13	-	88,88,88,88	0
55	MG	1H	3352	1/1	0.94	0.12	-	84,84,84,84	0
55	MG	1H	3532	1/1	0.98	0.18	-	91,91,91,91	0
55	MG	1H	3412	1/1	0.97	0.11	-	103,103,103,103	0
55	MG	1H	3373	1/1	0.86	0.19	-	87,87,87,87	0
55	MG	1G	1636	1/1	0.95	0.28	-	97,97,97,97	0
55	MG	14	3311	1/1	0.84	0.36	-	106,106,106,106	0
55	MG	1H	3301	1/1	0.79	0.28	-	93,93,93,93	0
55	MG	13	1652	1/1	0.93	0.37	-	98,98,98,98	0
55	MG	1H	3348	1/1	0.72	0.28	-	126,126,126,126	0
55	MG	1H	3321	1/1	0.88	0.24	-	88,88,88,88	0
55	MG	13	1618	1/1	0.96	0.23	-	86,86,86,86	0
55	MG	1G	1747	1/1	0.97	0.15	-	123,123,123,123	0
55	MG	1G	1631	1/1	0.95	0.26	-	81,81,81,81	0
55	MG	1H	3484	1/1	0.93	0.10	-	98,98,98,98	0
55	MG	16	212	1/1	0.93	0.15	-	126,126,126,126	0
55	MG	1G	1626	1/1	0.99	0.24	-	108,108,108,108	0
55	MG	14	3422	1/1	0.92	0.08	-	110,110,110,110	0
55	MG	1H	3237	1/1	0.91	0.33	-	99,99,99,99	0
55	MG	14	3195	1/1	0.91	0.25	-	103,103,103,103	0
55	MG	14	3282	1/1	0.93	0.26	-	77,77,77,77	0
55	MG	1H	3491	1/1	0.98	0.12	-	97,97,97,97	0
55	MG	14	3247	1/1	0.53	0.33	-	89,89,89,89	0
55	MG	14	3389	1/1	0.97	0.09	-	102,102,102,102	0
55	MG	1H	3466	1/1	0.99	0.19	-	78,78,78,78	0
55	MG	1H	3511	1/1	0.67	0.15	-	127,127,127,127	0
55	MG	14	3206	1/1	0.69	0.24	-	93,93,93,93	0
55	MG	14	3184	1/1	0.82	0.24	-	92,92,92,92	0
55	MG	1H	3069	1/1	0.92	0.22	-	86,86,86,86	0
55	MG	1H	3209	1/1	0.86	0.25	-	85,85,85,85	0
55	MG	14	3342	1/1	0.36	0.30	-	93,93,93,93	0
55	MG	14	3014	1/1	0.87	0.42	-	88,88,88,88	0
55	MG	14	3346	1/1	0.96	0.35	-	194,194,194,194	0
55	MG	1H	3093	1/1	0.99	0.27	-	67,67,67,67	0
55	MG	1H	3129	1/1	0.95	0.26	-	80,80,80,80	0
55	MG	1H	3452	1/1	0.95	0.10	-	86,86,86,86	0
55	MG	55	201	1/1	0.92	0.42	-	92,92,92,92	0
55	MG	1H	3229	1/1	0.80	0.27	-	86,86,86,86	0
55	MG	1G	1704	1/1	0.66	0.20	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3179	1/1	0.78	0.24	-	69,69,69,69	0
55	MG	14	3109	1/1	0.86	0.28	-	77,77,77,77	0
55	MG	1H	3150	1/1	0.96	0.31	-	81,81,81,81	0
55	MG	1H	3316	1/1	0.88	0.38	-	78,78,78,78	0
55	MG	14	3002	1/1	0.97	0.23	-	64,64,64,64	0
55	MG	14	3253	1/1	0.76	0.38	-	94,94,94,94	0
55	MG	14	3012	1/1	0.96	0.16	-	62,62,62,62	0
55	MG	14	3128	1/1	0.73	0.31	-	85,85,85,85	0
55	MG	13	1704	1/1	0.93	0.11	-	89,89,89,89	0
55	MG	1H	3152	1/1	0.82	0.39	-	82,82,82,82	0
55	MG	1H	3407	1/1	0.92	0.08	-	83,83,83,83	0
55	MG	1H	3364	1/1	0.86	0.17	-	101,101,101,101	0
55	MG	13	1680	1/1	0.92	0.40	-	160,160,160,160	0
55	MG	14	3080	1/1	0.90	0.18	-	66,66,66,66	0
55	MG	1H	3122	1/1	0.88	0.27	-	77,77,77,77	0
55	MG	1H	3244	1/1	0.94	0.35	-	75,75,75,75	0
55	MG	13	1665	1/1	0.83	0.19	-	106,106,106,106	0
55	MG	14	3228	1/1	0.96	0.39	-	93,93,93,93	0
55	MG	14	3105	1/1	0.91	0.19	-	82,82,82,82	0
55	MG	1H	3062	1/1	0.97	0.24	-	70,70,70,70	0
55	MG	1H	3512	1/1	0.93	0.26	-	103,103,103,103	0
55	MG	1H	3211	1/1	0.85	0.33	-	94,94,94,94	0
55	MG	1H	3399	1/1	0.84	0.18	-	109,109,109,109	0
55	MG	14	3464	1/1	0.79	0.23	-	122,122,122,122	0
55	MG	14	3366	1/1	0.94	0.09	-	71,71,71,71	0
55	MG	1G	1691	1/1	0.81	0.47	-	122,122,122,122	0
55	MG	13	1667	1/1	0.69	0.30	-	99,99,99,99	0
55	MG	1J	205	1/1	0.78	0.22	-	112,112,112,112	0
55	MG	14	3341	1/1	0.90	0.18	-	102,102,102,102	0
55	MG	3L	101	1/1	0.92	0.24	-	189,189,189,189	0
55	MG	1H	3344	1/1	0.68	0.52	-	95,95,95,95	0
55	MG	14	3136	1/1	0.73	0.18	-	109,109,109,109	0
55	MG	13	1695	1/1	0.84	0.17	-	108,108,108,108	0
55	MG	14	3010	1/1	0.99	0.19	-	57,57,57,57	0
55	MG	1H	3057	1/1	0.92	0.27	-	76,76,76,76	0
55	MG	14	3207	1/1	0.94	0.12	-	96,96,96,96	0
55	MG	1H	3049	1/1	0.92	0.24	-	78,78,78,78	0
55	MG	13	1653	1/1	0.88	0.10	-	97,97,97,97	0
55	MG	1G	1609	1/1	0.73	0.17	-	106,106,106,106	0
55	MG	1G	1656	1/1	0.92	0.31	-	104,104,104,104	0
55	MG	14	3192	1/1	0.95	0.19	-	74,74,74,74	0
55	MG	14	3226	1/1	0.66	0.19	-	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
55	MG	13	1636	1/1	0.82	0.23	-	100,100,100,100	0
55	MG	14	3076	1/1	0.89	0.20	-	68,68,68,68	0
55	MG	1H	3243	1/1	0.73	0.18	-	119,119,119,119	0
55	MG	1H	3196	1/1	0.94	0.29	-	106,106,106,106	0
55	MG	14	3471	1/1	0.87	0.08	-	109,109,109,109	0
55	MG	1H	3365	1/1	0.94	0.24	-	96,96,96,96	0
55	MG	1H	3274	1/1	0.95	0.12	-	97,97,97,97	0
55	MG	1H	3362	1/1	0.70	0.29	-	112,112,112,112	0
55	MG	14	3190	1/1	0.93	0.14	-	85,85,85,85	0
55	MG	1H	3170	1/1	0.98	0.13	-	69,69,69,69	0
55	MG	13	1627	1/1	0.97	0.15	-	79,79,79,79	0
55	MG	1H	3311	1/1	0.96	0.18	-	85,85,85,85	0
55	MG	13	1682	1/1	0.97	0.31	-	98,98,98,98	0
55	MG	1H	3206	1/1	0.89	0.31	-	89,89,89,89	0
55	MG	14	3485	1/1	0.92	0.10	-	73,73,73,73	0
55	MG	1G	1681	1/1	0.86	0.18	-	105,105,105,105	0
55	MG	14	3026	1/1	0.96	0.25	-	76,76,76,76	0
55	MG	1H	3076	1/1	0.92	0.29	-	74,74,74,74	0
55	MG	1H	3086	1/1	0.98	0.17	-	60,60,60,60	0
55	MG	14	3483	1/1	0.87	0.15	-	113,113,113,113	0
55	MG	1H	3251	1/1	0.95	0.44	-	76,76,76,76	0
55	MG	1H	3223	1/1	0.90	0.25	-	77,77,77,77	0
55	MG	14	3063	1/1	0.91	0.21	-	85,85,85,85	0
55	MG	1G	1628	1/1	0.66	0.42	-	95,95,95,95	0
55	MG	14	3255	1/1	0.90	0.22	-	107,107,107,107	0
55	MG	1H	3203	1/1	0.94	0.35	-	83,83,83,83	0
55	MG	1H	3438	1/1	0.98	0.15	-	69,69,69,69	0
55	MG	14	3321	1/1	0.81	0.39	-	93,93,93,93	0
55	MG	14	3274	1/1	0.82	0.19	-	88,88,88,88	0
55	MG	13	1727	1/1	0.77	0.08	-	130,130,130,130	0
55	MG	14	3224	1/1	0.83	0.26	-	87,87,87,87	0
55	MG	1G	1682	1/1	0.91	0.18	-	145,145,145,145	0
55	MG	13	1625	1/1	0.95	0.20	-	63,63,63,63	0
55	MG	1H	3021	1/1	0.97	0.19	-	61,61,61,61	0
55	MG	78	201	1/1	0.83	0.42	-	94,94,94,94	0
55	MG	1H	3147	1/1	0.92	0.43	-	76,76,76,76	0
55	MG	1J	211	1/1	0.87	0.12	-	133,133,133,133	0
55	MG	14	3204	1/1	0.96	0.07	-	104,104,104,104	0
55	MG	14	3310	1/1	0.85	0.11	-	107,107,107,107	0
55	MG	1H	3207	1/1	0.50	0.31	-	101,101,101,101	0
55	MG	13	1693	1/1	0.79	0.28	-	103,103,103,103	0
55	MG	1H	3006	1/1	0.97	0.30	-	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
55	MG	1H	3015	1/1	0.97	0.33	-	56,56,56,56	0
55	MG	1H	3330	1/1	0.88	0.38	-	91,91,91,91	0
55	MG	1H	3199	1/1	0.96	0.56	-	106,106,106,106	0
55	MG	14	3061	1/1	0.99	0.12	-	79,79,79,79	0
55	MG	1H	3092	1/1	0.95	0.19	-	79,79,79,79	0
55	MG	14	3317	1/1	0.58	0.28	-	92,92,92,92	0
55	MG	1H	3233	1/1	0.80	0.65	-	117,117,117,117	0
55	MG	1H	3453	1/1	0.90	0.09	-	89,89,89,89	0
55	MG	14	3182	1/1	0.96	0.16	-	79,79,79,79	0
55	MG	1G	1729	1/1	0.97	0.17	-	112,112,112,112	0
55	MG	Q8	101	1/1	0.90	0.28	-	95,95,95,95	0
55	MG	1H	3260	1/1	0.80	0.29	-	114,114,114,114	0
55	MG	13	1724	1/1	0.96	0.23	-	113,113,113,113	0
55	MG	14	3053	1/1	0.98	0.21	-	49,49,49,49	0
55	MG	13	1613	1/1	0.92	0.19	-	123,123,123,123	0
55	MG	1G	1674	1/1	0.92	0.20	-	106,106,106,106	0
55	MG	1H	3341	1/1	0.78	0.31	-	94,94,94,94	0
55	MG	14	3181	1/1	0.90	0.23	-	97,97,97,97	0
55	MG	1H	3174	1/1	0.78	0.33	-	80,80,80,80	0
55	MG	1G	1651	1/1	0.78	0.28	-	92,92,92,92	0
55	MG	1H	3158	1/1	0.59	0.41	-	93,93,93,93	0
55	MG	1G	1710	1/1	0.84	0.63	-	107,107,107,107	0
55	MG	1H	3189	1/1	0.91	0.11	-	83,83,83,83	0
55	MG	1H	3416	1/1	0.94	0.15	-	77,77,77,77	0
55	MG	13	1712	1/1	0.84	0.06	-	119,119,119,119	0
55	MG	14	3330	1/1	0.78	0.25	-	85,85,85,85	0
55	MG	14	3240	1/1	0.91	0.18	-	100,100,100,100	0
55	MG	13	1677	1/1	0.98	0.27	-	96,96,96,96	0
55	MG	14	3065	1/1	0.90	0.24	-	86,86,86,86	0
55	MG	13	1686	1/1	0.76	0.42	-	111,111,111,111	0
55	MG	14	3323	1/1	0.42	0.31	-	113,113,113,113	0
55	MG	14	3360	1/1	0.98	0.10	-	64,64,64,64	0
55	MG	1H	3528	1/1	0.94	0.06	-	115,115,115,115	0
55	MG	1G	1677	1/1	0.95	0.28	-	97,97,97,97	0
55	MG	14	3474	1/1	0.88	0.14	-	142,142,142,142	0
55	MG	1H	3271	1/1	0.98	0.16	-	89,89,89,89	0
55	MG	1H	3402	1/1	0.88	0.10	-	110,110,110,110	0
55	MG	1G	1663	1/1	0.88	0.20	-	110,110,110,110	0
55	MG	1H	3400	1/1	0.97	0.14	-	87,87,87,87	0
55	MG	1H	3082	1/1	0.99	0.12	-	66,66,66,66	0
55	MG	78	202	1/1	0.67	0.49	-	91,91,91,91	0
55	MG	14	3261	1/1	0.97	0.48	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1711	1/1	0.74	0.89	-	107,107,107,107	0
55	MG	14	3248	1/1	0.98	0.16	-	110,110,110,110	0
55	MG	14	3157	1/1	0.85	0.25	-	95,95,95,95	0
55	MG	14	3329	1/1	0.89	0.23	-	85,85,85,85	0
55	MG	1H	3171	1/1	0.96	0.23	-	70,70,70,70	0
55	MG	13	1654	1/1	0.91	0.13	-	104,104,104,104	0
55	MG	14	3292	1/1	0.95	0.23	-	104,104,104,104	0
55	MG	1H	3537	1/1	0.85	0.10	-	148,148,148,148	0
55	MG	1H	3162	1/1	0.89	0.29	-	87,87,87,87	0
55	MG	14	3345	1/1	0.93	0.19	-	116,116,116,116	0
55	MG	1H	3245	1/1	0.86	0.23	-	74,74,74,74	0
55	MG	1H	3303	1/1	0.90	0.19	-	88,88,88,88	0
55	MG	14	3022	1/1	0.94	0.11	-	60,60,60,60	0
55	MG	1H	3297	1/1	0.68	0.26	-	104,104,104,104	0
55	MG	1G	1698	1/1	0.88	0.57	-	86,86,86,86	0
55	MG	1H	3522	1/1	0.51	0.09	-	112,112,112,112	0
55	MG	1H	3234	1/1	0.97	0.28	-	89,89,89,89	0
55	MG	1G	1708	1/1	0.91	0.19	-	96,96,96,96	0
55	MG	1J	204	1/1	0.85	0.24	-	128,128,128,128	0
55	MG	13	1700	1/1	0.97	0.11	-	97,97,97,97	0
55	MG	14	3470	1/1	0.83	0.11	-	136,136,136,136	0
55	MG	14	3468	1/1	0.88	0.11	-	134,134,134,134	0
55	MG	14	3303	1/1	0.95	0.34	-	122,122,122,122	0
55	MG	14	3117	1/1	0.92	0.11	-	87,87,87,87	0
55	MG	13	1638	1/1	0.85	0.44	-	103,103,103,103	0
55	MG	1H	3145	1/1	0.93	0.28	-	84,84,84,84	0
55	MG	1H	3029	1/1	0.95	0.26	-	84,84,84,84	0
55	MG	1H	3060	1/1	0.86	0.29	-	79,79,79,79	0
55	MG	14	3165	1/1	0.93	0.15	-	90,90,90,90	0
55	MG	1H	3128	1/1	0.91	0.35	-	77,77,77,77	0
55	MG	1H	3217	1/1	0.88	0.24	-	85,85,85,85	0
55	MG	1H	3295	1/1	0.87	0.41	-	87,87,87,87	0
55	MG	13	1634	1/1	0.93	0.14	-	79,79,79,79	0
55	MG	2K	104	1/1	0.85	0.08	-	153,153,153,153	0
55	MG	13	1688	1/1	0.91	0.38	-	107,107,107,107	0
55	MG	1J	203	1/1	0.90	0.11	-	121,121,121,121	0
55	MG	1H	3280	1/1	0.76	0.20	-	97,97,97,97	0
55	MG	1H	3099	1/1	0.78	0.11	-	90,90,90,90	0
55	MG	1H	3198	1/1	0.87	0.23	-	58,58,58,58	0
55	MG	13	1617	1/1	0.85	0.21	-	99,99,99,99	0
55	MG	13	1714	1/1	0.95	0.07	-	120,120,120,120	0
55	MG	1H	3172	1/1	0.81	0.58	-	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
55	MG	1H	3497	1/1	0.80	0.09	-	152,152,152,152	0
55	MG	1G	1637	1/1	0.87	0.31	-	127,127,127,127	0
55	MG	1G	1670	1/1	0.65	0.32	-	115,115,115,115	0
55	MG	14	3428	1/1	0.99	0.11	-	92,92,92,92	0
55	MG	14	3327	1/1	0.91	0.15	-	101,101,101,101	0
55	MG	1H	3194	1/1	0.90	0.30	-	75,75,75,75	0
55	MG	1H	3377	1/1	0.92	0.19	-	66,66,66,66	0
55	MG	14	3277	1/1	0.91	0.15	-	68,68,68,68	0
55	MG	14	3340	1/1	0.88	0.25	-	103,103,103,103	0
55	MG	E5	102	1/1	0.93	0.34	-	116,116,116,116	0
55	MG	1H	3023	1/1	0.81	0.41	-	101,101,101,101	0
55	MG	14	3480	1/1	0.88	0.11	-	90,90,90,90	0
55	MG	1H	3347	1/1	0.79	0.37	-	117,117,117,117	0
55	MG	14	3052	1/1	0.95	0.27	-	74,74,74,74	0
55	MG	14	3314	1/1	0.82	0.14	-	111,111,111,111	0
55	MG	14	3326	1/1	0.66	0.51	-	103,103,103,103	0
55	MG	14	3196	1/1	0.84	0.26	-	107,107,107,107	0
55	MG	14	3418	1/1	0.98	0.11	-	70,70,70,70	0
55	MG	1G	1635	1/1	0.74	0.31	-	98,98,98,98	0
55	MG	1H	3202	1/1	0.97	0.21	-	75,75,75,75	0
55	MG	13	1679	1/1	0.89	0.25	-	101,101,101,101	0
55	MG	13	1699	1/1	0.86	0.05	-	137,137,137,137	0
55	MG	14	3191	1/1	0.96	0.30	-	97,97,97,97	0
55	MG	14	3466	1/1	0.88	0.06	-	104,104,104,104	0
55	MG	1H	3440	1/1	0.99	0.12	-	59,59,59,59	0
55	MG	1H	3184	1/1	0.91	0.12	-	66,66,66,66	0
55	MG	14	3257	1/1	0.66	0.29	-	109,109,109,109	0
55	MG	1H	3469	1/1	0.94	0.17	-	109,109,109,109	0
55	MG	1H	3008	1/1	0.95	0.26	-	74,74,74,74	0
55	MG	1G	1664	1/1	0.60	0.21	-	112,112,112,112	0
55	MG	14	3119	1/1	0.89	0.29	-	82,82,82,82	0
55	MG	13	1628	1/1	0.89	0.30	-	89,89,89,89	0
55	MG	13	1729	1/1	0.96	0.13	-	115,115,115,115	0
55	MG	13	1684	1/1	0.36	0.18	-	99,99,99,99	0
55	MG	14	3268	1/1	0.95	0.19	-	87,87,87,87	0
55	MG	1H	3351	1/1	0.76	0.44	-	114,114,114,114	0
55	MG	14	3328	1/1	0.68	0.25	-	103,103,103,103	0
55	MG	1H	3159	1/1	0.94	0.66	-	90,90,90,90	0
55	MG	13	1647	1/1	0.76	0.30	-	87,87,87,87	0
55	MG	14	3433	1/1	0.92	0.09	-	105,105,105,105	0
55	MG	14	3090	1/1	0.96	0.29	-	53,53,53,53	0
55	MG	14	3288	1/1	0.95	0.21	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3510	1/1	0.95	0.06	-	125,125,125,125	0
55	MG	1G	1676	1/1	0.71	0.21	-	129,129,129,129	0
55	MG	13	1609	1/1	0.85	0.21	-	130,130,130,130	0
55	MG	I8	102	1/1	0.96	0.44	-	73,73,73,73	0
55	MG	1G	1721	1/1	0.91	0.09	-	121,121,121,121	0
55	MG	1H	3272	1/1	0.94	0.15	-	97,97,97,97	0
55	MG	1H	3120	1/1	0.92	0.31	-	69,69,69,69	0
55	MG	3L	102	1/1	0.84	0.40	-	95,95,95,95	0
55	MG	13	1669	1/1	0.84	0.42	-	115,115,115,115	0
55	MG	1G	1655	1/1	0.98	0.17	-	88,88,88,88	0
55	MG	1H	3168	1/1	0.70	0.38	-	75,75,75,75	0
55	MG	1H	3451	1/1	0.76	0.21	-	123,123,123,123	0
55	MG	1H	3098	1/1	0.98	0.21	-	73,73,73,73	0
55	MG	1J	208	1/1	0.96	0.07	-	104,104,104,104	0
55	MG	14	3233	1/1	0.73	0.32	-	84,84,84,84	0
55	MG	1H	3135	1/1	0.70	0.60	-	102,102,102,102	0
55	MG	1H	3167	1/1	0.92	0.23	-	119,119,119,119	0
55	MG	1H	3324	1/1	0.82	0.27	-	96,96,96,96	0
55	MG	1H	3142	1/1	0.82	0.19	-	81,81,81,81	0
55	MG	1H	3448	1/1	0.98	0.21	-	79,79,79,79	0
55	MG	13	1664	1/1	0.92	0.18	-	142,142,142,142	0
55	MG	14	3423	1/1	0.90	0.14	-	101,101,101,101	0
55	MG	1H	3525	1/1	0.75	0.10	-	127,127,127,127	0
55	MG	1H	3055	1/1	0.98	0.22	-	55,55,55,55	0
55	MG	14	3331	1/1	0.86	0.66	-	79,79,79,79	0
55	MG	1H	3432	1/1	0.99	0.12	-	85,85,85,85	0
55	MG	14	3337	1/1	0.95	0.30	-	111,111,111,111	0
55	MG	1H	3442	1/1	0.92	0.11	-	97,97,97,97	0
55	MG	1G	1613	1/1	0.79	0.24	-	104,104,104,104	0
55	MG	14	3250	1/1	0.91	0.18	-	80,80,80,80	0
55	MG	14	3006	1/1	0.98	0.24	-	53,53,53,53	0
55	MG	14	3004	1/1	0.98	0.31	-	62,62,62,62	0
55	MG	1H	3536	1/1	0.93	0.04	-	130,130,130,130	0
55	MG	14	3443	1/1	0.93	0.07	-	106,106,106,106	0
55	MG	29	304	1/1	0.56	0.34	-	115,115,115,115	0
55	MG	1H	3018	1/1	0.98	0.21	-	76,76,76,76	0
55	MG	1G	1743	1/1	0.91	0.09	-	128,128,128,128	0
55	MG	1G	1707	1/1	0.96	0.21	-	91,91,91,91	0
55	MG	14	3270	1/1	0.85	0.15	-	88,88,88,88	0
55	MG	1G	1629	1/1	0.76	0.23	-	91,91,91,91	0
55	MG	14	3300	1/1	0.86	0.29	-	85,85,85,85	0
55	MG	16	207	1/1	0.92	0.29	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1658	1/1	0.89	0.37	-	84,84,84,84	0
55	MG	14	3189	1/1	0.95	0.29	-	98,98,98,98	0
55	MG	1H	3276	1/1	0.75	0.21	-	89,89,89,89	0
55	MG	14	3305	1/1	0.88	0.58	-	94,94,94,94	0
55	MG	13	1715	1/1	0.96	0.24	-	108,108,108,108	0
55	MG	13	1721	1/1	0.89	0.15	-	100,100,100,100	0
55	MG	1H	3045	1/1	0.95	0.23	-	104,104,104,104	0
55	MG	14	3067	1/1	0.92	0.15	-	66,66,66,66	0
55	MG	1H	3443	1/1	0.96	0.19	-	97,97,97,97	0
55	MG	14	3058	1/1	0.97	0.20	-	64,64,64,64	0
55	MG	14	3183	1/1	0.99	0.36	-	98,98,98,98	0
55	MG	1G	1621	1/1	0.90	0.13	-	90,90,90,90	0
55	MG	1H	3050	1/1	0.92	0.36	-	73,73,73,73	0
55	MG	14	3450	1/1	0.88	0.15	-	113,113,113,113	0
55	MG	13	1666	1/1	0.77	0.15	-	95,95,95,95	0
55	MG	14	3106	1/1	0.96	0.34	-	75,75,75,75	0
55	MG	14	3469	1/1	0.97	0.06	-	115,115,115,115	0
55	MG	1H	3527	1/1	0.94	0.14	-	118,118,118,118	0
55	MG	1H	3176	1/1	0.95	0.47	-	93,93,93,93	0
55	MG	C5	201	1/1	0.71	0.32	-	95,95,95,95	0
55	MG	14	3008	1/1	0.96	0.15	-	52,52,52,52	0
55	MG	14	3095	1/1	0.95	0.43	-	87,87,87,87	0
55	MG	1H	3414	1/1	0.99	0.14	-	51,51,51,51	0
55	MG	14	3066	1/1	0.93	0.21	-	82,82,82,82	0
55	MG	14	3149	1/1	0.77	0.33	-	81,81,81,81	0
55	MG	1H	3262	1/1	0.73	0.28	-	101,101,101,101	0
55	MG	1H	3320	1/1	0.89	0.51	-	106,106,106,106	0
55	MG	14	3343	1/1	0.90	0.40	-	83,83,83,83	0
55	MG	1H	3410	1/1	0.92	0.08	-	82,82,82,82	0
55	MG	14	3291	1/1	0.90	0.14	-	88,88,88,88	0
55	MG	14	3415	1/1	0.95	0.06	-	96,96,96,96	0
55	MG	1H	3240	1/1	0.85	0.38	-	91,91,91,91	0
55	MG	1H	3329	1/1	0.96	0.33	-	96,96,96,96	0
55	MG	1H	3177	1/1	0.97	0.27	-	69,69,69,69	0
55	MG	1H	3310	1/1	0.83	0.36	-	84,84,84,84	0
55	MG	1H	3068	1/1	0.97	0.39	-	72,72,72,72	0
55	MG	1G	1647	1/1	0.94	0.14	-	102,102,102,102	0
55	MG	1H	3535	1/1	0.97	0.08	-	115,115,115,115	0
55	MG	1H	3261	1/1	0.90	0.53	-	109,109,109,109	0
55	MG	14	3369	1/1	0.96	0.13	-	63,63,63,63	0
55	MG	1H	3546	1/1	0.82	0.19	-	89,89,89,89	0
55	MG	14	3239	1/1	0.93	0.13	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3541	1/1	0.94	0.12	-	89,89,89,89	0
55	MG	14	3299	1/1	0.73	0.40	-	138,138,138,138	0
55	MG	1H	3132	1/1	0.85	0.15	-	77,77,77,77	0
55	MG	14	3039	1/1	0.98	0.23	-	90,90,90,90	0
55	MG	1H	3009	1/1	0.97	0.30	-	67,67,67,67	0
55	MG	14	3437	1/1	0.84	0.12	-	98,98,98,98	0
55	MG	1H	3197	1/1	0.88	0.24	-	93,93,93,93	0
55	MG	1H	3270	1/1	0.85	0.38	-	92,92,92,92	0
55	MG	13	1663	1/1	0.80	0.35	-	108,108,108,108	0
55	MG	14	3234	1/1	0.69	0.32	-	96,96,96,96	0
55	MG	14	3454	1/1	0.95	0.11	-	96,96,96,96	0
55	MG	1H	3165	1/1	0.86	0.32	-	81,81,81,81	0
55	MG	14	3007	1/1	0.98	0.28	-	75,75,75,75	0
55	MG	1H	3074	1/1	0.96	0.38	-	63,63,63,63	0
55	MG	14	3104	1/1	0.80	0.39	-	96,96,96,96	0
55	MG	1H	3281	1/1	0.42	0.35	-	103,103,103,103	0
55	MG	1H	3434	1/1	0.97	0.06	-	109,109,109,109	0
55	MG	1H	3503	1/1	0.99	0.16	-	75,75,75,75	0
55	MG	14	3316	1/1	0.76	0.29	-	97,97,97,97	0
55	MG	1H	3242	1/1	0.51	0.34	-	107,107,107,107	0
55	MG	1H	3315	1/1	0.67	0.40	-	107,107,107,107	0
55	MG	13	1614	1/1	0.98	0.23	-	96,96,96,96	0
55	MG	25	201	1/1	0.92	0.07	-	129,129,129,129	0
55	MG	14	3225	1/1	0.90	0.35	-	94,94,94,94	0
55	MG	14	3435	1/1	0.91	0.11	-	123,123,123,123	0
55	MG	14	3380	1/1	0.93	0.09	-	92,92,92,92	0
55	MG	1H	3269	1/1	0.96	0.25	-	107,107,107,107	0
55	MG	1H	3370	1/1	0.77	0.45	-	87,87,87,87	0
55	MG	1H	3238	1/1	0.97	0.25	-	97,97,97,97	0
55	MG	1H	3002	1/1	0.99	0.30	-	61,61,61,61	0
55	MG	13	1676	1/1	0.91	0.30	-	120,120,120,120	0
55	MG	14	3297	1/1	0.72	0.20	-	81,81,81,81	0
55	MG	1H	3192	1/1	0.61	0.52	-	97,97,97,97	0
55	MG	1G	1686	1/1	0.91	0.24	-	121,121,121,121	0
55	MG	1H	3003	1/1	0.99	0.28	-	51,51,51,51	0
55	MG	14	3229	1/1	0.91	0.31	-	71,71,71,71	0
55	MG	14	3322	1/1	0.98	0.63	-	91,91,91,91	0
55	MG	1H	3437	1/1	0.99	0.14	-	94,94,94,94	0
55	MG	1H	3249	1/1	0.27	0.38	-	102,102,102,102	0
55	MG	14	3120	1/1	0.96	0.21	-	69,69,69,69	0
55	MG	1G	1672	1/1	0.91	0.33	-	111,111,111,111	0
55	MG	14	3455	1/1	0.83	0.19	-	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3424	1/1	0.86	0.10	-	113,113,113,113	0
55	MG	1H	3255	1/1	0.73	0.28	-	107,107,107,107	0
55	MG	1H	3267	1/1	0.93	0.40	-	95,95,95,95	0
55	MG	45	201	1/1	0.64	0.28	-	78,78,78,78	0
55	MG	14	3221	1/1	0.87	0.23	-	82,82,82,82	0
55	MG	14	3332	1/1	0.81	0.21	-	89,89,89,89	0
55	MG	14	3325	1/1	0.72	0.33	-	107,107,107,107	0
55	MG	13	1621	1/1	0.95	0.18	-	116,116,116,116	0
55	MG	14	3123	1/1	0.76	0.36	-	95,95,95,95	0
55	MG	1H	3408	1/1	0.94	0.08	-	102,102,102,102	0
55	MG	1H	3220	1/1	0.86	0.43	-	92,92,92,92	0
55	MG	1H	3257	1/1	0.92	0.41	-	102,102,102,102	0
55	MG	1H	3105	1/1	0.97	0.32	-	62,62,62,62	0
55	MG	1H	3307	1/1	0.65	0.27	-	105,105,105,105	0
55	MG	1H	3264	1/1	0.81	0.51	-	85,85,85,85	0
55	MG	13	1725	1/1	0.83	0.15	-	157,157,157,157	0
55	MG	13	1637	1/1	0.96	0.18	-	113,113,113,113	0
55	MG	14	3029	1/1	0.73	0.43	-	85,85,85,85	0
55	MG	14	3432	1/1	0.96	0.10	-	107,107,107,107	0
55	MG	1H	3169	1/1	0.99	0.19	-	68,68,68,68	0
55	MG	14	3461	1/1	0.97	0.22	-	88,88,88,88	0
55	MG	1H	3467	1/1	0.91	0.10	-	101,101,101,101	0
55	MG	14	3166	1/1	0.96	0.16	-	86,86,86,86	0
55	MG	1H	3482	1/1	0.94	0.18	-	99,99,99,99	0
55	MG	13	1689	1/1	0.71	0.38	-	102,102,102,102	0
55	MG	1H	3061	1/1	0.83	0.29	-	90,90,90,90	0
55	MG	1H	3275	1/1	0.94	0.23	-	85,85,85,85	0
55	MG	1G	1730	1/1	0.96	0.07	-	100,100,100,100	0
55	MG	14	3042	1/1	0.97	0.07	-	71,71,71,71	0
55	MG	1H	3508	1/1	0.87	0.14	-	122,122,122,122	0
55	MG	1H	3216	1/1	0.47	0.32	-	93,93,93,93	0
55	MG	14	3293	1/1	0.90	0.32	-	105,105,105,105	0
55	MG	14	3087	1/1	0.90	0.26	-	101,101,101,101	0
55	MG	1H	3247	1/1	0.93	0.17	-	89,89,89,89	0
55	MG	14	3097	1/1	0.64	0.27	-	94,94,94,94	0
55	MG	1G	1739	1/1	0.94	0.15	-	112,112,112,112	0
55	MG	14	3032	1/1	0.95	0.21	-	79,79,79,79	0
55	MG	1H	3014	1/1	0.95	0.29	-	69,69,69,69	0
55	MG	14	3249	1/1	0.70	0.28	-	106,106,106,106	0
55	MG	1G	1680	1/1	0.87	0.15	-	101,101,101,101	0
55	MG	13	1645	1/1	0.97	0.23	-	84,84,84,84	0
55	MG	13	1696	1/1	0.87	0.18	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1630	1/1	0.90	0.23	-	75,75,75,75	0
55	MG	1G	1652	1/1	0.95	0.35	-	100,100,100,100	0
55	MG	14	3082	1/1	0.97	0.34	-	100,100,100,100	0
55	MG	1H	3319	1/1	0.63	0.21	-	91,91,91,91	0
55	MG	14	3271	1/1	0.42	0.45	-	99,99,99,99	0
55	MG	1G	1705	1/1	0.79	0.18	-	110,110,110,110	0
55	MG	14	3267	1/1	0.75	0.14	-	99,99,99,99	0
55	MG	29	301	1/1	0.96	0.11	-	67,67,67,67	0
55	MG	14	3023	1/1	0.97	0.23	-	89,89,89,89	0
55	MG	1H	3213	1/1	0.73	0.36	-	80,80,80,80	0
55	MG	13	1602	1/1	0.98	0.15	-	88,88,88,88	0
55	MG	13	1713	1/1	0.97	0.11	-	94,94,94,94	0
55	MG	14	3336	1/1	0.86	0.63	-	102,102,102,102	0
55	MG	1H	3501	1/1	0.94	0.13	-	93,93,93,93	0
55	MG	1H	3283	1/1	0.94	0.54	-	104,104,104,104	0
55	MG	1H	3191	1/1	0.91	0.43	-	90,90,90,90	0
55	MG	1H	3294	1/1	0.75	0.44	-	91,91,91,91	0
55	MG	1H	3356	1/1	0.91	0.32	-	98,98,98,98	0
55	MG	1G	1646	1/1	0.89	0.17	-	81,81,81,81	0
55	MG	1H	3020	1/1	0.78	0.13	-	103,103,103,103	0
55	MG	1H	3205	1/1	0.88	0.45	-	101,101,101,101	0
55	MG	14	3442	1/1	0.94	0.27	-	84,84,84,84	0
55	MG	1G	1678	1/1	0.69	0.57	-	107,107,107,107	0
55	MG	1H	3367	1/1	0.82	0.23	-	97,97,97,97	0
55	MG	2L	102	1/1	0.92	0.16	-	113,113,113,113	0
55	MG	14	3333	1/1	0.90	0.49	-	96,96,96,96	0
55	MG	1G	1683	1/1	0.57	0.22	-	102,102,102,102	0
55	MG	1H	3366	1/1	0.89	0.27	-	113,113,113,113	0
55	MG	1H	3124	1/1	0.93	0.43	-	85,85,85,85	0
55	MG	1J	210	1/1	0.92	0.13	-	105,105,105,105	0
55	MG	1H	3495	1/1	0.97	0.08	-	122,122,122,122	0
55	MG	14	3405	1/1	0.97	0.11	-	65,65,65,65	0
55	MG	1H	3277	1/1	0.94	0.46	-	88,88,88,88	0
55	MG	14	3162	1/1	0.81	0.19	-	92,92,92,92	0
55	MG	1H	3524	1/1	0.89	0.33	-	123,123,123,123	0
55	MG	1H	3225	1/1	0.89	0.24	-	113,113,113,113	0
55	MG	1H	3038	1/1	0.98	0.28	-	56,56,56,56	0
55	MG	1H	3064	1/1	0.96	0.37	-	82,82,82,82	0
55	MG	1G	1696	1/1	0.17	0.33	-	112,112,112,112	0
55	MG	1H	3139	1/1	0.77	0.43	-	101,101,101,101	0
55	MG	1H	3190	1/1	0.95	0.21	-	98,98,98,98	0
55	MG	1H	3314	1/1	0.74	0.41	-	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
55	MG	1H	3292	1/1	0.95	0.22	-	100,100,100,100	0
55	MG	1H	3308	1/1	0.96	0.19	-	90,90,90,90	0
55	MG	1H	3431	1/1	0.85	0.19	-	127,127,127,127	0
55	MG	1G	1615	1/1	0.94	0.27	-	83,83,83,83	0
55	MG	1H	3230	1/1	0.76	0.39	-	91,91,91,91	0
55	MG	14	3430	1/1	0.93	0.07	-	114,114,114,114	0
55	MG	1H	3149	1/1	0.86	0.56	-	98,98,98,98	0
55	MG	14	3203	1/1	0.70	0.40	-	98,98,98,98	0
55	MG	1G	1737	1/1	0.78	0.23	-	147,147,147,147	0
55	MG	1H	3042	1/1	0.92	0.32	-	69,69,69,69	0
55	MG	1G	1715	1/1	0.81	0.29	-	116,116,116,116	0
55	MG	14	3387	1/1	0.90	0.07	-	77,77,77,77	0
55	MG	13	1635	1/1	0.70	0.50	-	106,106,106,106	0
55	MG	14	3197	1/1	0.76	0.33	-	105,105,105,105	0
55	MG	14	3444	1/1	0.66	0.09	-	113,113,113,113	0
55	MG	14	3001	1/1	0.80	0.13	-	84,84,84,84	0
55	MG	14	3018	1/1	0.92	0.22	-	81,81,81,81	0
55	MG	1H	3406	1/1	0.96	0.14	-	103,103,103,103	0
55	MG	14	3347	1/1	0.89	0.19	-	72,72,72,72	0
55	MG	1H	3144	1/1	0.87	0.45	-	86,86,86,86	0
55	MG	13	1675	1/1	0.62	0.33	-	127,127,127,127	0
55	MG	1H	3490	1/1	0.96	0.17	-	88,88,88,88	0
55	MG	1G	1619	1/1	0.96	0.20	-	92,92,92,92	0
55	MG	1G	1665	1/1	0.44	0.23	-	107,107,107,107	0
55	MG	1G	1699	1/1	0.92	0.14	-	157,157,157,157	0
55	MG	14	3051	1/1	0.99	0.35	-	78,78,78,78	0
55	MG	1H	3296	1/1	0.95	0.23	-	92,92,92,92	0
55	MG	14	3289	1/1	0.71	0.21	-	100,100,100,100	0
55	MG	1H	3037	1/1	0.83	0.20	-	78,78,78,78	0
55	MG	14	3099	1/1	0.96	0.24	-	75,75,75,75	0
55	MG	14	3361	1/1	0.97	0.20	-	75,75,75,75	0
55	MG	14	3417	1/1	0.81	0.07	-	119,119,119,119	0
55	MG	14	3130	1/1	0.95	0.25	-	85,85,85,85	0
55	MG	1H	3514	1/1	0.92	0.13	-	129,129,129,129	0
55	MG	14	3176	1/1	0.93	0.15	-	75,75,75,75	0
55	MG	1H	3313	1/1	0.86	0.51	-	100,100,100,100	0
55	MG	1G	1611	1/1	0.92	0.11	-	92,92,92,92	0
55	MG	1H	3353	1/1	0.73	0.42	-	100,100,100,100	0
55	MG	14	3138	1/1	0.82	0.26	-	90,90,90,90	0
55	MG	1H	3502	1/1	0.85	0.12	-	125,125,125,125	0
55	MG	5E	201	1/1	0.77	0.32	-	121,121,121,121	0
55	MG	M5	101	1/1	0.89	0.14	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1633	1/1	0.83	0.32	-	91,91,91,91	0
55	MG	1H	3222	1/1	0.87	0.19	-	83,83,83,83	0
55	MG	1H	3542	1/1	0.93	0.16	-	123,123,123,123	0
55	MG	14	3489	1/1	0.98	0.66	-	91,91,91,91	0
55	MG	14	3460	1/1	0.84	0.09	-	94,94,94,94	0
55	MG	14	3237	1/1	0.74	0.32	-	79,79,79,79	0
55	MG	1H	3420	1/1	0.96	0.14	-	71,71,71,71	0
55	MG	14	3304	1/1	0.84	0.35	-	85,85,85,85	0
55	MG	1H	3114	1/1	0.84	0.30	-	94,94,94,94	0
55	MG	1H	3411	1/1	0.87	0.09	-	110,110,110,110	0
55	MG	1H	3481	1/1	0.97	0.11	-	77,77,77,77	0
55	MG	1H	3333	1/1	0.54	0.43	-	97,97,97,97	0
55	MG	14	3324	1/1	0.44	0.19	-	119,119,119,119	0
55	MG	14	3258	1/1	0.77	0.24	-	78,78,78,78	0
55	MG	1H	3318	1/1	0.84	0.34	-	86,86,86,86	0
55	MG	1H	3035	1/1	0.95	0.48	-	98,98,98,98	0
55	MG	14	3003	1/1	0.93	0.25	-	67,67,67,67	0
55	MG	14	3135	1/1	0.99	0.43	-	101,101,101,101	0
55	MG	1H	3389	1/1	0.97	0.09	-	72,72,72,72	0
55	MG	14	3421	1/1	0.99	0.11	-	73,73,73,73	0
55	MG	1H	3022	1/1	0.98	0.20	-	83,83,83,83	0
55	MG	13	1649	1/1	0.97	0.25	-	121,121,121,121	0
55	MG	1H	3441	1/1	0.95	0.33	-	97,97,97,97	0
55	MG	1G	1731	1/1	0.80	0.07	-	117,117,117,117	0
55	MG	1H	3489	1/1	0.83	0.10	-	108,108,108,108	0
55	MG	14	3043	1/1	0.98	0.47	-	84,84,84,84	0
55	MG	14	3438	1/1	0.91	0.05	-	104,104,104,104	0
55	MG	13	1716	1/1	0.95	0.07	-	97,97,97,97	0
55	MG	1H	3071	1/1	0.75	0.67	-	80,80,80,80	0
55	MG	1H	3127	1/1	0.93	0.61	-	93,93,93,93	0
55	MG	14	3367	1/1	0.95	0.14	-	87,87,87,87	0
55	MG	1H	3460	1/1	0.95	0.09	-	94,94,94,94	0
55	MG	14	3033	1/1	0.97	0.26	-	83,83,83,83	0
55	MG	14	3318	1/1	0.81	0.31	-	102,102,102,102	0
55	MG	14	3306	1/1	0.49	0.55	-	92,92,92,92	0
55	MG	14	3278	1/1	0.91	0.23	-	82,82,82,82	0
55	MG	14	3193	1/1	0.85	0.20	-	90,90,90,90	0
55	MG	14	3379	1/1	0.98	0.09	-	99,99,99,99	0
55	MG	14	3145	1/1	0.94	0.27	-	75,75,75,75	0
55	MG	14	3187	1/1	0.97	0.21	-	103,103,103,103	0
55	MG	1H	3285	1/1	0.86	0.49	-	91,91,91,91	0
55	MG	14	3251	1/1	0.89	0.42	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3340	1/1	0.94	0.25	-	81,81,81,81	0
55	MG	1G	1668	1/1	0.92	0.34	-	99,99,99,99	0
55	MG	1H	3146	1/1	0.83	0.45	-	98,98,98,98	0
55	MG	14	3046	1/1	0.88	0.23	-	88,88,88,88	0
55	MG	13	1707	1/1	0.98	0.13	-	101,101,101,101	0
55	MG	1H	3345	1/1	0.79	0.27	-	104,104,104,104	0
55	MG	14	3009	1/1	0.95	0.23	-	67,67,67,67	0
55	MG	11	301	1/1	0.81	0.35	-	93,93,93,93	0
55	MG	14	3179	1/1	0.62	0.29	-	107,107,107,107	0
55	MG	1H	3464	1/1	0.98	0.09	-	86,86,86,86	0
55	MG	1H	3266	1/1	0.81	0.35	-	106,106,106,106	0
55	MG	14	3072	1/1	0.96	0.24	-	85,85,85,85	0
55	MG	1H	3298	1/1	0.89	0.35	-	114,114,114,114	0
55	MG	14	3363	1/1	0.98	0.13	-	73,73,73,73	0
55	MG	1H	3530	1/1	0.93	0.19	-	97,97,97,97	0
55	MG	13	1720	1/1	0.84	0.16	-	136,136,136,136	0
55	MG	14	3254	1/1	0.94	0.19	-	95,95,95,95	0
55	MG	1H	3305	1/1	0.89	0.54	-	107,107,107,107	0
55	MG	1H	3104	1/1	0.95	0.51	-	84,84,84,84	0
55	MG	1H	3500	1/1	0.95	0.14	-	87,87,87,87	0
55	MG	14	3245	1/1	0.98	0.13	-	109,109,109,109	0
55	MG	13	1610	1/1	0.91	0.10	-	104,104,104,104	0
55	MG	14	3309	1/1	0.96	0.14	-	85,85,85,85	0
55	MG	14	3211	1/1	0.46	0.38	-	101,101,101,101	0
55	MG	1H	3219	1/1	0.87	0.44	-	90,90,90,90	0
55	MG	1H	3398	1/1	0.58	0.09	-	110,110,110,110	0
55	MG	1H	3175	1/1	0.66	0.43	-	96,96,96,96	0
55	MG	1H	3095	1/1	0.94	0.33	-	72,72,72,72	0
55	MG	1H	3007	1/1	0.96	0.30	-	53,53,53,53	0
55	MG	13	1639	1/1	0.85	0.27	-	89,89,89,89	0
55	MG	13	1622	1/1	0.95	0.18	-	96,96,96,96	0
55	MG	1G	1741	1/1	0.90	0.08	-	140,140,140,140	0
55	MG	1G	1726	1/1	0.92	0.07	-	137,137,137,137	0
55	MG	13	1694	1/1	0.59	0.54	-	108,108,108,108	0
55	MG	1H	3188	1/1	0.94	0.30	-	88,88,88,88	0
55	MG	5E	202	1/1	0.83	0.21	-	109,109,109,109	0
55	MG	1H	3462	1/1	0.94	0.09	-	104,104,104,104	0
55	MG	14	3352	1/1	0.96	0.09	-	65,65,65,65	0
55	MG	14	3484	1/1	0.90	0.10	-	146,146,146,146	0
55	MG	14	3114	1/1	0.94	0.30	-	83,83,83,83	0
55	MG	1H	3125	1/1	0.99	0.22	-	93,93,93,93	0
55	MG	14	3377	1/1	0.96	0.09	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3533	1/1	0.94	0.18	-	88,88,88,88	0
55	MG	1G	1669	1/1	0.18	0.23	-	119,119,119,119	0
55	MG	14	3102	1/1	0.88	0.17	-	86,86,86,86	0
55	MG	1H	3138	1/1	0.91	0.18	-	82,82,82,82	0
55	MG	14	3478	1/1	0.95	0.23	-	102,102,102,102	0
55	MG	1H	3504	1/1	0.75	0.12	-	131,131,131,131	0
55	MG	1H	3317	1/1	0.95	0.34	-	87,87,87,87	0
55	MG	14	3113	1/1	0.67	0.22	-	85,85,85,85	0
55	MG	1H	3100	1/1	0.90	0.25	-	76,76,76,76	0
55	MG	14	3409	1/1	0.99	0.10	-	99,99,99,99	0
55	MG	14	3459	1/1	0.84	0.07	-	114,114,114,114	0
55	MG	13	1728	1/1	0.95	0.09	-	119,119,119,119	0
55	MG	1H	3515	1/1	0.94	0.06	-	125,125,125,125	0
55	MG	14	3273	1/1	0.94	0.20	-	92,92,92,92	0
55	MG	14	3094	1/1	0.89	0.14	-	68,68,68,68	0
55	MG	14	3419	1/1	0.85	0.07	-	104,104,104,104	0
55	MG	1H	3141	1/1	0.75	0.34	-	90,90,90,90	0
55	MG	14	3269	1/1	0.78	0.25	-	93,93,93,93	0
55	MG	1H	3109	1/1	0.92	0.11	-	57,57,57,57	0
55	MG	14	3290	1/1	0.96	0.18	-	102,102,102,102	0
55	MG	14	3213	1/1	0.69	0.27	-	108,108,108,108	0
55	MG	1H	3446	1/1	0.94	0.16	-	112,112,112,112	0
55	MG	14	3177	1/1	0.91	0.17	-	91,91,91,91	0
55	MG	1H	3523	1/1	0.92	0.08	-	135,135,135,135	0
55	MG	14	3434	1/1	0.95	0.11	-	102,102,102,102	0
55	MG	14	3127	1/1	0.96	0.17	-	87,87,87,87	0
55	MG	14	3212	1/1	0.76	0.21	-	94,94,94,94	0
55	MG	14	3232	1/1	0.91	0.10	-	86,86,86,86	0
55	MG	1G	1717	1/1	0.69	0.15	-	111,111,111,111	0
55	MG	1H	3355	1/1	0.72	0.28	-	92,92,92,92	0
55	MG	1H	3218	1/1	0.91	0.31	-	87,87,87,87	0
55	MG	1H	3499	1/1	0.86	0.09	-	116,116,116,116	0
55	MG	1G	1728	1/1	0.88	0.09	-	133,133,133,133	0
55	MG	1H	3394	1/1	0.92	0.15	-	119,119,119,119	0
55	MG	13	1691	1/1	0.88	0.13	-	98,98,98,98	0
55	MG	14	3069	1/1	0.96	0.45	-	86,86,86,86	0
55	MG	13	1623	1/1	0.87	0.22	-	104,104,104,104	0
55	MG	1H	3288	1/1	0.90	0.33	-	86,86,86,86	0
55	MG	14	3167	1/1	0.91	0.10	-	107,107,107,107	0
55	MG	1H	3409	1/1	0.91	0.18	-	84,84,84,84	0
55	MG	1H	3468	1/1	0.90	0.41	-	120,120,120,120	0
55	MG	1H	3024	1/1	0.89	0.43	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3214	1/1	0.90	0.62	-	94,94,94,94	0
55	MG	E5	101	1/1	0.95	0.16	-	73,73,73,73	0
55	MG	14	3238	1/1	0.83	0.26	-	153,153,153,153	0
55	MG	1H	3343	1/1	0.87	0.21	-	75,75,75,75	0
55	MG	13	1723	1/1	0.96	0.07	-	107,107,107,107	0
55	MG	1H	3470	1/1	0.96	0.15	-	98,98,98,98	0
55	MG	16	210	1/1	0.64	0.36	-	117,117,117,117	0
55	MG	1G	1612	1/1	0.68	0.20	-	108,108,108,108	0
55	MG	14	3388	1/1	0.95	0.11	-	80,80,80,80	0
55	MG	14	3298	1/1	0.93	0.75	-	88,88,88,88	0
55	MG	1H	3380	1/1	0.98	0.08	-	63,63,63,63	0
55	MG	14	3148	1/1	0.98	0.10	-	79,79,79,79	0
55	MG	1H	3039	1/1	0.97	0.27	-	55,55,55,55	0
55	MG	14	3262	1/1	0.94	0.13	-	84,84,84,84	0
55	MG	1G	1603	1/1	0.97	0.12	-	99,99,99,99	0
55	MG	13	1690	1/1	0.62	0.36	-	136,136,136,136	0
55	MG	14	3393	1/1	0.86	0.19	-	103,103,103,103	0
55	MG	14	3188	1/1	0.97	0.19	-	71,71,71,71	0
55	MG	1G	1723	1/1	0.83	0.20	-	131,131,131,131	0
55	MG	14	3132	1/1	0.90	0.23	-	90,90,90,90	0
55	MG	1H	3519	1/1	0.92	0.08	-	132,132,132,132	0
55	MG	1H	3164	1/1	0.89	0.21	-	95,95,95,95	0
55	MG	14	3045	1/1	0.98	0.28	-	66,66,66,66	0
55	MG	14	3378	1/1	0.94	0.12	-	99,99,99,99	0
55	MG	2L	103	1/1	0.71	0.21	-	109,109,109,109	0
55	MG	14	3364	1/1	0.97	0.04	-	91,91,91,91	0
55	MG	13	1601	1/1	0.96	0.14	-	110,110,110,110	0
55	MG	14	3386	1/1	0.97	0.13	-	67,67,67,67	0
55	MG	14	3147	1/1	0.77	0.19	-	115,115,115,115	0
55	MG	14	3398	1/1	0.98	0.14	-	109,109,109,109	0
55	MG	14	3272	1/1	0.93	0.45	-	94,94,94,94	0
55	MG	1H	3335	1/1	0.93	0.26	-	90,90,90,90	0
55	MG	1H	3444	1/1	0.86	0.14	-	111,111,111,111	0
55	MG	1H	3543	1/1	0.89	0.26	-	121,121,121,121	0
55	MG	14	3173	1/1	0.96	0.30	-	103,103,103,103	0
55	MG	1G	1714	1/1	0.91	0.12	-	115,115,115,115	0
55	MG	13	1641	1/1	0.88	0.31	-	117,117,117,117	0
55	MG	14	3071	1/1	0.90	0.15	-	95,95,95,95	0
55	MG	1G	1605	1/1	0.90	0.13	-	81,81,81,81	0
55	MG	14	3263	1/1	0.90	0.41	-	101,101,101,101	0
55	MG	1H	3278	1/1	0.90	0.33	-	79,79,79,79	0
55	MG	1G	1623	1/1	0.76	0.29	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1742	1/1	0.95	0.34	-	116,116,116,116	0
55	MG	1H	3476	1/1	0.89	0.19	-	106,106,106,106	0
55	MG	1G	1673	1/1	0.93	0.18	-	101,101,101,101	0
55	MG	1H	3304	1/1	0.85	0.31	-	84,84,84,84	0
55	MG	1H	3505	1/1	0.79	0.62	-	122,122,122,122	0
55	MG	1H	3091	1/1	0.85	0.17	-	81,81,81,81	0
55	MG	14	3431	1/1	0.94	0.05	-	106,106,106,106	0
55	MG	1G	1733	1/1	0.95	0.10	-	105,105,105,105	0
55	MG	14	3425	1/1	0.88	0.14	-	89,89,89,89	0
55	MG	1H	3033	1/1	0.95	0.18	-	113,113,113,113	0
55	MG	14	3092	1/1	0.96	0.21	-	84,84,84,84	0
55	MG	13	1644	1/1	0.80	0.26	-	91,91,91,91	0
55	MG	14	3412	1/1	0.91	0.07	-	91,91,91,91	0
55	MG	1G	1706	1/1	0.94	0.16	-	116,116,116,116	0
55	MG	1H	3326	1/1	0.89	0.21	-	85,85,85,85	0
55	MG	1H	3289	1/1	0.84	0.51	-	104,104,104,104	0
55	MG	14	3186	1/1	0.97	0.11	-	90,90,90,90	0
55	MG	14	3015	1/1	0.95	0.23	-	78,78,78,78	0
55	MG	1H	3282	1/1	0.84	0.28	-	87,87,87,87	0
55	MG	14	3159	1/1	0.96	0.17	-	66,66,66,66	0
55	MG	1H	3273	1/1	0.67	0.42	-	98,98,98,98	0
55	MG	14	3164	1/1	0.93	0.16	-	89,89,89,89	0
55	MG	14	3040	1/1	0.98	0.14	-	67,67,67,67	0
55	MG	14	3180	1/1	0.97	0.14	-	94,94,94,94	0
55	MG	3I	201	1/1	0.95	0.14	-	89,89,89,89	0
55	MG	14	3137	1/1	0.88	0.38	-	107,107,107,107	0
55	MG	14	3131	1/1	0.79	0.18	-	81,81,81,81	0
55	MG	14	3446	1/1	0.75	0.43	-	120,120,120,120	0
55	MG	14	3451	1/1	0.98	0.09	-	92,92,92,92	0
55	MG	14	3407	1/1	0.98	0.07	-	109,109,109,109	0
55	MG	13	1711	1/1	0.95	0.18	-	86,86,86,86	0
55	MG	1G	1693	1/1	0.42	0.43	-	106,106,106,106	0
55	MG	1H	3036	1/1	0.96	0.34	-	72,72,72,72	0
55	MG	14	3264	1/1	0.69	0.40	-	100,100,100,100	0
55	MG	1H	3306	1/1	0.94	0.27	-	109,109,109,109	0
55	MG	1H	3153	1/1	0.90	0.12	-	79,79,79,79	0
55	MG	14	3457	1/1	0.86	0.14	-	101,101,101,101	0
55	MG	14	3244	1/1	0.99	0.17	-	90,90,90,90	0
55	MG	14	3339	1/1	0.73	0.55	-	107,107,107,107	0
55	MG	1H	3456	1/1	0.97	0.07	-	86,86,86,86	0
55	MG	13	1646	1/1	0.70	0.29	-	100,100,100,100	0
55	MG	1H	3284	1/1	0.95	0.22	-	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
55	MG	14	3344	1/1	0.86	0.60	-	89,89,89,89	0
55	MG	1H	3509	1/1	0.91	0.05	-	126,126,126,126	0
55	MG	1H	3458	1/1	0.97	0.15	-	67,67,67,67	0
55	MG	14	3144	1/1	0.82	0.16	-	78,78,78,78	0
55	MG	14	3161	1/1	0.94	0.28	-	72,72,72,72	0
55	MG	14	3476	1/1	0.92	0.27	-	110,110,110,110	0
55	MG	1G	1659	1/1	0.96	0.20	-	97,97,97,97	0
55	MG	1H	3046	1/1	0.91	0.31	-	86,86,86,86	0
55	MG	1H	3263	1/1	0.66	0.31	-	78,78,78,78	0
55	MG	1H	3516	1/1	0.96	0.04	-	126,126,126,126	0
55	MG	13	1719	1/1	0.93	0.06	-	140,140,140,140	0
55	MG	1G	1709	1/1	0.86	0.27	-	111,111,111,111	0
55	MG	1H	3094	1/1	0.96	0.29	-	72,72,72,72	0
55	MG	1H	3328	1/1	0.81	0.19	-	94,94,94,94	0
55	MG	1H	3058	1/1	0.94	0.25	-	88,88,88,88	0
55	MG	14	3208	1/1	0.73	0.20	-	83,83,83,83	0
55	MG	1H	3478	1/1	0.94	0.07	-	99,99,99,99	0
55	MG	13	1671	1/1	0.90	0.28	-	155,155,155,155	0
55	MG	1G	1625	1/1	0.87	0.50	-	97,97,97,97	0
55	MG	1H	3102	1/1	0.95	0.21	-	82,82,82,82	0
55	MG	16	211	1/1	0.91	0.10	-	114,114,114,114	0
55	MG	1H	3052	1/1	0.91	0.30	-	72,72,72,72	0
55	MG	1H	3338	1/1	0.83	0.60	-	88,88,88,88	0
55	MG	1H	3239	1/1	0.91	0.36	-	71,71,71,71	0
55	MG	14	3391	1/1	0.96	0.25	-	80,80,80,80	0
55	MG	14	3151	1/1	0.92	0.20	-	79,79,79,79	0
55	MG	1H	3019	1/1	0.94	0.17	-	73,73,73,73	0
55	MG	13	1670	1/1	0.87	0.28	-	150,150,150,150	0
55	MG	1H	3312	1/1	0.83	0.40	-	106,106,106,106	0
55	MG	18	103	1/1	0.93	0.31	-	94,94,94,94	0
55	MG	1G	1734	1/1	0.88	0.12	-	114,114,114,114	0
55	MG	14	3074	1/1	0.87	0.24	-	97,97,97,97	0
55	MG	1H	3065	1/1	0.96	0.22	-	74,74,74,74	0
55	MG	14	3463	1/1	0.98	0.12	-	98,98,98,98	0
55	MG	14	3125	1/1	0.93	0.22	-	93,93,93,93	0
55	MG	1H	3291	1/1	0.91	0.37	-	120,120,120,120	0
55	MG	16	206	1/1	0.86	0.28	-	76,76,76,76	0
55	MG	14	3140	1/1	0.70	0.28	-	97,97,97,97	0
55	MG	1H	3336	1/1	0.68	0.27	-	103,103,103,103	0
55	MG	1H	3078	1/1	0.88	0.35	-	81,81,81,81	0
55	MG	1G	1744	1/1	0.64	0.20	-	126,126,126,126	0
55	MG	14	3219	1/1	0.81	0.12	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3136	1/1	0.52	0.36	-	96,96,96,96	0
55	MG	1H	3215	1/1	0.89	0.57	-	84,84,84,84	0
55	MG	1H	3494	1/1	0.91	0.07	-	88,88,88,88	0
55	MG	1H	3346	1/1	0.76	0.24	-	80,80,80,80	0
55	MG	14	3441	1/1	0.97	0.04	-	113,113,113,113	0
55	MG	1H	3545	1/1	0.96	0.24	-	71,71,71,71	0
55	MG	1H	3424	1/1	0.96	0.14	-	57,57,57,57	0
55	MG	1H	3252	1/1	0.91	0.22	-	76,76,76,76	0
55	MG	1H	3163	1/1	0.93	0.40	-	111,111,111,111	0
55	MG	14	3276	1/1	0.94	0.27	-	75,75,75,75	0
55	MG	14	3320	1/1	0.70	0.33	-	114,114,114,114	0
55	MG	13	1642	1/1	0.75	0.21	-	99,99,99,99	0
55	MG	1G	1675	1/1	0.91	0.29	-	111,111,111,111	0
55	MG	14	3458	1/1	0.99	0.22	-	94,94,94,94	0
55	MG	13	1722	1/1	0.93	0.10	-	103,103,103,103	0
55	MG	1G	1745	1/1	0.86	0.06	-	143,143,143,143	0
55	MG	13	1640	1/1	0.91	0.20	-	99,99,99,99	0
55	MG	1H	3227	1/1	0.77	0.48	-	83,83,83,83	0
55	MG	14	3098	1/1	0.73	0.45	-	86,86,86,86	0
55	MG	16	202	1/1	0.90	0.31	-	88,88,88,88	0
55	MG	1H	3187	1/1	0.82	0.44	-	103,103,103,103	0
55	MG	1G	1638	1/1	0.87	0.20	-	86,86,86,86	0
55	MG	14	3374	1/1	0.96	0.10	-	80,80,80,80	0
55	MG	2K	102	1/1	0.97	0.18	-	106,106,106,106	0
55	MG	1G	1689	1/1	0.97	0.21	-	126,126,126,126	0
55	MG	14	3335	1/1	0.81	0.24	-	93,93,93,93	0
55	MG	1H	3044	1/1	0.86	0.35	-	74,74,74,74	0
55	MG	1G	1732	1/1	0.97	0.18	-	113,113,113,113	0
55	MG	14	3122	1/1	0.95	0.15	-	81,81,81,81	0
55	MG	55	202	1/1	0.89	0.17	-	108,108,108,108	0
55	MG	16	208	1/1	0.92	0.25	-	76,76,76,76	0
55	MG	14	3281	1/1	0.83	0.25	-	98,98,98,98	0
55	MG	1H	3075	1/1	0.94	0.42	-	80,80,80,80	0
55	MG	14	3156	1/1	0.93	0.10	-	84,84,84,84	0
55	MG	1G	1624	1/1	0.91	0.17	-	101,101,101,101	0
55	MG	14	3057	1/1	0.97	0.20	-	63,63,63,63	0
55	MG	1H	3148	1/1	0.95	0.29	-	74,74,74,74	0
55	MG	1G	1666	1/1	0.81	0.28	-	99,99,99,99	0
55	MG	1H	3265	1/1	0.87	0.13	-	85,85,85,85	0
55	MG	14	3215	1/1	0.89	0.16	-	182,182,182,182	0
55	MG	1H	3212	1/1	0.92	0.16	-	97,97,97,97	0
55	MG	14	3338	1/1	0.95	0.19	-	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
55	MG	14	3139	1/1	0.94	0.25	-	102,102,102,102	0
55	MG	1H	3224	1/1	0.95	0.18	-	87,87,87,87	0
55	MG	1H	3028	1/1	0.95	0.38	-	93,93,93,93	0
55	MG	14	3073	1/1	0.98	0.20	-	82,82,82,82	0
55	MG	1H	3517	1/1	0.91	0.08	-	121,121,121,121	0
55	MG	14	3222	1/1	0.90	0.26	-	112,112,112,112	0
55	MG	14	3134	1/1	0.94	0.27	-	77,77,77,77	0
55	MG	14	3447	1/1	0.91	0.23	-	90,90,90,90	0
55	MG	1H	3178	1/1	0.61	0.57	-	92,92,92,92	0
55	MG	14	3295	1/1	0.74	0.45	-	103,103,103,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.