



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 1, 2016 – 06:30 PM EDT

PDB ID : 5IBB  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and cognate tRNA<sup>Val</sup> in the A-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2016-02-22  
Resolution : 2.96 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-20027939  
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-20027939

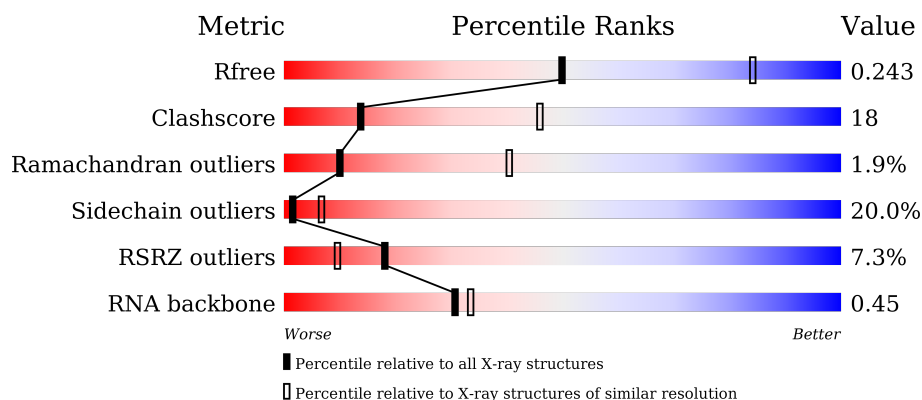
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



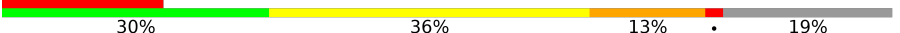
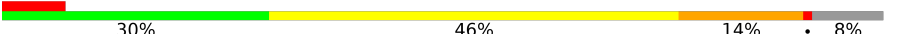
The reported resolution of this entry is 2.96 Å.

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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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	
1	1G	1522	
2	12	256	
2	1E	256	

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

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Mol	Chain	Length	Quality of chain
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	

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Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	I5	71	
52	M8	71	
53	J5	60	

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	

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
57	MG	13	1606	-	-	-	X
57	MG	13	1607	-	-	-	X
57	MG	13	1609	-	-	-	X
57	MG	13	1612	-	-	-	X
57	MG	13	1614	-	-	-	X
57	MG	13	1620	-	-	-	X
57	MG	13	1625	-	-	-	X
57	MG	13	1627	-	-	-	X
57	MG	13	1628	-	-	-	X
57	MG	13	1629	-	-	-	X
57	MG	13	1632	-	-	-	X
57	MG	13	1633	-	-	-	X
57	MG	13	1634	-	-	-	X
57	MG	13	1640	-	-	-	X
57	MG	13	1642	-	-	-	X
57	MG	13	1649	-	-	-	X
57	MG	13	1652	-	-	-	X
57	MG	13	1655	-	-	-	X
57	MG	13	1665	-	-	-	X
57	MG	13	1670	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1672	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	13	1681	-	-	-	X
57	MG	13	1683	-	-	-	X
57	MG	13	1685	-	-	-	X
57	MG	14	3014	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3016	-	-	-	X
57	MG	14	3023	-	-	-	X
57	MG	14	3027	-	-	-	X
57	MG	14	3029	-	-	-	X
57	MG	14	3031	-	-	-	X
57	MG	14	3033	-	-	-	X
57	MG	14	3036	-	-	-	X
57	MG	14	3039	-	-	-	X
57	MG	14	3046	-	-	-	X
57	MG	14	3055	-	-	-	X
57	MG	14	3058	-	-	-	X
57	MG	14	3060	-	-	-	X
57	MG	14	3061	-	-	-	X
57	MG	14	3070	-	-	-	X
57	MG	14	3078	-	-	-	X
57	MG	14	3079	-	-	-	X
57	MG	14	3085	-	-	-	X
57	MG	14	3086	-	-	-	X
57	MG	14	3087	-	-	-	X
57	MG	14	3089	-	-	-	X
57	MG	14	3091	-	-	-	X
57	MG	14	3096	-	-	-	X
57	MG	14	3100	-	-	-	X
57	MG	14	3104	-	-	-	X
57	MG	14	3109	-	-	-	X
57	MG	14	3110	-	-	-	X
57	MG	14	3113	-	-	-	X
57	MG	14	3114	-	-	-	X
57	MG	14	3116	-	-	-	X
57	MG	14	3121	-	-	-	X
57	MG	14	3123	-	-	-	X
57	MG	14	3124	-	-	-	X
57	MG	14	3126	-	-	-	X
57	MG	14	3127	-	-	-	X
57	MG	14	3129	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3135	-	-	-	X
57	MG	14	3137	-	-	-	X
57	MG	14	3144	-	-	-	X
57	MG	14	3146	-	-	-	X
57	MG	14	3148	-	-	-	X
57	MG	14	3149	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3156	-	-	-	X
57	MG	14	3160	-	-	-	X
57	MG	14	3167	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	14	3184	-	-	-	X
57	MG	14	3213	-	-	-	X
57	MG	14	3215	-	-	-	X
57	MG	14	3217	-	-	-	X
57	MG	14	3219	-	-	-	X
57	MG	14	3222	-	-	-	X
57	MG	14	3225	-	-	-	X
57	MG	14	3235	-	-	-	X
57	MG	14	3326	-	-	-	X
57	MG	14	3393	-	-	-	X
57	MG	14	3425	-	-	-	X
57	MG	16	201	-	-	-	X
57	MG	16	203	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1607	-	-	-	X
57	MG	1G	1610	-	-	-	X
57	MG	1G	1612	-	-	-	X
57	MG	1G	1614	-	-	-	X
57	MG	1G	1615	-	-	-	X
57	MG	1G	1622	-	-	-	X
57	MG	1G	1626	-	-	-	X
57	MG	1G	1627	-	-	-	X
57	MG	1G	1635	-	-	-	X
57	MG	1G	1655	-	-	-	X
57	MG	1G	1660	-	-	-	X
57	MG	1G	1661	-	-	-	X
57	MG	1G	1662	-	-	-	X
57	MG	1G	1666	-	-	-	X
57	MG	1H	3002	-	-	-	X
57	MG	1H	3014	-	-	-	X
57	MG	1H	3016	-	-	-	X
57	MG	1H	3024	-	-	-	X
57	MG	1H	3025	-	-	-	X
57	MG	1H	3026	-	-	-	X
57	MG	1H	3029	-	-	-	X
57	MG	1H	3033	-	-	-	X
57	MG	1H	3035	-	-	-	X
57	MG	1H	3036	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3038	-	-	-	X
57	MG	1H	3040	-	-	-	X
57	MG	1H	3042	-	-	-	X
57	MG	1H	3045	-	-	-	X
57	MG	1H	3046	-	-	-	X
57	MG	1H	3048	-	-	-	X
57	MG	1H	3050	-	-	-	X
57	MG	1H	3054	-	-	-	X
57	MG	1H	3055	-	-	-	X
57	MG	1H	3056	-	-	-	X
57	MG	1H	3058	-	-	-	X
57	MG	1H	3059	-	-	-	X
57	MG	1H	3060	-	-	-	X
57	MG	1H	3062	-	-	-	X
57	MG	1H	3066	-	-	-	X
57	MG	1H	3070	-	-	-	X
57	MG	1H	3071	-	-	-	X
57	MG	1H	3073	-	-	-	X
57	MG	1H	3085	-	-	-	X
57	MG	1H	3086	-	-	-	X
57	MG	1H	3088	-	-	-	X
57	MG	1H	3094	-	-	-	X
57	MG	1H	3095	-	-	-	X
57	MG	1H	3096	-	-	-	X
57	MG	1H	3097	-	-	-	X
57	MG	1H	3102	-	-	-	X
57	MG	1H	3104	-	-	-	X
57	MG	1H	3106	-	-	-	X
57	MG	1H	3109	-	-	-	X
57	MG	1H	3110	-	-	-	X
57	MG	1H	3113	-	-	-	X
57	MG	1H	3119	-	-	-	X
57	MG	1H	3124	-	-	-	X
57	MG	1H	3125	-	-	-	X
57	MG	1H	3141	-	-	-	X
57	MG	1H	3145	-	-	-	X
57	MG	1H	3152	-	-	-	X
57	MG	1H	3156	-	-	-	X
57	MG	1H	3165	-	-	-	X
57	MG	1H	3170	-	-	-	X
57	MG	1H	3176	-	-	-	X
57	MG	1H	3179	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3183	-	-	-	X
57	MG	1H	3187	-	-	-	X
57	MG	1H	3194	-	-	-	X
57	MG	1H	3196	-	-	-	X
57	MG	1H	3199	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3222	-	-	-	X
57	MG	1H	3231	-	-	-	X
57	MG	1H	3249	-	-	-	X
57	MG	1H	3256	-	-	-	X
57	MG	1H	3257	-	-	-	X
57	MG	1H	3264	-	-	-	X
57	MG	1H	3270	-	-	-	X
57	MG	1H	3281	-	-	-	X
57	MG	1H	3283	-	-	-	X
57	MG	1H	3284	-	-	-	X
57	MG	1H	3305	-	-	-	X
57	MG	1H	3308	-	-	-	X
57	MG	1H	3313	-	-	-	X
57	MG	1H	3331	-	-	-	X
57	MG	1H	3333	-	-	-	X
57	MG	1H	3340	-	-	-	X
57	MG	1H	3358	-	-	-	X
57	MG	1H	3378	-	-	-	X
57	MG	1H	3393	-	-	-	X
57	MG	1H	3402	-	-	-	X
57	MG	1H	3443	-	-	-	X
57	MG	1H	3522	-	-	-	X
57	MG	1H	3524	-	-	-	X
57	MG	1H	3538	-	-	-	X
57	MG	2I	301	-	-	-	X
57	MG	29	301	-	-	-	X
57	MG	29	302	-	-	-	X
57	MG	2K	101	-	-	-	X
57	MG	2L	101	-	-	-	X
57	MG	39	302	-	-	-	X
57	MG	98	201	-	-	-	X
57	MG	J8	101	-	-	-	X
58	SPE	13	1750	-	-	-	X
58	SPE	14	3447	-	-	-	X
58	SPE	14	3448	-	-	-	X
58	SPE	1J	208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	SF4	3E	301	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296743 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	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	235	Total	C	N	O	S	0	0	0
			1902	1215	340	342	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

- 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	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	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	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	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	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

- Molecule 22 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	0	0	0
			1540	688	274	506	72			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	296	527	76	1			

- Molecule 24 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1491	665	268	488	70			
24	3L	71	Total	C	N	O	P	0	0	0
			1513	675	272	495	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			462	207	96	138	21			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2841	Total	C	N	O	P	0	0	0
			61195	27234	11446	19674	2841			
26	14	2810	Total	C	N	O	P	0	0	0
			60535	26940	11330	19455	2810			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			
28	79	57	Total	C	N	O		0	0	0
			456	283	91	82				

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	202	Total	C	N	O	S	0	0	0
			1505	951	281	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	167	Total	C	N	O	S	0	0	0
			1283	815	239	228	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	136	Total	C	N	O	S	0	0	0
			1124	700	231	192	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			777	501	145	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O		0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O		0	0	0
			459	293	89	77				

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	61	Total	C	N	O	S	0	0	0
			479	299	86	89	5			
52	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	56	Total	C	N	O	S	0	0	0
			437	275	87	70	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
55	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 56 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	69	Total	C	N	O	P	0	0	0
			1469	656	262	482	69			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	98	1	Total	Mg	0	0
			1	1		
57	45	1	Total	Mg	0	0
			1	1		
57	19	1	Total	Mg	0	0
			1	1		
57	P8	1	Total	Mg	0	0
			1	1		
57	C5	1	Total	Mg	0	0
			1	1		
57	2I	1	Total	Mg	0	0
			1	1		
57	13	149	Total	Mg	0	0
			149	149		
57	1J	7	Total	Mg	0	0
			7	7		
57	5I	1	Total	Mg	0	0
			1	1		
57	35	2	Total	Mg	0	0
			2	2		
57	4L	2	Total	Mg	0	0
			2	2		
57	16	11	Total	Mg	0	0
			11	11		
57	42	1	Total	Mg	0	0
			1	1		
57	25	2	Total	Mg	0	0
			2	2		
57	M5	1	Total	Mg	0	0
			1	1		
57	21	2	Total	Mg	0	0
			2	2		
57	31	2	Total	Mg	0	0
			2	2		
57	Q8	1	Total	Mg	0	0
			1	1		

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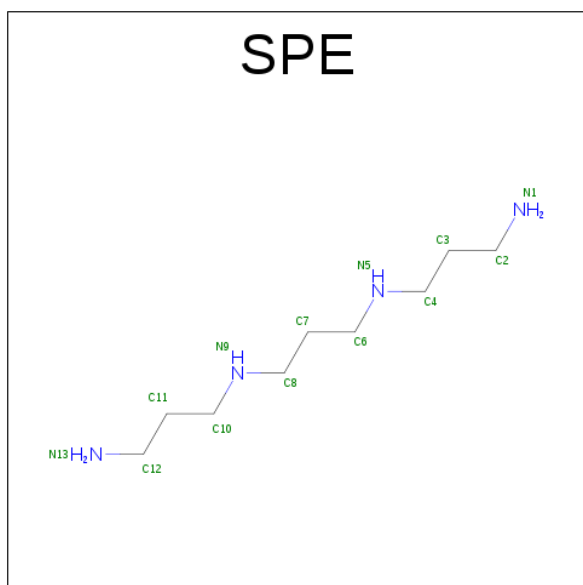
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	L8	1	Total 1	Mg 1	0	0
57	9A	1	Total 1	Mg 1	0	0
57	I8	1	Total 1	Mg 1	0	0
57	D8	1	Total 1	Mg 1	0	0
57	2A	1	Total 1	Mg 1	0	0
57	68	2	Total 2	Mg 2	0	0
57	29	3	Total 3	Mg 3	0	0
57	2K	4	Total 4	Mg 4	0	0
57	J8	1	Total 1	Mg 1	0	0
57	4A	1	Total 1	Mg 1	0	0
57	39	2	Total 2	Mg 2	0	0
57	1G	133	Total 133	Mg 133	0	0
57	4E	1	Total 1	Mg 1	0	0
57	11	3	Total 3	Mg 3	0	0
57	1H	546	Total 546	Mg 546	0	0
57	E5	1	Total 1	Mg 1	0	0
57	88	3	Total 3	Mg 3	0	0
57	5E	1	Total 1	Mg 1	0	0
57	14	446	Total 446	Mg 446	0	0
57	F8	1	Total 1	Mg 1	0	0
57	4K	1	Total 1	Mg 1	0	0

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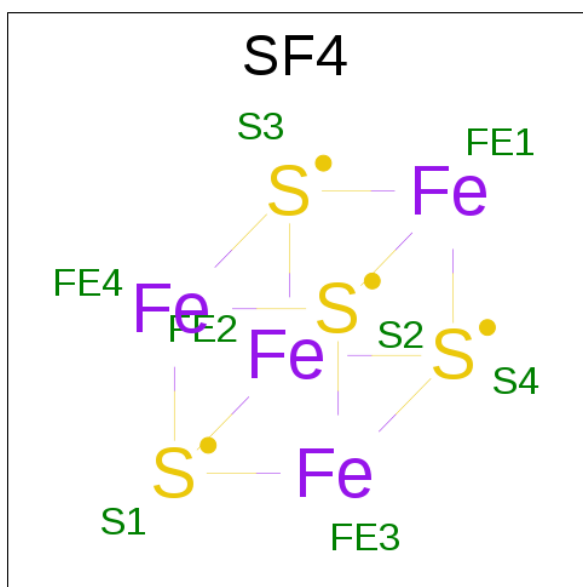
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	41	1	Total	Mg	0	0
			1	1		
57	2L	2	Total	Mg	0	0
			2	2		

- Molecule 58 is THERMINE (three-letter code: SPE) (formula:  $C_9H_{24}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	13	1	Total	C	N	0	0
			13	9	4		
58	1G	1	Total	C	N	0	0
			13	9	4		
58	14	1	Total	C	N	0	0
			13	9	4		
58	14	1	Total	C	N	0	0
			13	9	4		
58	1J	1	Total	C	N	0	0
			13	9	4		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C5	1	Total	Zn	0	0
			1	1		
60	5A	1	Total	Zn	0	0
			1	1		
60	G8	1	Total	Zn	0	0
			1	1		
60	5I	1	Total	Zn	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	304	Total	O	0	0
			304	304		
61	3E	1	Total	O	0	0
			1	1		
61	4E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1I	2	Total 2	O 2	0	0
61	2I	1	Total 1	O 1	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	2	Total 2	O 2	0	0
61	7I	2	Total 2	O 2	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	6	Total 6	O 6	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	11	Total 11	O 11	0	0
61	1H	1133	Total 1133	O 1133	0	0
61	16	15	Total 15	O 15	0	0
61	11	16	Total 16	O 16	0	0
61	21	8	Total 8	O 8	0	0
61	31	4	Total 4	O 4	0	0
61	58	1	Total 1	O 1	0	0
61	78	11	Total 11	O 11	0	0
61	98	2	Total 2	O 2	0	0
61	A8	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	I8	6	Total 6	O 6	0	0
61	K8	1	Total 1	O 1	0	0
61	L8	1	Total 1	O 1	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	391	Total 391	O 391	0	0
61	22	1	Total 1	O 1	0	0
61	42	1	Total 1	O 1	0	0
61	52	3	Total 3	O 3	0	0
61	3A	1	Total 1	O 1	0	0
61	7A	1	Total 1	O 1	0	0
61	9A	3	Total 3	O 3	0	0
61	BA	2	Total 2	O 2	0	0
61	4L	14	Total 14	O 14	0	0
61	14	1135	Total 1135	O 1135	0	0
61	1J	18	Total 18	O 18	0	0
61	19	8	Total 8	O 8	0	0
61	29	6	Total 6	O 6	0	0
61	39	6	Total 6	O 6	0	0
61	25	11	Total 11	O 11	0	0
61	35	9	Total 9	O 9	0	0

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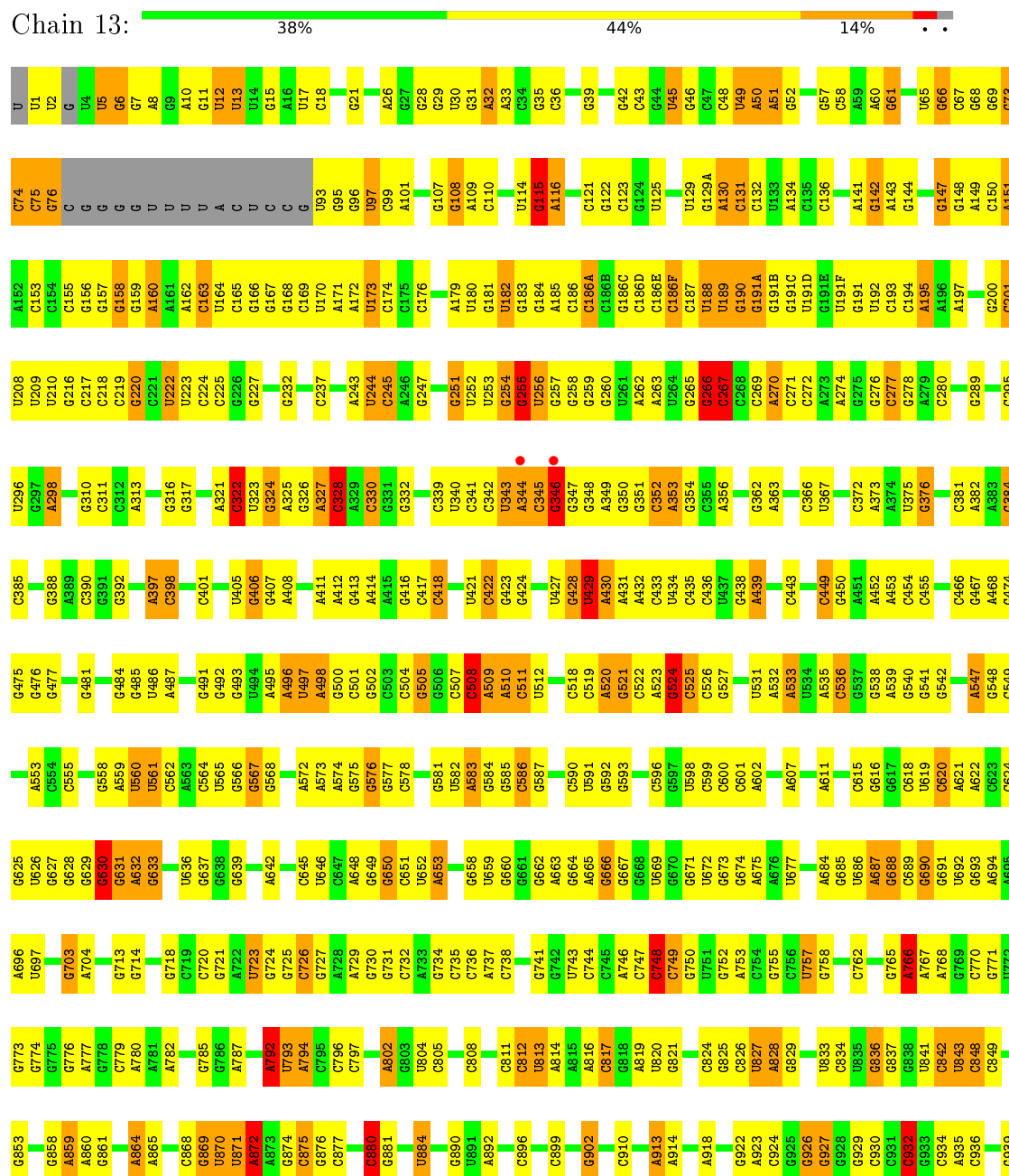
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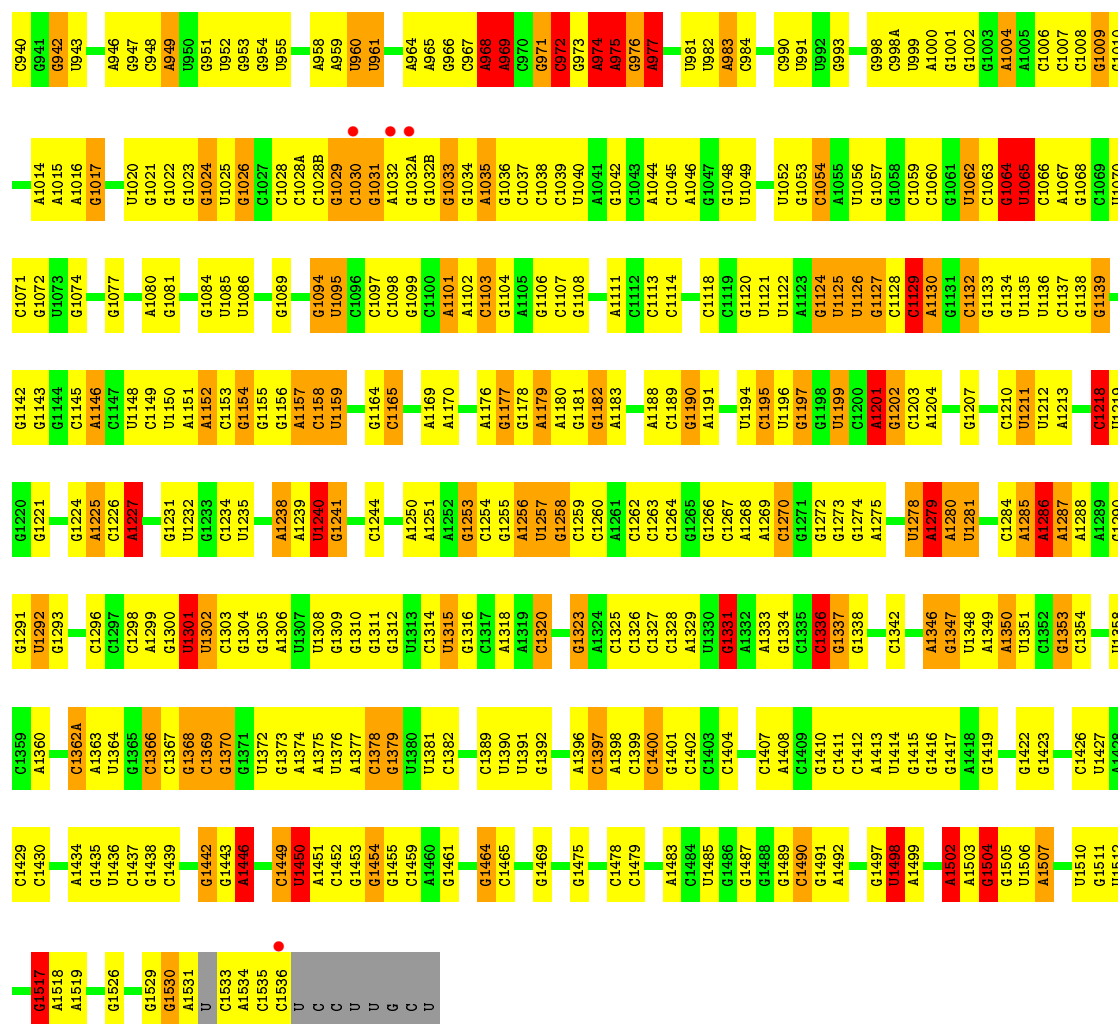
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	45	3	Total 3	O 3	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	A5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	E5	5	Total 5	O 5	0	0
61	F5	3	Total 3	O 3	0	0
61	H5	1	Total 1	O 1	0	0
61	M5	7	Total 7	O 7	0	0

### 3 Residue-property plots

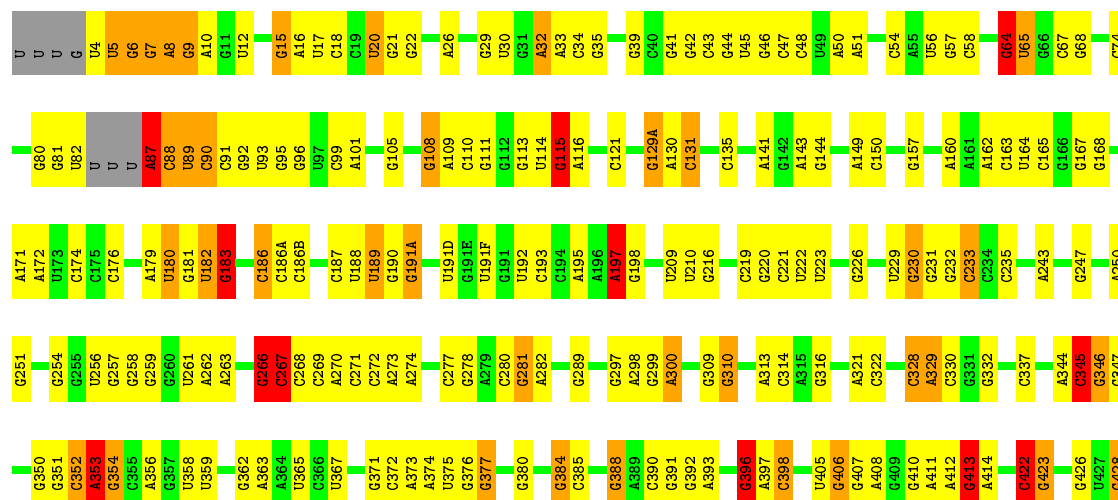
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16S ribosomal RNA

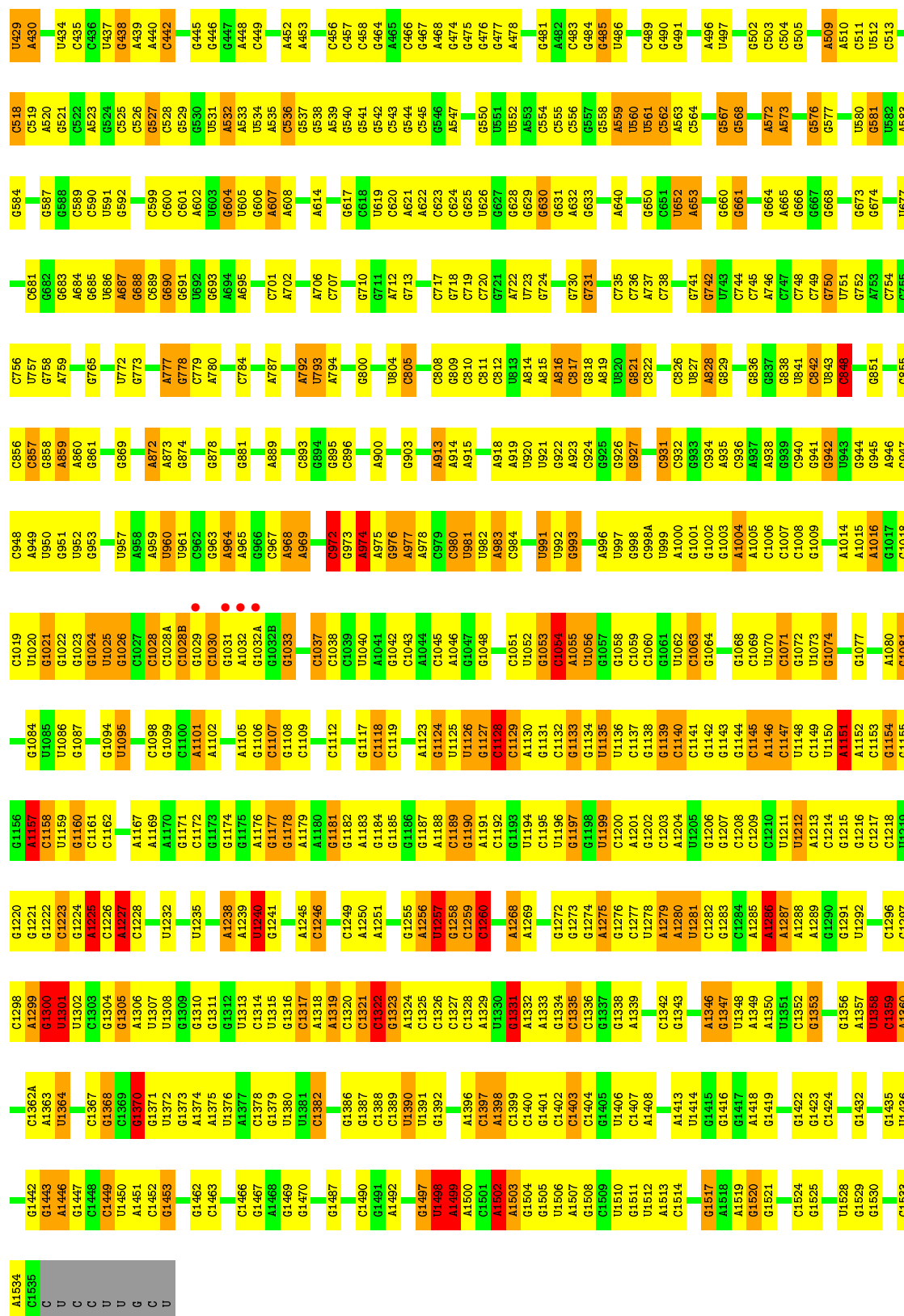




Chain 1G:  42% 43% 12% ..

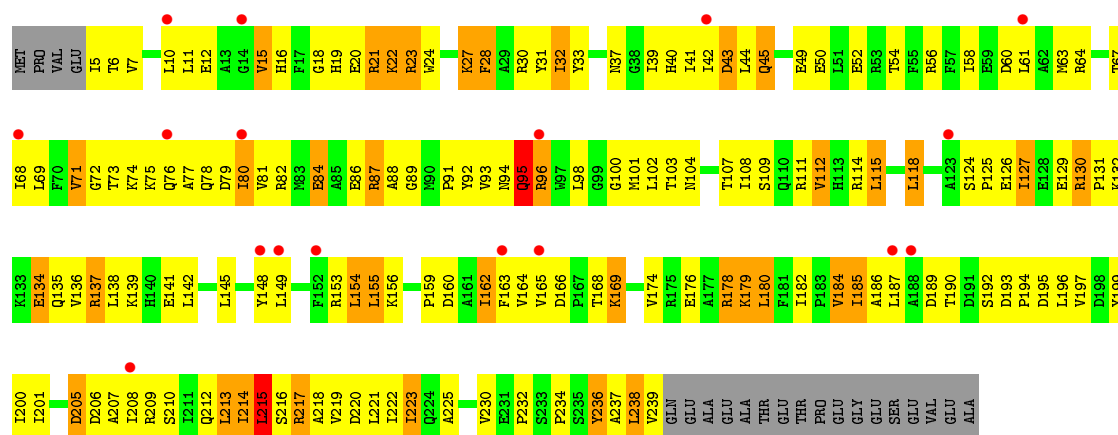




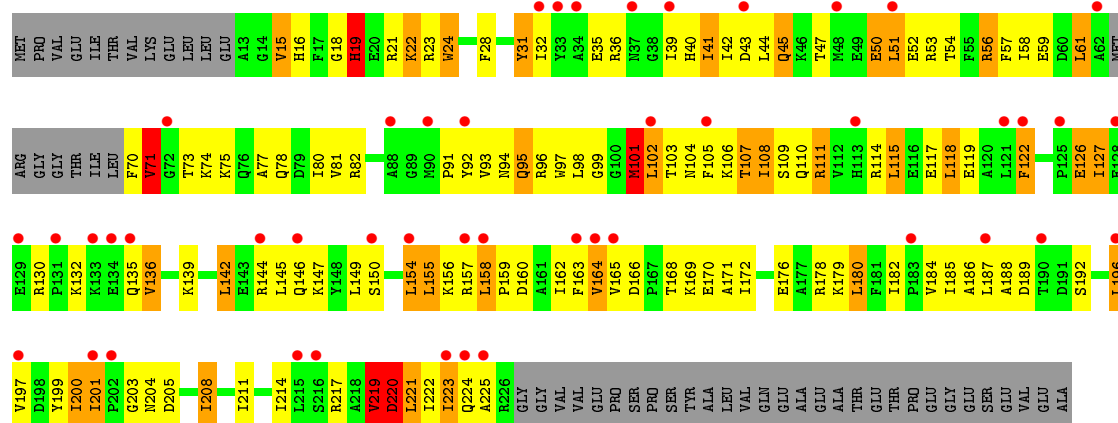


- Molecule 2: 30S ribosomal protein S2

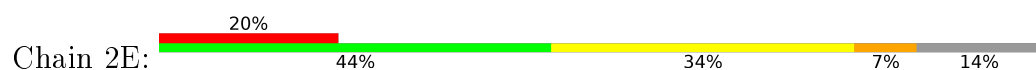




• Molecule 2: 30S ribosomal protein S2

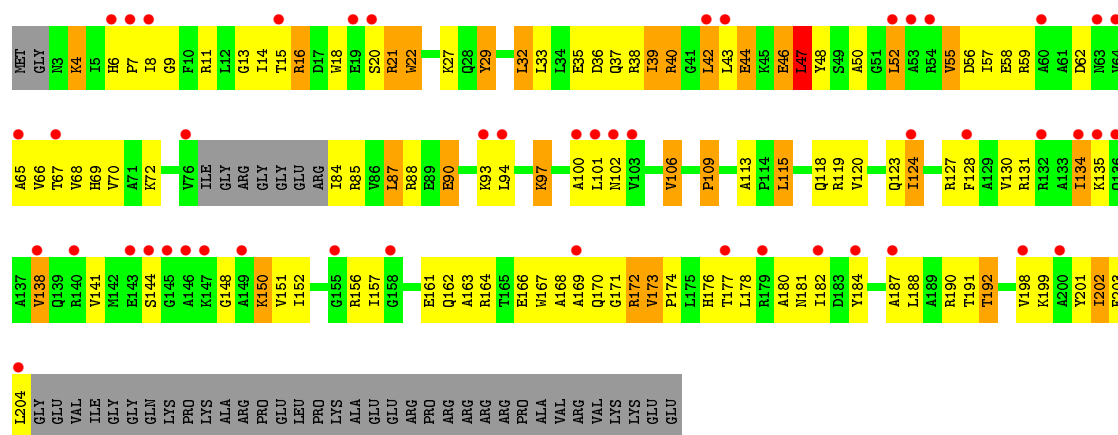


• Molecule 3: 30S ribosomal protein S3

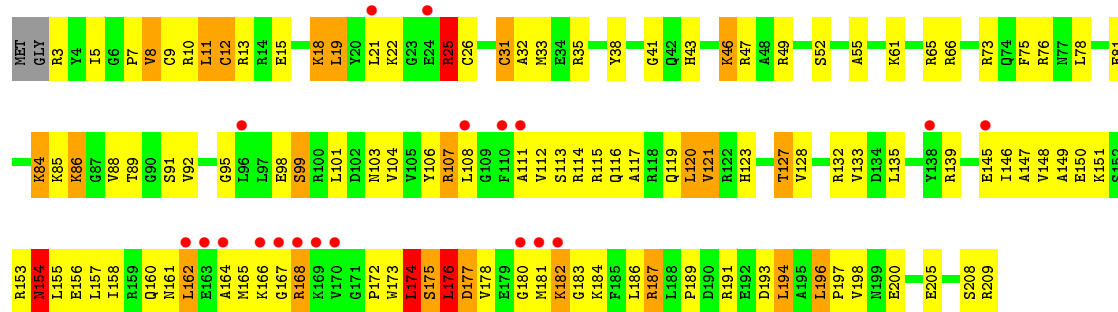
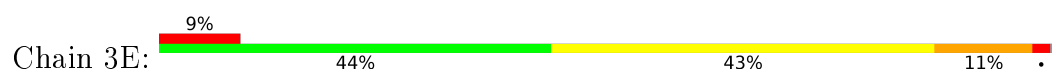


• Molecule 3: 30S ribosomal protein S3

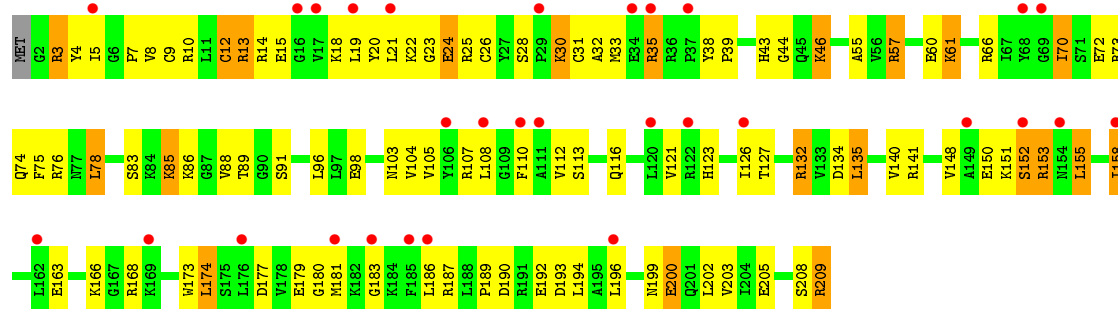




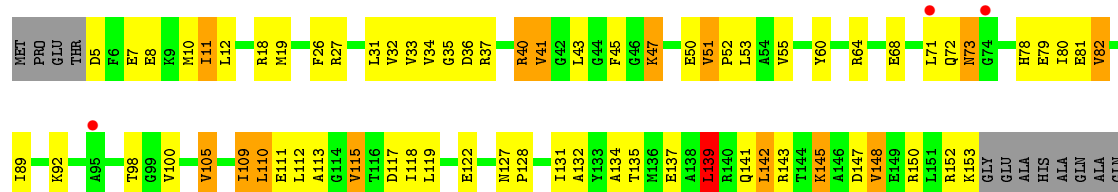
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

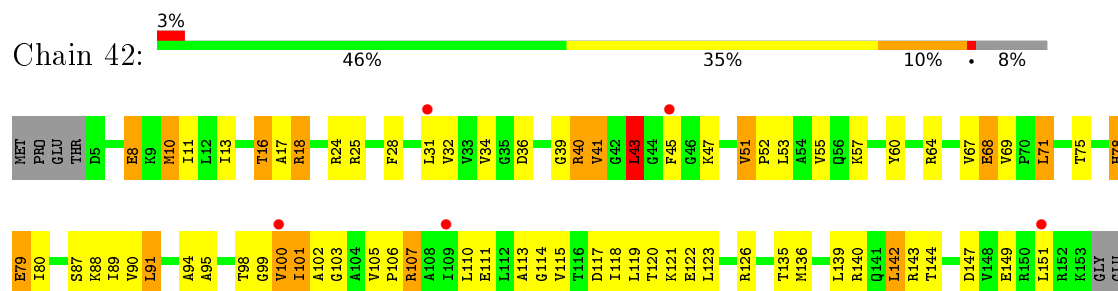


• Molecule 5: 30S ribosomal protein S5

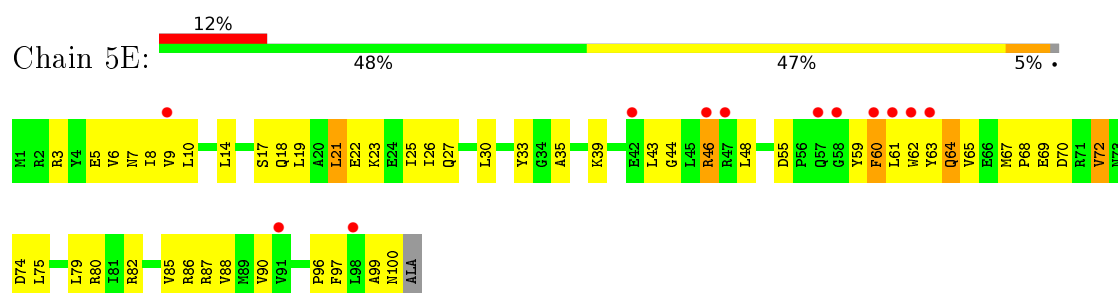


GLY

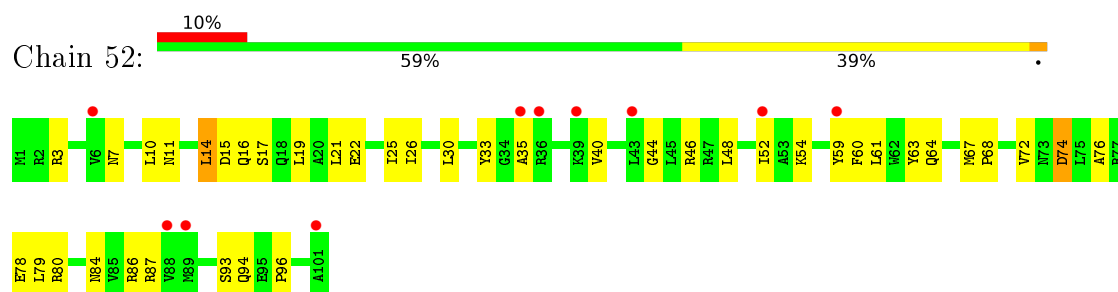
- Molecule 5: 30S ribosomal protein S5

ALA  
HIS  
ALA  
GLN  
ALA  
GLN  
GLY

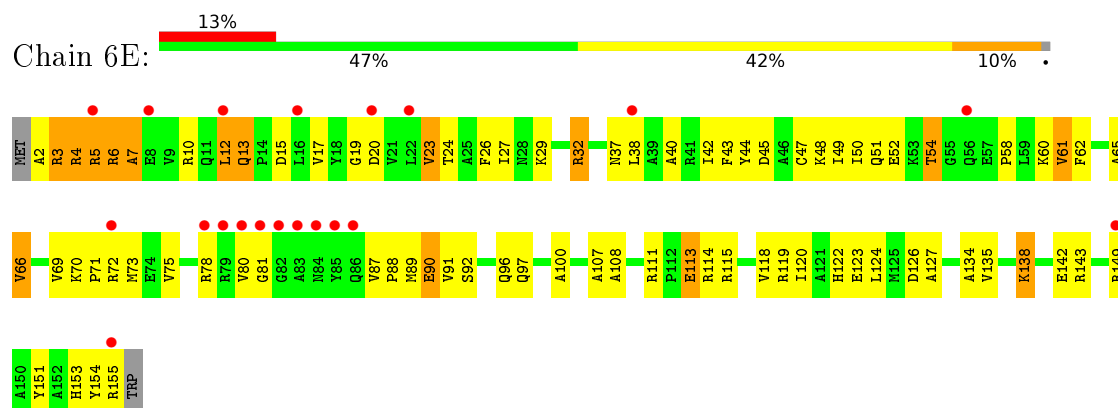
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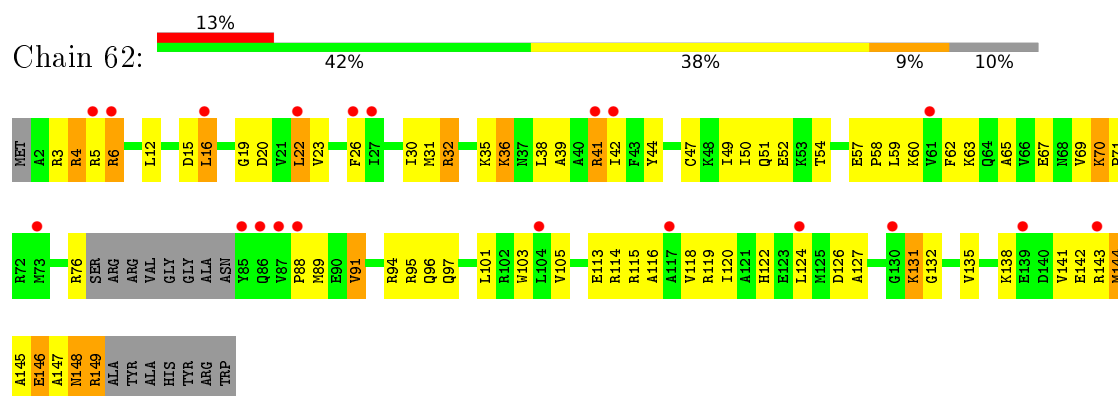
- Molecule 6: 30S ribosomal protein S6



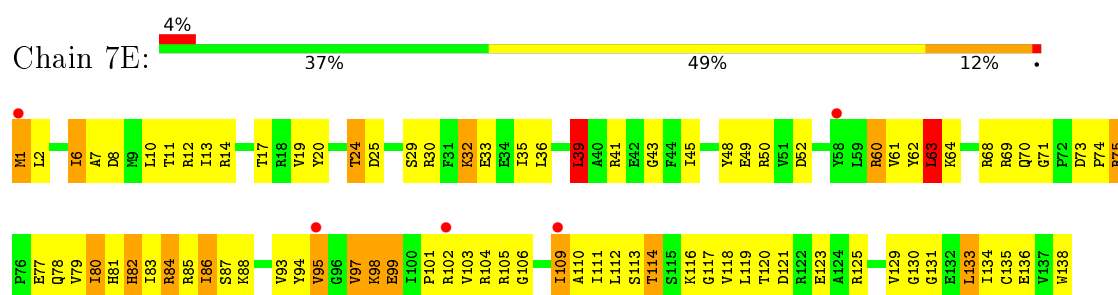
- Molecule 7: 30S ribosomal protein S7



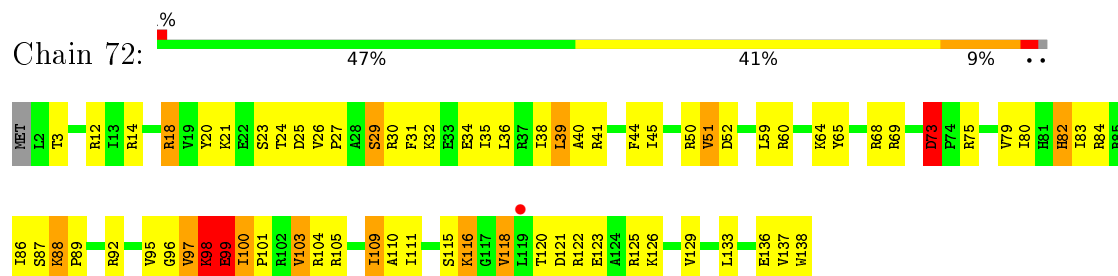
- Molecule 7: 30S ribosomal protein S7



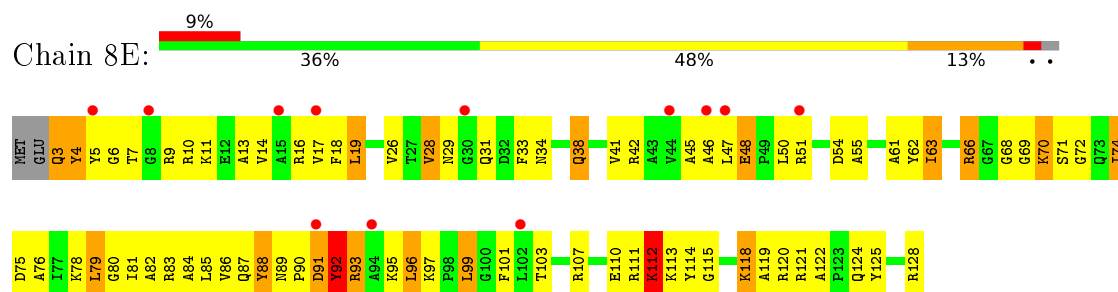
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

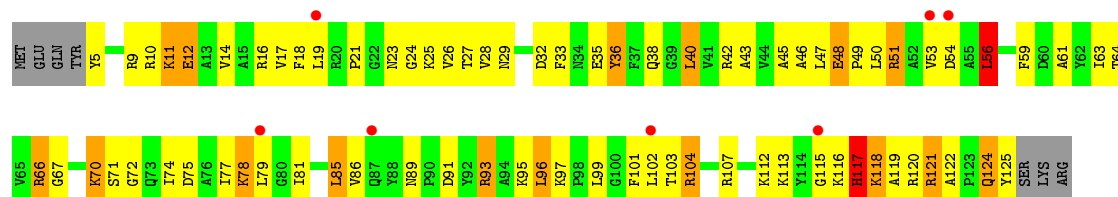


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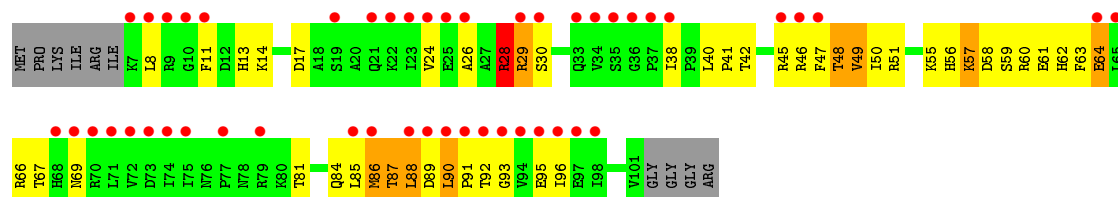


- Molecule 9: 30S ribosomal protein S9

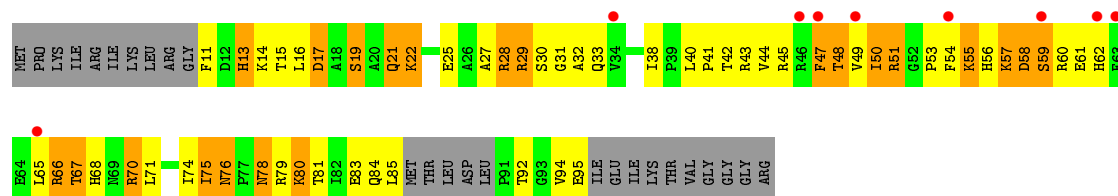
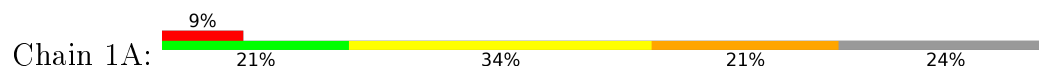




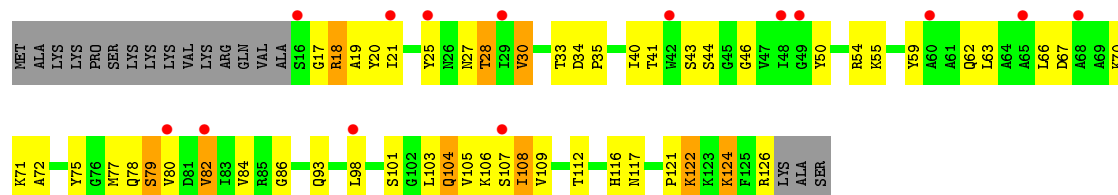
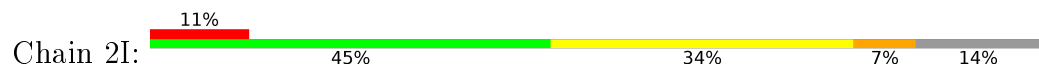
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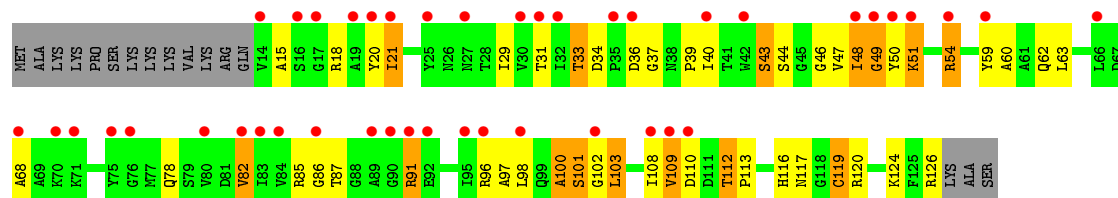
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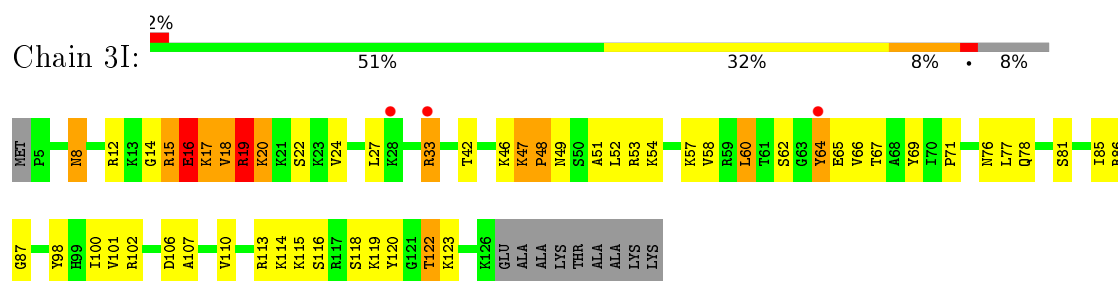
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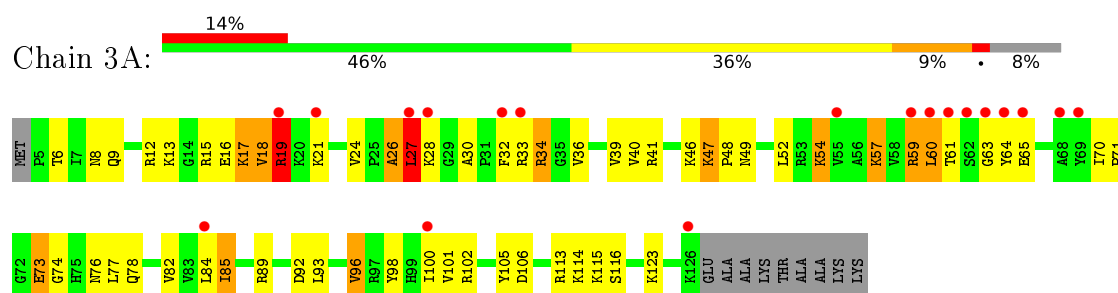
• Molecule 11: 30S ribosomal protein S11



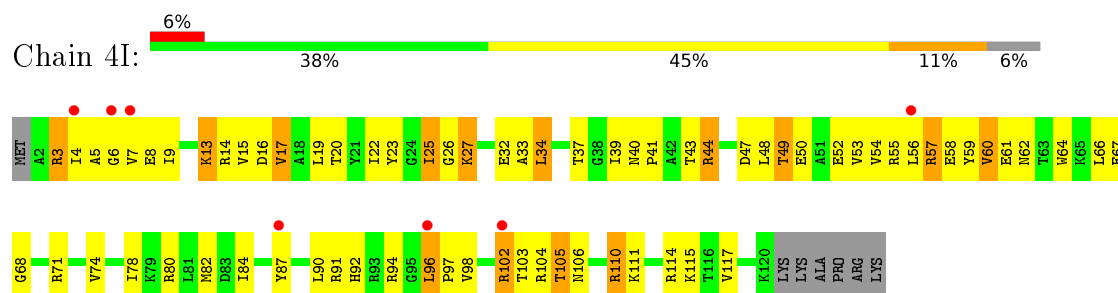
• Molecule 12: 30S ribosomal protein S12



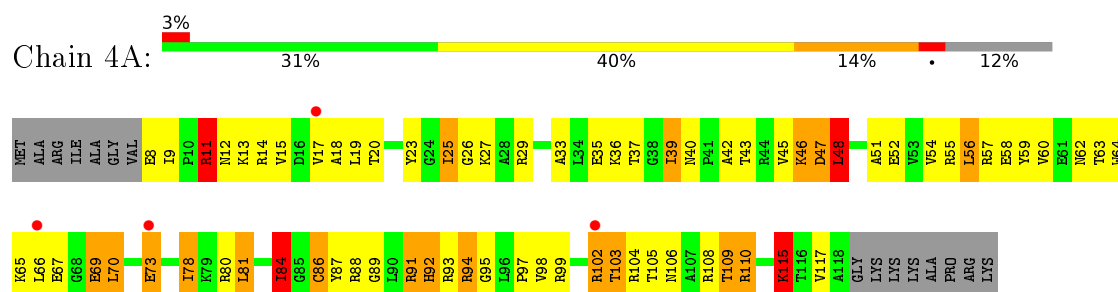
• Molecule 12: 30S ribosomal protein S12



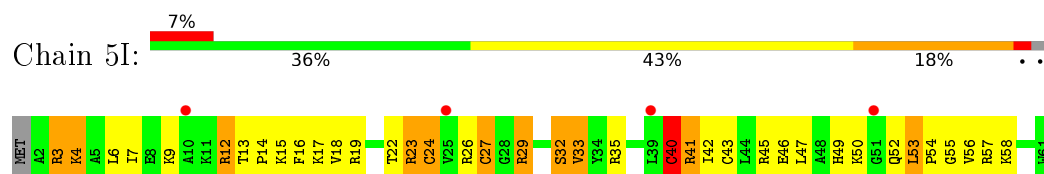
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

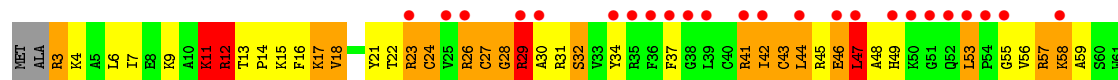


• Molecule 14: 30S ribosomal protein S14 type Z

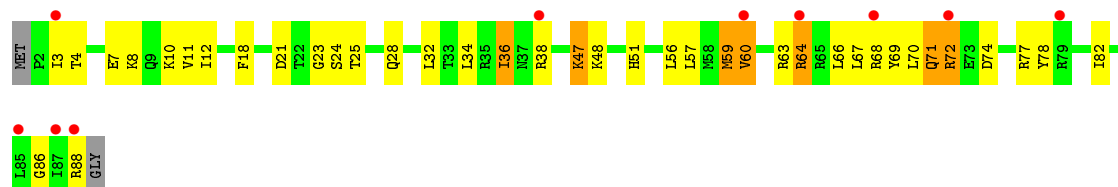


• Molecule 14: 30S ribosomal protein S14 type Z





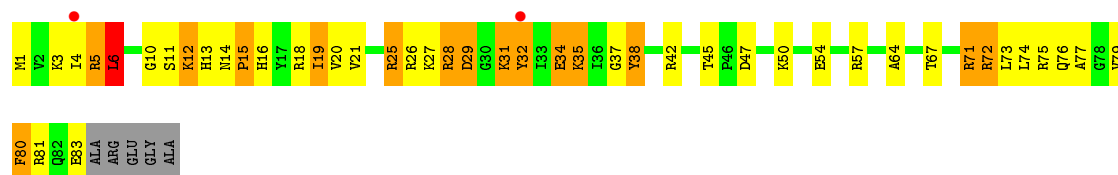
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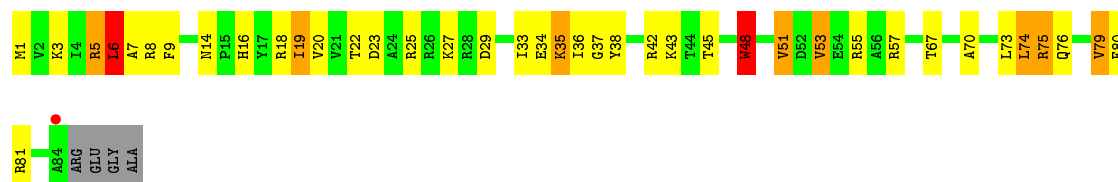
- Molecule 15: 30S ribosomal protein S15



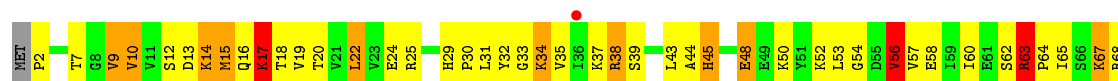
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



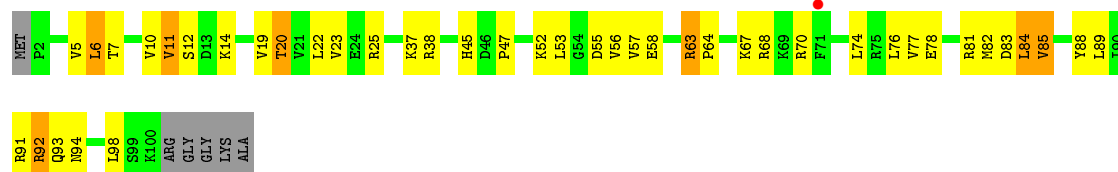
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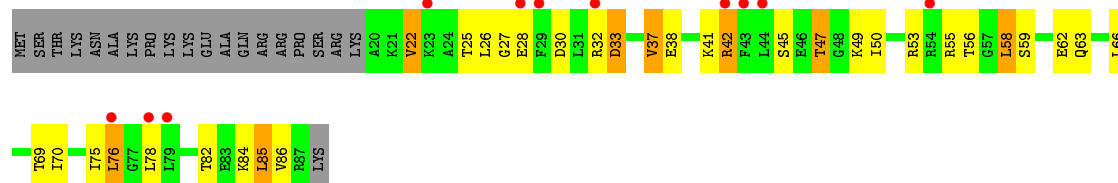




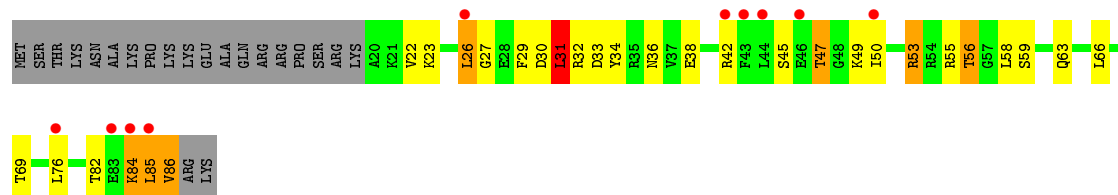
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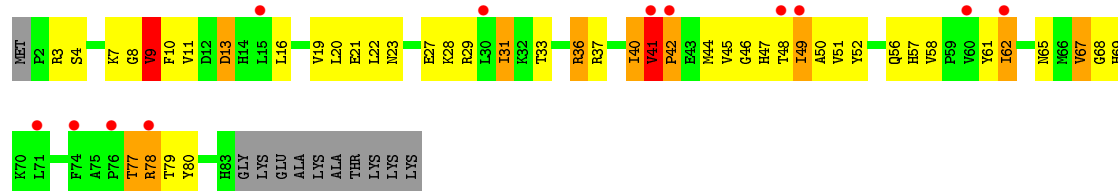
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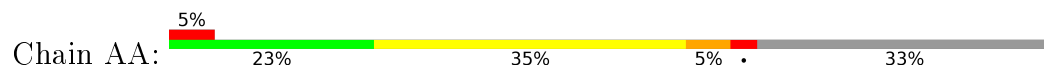
- Molecule 18: 30S ribosomal protein S18

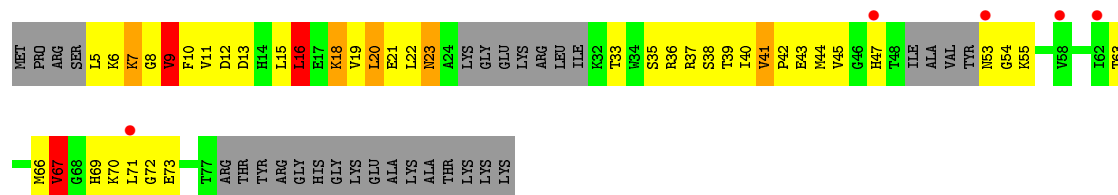


- Molecule 19: 30S ribosomal protein S19

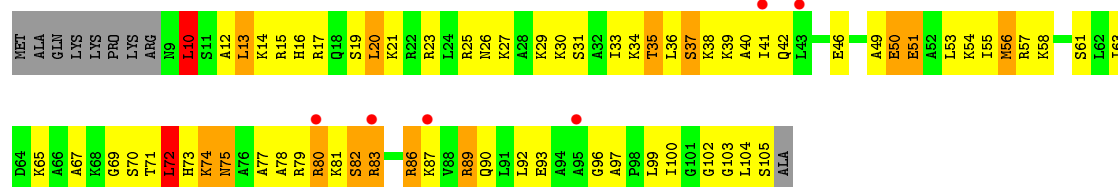


- Molecule 19: 30S ribosomal protein S19

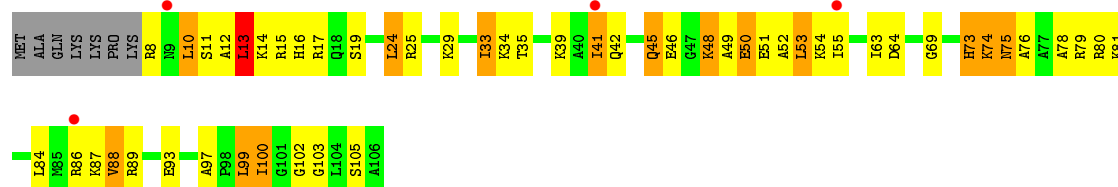




- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNAVal

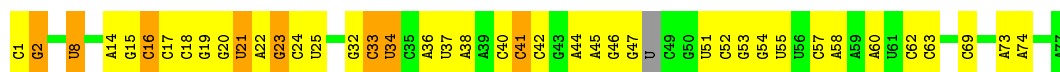




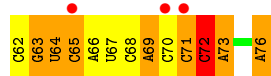
- Molecule 23: tRNA<sup>fMet</sup>



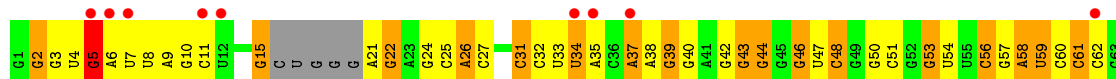
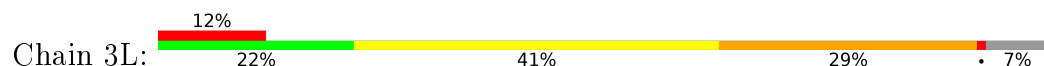
- Molecule 23: tRNA<sup>fMet</sup>



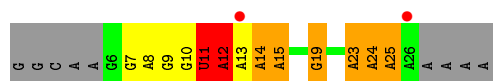
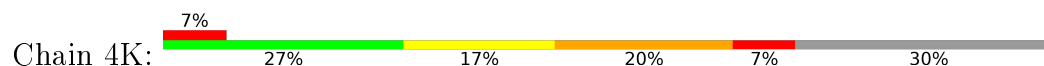
- Molecule 24: tRNA<sup>Val</sup>



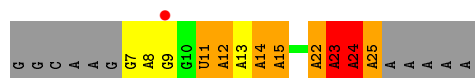
- Molecule 24: tRNA<sup>Val</sup>



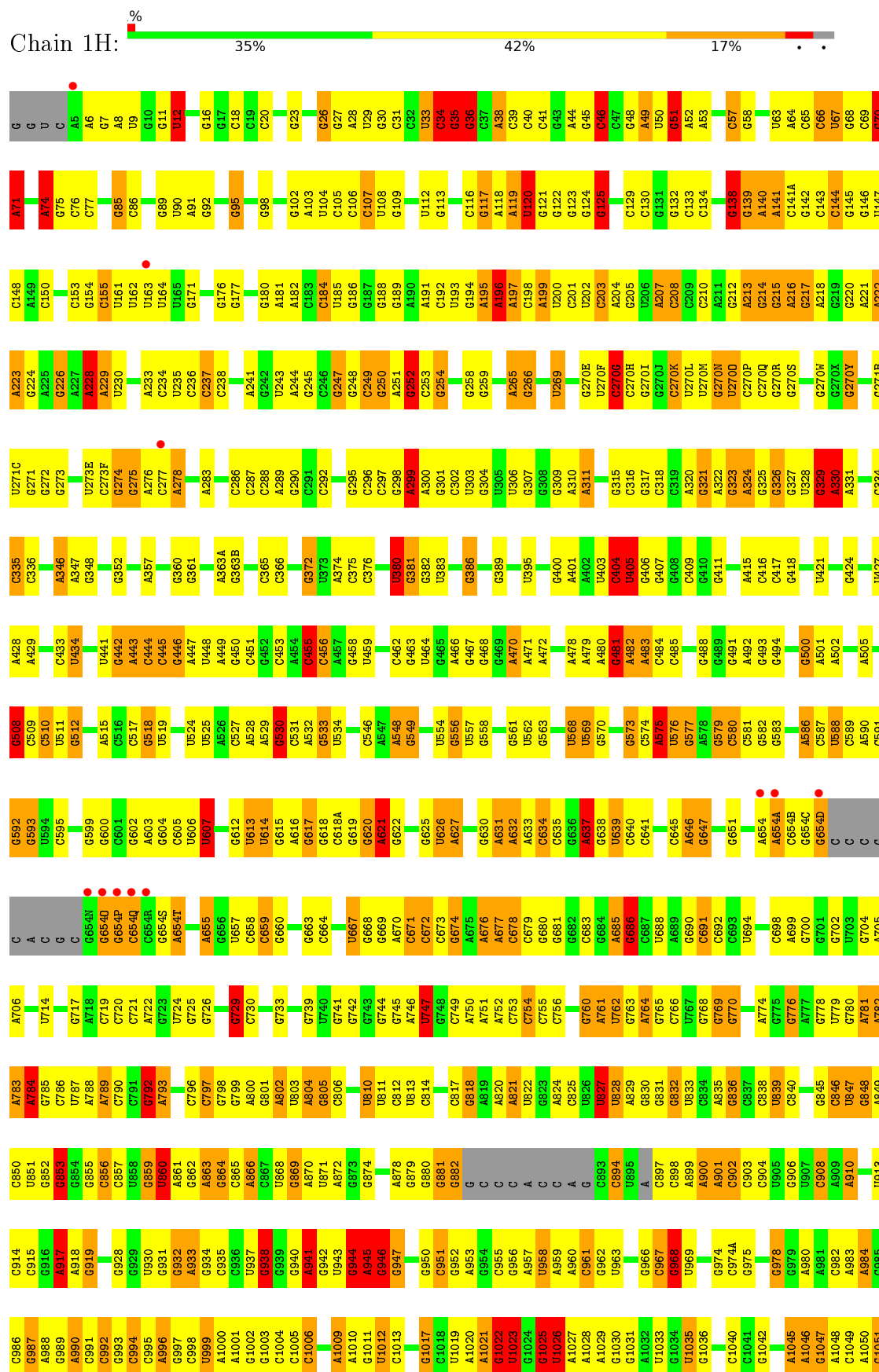
- Molecule 25: mRNA



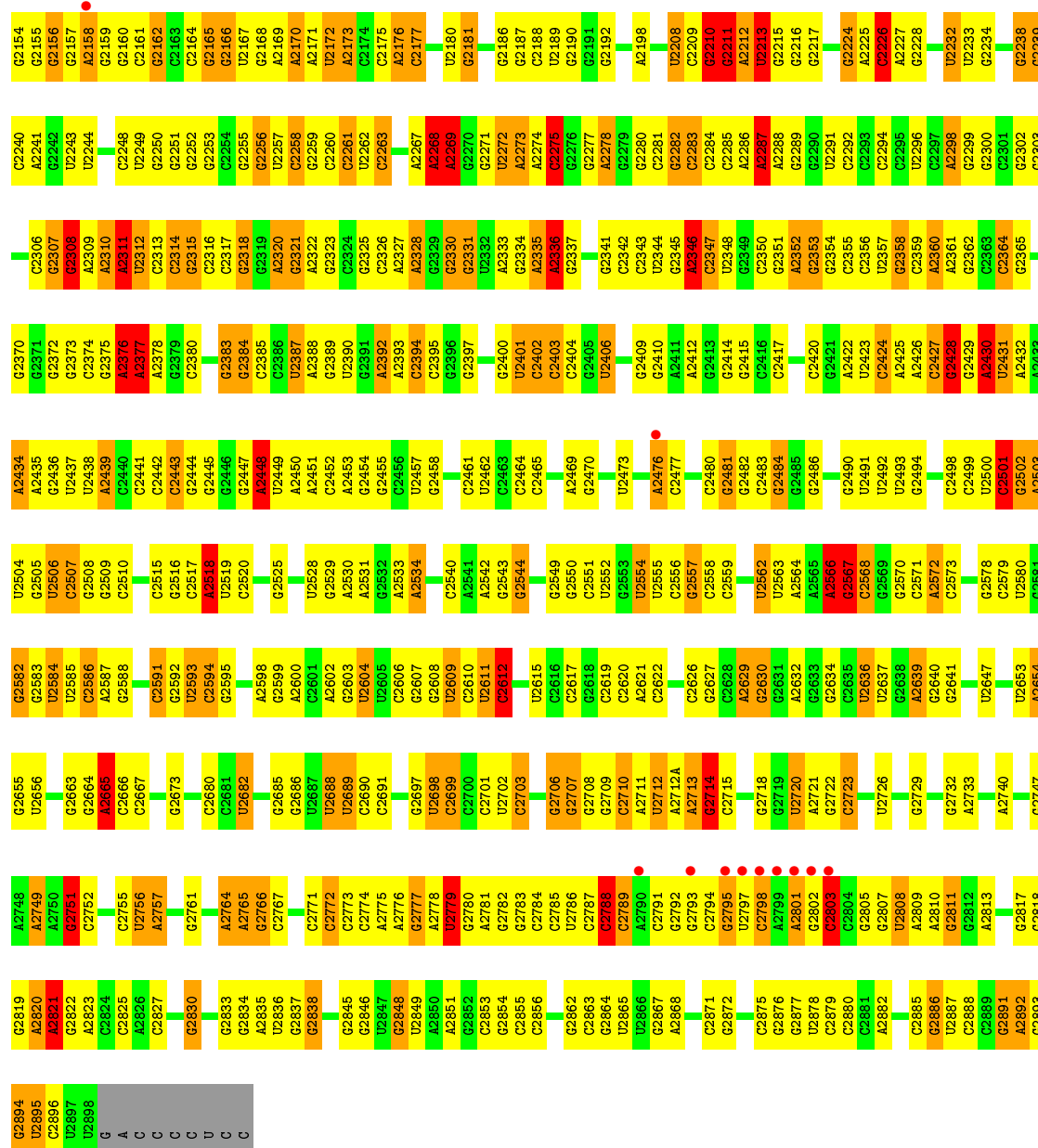
- Molecule 25: mRNA



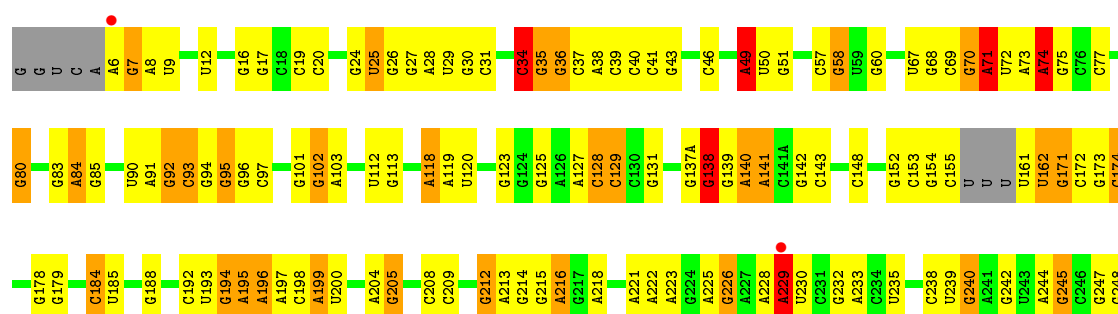
• Molecule 26: 23S ribosomal RNA



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C2085	U2016	A1937	U1833	G1772	A1669	A1603	G1539	G1475	C1403	C1330	G1261	C1196	C1124	G
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G2153	U2076		C1830			G1666		A1536	G1470	U1396	C1327		G1193	G1114



• Molecule 26: 23S ribosomal RNA

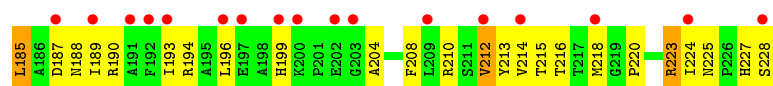


G1320	G1252	U165	A	G1025	G956	C	A819	A752	C662	G619	G549	G469	C385	C297	C249
A1321	A1253	U166	G	U1026	A957	C	A820	C753	C665	G620	G550	A470	G386	C297	G250
A1322	U1254	U167	U	A1027	U958	A	A821	C754	G666	A621	G556	A471	U387	G298	A251
U1255	U1256	U167	G	A1028	A959	C	U822	C755	U667	G622	G556	A472	G388	G299	G252
G1324	G1256	G169	C	A1029	A960	C	G823	C756	G668	G625	U557	G476	G389	G301	G253
G1325	C1257	G169	C	G1030	C961	C	G824	C756	G669	G625	G558	G476	G392	G302	G254
U1326	U1258	G170	U	G1031	G962	C	U825	G760	A670	U626	G559	G476	C392	C302	A255
G1327	G1259	G171	A	G1034	U963	C	U826	A761	C671	A627	C560	A479	C393	U603	A255
G1328	G1260	A1173	C	U1035	G963	C	U827	U762	C672	G630	G561	A480	A394	G304	G259
U1329	U1261	A1174	U	G1036	C966	U	U828	G763	C673	G631	U562	A481	U395	U305	A265
G1330	G1261	U1175	A	G1037	G967	A	A829	A764	G674	A631	G563	A482	G396	U306	G266
A1331	G1264	G1176	C	C1040	C970	C	G830	U767	A675	A632	U566	A483	C397	G307	G267
G1332	A1265	A1177	G	U1041	C971	C	G831	G768	A676	A633	A567	C486	C398	G308	C268
G1338	G1266	C1178	U	C1042	G972	A	G832	G769	A677	G634	U568	C486	C399	G309	U269
G1339	U1267	C1179	C	G1043	A973	A	U833	G770	C678	C635	U569	G489	A311	A310	U270
U1340	A1268	C1180	A	A1044	G974	C	C837	G771	C679	G636	G570	A489	G406	G312	A270B
U1341	U1269	C1181	U	G1045	C975	C	C838	G772	G680	A637	G571	A491	G406	G313	G270E
A1342	G1270	A1182	U	A	C976	C	U839	C773	U685	U639	A571	A492	C409	C314	U270F
G1345	G1271	G1183	G	A	G975	C	G840	A774	C687	C640	G572	G493	G410	G315	G270G
U1346	U1272	U1188	U	G1047	A980	C	A841	G775	C688	G641	G573	G494	G411	G316	G270H
A1347	U1273	A1189	G	A1048	A981	C	G842	G776	U694	G642	G574	G498	G412	A320	G270I
G1348	A1274	U1190	C	G1049	A982	C	G843	A777	U694	A643	U575	G499	A412	G321	U270L
A1349	U1275	U1191	A	U1051	A983	C	G844	U778	C697	C645	G576	A501	A415	A322	U270M
G1350	G1276	U1192	C	C	C	C	C845	G779	U697	A646	G577	A502	G418	G323	G270N
G1351	G1277	G1200	C	G	G887	C	C846	G780	U703	G647	C580	A503	U421	A324	U270O
U1352	G1280	C1201	A	A	A988	C	G847	A781	G704	G648	C581	U504	G439	G325	C270P
G1281	G1281	G1202	G	G	G989	C	G848	A782	G705	G649	G582	A505	G440	G326	C270Q
U1282	U1282	C1203	G	G	A990	C	A849	A783	A706	G650	G583	G508	U441	G327	G270R
G1283	A1204	A1204	A	C991	C991	C	C850	A784	A706	G651	G583	G509	G442	U328	G270S
A1359	U1205	U1205	U	U	U	C	G853	G785	G707	G651	G583	G509	G443	G329	G270T
A1360	G1209	G1209	G	C994	C994	C	G854	C786	G715	A654	A866	C509	C433	A330	G270U
G1364	U1210	A1210	U	C995	C995	C	G855	U787	G716	A654B	C587	C510	U434	G336	G270V
A1365	U1211	U1211	U	U922	U922	C	G859	A788	A717	G654B	U511	G512	C435	C336	G270X
A1366	G1212	G1212	G	C925	C925	C	U860	C790	A718	G654C	G512	A513	G439	G352	G271B
A1367	C1213	A1213	C	A926	A926	C	A861	C791	G719	G654D	A514	A514	G440	G353	U271C
G1368	A1214	A1214	C	G928	G928	C	G862	G792	C720	C	C516	A515	U441	G354	G271
C1295	C1295	C1295	U	A1000	A1000	C	A863	G793	G721	C	C517	C517	G442	G355	G272
G1296	G1296	G1296	A	G1002	G1002	C	G864	A793	A722	C	G597	C517	A443	G356	G273
C1297	C1297	C1297	G	G1003	G1003	C	C865	C796	A722	C	G598	C517	C444	C356	G273
G1371	G1219	G1219	A	C1004	C1004	C	A866	C797	A727	C	U525	U525	C445	G361	C273C
A1372	A1220	A1220	A	A1005	A1005	C	G867	G798	G728	A	A526	A526	C446	U362	C273D
G1299	G1299	G1299	G	G1006	G1006	C	U868	C799	G729	C	G527	G527	G450	G363	U273E
U1300	C1221	C1221	C	C1007	C1007	C	G869	A800	C730	C	A528	A528	G451	A363A	C273F
A1301	C1222	C1222	C	U1008	U1008	C	A870	G801	C731	C	G529	G529	G452	G363B	G274
A1302	G1224	G1224	G	A1009	A1009	C	U871	A802	A734	C	G530	G530	C453	G363C	G275
G1303	C1303	C1303	C	C	C	C	A872	G805	G737	C	U607	A532	A454	G363D	A276
C1304	G1229A	G1229A	C	G1010	G1010	C	G873	G805	G737	C	G533	G533	C455	U363E	C277
A1308	G1239	G1239	A	U1011	U1011	C	G874	G738	G745	C	C537	C537	C456	A363F	A278
G1309	U1240	U1240	U	U1012	U1012	C	G875	G739	U740	G654S	G539	G539	A457	C364	C279
U1312	A1241	A1241	C	C1013	C1013	C	U877	G741	G741	A654T	G540	G540	G458	G372	A283
G1385	G1151	G1151	A	G1014	G1014	C	U877	U811	G745	G656	G612	G612	U459	U380	C286
G1386	C1152	C1152	U	U1015	U1015	C	A878	U813	G745	U657	U613	U613	A460	G381	C287
C1387	U1153	U1153	U	U1019	U1019	C	G	C814	G746	G658	A616	A616	C461	G382	A288
U1316	A1247	A1247	U	A1020	A1020	C	G	C815	A746	G658	G617	G617	C462	U383	C289
A1317	G1248	G1248	A	U1021	U1021	C	G	C816	G747	G658	A547	A547	G467	U384	G290
G1389	U1249	U1249	A	G1022	G1022	C	G	C817	G748	G662	G618	G618	G467	G384	
U1390	G1250	G1250	A	U1023	U1023	C	G	C818	G748	G662	G618	G618	G467	G384	
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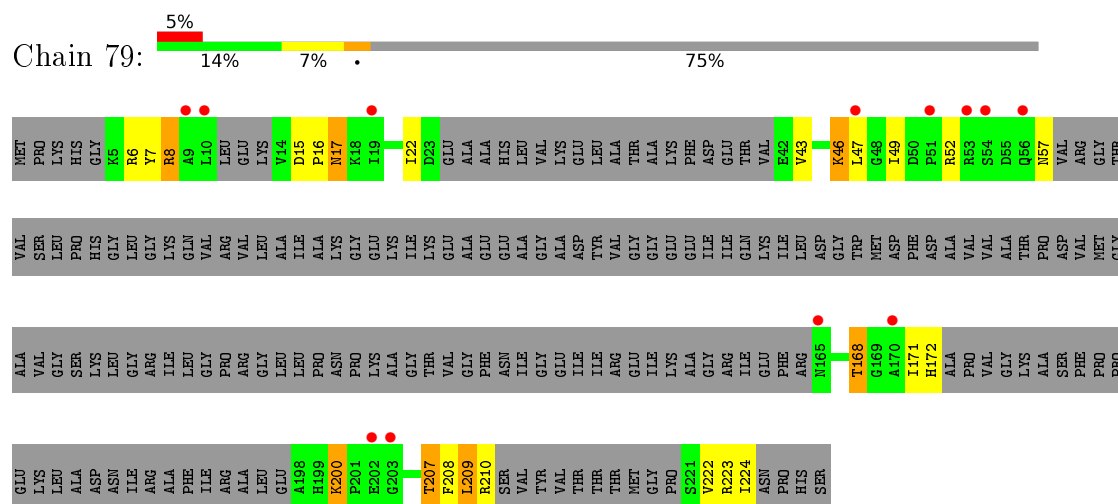




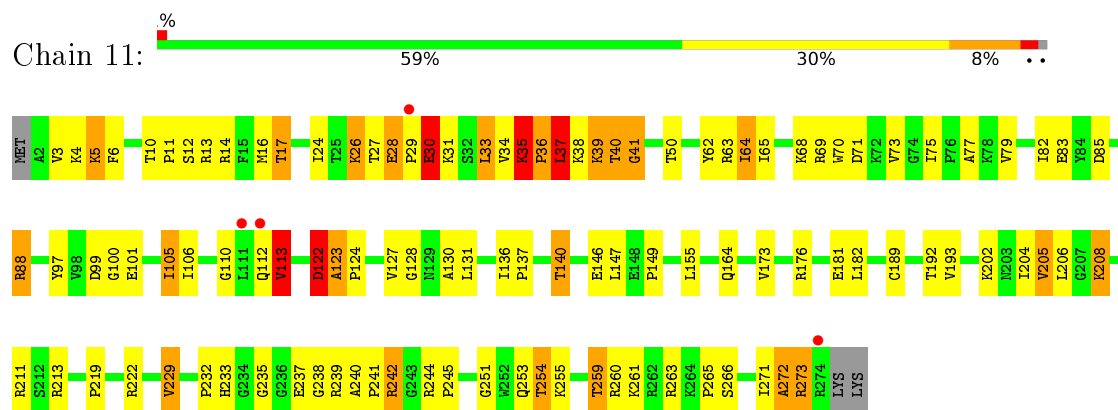




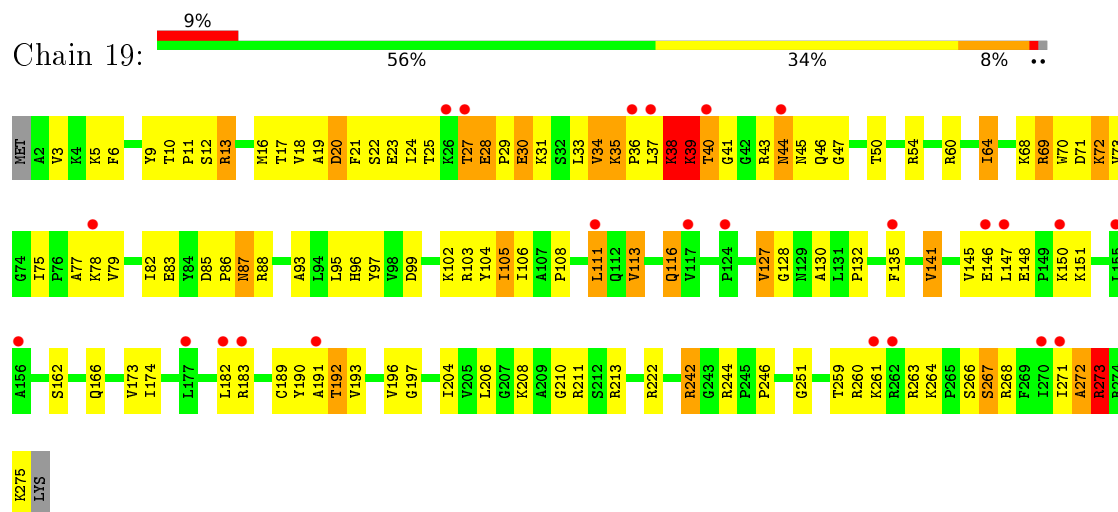
• Molecule 28: 50S ribosomal protein L1



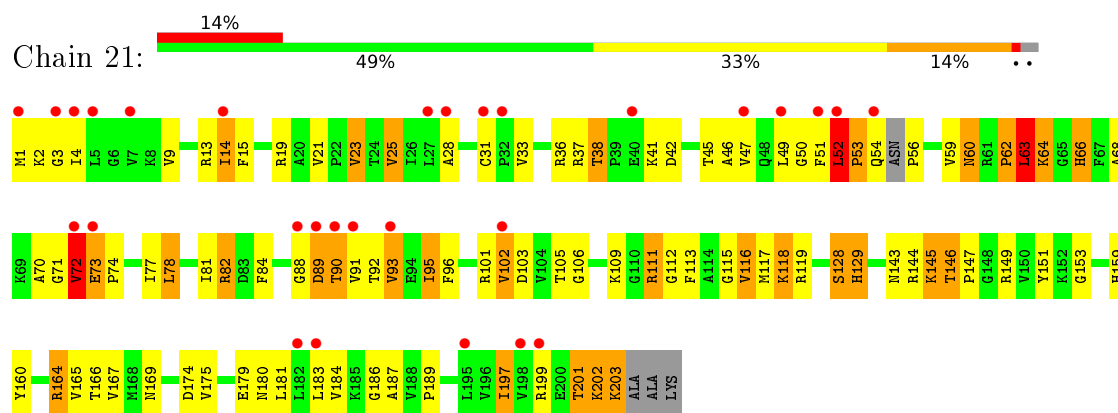
• Molecule 29: 50S ribosomal protein L2



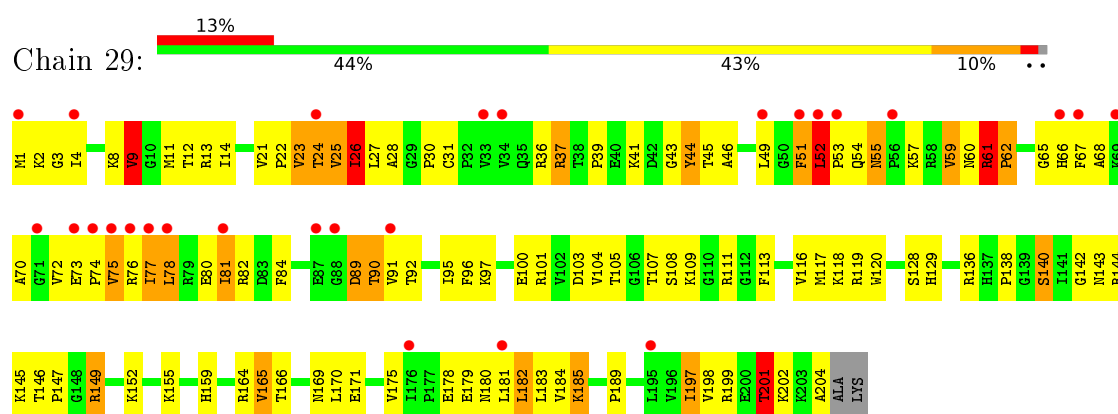
• Molecule 29: 50S ribosomal protein L2



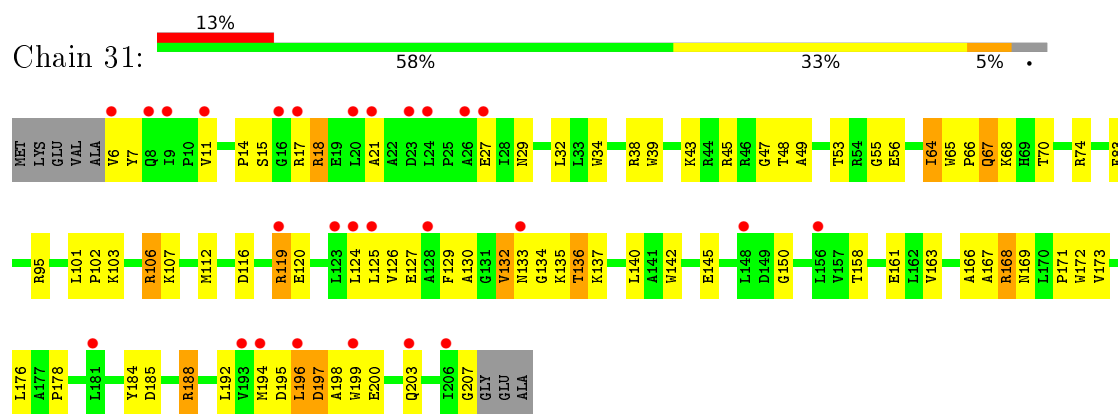
- Molecule 30: 50S ribosomal protein L3



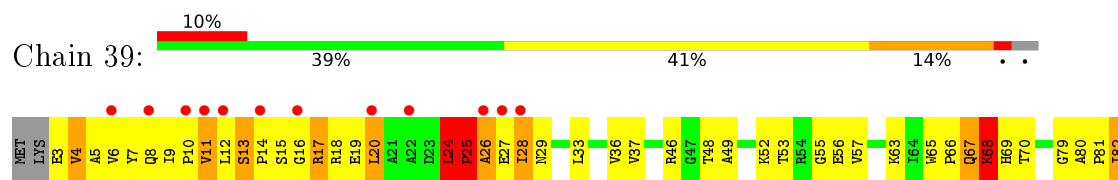
- Molecule 30: 50S ribosomal protein L3

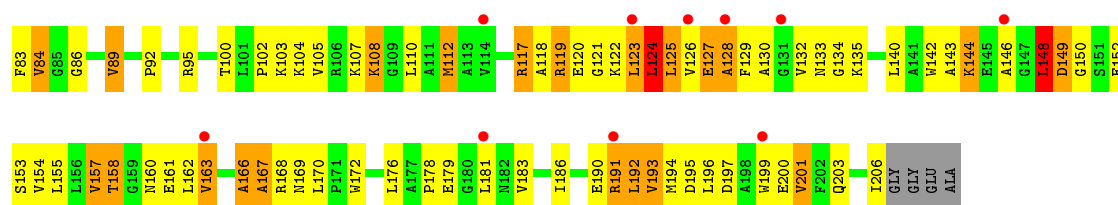


- Molecule 31: 50S ribosomal protein L4

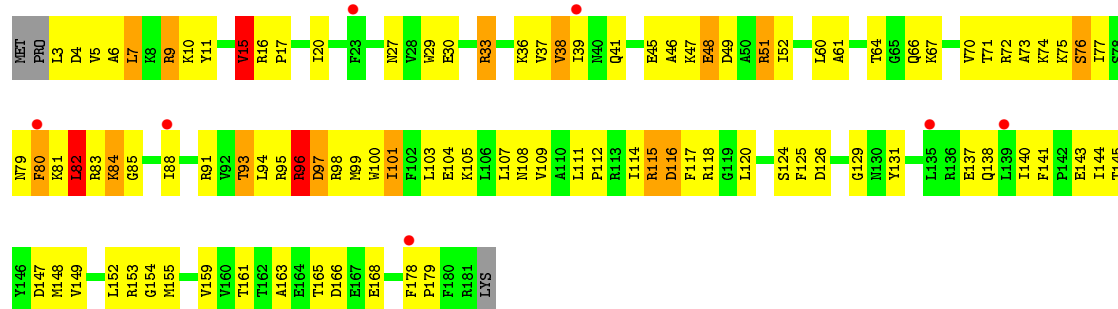
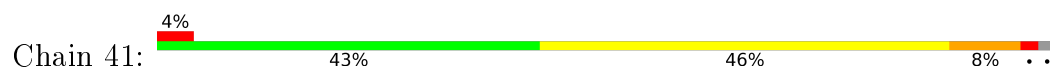


- Molecule 31: 50S ribosomal protein L4

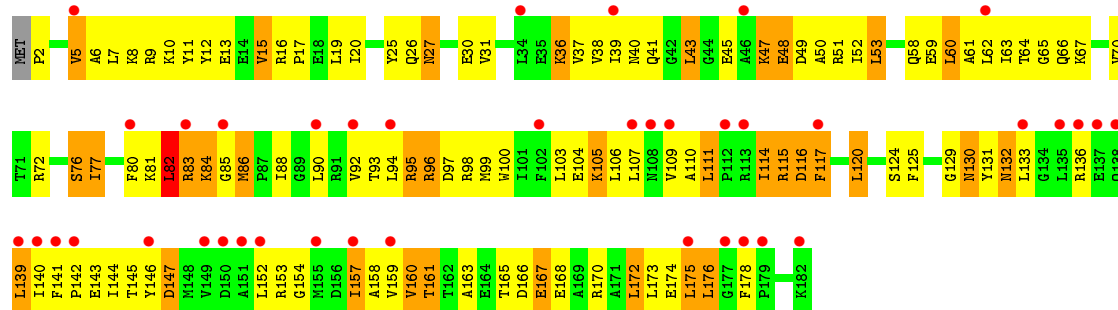




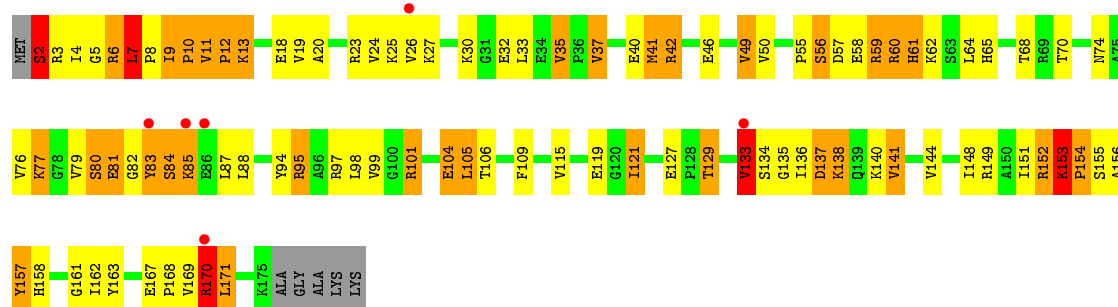
• Molecule 32: 50S ribosomal protein L5



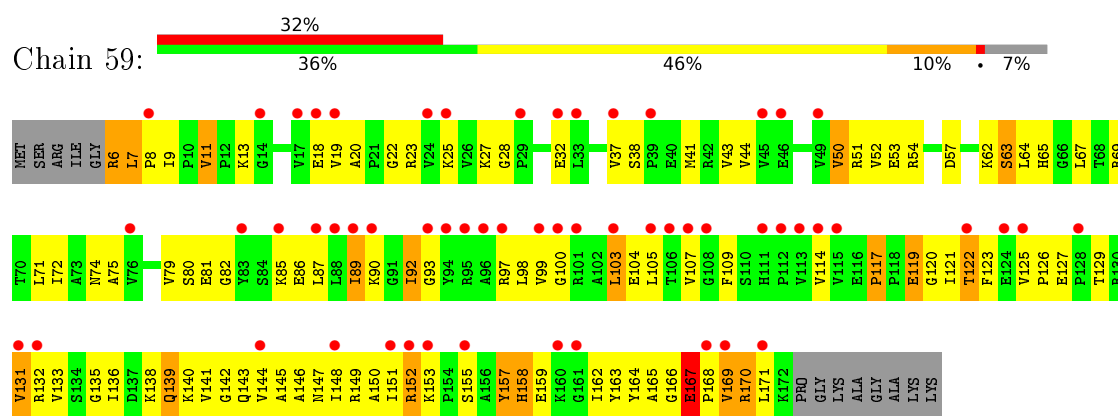
• Molecule 32: 50S ribosomal protein L5



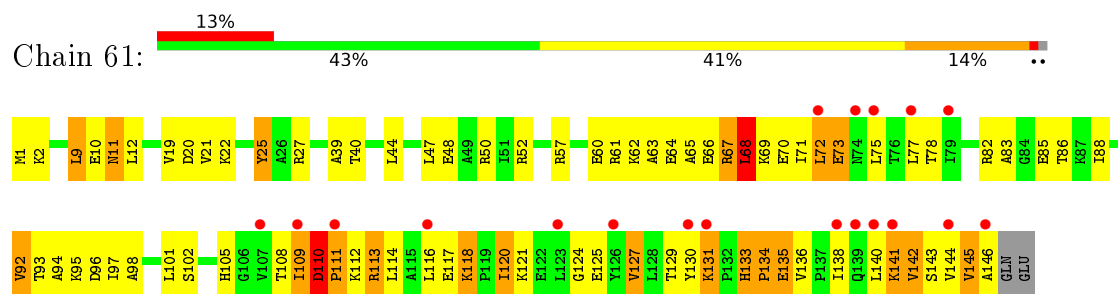
• Molecule 33: 50S ribosomal protein L6



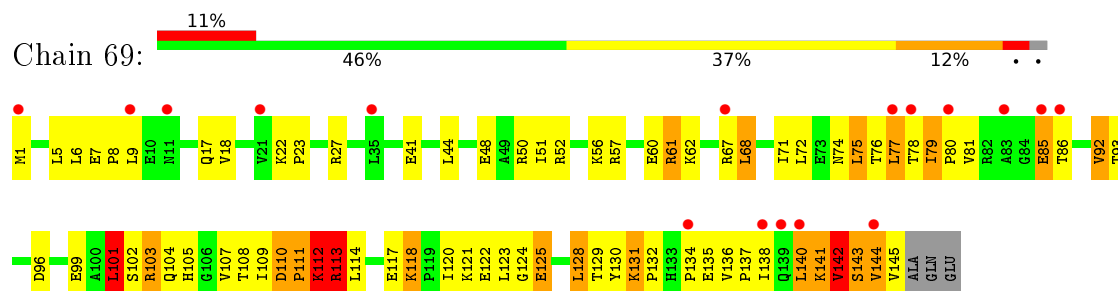
• Molecule 33: 50S ribosomal protein L6



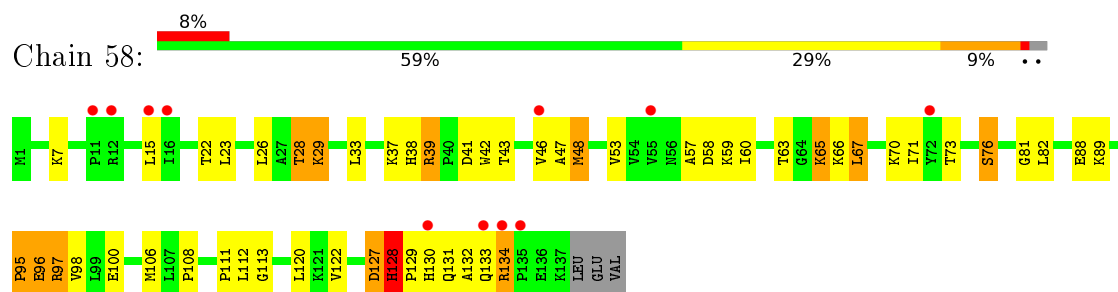
• Molecule 34: 50S ribosomal protein L9



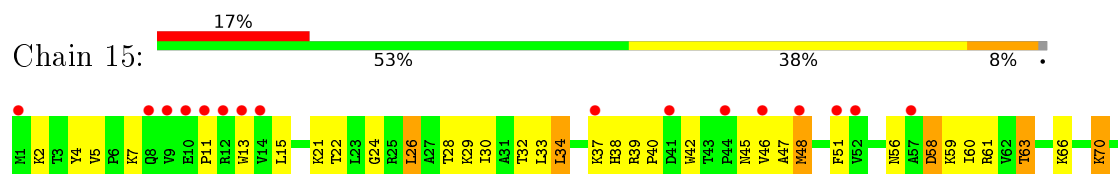
• Molecule 34: 50S ribosomal protein L9

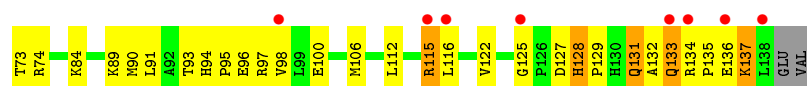


• Molecule 35: 50S ribosomal protein L13

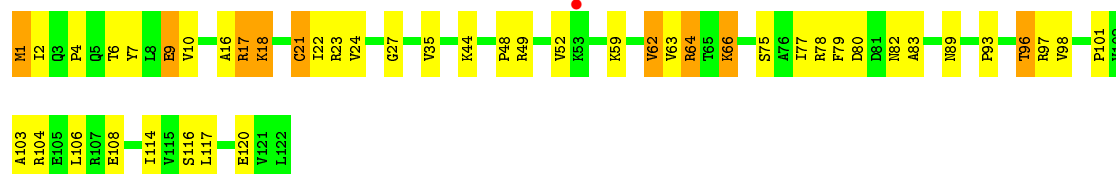


• Molecule 35: 50S ribosomal protein L13

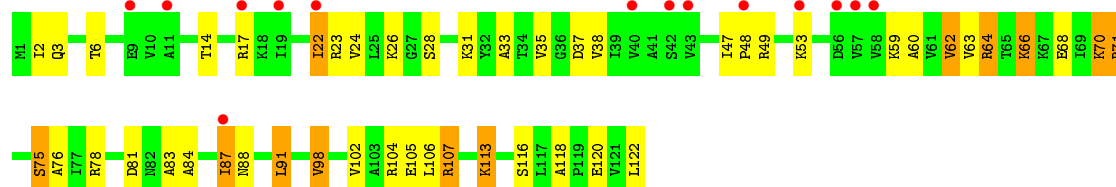




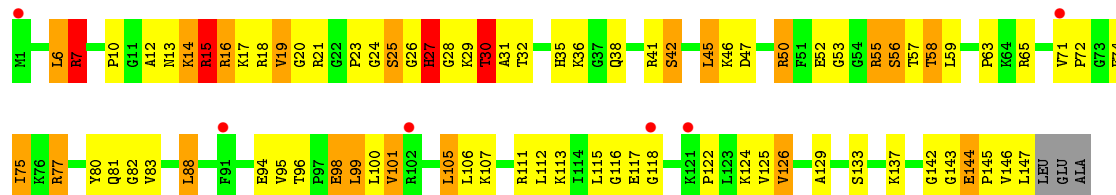
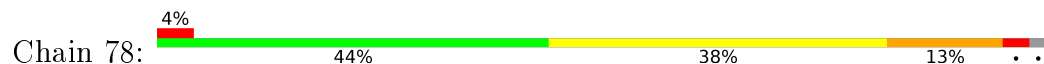
- Molecule 36: 50S ribosomal protein L14



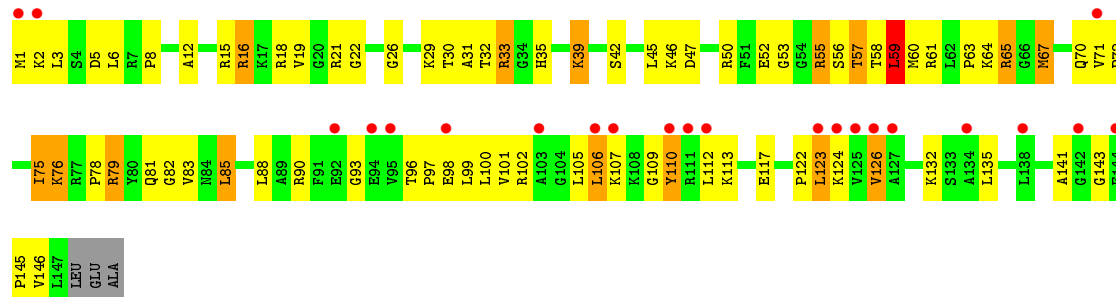
- Molecule 36: 50S ribosomal protein L14



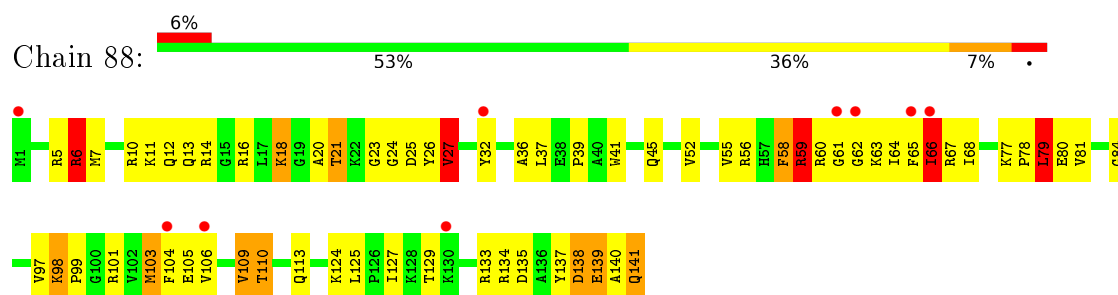
- Molecule 37: 50S ribosomal protein L15



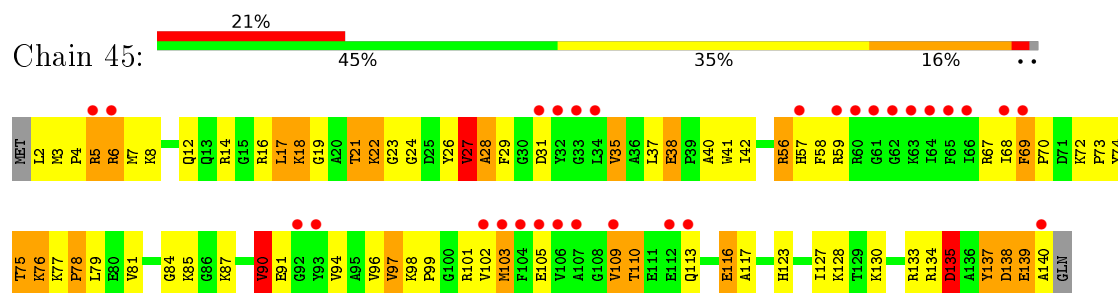
- Molecule 37: 50S ribosomal protein L15



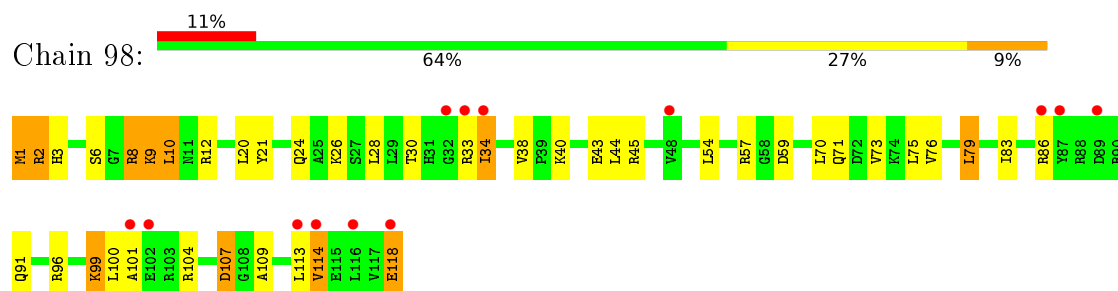
- Molecule 38: 50S ribosomal protein L16



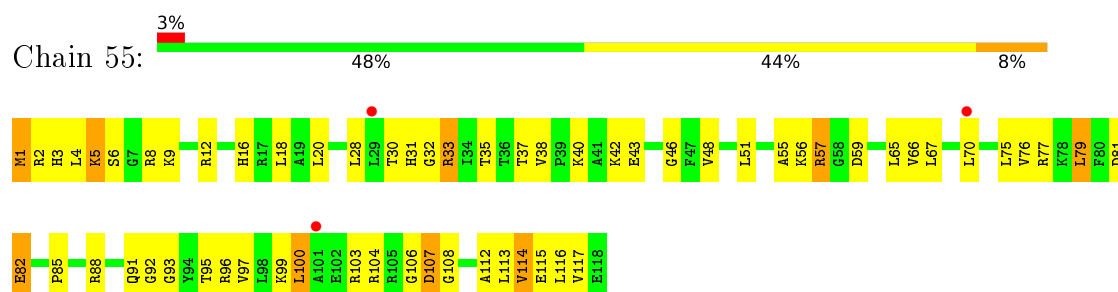
- Molecule 38: 50S ribosomal protein L16



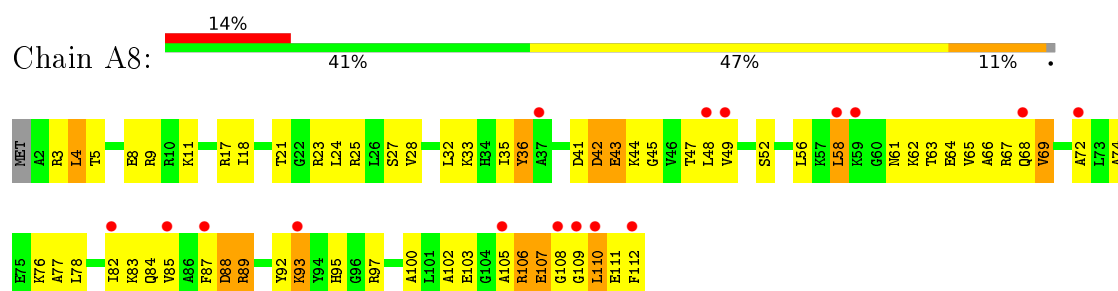
- Molecule 39: 50S ribosomal protein L17



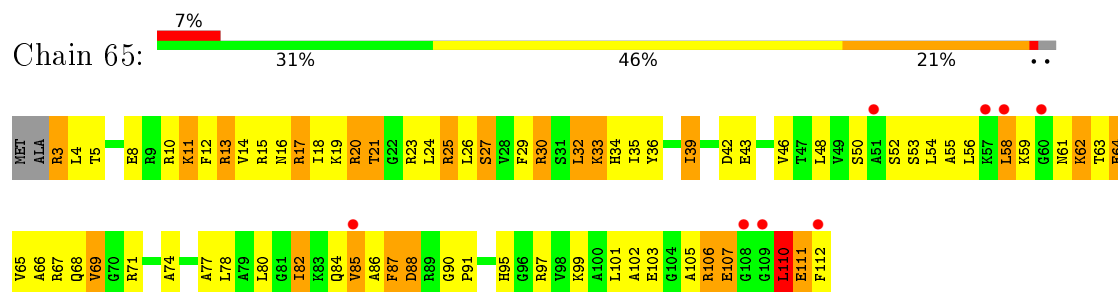
- Molecule 39: 50S ribosomal protein L17



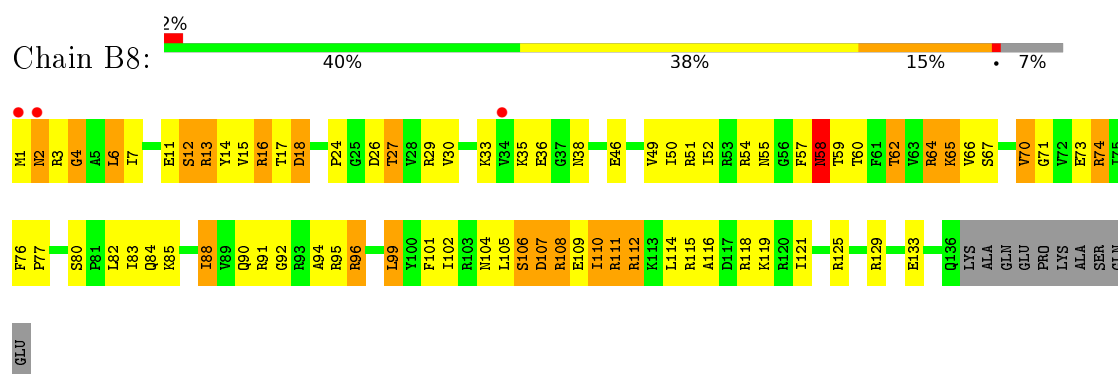
- Molecule 40: 50S ribosomal protein L18



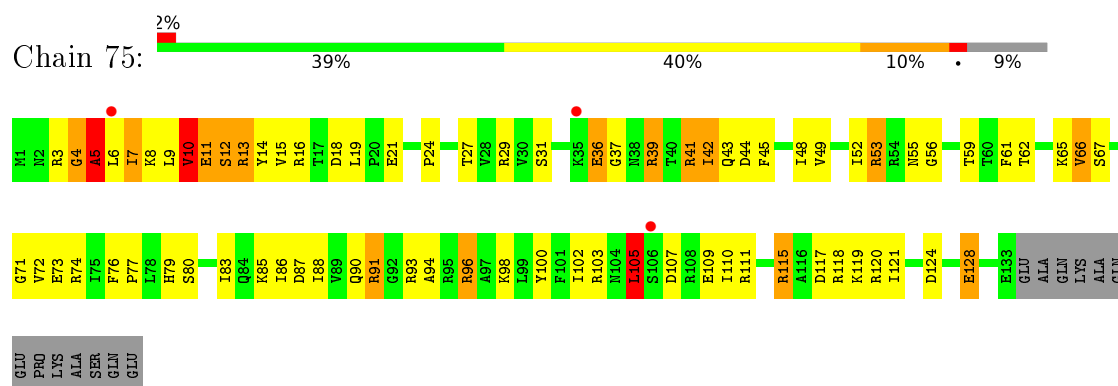
- Molecule 40: 50S ribosomal protein L18



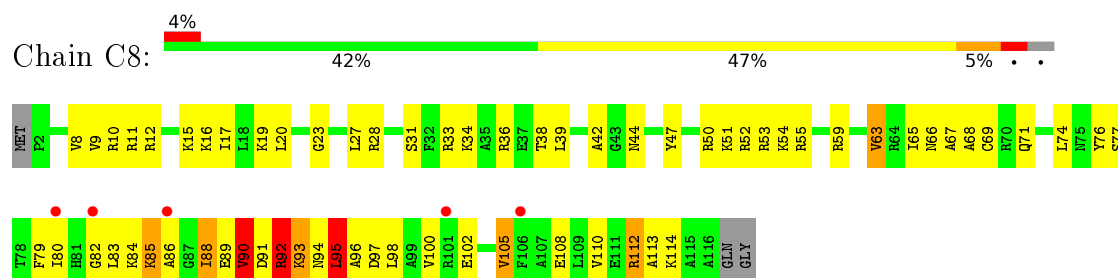
- Molecule 41: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L19



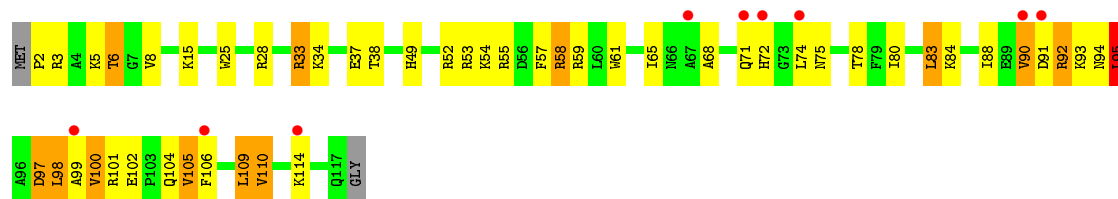
- Molecule 42: 50S ribosomal protein L20



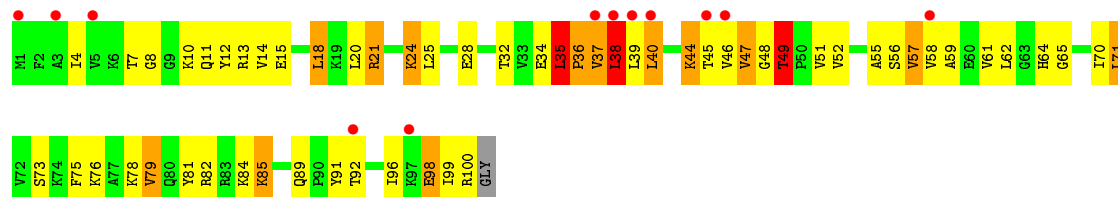
- Molecule 42: 50S ribosomal protein L20



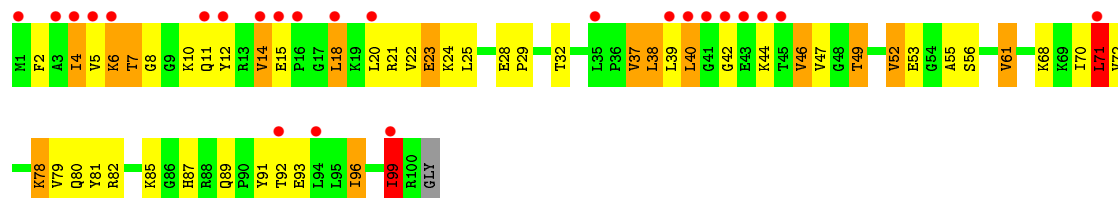




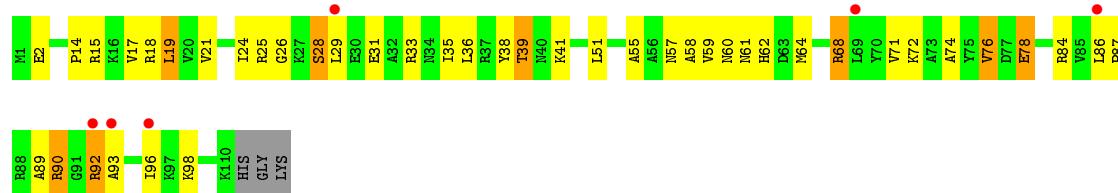
• Molecule 43: 50S ribosomal protein L21



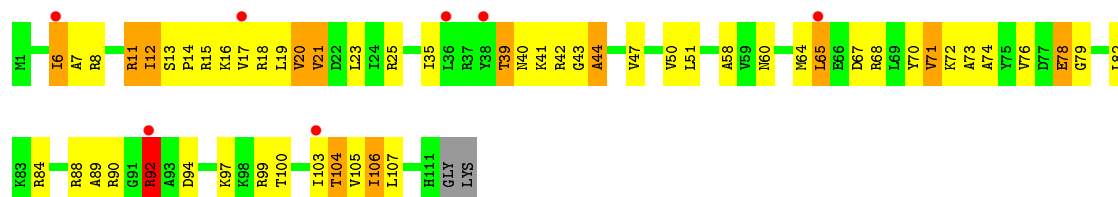
• Molecule 43: 50S ribosomal protein L21



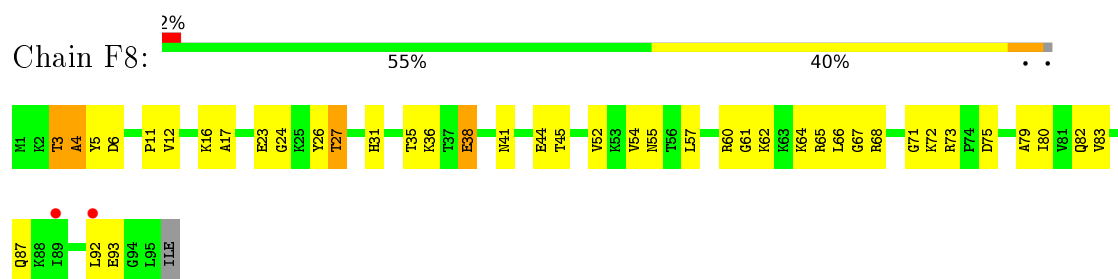
• Molecule 44: 50S ribosomal protein L22



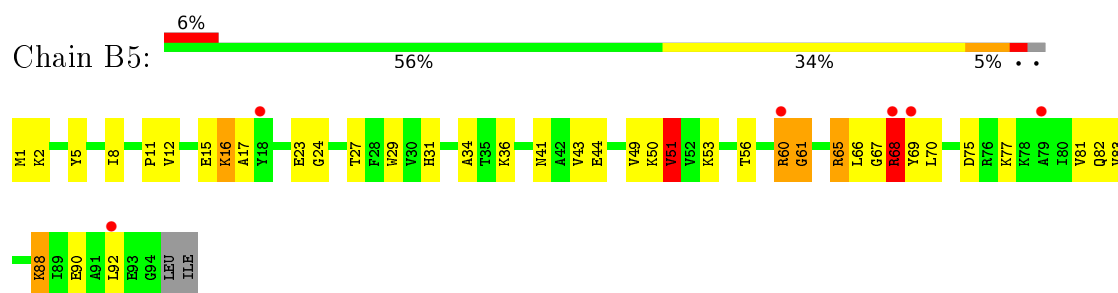
• Molecule 44: 50S ribosomal protein L22



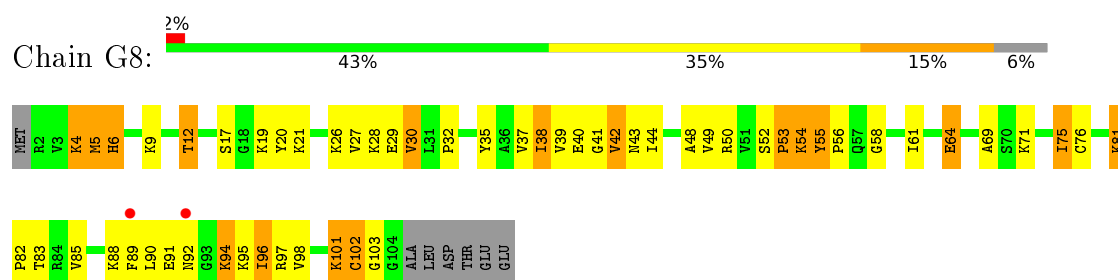
• Molecule 45: 50S ribosomal protein L23



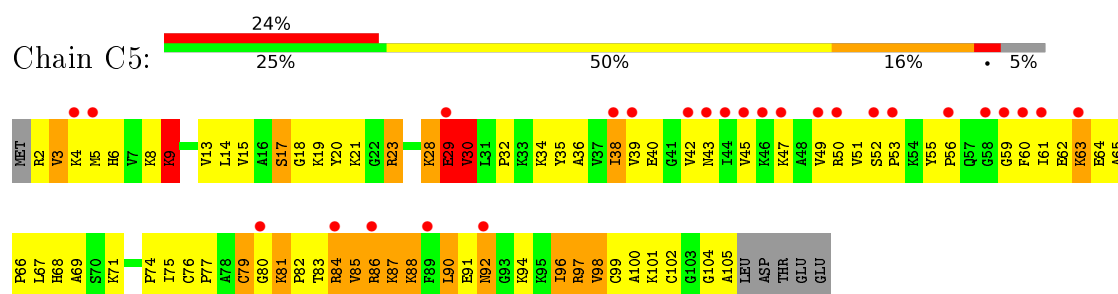
- Molecule 45: 50S ribosomal protein L23



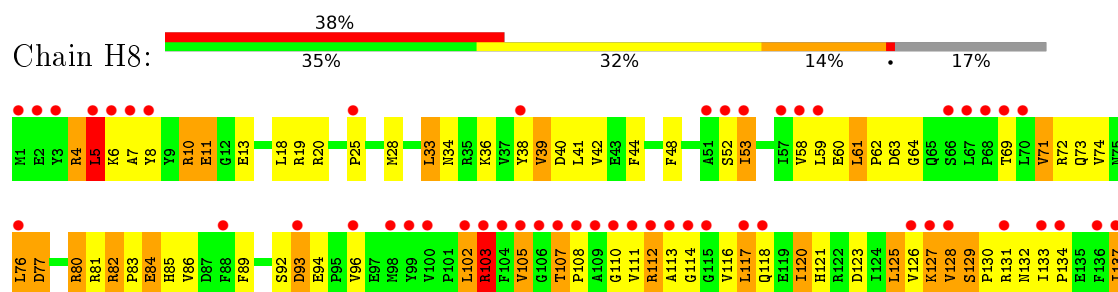
- Molecule 46: 50S ribosomal protein L24

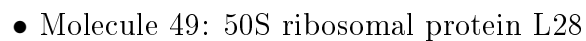
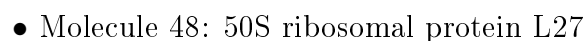
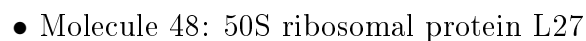
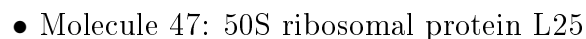


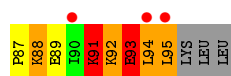
- Molecule 46: 50S ribosomal protein L24



- Molecule 47: 50S ribosomal protein L25







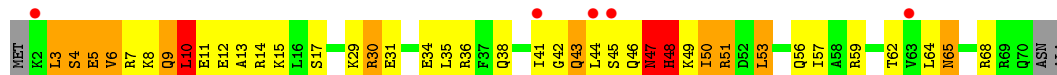
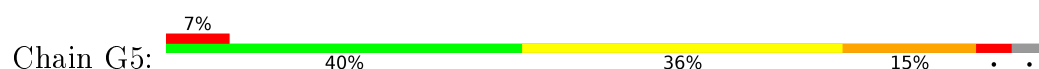
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



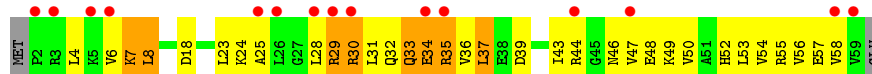
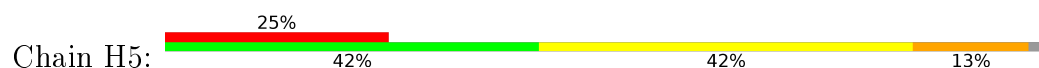
- Molecule 50: 50S ribosomal protein L29



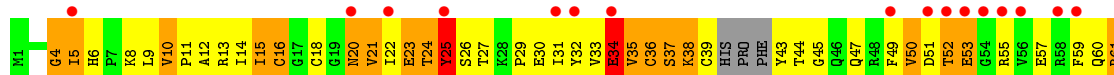
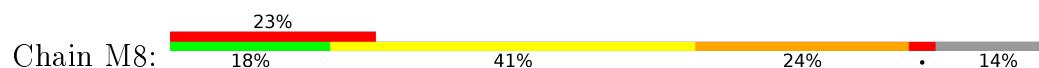
- Molecule 51: 50S ribosomal protein L30

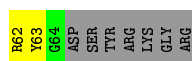


- Molecule 51: 50S ribosomal protein L30

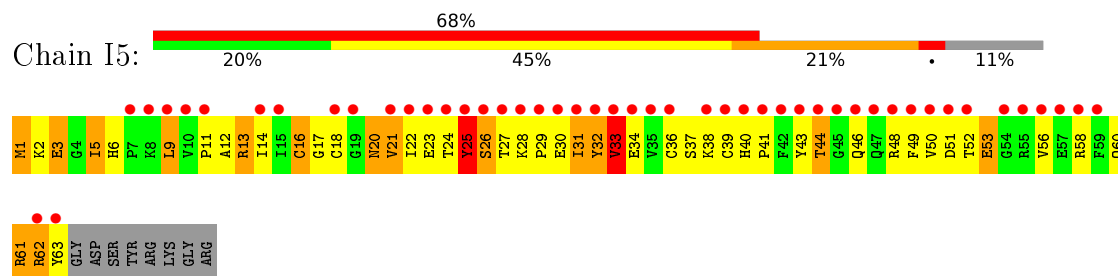


- Molecule 52: 50S ribosomal protein L31

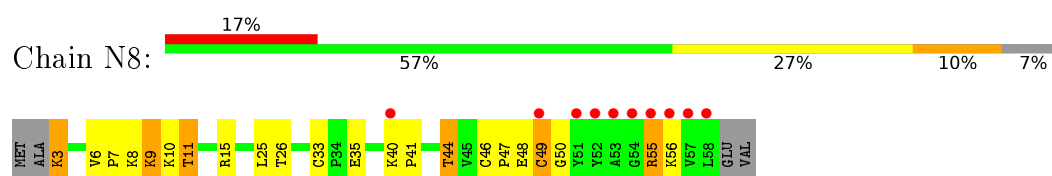




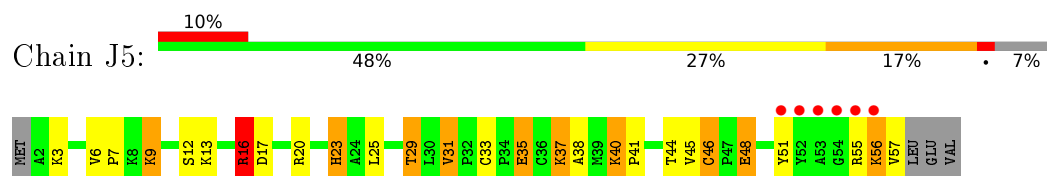
- Molecule 52: 50S ribosomal protein L31



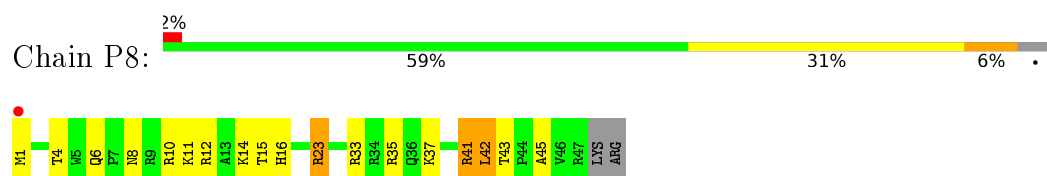
- Molecule 53: 50S ribosomal protein L32



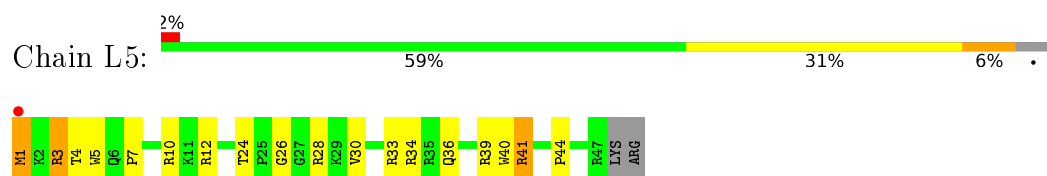
- Molecule 53: 50S ribosomal protein L32



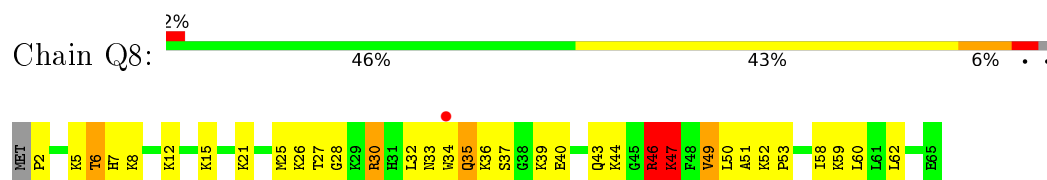
- Molecule 54: 50S ribosomal protein L34



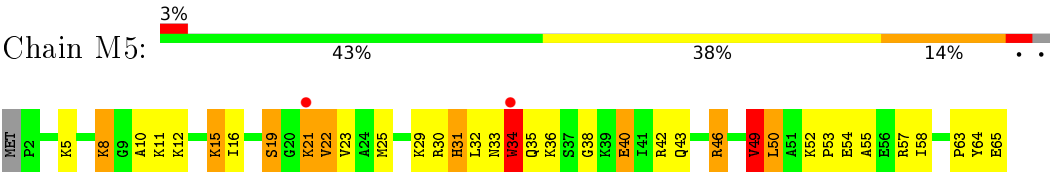
- Molecule 54: 50S ribosomal protein L34



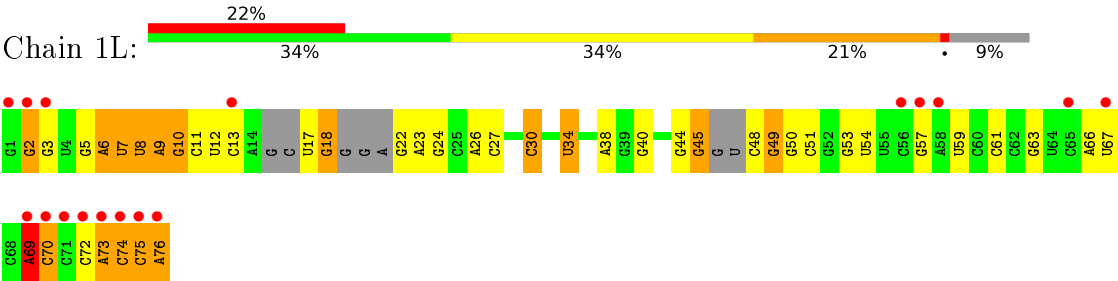
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



• Molecule 56: tRNAVal



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.50 Å 448.90 Å 620.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.68 – 2.96 146.68 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (146.68-2.96) 89.3 (146.68-2.96)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.96 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.201 , 0.243 0.202 , 0.243	Depositor DCC
$R_{free}$ test set	2000 reflections (0.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	296743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, H2U, SF4, MG, CM0, 6MZ, 4SU, 7MG, SPE, 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	0.67	6/35994 (0.0%)	1.30	243/56171 (0.4%)
1	1G	0.61	1/36236 (0.0%)	1.22	170/56555 (0.3%)
2	12	0.39	0/1727	0.70	1/2326 (0.0%)
2	1E	0.40	0/1936	0.66	1/2611 (0.0%)
3	22	0.62	1/1560 (0.1%)	0.65	1/2104 (0.0%)
3	2E	0.49	1/1629 (0.1%)	0.67	0/2195
4	32	0.45	0/1732	0.65	0/2318
4	3E	0.48	0/1728	0.73	4/2313 (0.2%)
5	42	0.46	0/1155	0.67	1/1555 (0.1%)
5	4E	0.46	0/1158	0.70	1/1559 (0.1%)
6	52	0.47	0/855	0.63	0/1154
6	5E	0.48	0/850	0.64	0/1147
7	62	0.42	0/1132	0.66	1/1514 (0.1%)
7	6E	0.45	0/1259	0.57	0/1686
8	72	0.41	0/1127	0.63	0/1517
8	7E	0.43	0/1135	0.71	1/1527 (0.1%)
9	82	0.41	0/971	0.74	1/1304 (0.1%)
9	8E	0.50	1/1019 (0.1%)	0.76	1/1367 (0.1%)
10	1A	0.74	2/658 (0.3%)	0.68	0/885
10	1I	0.41	0/767	0.72	2/1034 (0.2%)
11	2A	0.46	0/850	0.66	0/1150
11	2I	0.46	0/838	0.67	0/1133
12	3A	0.56	0/972	0.73	1/1301 (0.1%)
12	3I	0.61	0/972	0.79	0/1301
13	4A	0.42	0/903	0.69	1/1211 (0.1%)
13	4I	0.48	0/952	0.73	1/1277 (0.1%)
14	5A	0.46	0/495	0.89	2/657 (0.3%)
14	5I	0.63	2/500 (0.4%)	0.90	3/664 (0.5%)
15	6A	0.47	0/740	0.63	0/987
15	6I	0.47	0/740	0.70	0/987
16	7A	0.45	0/721	0.74	1/970 (0.1%)
16	7I	0.47	0/716	0.76	1/963 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.46	0/836	0.61	0/1117
17	8I	0.55	1/847 (0.1%)	0.77	1/1131 (0.1%)
18	9A	0.51	0/549	0.75	1/732 (0.1%)
18	9I	0.46	0/554	0.69	0/739
19	AA	0.43	0/490	0.75	2/662 (0.3%)
19	AI	0.42	0/676	0.79	1/910 (0.1%)
20	BA	0.40	0/764	0.71	0/1007
20	BI	0.56	1/748 (0.1%)	0.81	2/986 (0.2%)
21	1B	0.44	0/192	0.65	0/252
21	1F	0.44	0/203	0.67	0/266
22	1K	0.64	0/1595	1.19	11/2475 (0.4%)
23	2K	0.77	0/1721	1.38	7/2682 (0.3%)
23	2L	0.67	0/1698	1.28	12/2644 (0.5%)
24	3K	0.54	0/1663	1.20	16/2585 (0.6%)
24	3L	0.56	0/1689	1.16	11/2628 (0.4%)
25	4K	0.72	0/520	1.23	3/808 (0.4%)
25	4L	0.64	0/470	1.23	4/732 (0.5%)
26	14	0.81	39/67798 (0.1%)	1.49	1064/105832 (1.0%)
26	1H	0.95	95/68537 (0.1%)	1.67	1647/106989 (1.5%)
27	16	0.79	0/2928	1.48	37/4568 (0.8%)
27	1J	0.73	0/2928	1.34	23/4568 (0.5%)
28	71	0.32	0/1055	0.62	0/1425
28	79	0.31	0/459	0.58	0/608
29	11	0.68	1/2170 (0.0%)	0.94	6/2926 (0.2%)
29	19	0.61	0/2175	0.86	2/2933 (0.1%)
30	21	0.58	0/1537	0.92	3/2081 (0.1%)
30	29	0.53	0/1596	0.85	1/2153 (0.0%)
31	31	0.58	0/1620	0.78	2/2194 (0.1%)
31	39	0.54	1/1637 (0.1%)	0.84	2/2218 (0.1%)
32	41	0.51	1/1481 (0.1%)	0.71	1/1994 (0.1%)
32	49	0.42	0/1492	0.72	3/2008 (0.1%)
33	51	0.54	0/1354	0.95	5/1833 (0.3%)
33	59	0.36	0/1308	0.67	2/1771 (0.1%)
34	61	0.46	0/1151	0.80	4/1558 (0.3%)
34	69	0.45	0/1146	0.75	2/1551 (0.1%)
35	15	0.47	1/1131 (0.1%)	0.72	0/1525
35	58	0.52	0/1123	0.74	1/1514 (0.1%)
36	25	0.51	0/942	0.70	0/1269
36	68	0.54	0/942	0.74	0/1269
37	35	0.55	0/1139	0.90	3/1514 (0.2%)
37	78	0.64	0/1139	1.03	6/1514 (0.4%)
38	45	0.65	2/1125 (0.2%)	0.83	1/1505 (0.1%)
38	88	0.71	0/1138	0.92	2/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	55	0.50	0/981	0.78	1/1312 (0.1%)
39	98	0.51	0/981	0.78	0/1312
40	65	0.52	0/886	0.83	0/1180
40	A8	0.56	0/891	0.78	0/1187
41	75	0.53	0/1123	0.83	4/1500 (0.3%)
41	B8	0.52	0/1138	0.82	1/1521 (0.1%)
42	85	0.52	0/977	0.73	0/1301
42	C8	0.57	0/968	0.85	4/1289 (0.3%)
43	95	0.49	0/781	0.81	1/1048 (0.1%)
43	D8	0.54	0/785	0.86	2/1052 (0.2%)
44	A5	0.54	0/897	0.76	1/1204 (0.1%)
44	E8	0.58	0/886	0.81	1/1189 (0.1%)
45	B5	0.53	0/749	0.72	1/1007 (0.1%)
45	F8	0.59	0/757	0.77	1/1017 (0.1%)
46	C5	0.54	0/807	0.89	0/1076
46	G8	0.64	0/790	0.93	3/1055 (0.3%)
47	D5	0.50	2/1103 (0.2%)	0.80	2/1494 (0.1%)
47	H8	0.48	0/1395	0.77	2/1890 (0.1%)
48	E5	0.62	0/611	0.83	0/814
48	I8	0.60	0/619	0.84	1/825 (0.1%)
49	F5	0.57	0/744	0.94	4/989 (0.4%)
49	J8	0.61	0/744	0.89	1/989 (0.1%)
50	G5	0.51	0/578	0.81	1/766 (0.1%)
50	K8	0.65	0/577	0.88	1/763 (0.1%)
51	H5	0.49	0/464	0.66	0/623
51	L8	0.49	0/464	0.73	0/623
52	I5	0.41	0/527	0.84	0/709
52	M8	0.54	0/486	0.87	2/652 (0.3%)
53	J5	0.51	0/448	0.83	1/606 (0.2%)
53	N8	0.58	0/451	0.75	0/610
54	L5	0.61	0/409	0.75	0/540
54	P8	0.78	0/409	0.96	3/540 (0.6%)
55	M5	0.61	1/524 (0.2%)	0.91	1/691 (0.1%)
55	Q8	0.67	0/524	0.96	2/691 (0.3%)
56	1L	0.53	0/1592	1.05	1/2472 (0.0%)
All	All	0.73	159/317359 (0.1%)	1.32	3368/475179 (0.7%)

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	5
2	1E	0	3
3	22	0	1
3	2E	0	1
4	32	0	2
4	3E	0	2
7	6E	0	1
8	72	0	2
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1I	0	2
11	2A	0	2
12	3I	0	6
13	4A	0	4
13	4I	0	2
14	5A	0	5
14	5I	0	1
16	7I	0	1
17	8I	0	1
18	9I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	2
28	71	0	1
29	11	0	3
29	19	0	4
30	21	0	5
30	29	0	3
31	31	0	1
31	39	0	9
32	41	0	3
32	49	0	3
33	51	0	7
33	59	0	2
34	61	0	3
34	69	0	5
35	58	0	1
36	68	0	1
37	35	0	5
37	78	0	4
38	45	0	3
38	88	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	3
41	75	0	3
41	B8	0	4
42	85	0	4
42	C8	0	3
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	1
46	C5	0	2
46	G8	0	4
47	D5	0	3
47	H8	0	3
49	F5	0	2
49	J8	0	4
50	G5	0	2
50	K8	0	2
52	I5	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	180

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	22	173	VAL	C-N	19.50	1.71	1.34
10	1A	38	ILE	C-N	14.98	1.62	1.34
26	1H	1698	A	N9-C4	-11.67	1.30	1.37
26	1H	783	A	N3-C4	-10.65	1.28	1.34
20	BI	97	ALA	C-N	10.36	1.53	1.34

The worst 5 of 3368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-25.58	110.65	126.00
26	1H	945	A	N1-C6-N6	24.24	133.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	945	A	C6-C5-N7	-23.79	115.65	132.30
26	1H	945	A	C5-N7-C8	-20.19	93.80	103.90
26	1H	1899	G	N3-C4-C5	19.48	138.34	128.60

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	236	TYR	Peptide
2	1E	95	GLN	Peptide
3	2E	78	GLY	Peptide
4	3E	154	ASN	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	32157	0	16234	740	0
1	1G	32371	0	16342	723	0
2	12	1696	0	1730	124	0
2	1E	1902	0	1949	157	0
3	22	1537	0	1603	116	0
3	2E	1605	0	1668	76	0
4	32	1702	0	1764	95	0
4	3E	1698	0	1760	125	0
5	42	1139	0	1202	85	0
5	4E	1142	0	1204	68	0
6	52	842	0	857	26	0
6	5E	837	0	852	39	0
7	62	1120	0	1167	82	0
7	6E	1242	0	1286	80	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	92	0
9	82	953	0	983	106	0
9	8E	1000	0	1031	100	0
10	1A	646	0	662	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1I	754	0	769	44	0
11	2A	835	0	847	42	0
11	2I	823	0	832	33	0
12	3A	956	0	1046	64	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	72	0
13	4I	942	0	997	76	0
14	5A	486	0	525	65	0
14	5I	491	0	532	49	0
15	6A	729	0	768	33	0
15	6I	729	0	768	38	0
16	7A	705	0	725	58	0
16	7I	700	0	720	77	0
17	8A	823	0	891	32	0
17	8I	834	0	904	84	0
18	9A	544	0	605	26	0
18	9I	549	0	607	33	0
19	AA	481	0	468	39	0
19	AI	661	0	683	55	0
20	BA	762	0	861	44	0
20	BI	746	0	843	98	0
21	1B	188	0	195	12	0
21	1F	199	0	208	19	0
22	1K	1540	0	787	25	0
23	2K	1646	0	843	25	0
23	2L	1626	0	836	27	0
24	3K	1491	0	761	59	0
24	3L	1513	0	770	36	0
25	4K	462	0	230	11	0
25	4L	417	0	207	12	0
26	14	60535	0	30516	1083	0
26	1H	61195	0	30847	1151	0
27	16	2617	0	1328	54	0
27	1J	2617	0	1328	88	0
28	7I	1033	0	1048	71	0
28	79	456	0	460	21	0
29	11	2120	0	2197	112	0
29	19	2125	0	2199	96	0
30	21	1505	0	1526	85	0
30	29	1563	0	1629	139	0
31	31	1585	0	1632	61	0
31	39	1602	0	1649	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	41	1457	0	1514	101	0
32	49	1468	0	1520	112	0
33	51	1328	0	1396	108	0
33	59	1283	0	1352	87	0
34	61	1136	0	1223	75	0
34	69	1131	0	1218	60	0
35	15	1104	0	1180	56	0
35	58	1096	0	1169	52	0
36	25	932	0	996	42	0
36	68	932	0	996	40	0
37	35	1122	0	1206	76	0
37	78	1122	0	1206	84	0
38	45	1104	0	1159	88	0
38	88	1117	0	1168	67	0
39	55	967	0	1033	45	0
39	98	967	0	1033	33	0
40	65	876	0	938	99	0
40	A8	881	0	943	58	0
41	75	1109	0	1170	74	0
41	B8	1124	0	1179	78	0
42	85	959	0	1019	59	0
42	C8	950	0	1011	85	0
43	95	770	0	838	48	0
43	D8	774	0	849	58	0
44	A5	886	0	948	38	0
44	E8	876	0	941	43	0
45	B5	735	0	785	37	0
45	F8	743	0	794	30	0
46	C5	794	0	886	81	0
46	G8	777	0	857	42	0
47	D5	1079	0	1088	86	0
47	H8	1365	0	1391	106	0
48	E5	603	0	620	36	0
48	I8	611	0	631	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	58	0
50	G5	576	0	625	33	0
50	K8	575	0	634	42	0
51	H5	459	0	512	41	0
51	L8	459	0	512	18	0
52	I5	515	0	514	46	0
52	M8	479	0	475	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	J5	434	0	454	25	0
53	N8	437	0	460	21	0
54	L5	401	0	436	15	0
54	P8	401	0	436	9	0
55	M5	516	0	582	32	0
55	Q8	516	0	582	32	0
56	1L	1469	0	752	37	0
57	11	3	0	0	0	0
57	13	149	0	0	0	0
57	14	446	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	133	0	0	0	0
57	1H	546	0	0	0	0
57	1J	7	0	0	0	0
57	21	2	0	0	0	0
57	25	2	0	0	0	0
57	29	3	0	0	0	0
57	2A	1	0	0	0	0
57	2I	1	0	0	0	0
57	2K	4	0	0	0	0
57	2L	2	0	0	0	0
57	31	2	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	1	0	0	0	0
57	4A	1	0	0	0	0
57	4E	1	0	0	0	0
57	4K	1	0	0	0	0
57	4L	2	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	68	2	0	0	0	0
57	88	3	0	0	0	0
57	98	1	0	0	0	0
57	9A	1	0	0	0	0
57	C5	1	0	0	0	0
57	D8	1	0	0	0	0
57	E5	1	0	0	0	0
57	F8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	I8	1	0	0	0	0
57	J8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	13	0	22	3	0
58	14	26	0	46	11	0
58	1G	13	0	24	0	0
58	1J	13	0	24	1	0
59	32	8	0	0	1	0
59	3E	8	0	0	3	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	16	0	0	6	0
61	13	304	0	0	17	0
61	14	1135	0	0	56	0
61	16	15	0	0	1	0
61	19	8	0	0	0	0
61	1G	391	0	0	17	0
61	1H	1133	0	0	86	0
61	1I	2	0	0	0	0
61	1J	18	0	0	1	0
61	1K	1	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	25	11	0	0	1	0
61	29	6	0	0	0	0
61	2I	1	0	0	0	0
61	2K	6	0	0	0	0
61	31	4	0	0	0	0
61	35	9	0	0	4	0
61	39	6	0	0	0	0
61	3A	1	0	0	0	0
61	3E	1	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	45	3	0	0	0	0
61	4E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	4K	11	0	0	0	0
61	4L	14	0	0	1	0
61	52	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	11	0	0	5	0
61	7A	1	0	0	0	0
61	7I	2	0	0	1	0
61	85	1	0	0	0	0
61	98	2	0	0	0	0
61	9A	3	0	0	3	0
61	A5	1	0	0	0	0
61	A8	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	2	0	0	0	0
61	C5	3	0	0	0	0
61	E5	5	0	0	0	0
61	E8	1	0	0	0	0
61	F5	3	0	0	0	0
61	F8	1	0	0	0	0
61	H5	1	0	0	0	0
61	I8	6	0	0	1	0
61	K8	1	0	0	0	0
61	L8	1	0	0	1	0
61	M5	7	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296743	0	197188	8827	0

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

The worst 5 of 8827 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)
3:22:173:VAL:C	3:22:174:PRO:N	1.71	1.38
4:3E:25:ARG:NH1	59:3E:301:SF4:S3	2.12	1.23
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.07	1.14
44:E8:89:ALA:O	44:E8:92:ARG:NH1	1.81	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:45:27:VAL:HB	38:45:28:ALA:HA	1.12	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	172 (85%)	25 (12%)	6 (3%)	5	26
2	1E	231/256 (90%)	188 (81%)	41 (18%)	2 (1%)	21	61
3	22	191/239 (80%)	167 (87%)	24 (13%)	0	100	100
3	2E	203/239 (85%)	181 (89%)	22 (11%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	34	74
4	3E	205/209 (98%)	190 (93%)	15 (7%)	0	100	100
5	42	147/162 (91%)	140 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	140 (95%)	6 (4%)	1 (1%)	26	67
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	125 (93%)	7 (5%)	3 (2%)	8	35
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	26	67
9	82	119/128 (93%)	101 (85%)	17 (14%)	1 (1%)	24	64
9	8E	124/128 (97%)	101 (82%)	19 (15%)	4 (3%)	5	24
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	93/105 (89%)	82 (88%)	10 (11%)	1 (1%)	17	56
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	11	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	21	61
12	3A	120/132 (91%)	101 (84%)	14 (12%)	5 (4%)	3	17
12	3I	120/132 (91%)	106 (88%)	11 (9%)	3 (2%)	7	31
13	4A	109/126 (86%)	98 (90%)	9 (8%)	2 (2%)	11	42
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	11	42
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	5	22
15	6A	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	6I	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	16	53
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	9	38
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	13	47
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	4	21
19	AI	80/93 (86%)	67 (84%)	8 (10%)	5 (6%)	2	8
20	BA	97/106 (92%)	85 (88%)	10 (10%)	2 (2%)	9	37
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	116 (90%)	12 (9%)	1 (1%)	24	64
28	79	45/229 (20%)	40 (89%)	4 (9%)	1 (2%)	8	35
29	11	271/276 (98%)	241 (89%)	21 (8%)	9 (3%)	5	23
29	19	272/276 (99%)	243 (89%)	25 (9%)	4 (2%)	13	47
30	21	200/206 (97%)	154 (77%)	37 (18%)	9 (4%)	3	15
30	29	202/206 (98%)	155 (77%)	35 (17%)	12 (6%)	2	9
31	31	200/210 (95%)	179 (90%)	18 (9%)	3 (2%)	13	47
31	39	202/210 (96%)	159 (79%)	35 (17%)	8 (4%)	4	18
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	11	43
32	49	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	30	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	51	172/180 (96%)	138 (80%)	23 (13%)	11 (6%)	2	7
33	59	165/180 (92%)	129 (78%)	30 (18%)	6 (4%)	4	21
34	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	9	37
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	9	37
35	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	26	67
35	58	135/140 (96%)	115 (85%)	17 (13%)	3 (2%)	8	35
36	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	117 (81%)	27 (19%)	1 (1%)	26	67
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	2	11
38	45	137/141 (97%)	115 (84%)	19 (14%)	3 (2%)	8	35
38	88	139/141 (99%)	121 (87%)	12 (9%)	6 (4%)	3	16
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	61
39	98	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	43
40	65	108/112 (96%)	91 (84%)	16 (15%)	1 (1%)	21	61
40	A8	109/112 (97%)	92 (84%)	15 (14%)	2 (2%)	11	42
41	75	131/146 (90%)	120 (92%)	8 (6%)	3 (2%)	8	34
41	B8	134/146 (92%)	120 (90%)	12 (9%)	2 (2%)	13	47
42	85	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
42	C8	113/118 (96%)	105 (93%)	3 (3%)	5 (4%)	3	16
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	5	25
43	D8	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	9	38
44	A5	109/113 (96%)	103 (94%)	5 (5%)	1 (1%)	21	61
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	8	35
45	F8	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	17	56
46	C5	102/110 (93%)	71 (70%)	24 (24%)	7 (7%)	1	6
46	G8	101/110 (92%)	82 (81%)	15 (15%)	4 (4%)	4	18
47	D5	127/206 (62%)	102 (80%)	21 (16%)	4 (3%)	5	25
47	H8	168/206 (82%)	132 (79%)	32 (19%)	4 (2%)	7	33
48	E5	74/85 (87%)	66 (89%)	7 (10%)	1 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	I8	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	15	51
49	F5	92/98 (94%)	80 (87%)	11 (12%)	1 (1%)	17	56
49	J8	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	8	35
50	G5	67/72 (93%)	62 (92%)	2 (3%)	3 (4%)	3	15
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	3	15
51	H5	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	I5	61/71 (86%)	28 (46%)	28 (46%)	5 (8%)	1	4
52	M8	57/71 (80%)	39 (68%)	13 (23%)	5 (9%)	1	4
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	M5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	24
55	Q8	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	3	14
All	All	11163/12404 (90%)	9756 (87%)	1192 (11%)	215 (2%)	10	40

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	111	ARG
18	9I	22	VAL
19	AI	41	VAL
30	21	77	ILE
37	78	25	SER

### 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	179/220 (81%)	136 (76%)	43 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	202/220 (92%)	152 (75%)	50 (25%)	1	3
3	22	154/188 (82%)	119 (77%)	35 (23%)	1	4
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	6
4	32	180/181 (99%)	151 (84%)	29 (16%)	3	12
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	5
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	4
5	4E	115/123 (94%)	93 (81%)	22 (19%)	2	8
6	52	90/90 (100%)	79 (88%)	11 (12%)	6	23
6	5E	90/90 (100%)	82 (91%)	8 (9%)	12	39
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	6
7	6E	125/127 (98%)	101 (81%)	24 (19%)	2	8
8	72	118/119 (99%)	94 (80%)	24 (20%)	1	6
8	7E	119/119 (100%)	96 (81%)	23 (19%)	2	8
9	82	92/99 (93%)	67 (73%)	25 (27%)	0	2
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	6
10	1A	71/92 (77%)	46 (65%)	25 (35%)	0	1
10	1I	81/92 (88%)	66 (82%)	15 (18%)	2	9
11	2A	85/99 (86%)	69 (81%)	16 (19%)	2	8
11	2I	84/99 (85%)	69 (82%)	15 (18%)	2	9
12	3A	103/109 (94%)	84 (82%)	19 (18%)	2	9
12	3I	103/109 (94%)	86 (84%)	17 (16%)	3	12
13	4A	91/101 (90%)	62 (68%)	29 (32%)	0	1
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	4
14	5A	49/50 (98%)	26 (53%)	23 (47%)	0	0
14	5I	49/50 (98%)	35 (71%)	14 (29%)	0	2
15	6A	79/80 (99%)	74 (94%)	5 (6%)	22	58
15	6I	79/80 (99%)	70 (89%)	9 (11%)	7	26
16	7A	72/74 (97%)	60 (83%)	12 (17%)	3	11
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2	11
17	8I	95/97 (98%)	72 (76%)	23 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	45 (78%)	13 (22%)	1	4
18	9I	58/77 (75%)	43 (74%)	15 (26%)	0	2
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	5
19	AI	72/80 (90%)	60 (83%)	12 (17%)	3	11
20	BA	76/82 (93%)	56 (74%)	20 (26%)	0	2
20	BI	75/82 (92%)	57 (76%)	18 (24%)	1	3
21	1B	17/22 (77%)	13 (76%)	4 (24%)	1	3
21	1F	18/22 (82%)	15 (83%)	3 (17%)	3	11
28	71	109/181 (60%)	84 (77%)	25 (23%)	1	4
28	79	48/181 (26%)	37 (77%)	11 (23%)	1	4
29	11	214/218 (98%)	189 (88%)	25 (12%)	7	25
29	19	214/218 (98%)	179 (84%)	35 (16%)	3	12
30	21	155/166 (93%)	121 (78%)	34 (22%)	1	5
30	29	165/166 (99%)	145 (88%)	20 (12%)	6	23
31	31	161/166 (97%)	139 (86%)	22 (14%)	4	18
31	39	163/166 (98%)	129 (79%)	34 (21%)	1	6
32	41	153/156 (98%)	131 (86%)	22 (14%)	4	16
32	49	153/156 (98%)	112 (73%)	41 (27%)	0	2
33	51	143/148 (97%)	104 (73%)	39 (27%)	0	2
33	59	139/148 (94%)	113 (81%)	26 (19%)	2	9
34	61	122/124 (98%)	97 (80%)	25 (20%)	1	6
34	69	122/124 (98%)	93 (76%)	29 (24%)	1	3
35	15	117/119 (98%)	100 (86%)	17 (14%)	4	16
35	58	116/119 (98%)	100 (86%)	16 (14%)	4	18
36	25	100/100 (100%)	83 (83%)	17 (17%)	2	11
36	68	100/100 (100%)	88 (88%)	12 (12%)	6	24
37	35	114/116 (98%)	89 (78%)	25 (22%)	1	5
37	78	114/116 (98%)	91 (80%)	23 (20%)	1	6
38	45	109/111 (98%)	82 (75%)	27 (25%)	1	3
38	88	110/111 (99%)	92 (84%)	18 (16%)	3	12
39	55	101/101 (100%)	86 (85%)	15 (15%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	98	101/101 (100%)	85 (84%)	16 (16%)	3	13
40	65	87/88 (99%)	57 (66%)	30 (34%)	0	1
40	A8	87/88 (99%)	72 (83%)	15 (17%)	2	10
41	75	117/127 (92%)	98 (84%)	19 (16%)	3	12
41	B8	117/127 (92%)	90 (77%)	27 (23%)	1	4
42	85	93/94 (99%)	78 (84%)	15 (16%)	3	12
42	C8	92/94 (98%)	80 (87%)	12 (13%)	5	20
43	95	81/82 (99%)	60 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	60 (73%)	22 (27%)	0	2
44	A5	91/92 (99%)	74 (81%)	17 (19%)	2	9
44	E8	90/92 (98%)	80 (89%)	10 (11%)	8	27
45	B5	74/78 (95%)	64 (86%)	10 (14%)	5	18
45	F8	75/78 (96%)	69 (92%)	6 (8%)	15	45
46	C5	85/91 (93%)	62 (73%)	23 (27%)	0	2
46	G8	83/91 (91%)	65 (78%)	18 (22%)	1	5
47	D5	118/179 (66%)	90 (76%)	28 (24%)	1	3
47	H8	151/179 (84%)	112 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	5	20
48	I8	62/67 (92%)	53 (86%)	9 (14%)	4	16
49	F5	79/83 (95%)	65 (82%)	14 (18%)	2	10
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	10
50	G5	63/67 (94%)	42 (67%)	21 (33%)	0	1
50	K8	64/67 (96%)	48 (75%)	16 (25%)	1	3
51	H5	50/52 (96%)	39 (78%)	11 (22%)	1	5
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1	7
52	I5	57/63 (90%)	39 (68%)	18 (32%)	0	1
52	M8	52/63 (82%)	33 (64%)	19 (36%)	0	1
53	J5	48/52 (92%)	34 (71%)	14 (29%)	0	2
53	N8	49/52 (94%)	39 (80%)	10 (20%)	1	6
54	L5	38/42 (90%)	33 (87%)	5 (13%)	5	20
54	P8	38/42 (90%)	32 (84%)	6 (16%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	M5	54/55 (98%)	42 (78%)	12 (22%)	1	4
55	Q8	54/55 (98%)	48 (89%)	6 (11%)	8	27
All	All	9419/10256 (92%)	7533 (80%)	1886 (20%)	1	7

5 of 1886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	K8	28	LYS
6	52	74	ASP
46	C5	79	CYS
52	M8	21	VAL
3	22	4	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	135	GLN
11	2A	117	ASN
32	49	130	ASN
2	12	16	HIS
38	45	123	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	348 (23%)	34 (2%)
1	1G	1505/1522 (98%)	323 (21%)	33 (2%)
22	1K	67/76 (88%)	36 (53%)	4 (5%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	75/77 (97%)	10 (13%)	2 (2%)
24	3K	67/76 (88%)	37 (55%)	3 (4%)
24	3L	69/76 (90%)	32 (46%)	1 (1%)
25	4K	19/30 (63%)	12 (63%)	2 (10%)
25	4L	18/30 (60%)	10 (55%)	2 (11%)
26	14	2803/2917 (96%)	638 (22%)	37 (1%)
26	1H	2836/2917 (97%)	590 (20%)	43 (1%)
27	16	121/122 (99%)	24 (19%)	0
27	1J	121/122 (99%)	34 (28%)	2 (1%)
56	1L	65/76 (85%)	24 (36%)	2 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9335/9640 (96%)	2138 (22%)	166 (1%)

5 of 2138 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	12	U
1	13	13	U

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	1900	A
1	1G	250	A
26	14	2402	C
26	1H	2172	U
26	1H	2481	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	H2U	1K	17	22	17,21,22	2.23	4 (23%)	23,30,33	2.84	5 (21%)
22	CM0	1K	34	22	15,26,27	3.42	4 (26%)	18,37,40	1.96	2 (11%)
22	6MZ	1K	37	22	17,25,26	2.21	3 (17%)	15,36,39	3.26	3 (20%)
22	5MU	1K	54	22	13,22,23	1.67	2 (15%)	16,32,35	1.74	1 (6%)
22	PSU	1K	55	22	15,21,22	1.17	1 (6%)	16,30,33	2.47	3 (18%)
56	5MU	1L	54	56	13,22,23	1.72	2 (15%)	16,32,35	1.45	1 (6%)
56	PSU	1L	55	56	15,21,22	1.25	1 (6%)	16,30,33	2.42	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	OMC	2K	33	23	15,22,23	2.17	4 (26%)	20,31,34	2.36	3 (15%)
23	7MG	2K	47	23	20,26,27	3.34	6 (30%)	23,39,42	2.14	7 (30%)
23	5MU	2K	55	57,23	13,22,23	1.70	2 (15%)	16,32,35	1.35	1 (6%)
23	PSU	2K	56	23	15,21,22	1.08	2 (13%)	16,30,33	1.72	3 (18%)
23	4SU	2K	8	23	12,21,22	3.26	2 (16%)	15,30,33	0.80	1 (6%)
23	OMC	2L	33	23	15,22,23	2.29	4 (26%)	20,31,34	1.33	2 (10%)
23	7MG	2L	47	23	20,26,27	3.42	5 (25%)	23,39,42	2.53	7 (30%)
23	5MU	2L	55	23	13,22,23	1.71	2 (15%)	16,32,35	1.59	1 (6%)
23	PSU	2L	56	23	15,21,22	1.09	1 (6%)	16,30,33	1.92	3 (18%)
23	4SU	2L	8	23	12,21,22	3.45	2 (16%)	15,30,33	0.68	0

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	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	CM0	1K	34	22	-	0/6/30/31	0/2/2/2
22	6MZ	1K	37	22	-	0/5/27/28	0/3/3/3
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/3/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2K	55	57,23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C5-C4	-5.90	1.23	1.39
23	2L	47	7MG	C5-C4	-5.04	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	17	H2U	C6-N1	-3.70	1.42	1.47
22	1K	37	6MZ	C5-C4	-3.42	1.32	1.40
56	1L	54	5MU	C4-N3	-3.12	1.27	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	6MZ	N3-C2-N1	-11.45	119.88	128.87
23	2L	47	7MG	C5-C4-N3	-9.06	117.52	126.74
22	1K	17	H2U	C4-N3-C2	-6.99	119.43	125.77
23	2K	47	7MG	C5-C4-N3	-5.18	121.47	126.74
22	1K	55	PSU	C5-C1'-C2'	-5.07	106.83	115.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	17	H2U	2	0
22	1K	34	CM0	1	0
22	1K	54	5MU	1	0
22	1K	55	PSU	2	0
56	1L	54	5MU	1	0
23	2K	33	OMC	1	0
23	2K	47	7MG	2	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	3	0
23	2L	47	7MG	1	0
23	2L	55	5MU	3	0
23	2L	8	4SU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1355 ligands modelled in this entry, 1348 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SPE	13	1750	1	12,12,12	0.50	0	11,11,11	1.06	1 (9%)
58	SPE	14	3447	26	12,12,12	0.59	0	11,11,11	0.83	0
58	SPE	14	3448	-	12,12,12	0.72	0	11,11,11	1.09	1 (9%)
58	SPE	1G	1734	-	12,12,12	0.41	0	11,11,11	0.91	0
58	SPE	1J	208	-	12,12,12	0.41	0	11,11,11	0.87	0
59	SF4	32	301	4	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	3E	301	4	0,12,12	0.00	-	0,24,24	0.00	-

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
58	SPE	13	1750	1	-	0/10/10/10	0/0/0/0
58	SPE	14	3447	26	-	0/10/10/10	0/0/0/0
58	SPE	14	3448	-	-	0/10/10/10	0/0/0/0
58	SPE	1G	1734	-	-	0/10/10/10	0/0/0/0
58	SPE	1J	208	-	-	0/10/10/10	0/0/0/0
59	SF4	32	301	4	-	0/0/48/48	0/6/5/5
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1750	SPE	C11-C10-N9	-2.66	105.58	112.04
58	14	3448	SPE	C11-C10-N9	-2.62	105.69	112.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	13	1750	SPE	3	0
58	14	3447	SPE	5	0
58	14	3448	SPE	6	0
58	1J	208	SPE	1	0
59	32	301	SF4	1	0
59	3E	301	SF4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	22	1
10	1A	1
25	4K	1
2	1E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1E	78:GLN	C	79:ASP	N	4.14
1	4K	25:A	O3'	26:A	P	3.23
1	22	173:VAL	C	174:PRO	N	1.71
1	1A	38:ILE	C	39:PRO	N	1.62

## 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	1496/1522 (98%)	-0.39	6 (0%) 93 83	57, 98, 164, 235	0
1	1G	1506/1522 (98%)	-0.44	4 (0%) 94 87	68, 105, 166, 238	0
2	12	207/256 (80%)	1.11	46 (22%) 1 1	121, 148, 168, 185	0
2	1E	235/256 (91%)	0.45	17 (7%) 18 10	108, 135, 160, 171	0
3	22	195/239 (81%)	1.28	48 (24%) 1 1	113, 131, 152, 164	0
3	2E	205/239 (85%)	1.22	47 (22%) 1 1	85, 107, 142, 149	0
4	32	208/209 (99%)	0.84	30 (14%) 3 2	84, 101, 123, 132	0
4	3E	207/209 (99%)	0.55	19 (9%) 11 6	77, 103, 125, 133	0
5	42	149/162 (91%)	0.17	5 (3%) 49 30	91, 111, 128, 149	0
5	4E	149/162 (91%)	0.22	3 (2%) 68 48	79, 98, 118, 135	0
6	52	101/101 (100%)	0.83	10 (9%) 9 5	81, 97, 110, 131	0
6	5E	100/101 (99%)	0.89	12 (12%) 6 3	83, 99, 113, 123	0
7	62	140/156 (89%)	0.88	20 (14%) 4 2	103, 119, 131, 138	0
7	6E	154/156 (98%)	0.98	20 (12%) 5 2	98, 113, 138, 162	0
8	72	137/138 (99%)	-0.18	1 (0%) 89 76	90, 114, 125, 128	0
8	7E	138/138 (100%)	0.05	5 (3%) 46 28	87, 102, 113, 120	0
9	82	121/128 (94%)	0.40	7 (5%) 26 14	101, 144, 160, 164	0
9	8E	126/128 (98%)	0.66	12 (9%) 10 5	84, 133, 153, 157	0
10	1A	80/105 (76%)	0.31	9 (11%) 7 3	111, 138, 152, 156	0
10	1I	95/105 (90%)	2.01	48 (50%) 0 0	80, 127, 155, 159	0
11	2A	113/129 (87%)	1.70	43 (38%) 0 0	78, 103, 117, 120	0
11	2I	111/129 (86%)	0.92	14 (12%) 5 2	70, 99, 115, 125	0
12	3A	122/132 (92%)	0.84	19 (15%) 3 1	74, 91, 116, 132	0
12	3I	122/132 (92%)	0.29	3 (2%) 61 39	65, 76, 103, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	111/126 (88%)	0.34	4 (3%) 46 28	102, 129, 143, 152	0
13	4I	119/126 (94%)	0.30	7 (5%) 26 14	87, 111, 129, 139	0
14	5A	59/61 (96%)	1.73	24 (40%) 0 0	118, 129, 141, 142	0
14	5I	60/61 (98%)	0.42	4 (6%) 21 11	83, 97, 112, 119	0
15	6A	87/89 (97%)	-0.03	0 100 100	79, 100, 115, 117	0
15	6I	87/89 (97%)	0.81	10 (11%) 6 3	75, 94, 109, 116	0
16	7A	84/88 (95%)	0.03	1 (1%) 81 63	85, 98, 119, 145	0
16	7I	83/88 (94%)	0.14	2 (2%) 62 41	91, 107, 132, 147	0
17	8A	99/105 (94%)	0.14	1 (1%) 84 67	89, 100, 117, 120	0
17	8I	100/105 (95%)	0.30	3 (3%) 54 33	81, 98, 108, 115	0
18	9A	67/88 (76%)	0.85	10 (14%) 3 1	87, 101, 125, 129	0
18	9I	68/88 (77%)	0.94	11 (16%) 3 1	85, 100, 125, 128	0
19	AA	62/93 (66%)	0.26	5 (8%) 15 7	118, 142, 155, 158	0
19	AI	82/93 (88%)	0.76	12 (14%) 3 1	95, 110, 128, 136	0
20	BA	99/106 (93%)	0.44	4 (4%) 42 25	85, 104, 128, 140	0
20	BI	97/106 (91%)	0.25	6 (6%) 24 13	103, 117, 139, 145	0
21	1B	22/27 (81%)	0.93	3 (13%) 4 2	110, 116, 124, 134	0
21	1F	23/27 (85%)	0.77	3 (13%) 5 2	90, 98, 106, 108	0
22	1K	67/76 (88%)	0.63	7 (10%) 8 4	80, 167, 196, 203	0
23	2K	72/77 (93%)	-0.20	1 (1%) 78 59	68, 89, 116, 129	0
23	2L	71/77 (92%)	-0.03	0 100 100	78, 100, 132, 145	0
24	3K	70/76 (92%)	0.67	11 (15%) 3 1	71, 198, 222, 224	0
24	3L	71/76 (93%)	0.67	9 (12%) 5 2	78, 191, 215, 218	0
25	4K	21/30 (70%)	0.82	2 (9%) 10 5	69, 129, 212, 213	0
25	4L	19/30 (63%)	0.26	1 (5%) 30 17	85, 144, 210, 210	0
26	14	2810/2917 (96%)	-0.10	30 (1%) 82 65	54, 81, 180, 237	0
26	1H	2841/2917 (97%)	-0.10	27 (0%) 84 67	44, 70, 166, 244	0
27	16	122/122 (100%)	-0.65	1 (0%) 87 73	65, 87, 105, 180	0
27	1J	122/122 (100%)	-0.71	0 100 100	79, 106, 125, 185	0
28	71	133/229 (58%)	2.14	59 (44%) 0 0	137, 194, 219, 229	0
28	79	57/229 (24%)	0.85	12 (21%) 1 1	136, 178, 198, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	11	273/276 (98%)	0.34	4 (1%) 76 57	44, 62, 78, 94	0
29	19	274/276 (99%)	0.84	24 (8%) 12 6	50, 72, 87, 102	0
30	21	202/206 (98%)	0.88	29 (14%) 3 2	49, 82, 115, 123	0
30	29	204/206 (99%)	0.78	27 (13%) 4 2	57, 88, 125, 135	0
31	31	202/210 (96%)	0.75	27 (13%) 4 2	46, 75, 108, 123	0
31	39	204/210 (97%)	0.66	22 (10%) 8 4	57, 95, 139, 164	0
32	41	179/182 (98%)	0.35	7 (3%) 43 25	75, 95, 124, 138	0
32	49	181/182 (99%)	1.05	40 (22%) 1 1	99, 118, 142, 156	0
33	51	174/180 (96%)	0.09	6 (3%) 49 30	76, 99, 116, 128	0
33	59	167/180 (92%)	1.59	57 (34%) 0 0	123, 190, 216, 225	0
34	61	146/148 (98%)	0.75	19 (13%) 5 2	75, 119, 134, 148	0
34	69	145/148 (97%)	0.57	17 (11%) 6 3	80, 115, 138, 144	0
35	15	138/140 (98%)	1.03	24 (17%) 2 1	76, 98, 124, 139	0
35	58	137/140 (97%)	0.56	11 (8%) 15 8	64, 84, 113, 134	0
36	25	122/122 (100%)	0.78	14 (11%) 6 3	68, 81, 97, 107	0
36	68	122/122 (100%)	0.49	1 (0%) 87 73	57, 72, 87, 93	0
37	35	147/150 (98%)	0.89	22 (14%) 3 1	59, 93, 121, 133	0
37	78	147/150 (98%)	0.32	6 (4%) 41 24	46, 77, 98, 106	0
38	45	139/141 (98%)	1.16	29 (20%) 1 1	70, 94, 112, 126	0
38	88	141/141 (100%)	0.46	9 (6%) 23 12	57, 74, 97, 117	0
39	55	118/118 (100%)	0.17	3 (2%) 61 39	61, 77, 92, 109	0
39	98	118/118 (100%)	0.79	13 (11%) 7 4	58, 76, 94, 104	0
40	65	110/112 (98%)	0.61	8 (7%) 18 9	82, 100, 119, 130	0
40	A8	111/112 (99%)	1.02	16 (14%) 3 2	73, 86, 104, 112	0
41	75	133/146 (91%)	0.17	3 (2%) 64 43	76, 88, 117, 142	0
41	B8	136/146 (93%)	0.05	3 (2%) 65 44	66, 83, 121, 152	0
42	85	116/118 (98%)	0.66	9 (7%) 16 8	65, 91, 116, 123	0
42	C8	115/118 (97%)	0.37	5 (4%) 39 23	57, 75, 96, 106	0
43	95	100/101 (99%)	1.24	24 (24%) 1 1	65, 108, 126, 132	0
43	D8	100/101 (99%)	0.91	12 (12%) 6 3	56, 92, 111, 125	0
44	A5	111/113 (98%)	0.62	7 (6%) 23 12	62, 73, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	E8	110/113 (97%)	0.48	6 (5%) 29 16	57, 69, 90, 101	0
45	B5	94/96 (97%)	0.40	6 (6%) 23 12	66, 80, 103, 111	0
45	F8	95/96 (98%)	0.13	2 (2%) 67 46	50, 66, 91, 99	0
46	C5	104/110 (94%)	1.58	26 (25%) 1 1	84, 110, 143, 150	0
46	G8	103/110 (93%)	0.22	2 (1%) 70 50	74, 91, 118, 125	0
47	D5	133/206 (64%)	1.69	49 (36%) 0 0	93, 123, 150, 159	0
47	H8	170/206 (82%)	2.14	78 (45%) 0 0	77, 112, 191, 198	0
48	E5	76/85 (89%)	0.06	1 (1%) 79 61	58, 82, 94, 108	0
48	I8	77/85 (90%)	-0.16	3 (3%) 43 25	54, 70, 87, 98	0
49	F5	94/98 (95%)	0.67	5 (5%) 30 17	61, 76, 117, 123	0
49	J8	94/98 (95%)	0.54	5 (5%) 30 17	49, 70, 115, 135	0
50	G5	69/72 (95%)	0.65	5 (7%) 18 10	77, 96, 113, 130	0
50	K8	68/72 (94%)	0.07	1 (1%) 76 57	60, 76, 94, 124	0
51	H5	58/60 (96%)	1.36	15 (25%) 1 1	73, 90, 118, 123	0
51	L8	58/60 (96%)	0.09	0 100 100	59, 75, 94, 101	0
52	I5	63/71 (88%)	3.51	48 (76%) 0 0	133, 174, 191, 195	0
52	M8	61/71 (85%)	1.39	16 (26%) 1 1	96, 137, 167, 174	0
53	J5	56/60 (93%)	0.62	6 (10%) 8 4	57, 81, 130, 140	0
53	N8	56/60 (93%)	1.23	10 (17%) 2 1	50, 83, 145, 155	0
54	L5	47/49 (95%)	0.19	1 (2%) 67 46	51, 61, 82, 96	0
54	P8	47/49 (95%)	0.06	1 (2%) 67 46	44, 53, 68, 89	0
55	M5	64/65 (98%)	0.53	2 (3%) 52 33	64, 76, 89, 114	0
55	Q8	64/65 (98%)	0.06	1 (1%) 74 55	52, 64, 78, 91	0
56	1L	67/76 (88%)	1.42	17 (25%) 1 1	98, 180, 207, 210	0
All	All	20742/22044 (94%)	0.31	1522 (7%) 18 9	44, 93, 167, 244	0

The worst 5 of 1522 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	15.3
46	C5	59	GLY	14.9
52	I5	52	THR	11.4
43	D8	37	VAL	11.2
26	14	2901	C	11.2

## 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
23	7MG	2L	47	24/25	0.84	0.16	-	92,112,117,118	0
23	7MG	2K	47	24/25	0.94	0.12	-	90,98,109,111	0
23	5MU	2L	55	21/22	0.95	0.09	-	111,115,122,127	0
23	OMC	2L	33	21/22	0.90	0.18	-	83,94,97,100	0
23	4SU	2K	8	20/21	0.95	0.14	-	84,88,92,94	0
23	PSU	2K	56	20/21	0.92	0.11	-	93,98,106,114	0
22	5MU	1K	54	21/22	0.92	0.19	-	100,106,117,129	0
22	H2U	1K	17	20/21	0.81	0.12	-	119,145,154,154	0
22	PSU	1K	55	20/21	0.84	0.25	-	102,116,131,132	0
56	PSU	1L	55	20/21	0.73	0.29	-	118,133,146,147	0
22	6MZ	1K	37	23/24	0.97	0.13	-	61,79,86,90	0
23	PSU	2L	56	20/21	0.92	0.10	-	105,114,120,120	0
56	5MU	1L	54	21/22	0.91	0.22	-	117,124,131,143	0
23	OMC	2K	33	21/22	0.96	0.17	-	72,79,82,89	0
23	4SU	2L	8	20/21	0.93	0.15	-	104,106,109,112	0
22	CM0	1K	34	25/26	0.95	0.13	-	72,89,106,107	0
23	5MU	2K	55	21/22	0.95	0.12	-	99,102,106,113	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3187	1/1	0.75	1.23	85.41	81,81,81,81	0
57	MG	1H	3038	1/1	0.83	0.61	83.25	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3094	1/1	0.88	0.51	43.63	68,68,68,68	0
57	MG	13	1672	1/1	0.54	0.80	41.98	91,91,91,91	0
57	MG	1H	3042	1/1	0.87	0.41	39.77	67,67,67,67	0
57	MG	1H	3026	1/1	0.92	0.40	38.12	52,52,52,52	0
57	MG	1H	3036	1/1	0.72	0.76	37.80	70,70,70,70	0
57	MG	14	3060	1/1	0.96	0.56	36.13	56,56,56,56	0
57	MG	13	1640	1/1	0.97	0.48	35.55	77,77,77,77	0
57	MG	14	3148	1/1	0.73	0.37	34.46	63,63,63,63	0
57	MG	1H	3016	1/1	0.92	0.39	34.45	47,47,47,47	0
57	MG	1H	3102	1/1	0.86	0.60	29.67	66,66,66,66	0
57	MG	14	3031	1/1	0.59	0.45	29.09	86,86,86,86	0
57	MG	14	3184	1/1	0.89	0.62	28.63	65,65,65,65	0
57	MG	14	3087	1/1	0.71	0.55	28.37	58,58,58,58	0
57	MG	1G	1615	1/1	0.92	0.39	28.10	91,91,91,91	0
57	MG	14	3149	1/1	0.83	0.68	27.10	71,71,71,71	0
57	MG	1H	3097	1/1	0.89	0.49	26.99	83,83,83,83	0
57	MG	1H	3070	1/1	0.87	0.41	26.68	56,56,56,56	0
57	MG	14	3109	1/1	0.98	0.53	25.67	74,74,74,74	0
57	MG	1G	1622	1/1	0.91	0.36	25.49	85,85,85,85	0
57	MG	13	1632	1/1	0.86	0.39	25.19	90,90,90,90	0
57	MG	1H	3145	1/1	0.86	0.63	24.97	62,62,62,62	0
57	MG	14	3033	1/1	0.94	0.67	24.94	75,75,75,75	0
57	MG	1H	3257	1/1	0.93	0.36	24.94	51,51,51,51	0
57	MG	1H	3086	1/1	0.72	0.40	24.68	66,66,66,66	0
57	MG	1H	3073	1/1	0.92	0.58	23.96	59,59,59,59	0
57	MG	1H	3056	1/1	0.87	0.43	22.24	73,73,73,73	0
57	MG	13	1625	1/1	0.75	0.32	21.35	93,93,93,93	0
57	MG	14	3124	1/1	0.95	0.36	21.03	82,82,82,82	0
57	MG	13	1628	1/1	0.97	0.39	20.96	79,79,79,79	0
57	MG	1H	3217	1/1	0.60	0.42	20.66	80,80,80,80	0
57	MG	1G	1660	1/1	0.92	0.38	20.63	72,72,72,72	0
57	MG	1H	3176	1/1	0.90	0.35	20.60	62,62,62,62	0
57	MG	1H	3124	1/1	0.86	0.52	20.52	73,73,73,73	0
57	MG	14	3089	1/1	0.96	0.44	20.00	79,79,79,79	0
57	MG	1H	3109	1/1	0.91	0.34	18.94	79,79,79,79	0
57	MG	13	1620	1/1	0.87	0.29	18.75	57,57,57,57	0
57	MG	14	3085	1/1	0.83	0.48	18.71	81,81,81,81	0
57	MG	13	1629	1/1	0.94	0.34	18.68	56,56,56,56	0
57	MG	14	3137	1/1	0.77	0.43	18.59	68,68,68,68	0
57	MG	1H	3152	1/1	0.91	0.31	18.54	51,51,51,51	0
57	MG	14	3110	1/1	0.75	0.52	18.30	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1607	1/1	0.87	0.27	18.29	92,92,92,92	0
57	MG	1H	3058	1/1	0.77	0.43	17.95	77,77,77,77	0
57	MG	1G	1614	1/1	0.97	0.29	17.13	82,82,82,82	0
57	MG	13	1681	1/1	0.76	0.29	17.10	86,86,86,86	0
57	MG	1H	3179	1/1	0.77	0.41	17.02	67,67,67,67	0
57	MG	14	3014	1/1	0.95	0.33	16.92	62,62,62,62	0
57	MG	1H	3014	1/1	0.98	0.39	16.70	43,43,43,43	0
57	MG	1H	3104	1/1	0.65	0.29	16.69	88,88,88,88	0
57	MG	1H	3085	1/1	0.79	0.43	16.44	75,75,75,75	0
57	MG	1G	1635	1/1	0.92	0.26	16.36	102,102,102,102	0
57	MG	14	3170	1/1	0.95	0.34	16.34	87,87,87,87	0
57	MG	13	1634	1/1	0.94	0.31	16.08	78,78,78,78	0
57	MG	1H	3040	1/1	0.96	0.33	15.74	36,36,36,36	0
57	MG	2L	101	1/1	0.96	0.54	15.44	77,77,77,77	0
57	MG	1H	3199	1/1	0.71	0.42	15.26	78,78,78,78	0
57	MG	1H	3095	1/1	0.60	0.34	15.24	69,69,69,69	0
57	MG	14	3104	1/1	0.83	0.19	15.21	84,84,84,84	0
57	MG	1H	3055	1/1	0.96	0.26	15.11	60,60,60,60	0
57	MG	J8	101	1/1	0.89	0.62	14.39	79,79,79,79	0
57	MG	1H	3222	1/1	0.72	0.40	14.39	64,64,64,64	0
57	MG	14	3123	1/1	0.92	0.39	13.89	60,60,60,60	0
57	MG	1H	3283	1/1	0.97	0.35	13.72	146,146,146,146	0
57	MG	1G	1661	1/1	0.90	0.28	13.55	75,75,75,75	0
57	MG	1H	3196	1/1	0.95	0.18	13.41	56,56,56,56	0
57	MG	1H	3071	1/1	0.96	0.41	13.37	57,57,57,57	0
57	MG	13	1652	1/1	0.92	0.22	13.22	68,68,68,68	0
57	MG	14	3091	1/1	0.94	0.42	13.14	66,66,66,66	0
57	MG	14	3070	1/1	0.96	0.33	13.11	82,82,82,82	0
57	MG	14	3127	1/1	0.91	0.36	12.99	62,62,62,62	0
57	MG	14	3129	1/1	0.87	0.48	12.92	75,75,75,75	0
57	MG	14	3100	1/1	0.95	0.31	12.52	61,61,61,61	0
57	MG	14	3113	1/1	0.89	0.31	12.36	57,57,57,57	0
57	MG	13	1671	1/1	0.90	0.24	12.32	100,100,100,100	0
57	MG	14	3167	1/1	0.89	0.29	12.12	76,76,76,76	0
57	MG	1H	3059	1/1	0.92	0.42	12.09	72,72,72,72	0
57	MG	1H	3256	1/1	0.95	0.29	11.60	67,67,67,67	0
57	MG	1H	3194	1/1	0.90	0.27	11.47	71,71,71,71	0
57	MG	14	3039	1/1	0.89	0.41	11.30	65,65,65,65	0
57	MG	1H	3113	1/1	0.86	0.26	11.29	64,64,64,64	0
57	MG	1H	3050	1/1	0.97	0.30	11.04	54,54,54,54	0
57	MG	13	1609	1/1	0.90	0.25	10.93	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1627	1/1	0.96	0.24	10.85	85,85,85,85	0
57	MG	14	3078	1/1	0.86	0.36	10.61	64,64,64,64	0
57	MG	14	3086	1/1	0.64	0.26	10.53	64,64,64,64	0
57	MG	1H	3231	1/1	0.86	0.22	10.34	67,67,67,67	0
57	MG	14	3425	1/1	0.53	0.38	10.20	92,92,92,92	0
57	MG	14	3023	1/1	0.97	0.42	10.15	82,82,82,82	0
57	MG	14	3215	1/1	0.83	0.40	10.02	76,76,76,76	0
57	MG	13	1670	1/1	0.85	0.31	9.85	92,92,92,92	0
57	MG	14	3046	1/1	0.92	0.42	9.74	76,76,76,76	0
57	MG	1H	3060	1/1	0.96	0.33	9.53	51,51,51,51	0
57	MG	14	3061	1/1	0.98	0.66	9.50	56,56,56,56	0
57	MG	1H	3033	1/1	0.90	0.23	9.31	73,73,73,73	0
57	MG	29	301	1/1	0.94	0.54	9.27	69,69,69,69	0
57	MG	13	1655	1/1	0.93	0.26	9.19	64,64,64,64	0
58	SPE	14	3447	13/13	0.87	0.36	8.97	70,76,79,79	0
57	MG	1H	3002	1/1	0.92	0.40	8.94	82,82,82,82	0
57	MG	14	3114	1/1	0.99	0.43	8.89	63,63,63,63	0
57	MG	14	3225	1/1	0.86	0.31	8.87	87,87,87,87	0
57	MG	1G	1610	1/1	0.90	0.25	8.75	69,69,69,69	0
57	MG	1H	3378	1/1	0.81	0.24	8.71	75,75,75,75	0
57	MG	1H	3096	1/1	0.93	0.31	8.67	53,53,53,53	0
57	MG	14	3213	1/1	0.84	0.42	8.63	85,85,85,85	0
57	MG	13	1606	1/1	0.91	0.33	8.56	77,77,77,77	0
57	MG	1H	3035	1/1	0.97	0.33	8.46	80,80,80,80	0
57	MG	14	3027	1/1	0.82	0.25	8.30	76,76,76,76	0
57	MG	13	1649	1/1	0.90	0.23	8.05	72,72,72,72	0
57	MG	1H	3284	1/1	0.86	0.34	7.97	71,71,71,71	0
57	MG	1H	3141	1/1	0.90	0.31	7.96	66,66,66,66	0
57	MG	13	1607	1/1	0.97	0.26	7.53	80,80,80,80	0
58	SPE	14	3448	13/13	0.82	0.28	7.31	68,79,87,89	0
57	MG	1H	3183	1/1	0.82	0.26	7.29	73,73,73,73	0
57	MG	14	3079	1/1	0.98	0.34	7.26	61,61,61,61	0
57	MG	1G	1627	1/1	0.97	0.21	7.23	77,77,77,77	0
57	MG	1H	3062	1/1	0.87	0.26	7.18	40,40,40,40	0
57	MG	1H	3170	1/1	0.93	0.27	7.15	79,79,79,79	0
57	MG	14	3126	1/1	0.87	0.22	7.10	75,75,75,75	0
57	MG	13	1685	1/1	0.71	0.20	6.81	72,72,72,72	0
57	MG	13	1614	1/1	0.79	0.28	6.76	88,88,88,88	0
57	MG	1H	3088	1/1	0.81	0.23	6.74	61,61,61,61	0
57	MG	1H	3249	1/1	0.88	0.30	6.70	68,68,68,68	0
57	MG	1H	3119	1/1	0.90	0.21	6.66	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	16	201	1/1	0.91	0.17	6.59	83,83,83,83	0
57	MG	1H	3046	1/1	0.96	0.24	6.58	49,49,49,49	0
57	MG	1H	3340	1/1	0.82	0.31	6.51	70,70,70,70	0
57	MG	1H	3110	1/1	0.96	0.26	6.44	65,65,65,65	0
57	MG	19	301	1/1	0.93	0.40	6.27	57,57,57,57	0
57	MG	14	3133	1/1	0.82	0.30	6.21	58,58,58,58	0
57	MG	14	3058	1/1	0.95	0.27	6.17	83,83,83,83	0
57	MG	14	3016	1/1	0.91	0.35	6.13	63,63,63,63	0
57	MG	1H	3305	1/1	0.96	0.23	6.13	71,71,71,71	0
57	MG	14	3121	1/1	0.95	0.29	6.11	55,55,55,55	0
57	MG	14	3036	1/1	0.96	0.26	6.05	47,47,47,47	0
57	MG	14	3222	1/1	0.81	0.29	6.01	73,73,73,73	0
57	MG	1G	1662	1/1	0.87	0.19	5.98	99,99,99,99	0
57	MG	13	1676	1/1	0.97	0.18	5.90	104,104,104,104	0
57	MG	14	3146	1/1	0.92	0.30	5.87	51,51,51,51	0
57	MG	14	3393	1/1	0.74	0.24	5.77	103,103,103,103	0
57	MG	1H	3156	1/1	0.93	0.27	5.66	66,66,66,66	0
57	MG	14	3219	1/1	0.72	0.20	5.66	77,77,77,77	0
57	MG	1H	3025	1/1	0.91	0.25	5.46	48,48,48,48	0
57	MG	1H	3125	1/1	0.76	0.22	5.32	63,63,63,63	0
57	MG	14	3135	1/1	0.98	0.21	5.19	69,69,69,69	0
57	MG	1G	1655	1/1	0.86	0.25	5.07	77,77,77,77	0
57	MG	1H	3281	1/1	0.84	0.21	4.98	67,67,67,67	0
57	MG	2K	101	1/1	0.90	0.31	4.95	63,63,63,63	0
57	MG	1H	3270	1/1	0.81	0.35	4.86	61,61,61,61	0
57	MG	14	3055	1/1	0.95	0.30	4.85	50,50,50,50	0
58	SPE	13	1750	13/13	0.85	0.24	4.83	60,77,82,87	0
58	SPE	1J	208	13/13	0.80	0.22	4.82	94,98,105,105	0
57	MG	14	3116	1/1	0.83	0.28	4.81	66,66,66,66	0
57	MG	13	1665	1/1	0.86	0.19	4.72	69,69,69,69	0
57	MG	1H	3402	1/1	0.89	0.20	4.61	63,63,63,63	0
57	MG	1G	1666	1/1	0.96	0.20	4.61	78,78,78,78	0
57	MG	1H	3165	1/1	0.80	0.20	4.57	59,59,59,59	0
57	MG	1H	3443	1/1	0.88	0.22	4.49	69,69,69,69	0
57	MG	1H	3029	1/1	0.96	0.21	4.38	63,63,63,63	0
57	MG	29	302	1/1	0.77	0.27	4.35	75,75,75,75	0
57	MG	13	1683	1/1	0.73	0.25	4.13	68,68,68,68	0
57	MG	13	1633	1/1	0.89	0.21	4.12	87,87,87,87	0
57	MG	13	1612	1/1	0.96	0.21	4.11	76,76,76,76	0
57	MG	14	3144	1/1	0.96	0.31	4.07	56,56,56,56	0
57	MG	1H	3524	1/1	0.80	0.23	4.01	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3048	1/1	0.82	0.25	3.97	43,43,43,43	0
57	MG	1H	3106	1/1	0.84	0.18	3.91	68,68,68,68	0
57	MG	2I	301	1/1	0.96	0.25	3.84	62,62,62,62	0
57	MG	1H	3308	1/1	0.77	0.36	3.78	56,56,56,56	0
57	MG	1H	3054	1/1	0.96	0.29	3.76	37,37,37,37	0
57	MG	14	3029	1/1	0.94	0.23	3.61	73,73,73,73	0
57	MG	1H	3066	1/1	0.92	0.18	3.49	65,65,65,65	0
57	MG	39	302	1/1	0.58	0.30	3.48	67,67,67,67	0
57	MG	1H	3264	1/1	0.96	0.26	3.42	59,59,59,59	0
57	MG	14	3156	1/1	0.91	0.16	3.40	71,71,71,71	0
57	MG	1H	3024	1/1	0.93	0.23	3.37	51,51,51,51	0
57	MG	1G	1612	1/1	0.91	0.19	3.28	82,82,82,82	0
57	MG	1H	3522	1/1	0.77	0.25	3.24	86,86,86,86	0
57	MG	1H	3393	1/1	0.89	0.20	3.10	52,52,52,52	0
57	MG	1H	3538	1/1	0.85	0.21	3.09	61,61,61,61	0
57	MG	98	201	1/1	1.00	0.28	3.02	61,61,61,61	0
57	MG	1G	1626	1/1	0.94	0.25	2.96	68,68,68,68	0
57	MG	14	3326	1/1	0.82	0.25	2.90	66,66,66,66	0
57	MG	14	3096	1/1	0.98	0.24	2.71	50,50,50,50	0
57	MG	14	3235	1/1	0.95	0.26	2.68	54,54,54,54	0
57	MG	1H	3313	1/1	0.78	0.18	2.65	74,74,74,74	0
57	MG	1H	3331	1/1	0.86	0.23	2.61	53,53,53,53	0
57	MG	1H	3045	1/1	0.93	0.22	2.38	42,42,42,42	0
57	MG	1H	3358	1/1	0.90	0.20	2.37	62,62,62,62	0
57	MG	1H	3333	1/1	0.98	0.21	2.20	67,67,67,67	0
57	MG	16	203	1/1	0.80	0.12	2.17	78,78,78,78	0
57	MG	14	3160	1/1	0.89	0.33	2.15	92,92,92,92	0
57	MG	14	3217	1/1	0.77	0.19	2.08	72,72,72,72	0
57	MG	13	1642	1/1	0.85	0.17	2.00	72,72,72,72	0
57	MG	13	1639	1/1	0.94	0.17	1.99	73,73,73,73	0
57	MG	1H	3065	1/1	0.88	0.19	1.93	50,50,50,50	0
57	MG	14	3433	1/1	0.87	0.23	1.91	60,60,60,60	0
57	MG	1H	3166	1/1	0.92	0.27	1.86	56,56,56,56	0
57	MG	1G	1664	1/1	0.96	0.20	1.85	76,76,76,76	0
57	MG	13	1693	1/1	0.83	0.20	1.80	65,65,65,65	0
57	MG	1H	3451	1/1	0.87	0.20	1.66	59,59,59,59	0
57	MG	1G	1631	1/1	0.94	0.14	1.62	82,82,82,82	0
57	MG	14	3310	1/1	0.90	0.24	1.59	58,58,58,58	0
57	MG	1H	3116	1/1	0.90	0.18	1.53	82,82,82,82	0
57	MG	9A	101	1/1	0.79	0.24	1.52	115,115,115,115	0
57	MG	14	3327	1/1	0.95	0.21	1.50	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3005	1/1	0.89	0.31	1.40	50,50,50,50	0
57	MG	1H	3273	1/1	0.78	0.14	1.38	69,69,69,69	0
57	MG	1H	3154	1/1	0.69	0.14	1.35	66,66,66,66	0
57	MG	1H	3057	1/1	0.96	0.26	1.34	72,72,72,72	0
57	MG	13	1619	1/1	0.89	0.22	1.32	53,53,53,53	0
57	MG	14	3298	1/1	0.90	0.20	1.31	62,62,62,62	0
57	MG	5E	201	1/1	0.97	0.28	1.24	75,75,75,75	0
57	MG	14	3444	1/1	0.83	0.20	1.23	75,75,75,75	0
57	MG	1H	3416	1/1	0.66	0.21	1.05	72,72,72,72	0
57	MG	14	3266	1/1	0.88	0.21	1.00	52,52,52,52	0
57	MG	14	3237	1/1	0.91	0.21	0.99	65,65,65,65	0
57	MG	14	3248	1/1	0.84	0.18	0.99	72,72,72,72	0
57	MG	14	3088	1/1	0.94	0.18	0.96	53,53,53,53	0
57	MG	1H	3225	1/1	0.92	0.20	0.85	74,74,74,74	0
57	MG	14	3330	1/1	0.98	0.19	0.83	56,56,56,56	0
57	MG	1H	3343	1/1	0.95	0.20	0.81	44,44,44,44	0
57	MG	14	3302	1/1	0.98	0.20	0.74	73,73,73,73	0
57	MG	1H	3383	1/1	0.96	0.22	0.74	54,54,54,54	0
57	MG	1H	3140	1/1	0.90	0.21	0.73	40,40,40,40	0
57	MG	14	3231	1/1	0.90	0.17	0.73	90,90,90,90	0
57	MG	1H	3075	1/1	0.85	0.19	0.69	61,61,61,61	0
57	MG	1H	3081	1/1	0.97	0.16	0.68	55,55,55,55	0
57	MG	1G	1629	1/1	0.91	0.14	0.64	97,97,97,97	0
57	MG	1H	3376	1/1	0.98	0.19	0.63	48,48,48,48	0
57	MG	1H	3534	1/1	0.88	0.20	0.59	44,44,44,44	0
57	MG	1H	3349	1/1	0.91	0.19	0.56	67,67,67,67	0
57	MG	1H	3329	1/1	0.91	0.20	0.56	50,50,50,50	0
57	MG	14	3122	1/1	0.94	0.29	0.56	84,84,84,84	0
57	MG	14	3034	1/1	0.94	0.24	0.50	48,48,48,48	0
57	MG	14	3301	1/1	0.93	0.21	0.47	58,58,58,58	0
57	MG	14	3072	1/1	0.87	0.16	0.44	57,57,57,57	0
57	MG	14	3021	1/1	0.81	0.15	0.36	76,76,76,76	0
57	MG	4A	201	1/1	0.86	0.21	0.34	96,96,96,96	0
57	MG	1H	3441	1/1	0.93	0.17	0.33	61,61,61,61	0
57	MG	1G	1674	1/1	0.91	0.17	0.30	71,71,71,71	0
57	MG	14	3076	1/1	0.93	0.17	0.26	89,89,89,89	0
57	MG	13	1669	1/1	0.54	0.13	0.21	121,121,121,121	0
57	MG	14	3255	1/1	0.96	0.22	0.13	53,53,53,53	0
57	MG	14	3154	1/1	0.89	0.15	0.13	87,87,87,87	0
57	MG	14	3181	1/1	0.95	0.16	0.08	65,65,65,65	0
57	MG	1G	1699	1/1	0.89	0.12	0.07	105,105,105,105	0
57	MG	1H	3063	1/1	0.96	0.17	0.05	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3157	1/1	0.77	0.14	0.05	73,73,73,73	0
57	MG	1G	1637	1/1	0.89	0.12	0.04	113,113,113,113	0
57	MG	14	3305	1/1	0.95	0.18	-0.01	70,70,70,70	0
57	MG	1H	3480	1/1	0.68	0.17	-0.02	75,75,75,75	0
57	MG	14	3249	1/1	0.91	0.20	-0.02	60,60,60,60	0
57	MG	14	3142	1/1	0.92	0.20	-0.06	76,76,76,76	0
57	MG	1H	3032	1/1	0.93	0.19	-0.08	56,56,56,56	0
57	MG	14	3322	1/1	0.94	0.18	-0.20	46,46,46,46	0
57	MG	1G	1656	1/1	0.91	0.14	-0.21	70,70,70,70	0
57	MG	1H	3392	1/1	0.88	0.19	-0.23	50,50,50,50	0
57	MG	13	1734	1/1	0.56	0.15	-0.23	118,118,118,118	0
57	MG	1H	3174	1/1	0.95	0.20	-0.27	37,37,37,37	0
57	MG	88	201	1/1	0.89	0.16	-0.31	78,78,78,78	0
57	MG	14	3315	1/1	0.91	0.15	-0.42	87,87,87,87	0
57	MG	1G	1724	1/1	0.78	0.16	-0.43	94,94,94,94	0
57	MG	14	3319	1/1	0.83	0.16	-0.43	64,64,64,64	0
57	MG	13	1705	1/1	0.98	0.14	-0.43	66,66,66,66	0
57	MG	1J	204	1/1	0.99	0.12	-0.47	88,88,88,88	0
57	MG	14	3026	1/1	0.93	0.12	-0.47	69,69,69,69	0
57	MG	14	3333	1/1	0.85	0.16	-0.48	79,79,79,79	0
57	MG	13	1611	1/1	0.98	0.11	-0.49	85,85,85,85	0
57	MG	1H	3195	1/1	0.89	0.16	-0.54	59,59,59,59	0
57	MG	1H	3242	1/1	0.88	0.12	-0.57	74,74,74,74	0
57	MG	1H	3299	1/1	0.90	0.13	-0.59	78,78,78,78	0
57	MG	14	3375	1/1	0.90	0.13	-0.66	97,97,97,97	0
57	MG	1G	1675	1/1	0.81	0.18	-0.68	78,78,78,78	0
57	MG	14	3396	1/1	0.85	0.14	-0.69	63,63,63,63	0
57	MG	13	1713	1/1	0.91	0.12	-0.76	102,102,102,102	0
57	MG	1H	3338	1/1	0.87	0.17	-0.76	63,63,63,63	0
57	MG	1H	3404	1/1	0.98	0.17	-0.77	50,50,50,50	0
57	MG	14	3019	1/1	0.95	0.18	-0.77	53,53,53,53	0
57	MG	14	3263	1/1	0.72	0.20	-0.78	67,67,67,67	0
57	MG	1H	3372	1/1	0.89	0.14	-0.79	56,56,56,56	0
57	MG	14	3264	1/1	0.94	0.16	-0.86	66,66,66,66	0
57	MG	14	3239	1/1	0.97	0.15	-0.89	56,56,56,56	0
57	MG	1H	3137	1/1	0.90	0.17	-0.91	57,57,57,57	0
57	MG	1G	1608	1/1	0.95	0.10	-0.94	111,111,111,111	0
57	MG	1H	3023	1/1	0.91	0.12	-0.94	72,72,72,72	0
57	MG	16	205	1/1	0.89	0.10	-0.96	66,66,66,66	0
57	MG	13	1695	1/1	0.94	0.12	-0.97	84,84,84,84	0
59	SF4	3E	301	8/8	0.99	0.17	-0.97	86,90,100,103	0
57	MG	2I	201	1/1	0.96	0.14	-0.97	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
57	MG	13	1637	1/1	0.88	0.11	-0.97	79,79,79,79	0
57	MG	1J	202	1/1	0.88	0.09	-0.98	84,84,84,84	0
57	MG	14	3147	1/1	0.65	0.10	-1.07	69,69,69,69	0
57	MG	16	207	1/1	0.91	0.08	-1.07	84,84,84,84	0
60	ZN	5I	102	1/1	0.98	0.11	-1.13	98,98,98,98	0
57	MG	1H	3446	1/1	0.88	0.16	-1.14	44,44,44,44	0
60	ZN	5A	101	1/1	0.99	0.09	-1.14	123,123,123,123	0
57	MG	14	3295	1/1	0.50	0.15	-1.15	72,72,72,72	0
57	MG	2A	201	1/1	0.97	0.16	-1.17	84,84,84,84	0
57	MG	42	201	1/1	0.85	0.12	-1.19	116,116,116,116	0
57	MG	1G	1606	1/1	0.91	0.13	-1.19	84,84,84,84	0
58	SPE	1G	1734	13/13	0.84	0.10	-1.21	98,101,104,105	0
57	MG	1H	3332	1/1	0.85	0.15	-1.22	50,50,50,50	0
57	MG	1H	3151	1/1	0.93	0.13	-1.28	59,59,59,59	0
57	MG	14	3240	1/1	0.88	0.15	-1.29	66,66,66,66	0
60	ZN	G8	201	1/1	0.96	0.10	-1.32	131,131,131,131	0
59	SF4	32	301	8/8	0.99	0.15	-1.35	90,99,108,116	0
57	MG	14	3374	1/1	0.95	0.13	-1.35	79,79,79,79	0
57	MG	13	1738	1/1	0.20	0.10	-1.38	104,104,104,104	0
57	MG	1G	1668	1/1	0.89	0.12	-1.38	90,90,90,90	0
57	MG	1H	3135	1/1	0.97	0.20	-1.39	42,42,42,42	0
57	MG	14	3385	1/1	0.87	0.14	-1.39	92,92,92,92	0
57	MG	1H	3290	1/1	0.97	0.13	-1.43	87,87,87,87	0
57	MG	1H	3535	1/1	0.96	0.11	-1.46	92,92,92,92	0
57	MG	39	301	1/1	0.93	0.13	-1.48	95,95,95,95	0
57	MG	13	1724	1/1	0.94	0.12	-1.49	77,77,77,77	0
57	MG	14	3435	1/1	0.90	0.11	-1.51	69,69,69,69	0
57	MG	13	1624	1/1	0.90	0.12	-1.53	93,93,93,93	0
57	MG	13	1656	1/1	0.96	0.14	-1.56	65,65,65,65	0
57	MG	14	3117	1/1	0.92	0.14	-1.56	58,58,58,58	0
57	MG	1H	3411	1/1	0.85	0.08	-1.58	106,106,106,106	0
57	MG	14	3279	1/1	0.94	0.17	-1.58	59,59,59,59	0
57	MG	14	3183	1/1	0.93	0.12	-1.59	82,82,82,82	0
57	MG	1H	3139	1/1	0.79	0.14	-1.65	54,54,54,54	0
57	MG	41	201	1/1	0.84	0.11	-1.66	62,62,62,62	0
57	MG	14	3238	1/1	0.89	0.15	-1.67	70,70,70,70	0
57	MG	14	3290	1/1	0.85	0.15	-1.68	77,77,77,77	0
57	MG	13	1694	1/1	0.96	0.16	-1.70	61,61,61,61	0
57	MG	1G	1686	1/1	0.75	0.12	-1.72	91,91,91,91	0
57	MG	1H	3526	1/1	0.64	0.08	-1.73	134,134,134,134	0
57	MG	14	3251	1/1	0.98	0.18	-1.73	60,60,60,60	0
57	MG	1H	3519	1/1	0.81	0.12	-1.74	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
57	MG	1H	3341	1/1	0.96	0.18	-1.74	48,48,48,48	0
57	MG	14	3267	1/1	0.96	0.16	-1.78	52,52,52,52	0
57	MG	14	3386	1/1	0.90	0.06	-1.84	88,88,88,88	0
57	MG	14	3253	1/1	0.98	0.18	-1.88	63,63,63,63	0
57	MG	14	3271	1/1	0.98	0.14	-1.90	63,63,63,63	0
57	MG	14	3407	1/1	0.58	0.09	-1.91	91,91,91,91	0
57	MG	1H	3391	1/1	0.90	0.10	-2.02	68,68,68,68	0
57	MG	1H	3464	1/1	0.94	0.18	-2.09	48,48,48,48	0
57	MG	1G	1730	1/1	0.84	0.10	-2.11	104,104,104,104	0
57	MG	D8	401	1/1	0.98	0.14	-2.12	70,70,70,70	0
57	MG	14	3268	1/1	0.96	0.11	-2.21	72,72,72,72	0
57	MG	13	1704	1/1	0.78	0.08	-2.28	107,107,107,107	0
57	MG	1H	3434	1/1	0.96	0.13	-2.31	61,61,61,61	0
57	MG	14	3354	1/1	0.85	0.11	-2.34	84,84,84,84	0
57	MG	1G	1602	1/1	0.92	0.11	-2.35	81,81,81,81	0
57	MG	1H	3465	1/1	0.72	0.18	-2.46	48,48,48,48	0
57	MG	1H	3466	1/1	0.97	0.12	-2.49	63,63,63,63	0
57	MG	1H	3342	1/1	0.94	0.16	-2.52	42,42,42,42	0
57	MG	13	1725	1/1	0.82	0.12	-2.52	83,83,83,83	0
57	MG	M5	101	1/1	0.85	0.10	-2.53	86,86,86,86	0
57	MG	1H	3357	1/1	0.90	0.12	-2.57	75,75,75,75	0
57	MG	1H	3413	1/1	0.98	0.10	-2.60	51,51,51,51	0
57	MG	14	3186	1/1	0.90	0.12	-2.62	76,76,76,76	0
57	MG	1H	3368	1/1	0.88	0.15	-2.63	56,56,56,56	0
57	MG	1H	3442	1/1	0.95	0.17	-2.65	44,44,44,44	0
57	MG	14	3312	1/1	0.92	0.14	-2.66	64,64,64,64	0
57	MG	14	3280	1/1	0.95	0.13	-2.73	80,80,80,80	0
57	MG	1H	3346	1/1	0.95	0.14	-2.82	53,53,53,53	0
57	MG	14	3292	1/1	0.98	0.08	-2.85	66,66,66,66	0
57	MG	1G	1704	1/1	0.88	0.08	-2.86	113,113,113,113	0
57	MG	14	3256	1/1	0.96	0.17	-2.92	52,52,52,52	0
57	MG	1H	3167	1/1	0.90	0.14	-2.96	60,60,60,60	0
57	MG	1G	1678	1/1	0.94	0.07	-3.08	97,97,97,97	0
57	MG	1H	3164	1/1	0.86	0.14	-3.13	64,64,64,64	0
57	MG	5I	101	1/1	0.89	0.08	-3.13	80,80,80,80	0
57	MG	1H	3542	1/1	0.89	0.10	-3.16	67,67,67,67	0
57	MG	14	3410	1/1	0.89	0.07	-3.23	111,111,111,111	0
57	MG	14	3428	1/1	0.74	0.07	-3.26	126,126,126,126	0
57	MG	14	3258	1/1	0.82	0.16	-3.27	54,54,54,54	0
57	MG	13	1696	1/1	0.93	0.05	-3.36	94,94,94,94	0
57	MG	1G	1684	1/1	0.79	0.04	-3.47	113,113,113,113	0
57	MG	1H	3353	1/1	0.96	0.13	-3.47	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3306	1/1	0.98	0.13	-3.49	68,68,68,68	0
57	MG	1G	1632	1/1	0.80	0.05	-3.58	99,99,99,99	0
57	MG	14	3250	1/1	0.92	0.12	-3.59	57,57,57,57	0
57	MG	1H	3414	1/1	0.97	0.13	-3.65	59,59,59,59	0
57	MG	1H	3457	1/1	0.90	0.15	-3.65	41,41,41,41	0
57	MG	14	3242	1/1	0.96	0.12	-3.66	62,62,62,62	0
57	MG	1H	3439	1/1	0.97	0.12	-3.68	50,50,50,50	0
57	MG	14	3286	1/1	0.63	0.11	-3.71	72,72,72,72	0
57	MG	14	3257	1/1	0.98	0.17	-3.79	52,52,52,52	0
57	MG	1G	1677	1/1	0.79	0.07	-3.97	100,100,100,100	0
57	MG	1H	3359	1/1	0.90	0.15	-3.99	40,40,40,40	0
57	MG	11	302	1/1	0.95	0.11	-4.03	41,41,41,41	0
57	MG	13	1702	1/1	0.85	0.07	-4.07	86,86,86,86	0
57	MG	14	3381	1/1	0.82	0.09	-4.08	99,99,99,99	0
57	MG	14	3265	1/1	0.95	0.13	-4.12	56,56,56,56	0
57	MG	11	303	1/1	0.98	0.07	-4.13	47,47,47,47	0
57	MG	14	3118	1/1	0.93	0.09	-4.15	73,73,73,73	0
57	MG	14	3259	1/1	0.93	0.14	-4.17	69,69,69,69	0
57	MG	14	3338	1/1	0.95	0.06	-4.22	65,65,65,65	0
57	MG	1G	1646	1/1	0.89	0.07	-4.26	83,83,83,83	0
57	MG	1H	3381	1/1	0.70	0.13	-4.29	59,59,59,59	0
57	MG	1H	3461	1/1	0.98	0.14	-4.29	48,48,48,48	0
57	MG	1H	3384	1/1	0.96	0.13	-4.40	53,53,53,53	0
57	MG	14	3373	1/1	0.90	0.10	-4.49	90,90,90,90	0
57	MG	14	3272	1/1	0.99	0.10	-4.54	65,65,65,65	0
57	MG	1G	1645	1/1	0.75	0.06	-4.54	93,93,93,93	0
57	MG	1H	3481	1/1	0.93	0.12	-4.59	53,53,53,53	0
57	MG	14	3331	1/1	0.97	0.11	-4.61	60,60,60,60	0
57	MG	14	3341	1/1	0.97	0.14	-4.61	49,49,49,49	0
57	MG	14	3245	1/1	0.81	0.08	-4.68	82,82,82,82	0
57	MG	13	1719	1/1	0.95	0.11	-4.69	53,53,53,53	0
57	MG	1H	3326	1/1	0.94	0.12	-4.69	47,47,47,47	0
57	MG	1H	3351	1/1	0.99	0.11	-4.72	59,59,59,59	0
57	MG	13	1715	1/1	0.98	0.12	-4.78	65,65,65,65	0
57	MG	1H	3344	1/1	0.95	0.13	-4.80	46,46,46,46	0
57	MG	14	3285	1/1	0.86	0.09	-4.91	71,71,71,71	0
57	MG	1H	3387	1/1	0.90	0.16	-4.96	48,48,48,48	0
57	MG	1H	3405	1/1	0.78	0.12	-5.40	65,65,65,65	0
57	MG	1H	3456	1/1	0.90	0.15	-5.56	42,42,42,42	0
57	MG	1H	3382	1/1	0.96	0.10	-5.69	48,48,48,48	0
57	MG	1H	3355	1/1	0.90	0.07	-5.69	57,57,57,57	0
57	MG	1H	3520	1/1	0.77	0.10	-5.76	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
57	MG	14	3316	1/1	0.85	0.13	-5.81	83,83,83,83	0
57	MG	1H	3363	1/1	0.92	0.08	-5.96	56,56,56,56	0
57	MG	1H	3410	1/1	0.93	0.12	-6.22	55,55,55,55	0
57	MG	1H	3377	1/1	0.95	0.09	-6.27	45,45,45,45	0
57	MG	1H	3489	1/1	0.87	0.07	-6.48	88,88,88,88	0
57	MG	14	3320	1/1	0.97	0.07	-6.61	75,75,75,75	0
57	MG	14	3269	1/1	0.90	0.08	-6.84	86,86,86,86	0
57	MG	14	3324	1/1	0.97	0.12	-7.00	64,64,64,64	0
57	MG	1H	3472	1/1	0.90	0.07	-7.11	73,73,73,73	0
57	MG	1H	3448	1/1	0.89	0.12	-7.27	66,66,66,66	0
57	MG	1H	3385	1/1	0.98	0.07	-7.33	61,61,61,61	0
57	MG	1H	3500	1/1	0.99	0.09	-7.73	52,52,52,52	0
57	MG	14	3376	1/1	0.79	0.11	-7.85	83,83,83,83	0
57	MG	14	3418	1/1	0.69	0.05	-8.42	89,89,89,89	0
57	MG	1H	3540	1/1	0.95	0.11	-8.70	45,45,45,45	0
57	MG	1H	3444	1/1	0.74	0.14	-9.96	53,53,53,53	0
57	MG	1H	3348	1/1	0.81	0.14	-10.07	49,49,49,49	0
57	MG	1H	3508	1/1	0.98	0.04	-10.09	74,74,74,74	0
57	MG	1H	3379	1/1	0.87	0.09	-10.24	65,65,65,65	0
57	MG	14	3377	1/1	0.88	0.06	-10.51	84,84,84,84	0
57	MG	14	3261	1/1	0.97	0.06	-10.55	63,63,63,63	0
57	MG	1H	3409	1/1	0.92	0.09	-10.66	69,69,69,69	0
57	MG	1H	3515	1/1	0.97	0.08	-10.67	76,76,76,76	0
57	MG	14	3422	1/1	0.85	0.08	-11.80	96,96,96,96	0
57	MG	14	3053	1/1	0.68	0.08	-12.42	72,72,72,72	0
57	MG	13	1644	1/1	0.93	0.06	-13.28	82,82,82,82	0
57	MG	13	1723	1/1	0.98	0.06	-16.55	62,62,62,62	0
57	MG	14	3335	1/1	0.99	0.06	-16.61	66,66,66,66	0
57	MG	1H	3504	1/1	0.97	0.06	-20.73	47,47,47,47	0
57	MG	14	3007	1/1	0.75	0.66	-	72,72,72,72	0
57	MG	1H	3291	1/1	0.97	0.20	-	78,78,78,78	0
57	MG	13	1688	1/1	0.50	0.34	-	104,104,104,104	0
57	MG	14	3323	1/1	0.98	0.07	-	64,64,64,64	0
57	MG	1H	3271	1/1	0.92	0.32	-	77,77,77,77	0
57	MG	1H	3227	1/1	0.72	0.42	-	79,79,79,79	0
57	MG	1H	3440	1/1	0.68	0.05	-	95,95,95,95	0
57	MG	1H	3533	1/1	0.97	0.12	-	103,103,103,103	0
57	MG	1G	1623	1/1	0.87	0.50	-	75,75,75,75	0
57	MG	1H	3490	1/1	0.94	0.09	-	69,69,69,69	0
57	MG	13	1650	1/1	0.69	0.41	-	85,85,85,85	0
57	MG	1H	3278	1/1	0.75	0.31	-	83,83,83,83	0
57	MG	1G	1717	1/1	0.90	0.07	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3210	1/1	0.62	0.21	-	78,78,78,78	0
57	MG	1G	1692	1/1	0.54	0.12	-	99,99,99,99	0
57	MG	14	3409	1/1	0.90	0.04	-	83,83,83,83	0
57	MG	13	1714	1/1	0.97	0.09	-	101,101,101,101	0
57	MG	14	3291	1/1	0.91	0.06	-	90,90,90,90	0
57	MG	14	3073	1/1	0.94	0.31	-	48,48,48,48	0
57	MG	1G	1640	1/1	0.94	0.24	-	92,92,92,92	0
57	MG	14	3168	1/1	0.82	0.27	-	87,87,87,87	0
57	MG	1G	1639	1/1	0.94	0.12	-	103,103,103,103	0
57	MG	14	3212	1/1	0.88	0.18	-	80,80,80,80	0
57	MG	14	3101	1/1	0.90	0.26	-	90,90,90,90	0
57	MG	13	1716	1/1	0.96	0.08	-	100,100,100,100	0
57	MG	14	3307	1/1	0.90	0.10	-	78,78,78,78	0
57	MG	14	3166	1/1	0.90	0.77	-	82,82,82,82	0
57	MG	14	3321	1/1	0.85	0.11	-	78,78,78,78	0
57	MG	1H	3427	1/1	0.95	0.05	-	76,76,76,76	0
57	MG	14	3247	1/1	0.98	0.17	-	56,56,56,56	0
57	MG	1H	3364	1/1	0.96	0.15	-	47,47,47,47	0
57	MG	14	3010	1/1	0.94	0.27	-	50,50,50,50	0
57	MG	1H	3043	1/1	0.96	0.42	-	66,66,66,66	0
57	MG	13	1601	1/1	0.97	0.32	-	74,74,74,74	0
57	MG	14	3293	1/1	0.62	0.14	-	90,90,90,90	0
57	MG	14	3025	1/1	0.76	0.28	-	80,80,80,80	0
57	MG	1H	3367	1/1	0.95	0.16	-	63,63,63,63	0
57	MG	13	1660	1/1	0.91	0.65	-	85,85,85,85	0
57	MG	1H	3072	1/1	0.74	0.67	-	72,72,72,72	0
57	MG	1H	3028	1/1	0.93	0.43	-	62,62,62,62	0
57	MG	14	3038	1/1	0.96	0.37	-	69,69,69,69	0
57	MG	1H	3458	1/1	0.94	0.10	-	45,45,45,45	0
57	MG	14	3004	1/1	0.86	0.24	-	73,73,73,73	0
57	MG	1H	3395	1/1	0.87	0.07	-	74,74,74,74	0
57	MG	13	1654	1/1	0.57	0.09	-	113,113,113,113	0
57	MG	14	3083	1/1	0.71	0.69	-	87,87,87,87	0
57	MG	1G	1652	1/1	0.74	0.33	-	94,94,94,94	0
57	MG	14	3214	1/1	0.94	0.34	-	94,94,94,94	0
57	MG	1H	3250	1/1	0.71	0.38	-	93,93,93,93	0
57	MG	14	3270	1/1	0.88	0.13	-	86,86,86,86	0
57	MG	1G	1621	1/1	0.77	0.75	-	86,86,86,86	0
57	MG	13	1636	1/1	0.91	0.27	-	103,103,103,103	0
57	MG	25	202	1/1	0.86	0.17	-	110,110,110,110	0
57	MG	1G	1625	1/1	0.89	0.12	-	98,98,98,98	0
57	MG	14	3399	1/1	0.67	0.07	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1708	1/1	0.66	0.22	-	108,108,108,108	0
57	MG	14	3203	1/1	0.87	0.74	-	95,95,95,95	0
57	MG	1H	3052	1/1	0.96	0.35	-	50,50,50,50	0
57	MG	14	3394	1/1	0.90	0.05	-	112,112,112,112	0
57	MG	14	3416	1/1	0.93	0.23	-	100,100,100,100	0
57	MG	1H	3311	1/1	0.83	0.20	-	93,93,93,93	0
57	MG	13	1707	1/1	0.95	0.18	-	83,83,83,83	0
57	MG	1H	3494	1/1	0.87	0.05	-	102,102,102,102	0
57	MG	1H	3161	1/1	0.80	0.33	-	93,93,93,93	0
57	MG	1H	3220	1/1	0.84	0.16	-	89,89,89,89	0
57	MG	14	3112	1/1	0.78	0.43	-	99,99,99,99	0
57	MG	1H	3191	1/1	0.85	0.29	-	72,72,72,72	0
57	MG	14	3282	1/1	0.88	0.11	-	97,97,97,97	0
57	MG	14	3163	1/1	0.79	0.85	-	84,84,84,84	0
57	MG	14	3390	1/1	0.91	0.31	-	89,89,89,89	0
57	MG	14	3050	1/1	0.95	0.48	-	77,77,77,77	0
57	MG	14	3141	1/1	0.93	0.22	-	76,76,76,76	0
57	MG	13	1697	1/1	0.79	0.11	-	82,82,82,82	0
57	MG	14	3383	1/1	0.82	0.28	-	74,74,74,74	0
57	MG	1G	1672	1/1	0.95	0.09	-	86,86,86,86	0
57	MG	1H	3129	1/1	0.95	0.51	-	69,69,69,69	0
57	MG	13	1747	1/1	0.83	0.06	-	111,111,111,111	0
57	MG	1H	3209	1/1	0.87	0.42	-	52,52,52,52	0
57	MG	1H	3468	1/1	0.91	0.09	-	85,85,85,85	0
57	MG	1H	3275	1/1	0.86	0.61	-	67,67,67,67	0
57	MG	1G	1702	1/1	0.68	0.08	-	101,101,101,101	0
57	MG	14	3227	1/1	0.87	0.11	-	95,95,95,95	0
57	MG	1H	3503	1/1	0.88	0.10	-	90,90,90,90	0
57	MG	13	1703	1/1	0.96	0.04	-	69,69,69,69	0
57	MG	1H	3253	1/1	0.92	0.67	-	71,71,71,71	0
57	MG	1H	3334	1/1	0.94	0.21	-	42,42,42,42	0
57	MG	1H	3251	1/1	0.91	0.22	-	77,77,77,77	0
57	MG	14	3283	1/1	0.85	0.07	-	95,95,95,95	0
57	MG	13	1645	1/1	0.58	0.31	-	78,78,78,78	0
57	MG	13	1666	1/1	0.74	0.31	-	88,88,88,88	0
57	MG	1G	1667	1/1	0.86	0.08	-	103,103,103,103	0
57	MG	1H	3463	1/1	0.82	0.20	-	53,53,53,53	0
57	MG	1H	3115	1/1	0.73	0.92	-	84,84,84,84	0
57	MG	14	3012	1/1	0.96	0.42	-	60,60,60,60	0
57	MG	14	3411	1/1	0.59	0.25	-	95,95,95,95	0
57	MG	14	3438	1/1	0.46	0.22	-	96,96,96,96	0
57	MG	14	3344	1/1	0.97	0.11	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1671	1/1	0.84	0.21	-	88,88,88,88	0
57	MG	1H	3486	1/1	0.96	0.06	-	83,83,83,83	0
57	MG	1H	3474	1/1	0.83	0.12	-	76,76,76,76	0
57	MG	1G	1679	1/1	0.85	0.15	-	73,73,73,73	0
57	MG	14	3304	1/1	0.93	0.13	-	86,86,86,86	0
57	MG	14	3318	1/1	0.87	0.09	-	90,90,90,90	0
57	MG	1H	3018	1/1	0.97	0.50	-	55,55,55,55	0
57	MG	14	3158	1/1	0.81	0.37	-	76,76,76,76	0
57	MG	1H	3144	1/1	0.96	0.42	-	64,64,64,64	0
57	MG	1H	3136	1/1	0.98	0.17	-	45,45,45,45	0
57	MG	14	3357	1/1	0.79	0.14	-	107,107,107,107	0
57	MG	1H	3223	1/1	0.82	0.24	-	80,80,80,80	0
57	MG	14	3421	1/1	0.87	0.21	-	110,110,110,110	0
57	MG	16	209	1/1	0.97	0.03	-	68,68,68,68	0
57	MG	1H	3092	1/1	0.88	0.17	-	74,74,74,74	0
57	MG	13	1630	1/1	0.70	0.26	-	87,87,87,87	0
57	MG	1H	3510	1/1	0.35	0.18	-	88,88,88,88	0
57	MG	1H	3132	1/1	0.98	0.27	-	88,88,88,88	0
57	MG	14	3228	1/1	0.77	0.47	-	83,83,83,83	0
57	MG	14	3366	1/1	0.95	0.07	-	85,85,85,85	0
57	MG	14	3296	1/1	0.89	0.11	-	114,114,114,114	0
57	MG	14	3408	1/1	0.84	0.09	-	90,90,90,90	0
57	MG	14	3275	1/1	0.86	0.16	-	70,70,70,70	0
57	MG	1H	3437	1/1	0.85	0.12	-	65,65,65,65	0
57	MG	14	3131	1/1	0.78	0.36	-	70,70,70,70	0
57	MG	1H	3010	1/1	0.56	0.25	-	78,78,78,78	0
57	MG	1H	3198	1/1	0.51	0.22	-	108,108,108,108	0
57	MG	1H	3545	1/1	0.84	0.08	-	84,84,84,84	0
57	MG	1H	3254	1/1	0.91	0.92	-	75,75,75,75	0
57	MG	1H	3327	1/1	0.83	0.11	-	65,65,65,65	0
57	MG	1H	3252	1/1	0.91	0.49	-	81,81,81,81	0
57	MG	1J	205	1/1	0.64	0.10	-	87,87,87,87	0
57	MG	13	1616	1/1	0.89	0.29	-	82,82,82,82	0
57	MG	14	3150	1/1	0.95	0.19	-	81,81,81,81	0
57	MG	1H	3108	1/1	0.85	0.33	-	69,69,69,69	0
57	MG	1H	3017	1/1	0.95	0.29	-	53,53,53,53	0
57	MG	4E	201	1/1	0.76	0.46	-	85,85,85,85	0
57	MG	1G	1609	1/1	0.93	0.44	-	96,96,96,96	0
57	MG	1H	3101	1/1	0.79	0.14	-	65,65,65,65	0
57	MG	1H	3263	1/1	0.67	0.48	-	91,91,91,91	0
57	MG	1H	3478	1/1	0.77	0.07	-	83,83,83,83	0
57	MG	1H	3418	1/1	0.90	0.11	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3437	1/1	0.64	0.12	-	93,93,93,93	0
57	MG	14	3395	1/1	0.69	0.08	-	118,118,118,118	0
57	MG	14	3244	1/1	0.98	0.19	-	44,44,44,44	0
57	MG	14	3204	1/1	0.91	0.27	-	83,83,83,83	0
57	MG	13	1729	1/1	0.84	0.16	-	90,90,90,90	0
57	MG	14	3169	1/1	0.94	0.14	-	53,53,53,53	0
57	MG	13	1720	1/1	0.91	0.07	-	88,88,88,88	0
57	MG	1H	3476	1/1	0.96	0.06	-	83,83,83,83	0
57	MG	13	1641	1/1	0.96	0.26	-	68,68,68,68	0
57	MG	14	3075	1/1	0.85	0.35	-	89,89,89,89	0
57	MG	1H	3469	1/1	0.95	0.11	-	68,68,68,68	0
57	MG	1H	3415	1/1	0.81	0.06	-	95,95,95,95	0
57	MG	14	3140	1/1	0.74	0.35	-	89,89,89,89	0
57	MG	1G	1647	1/1	0.77	0.26	-	102,102,102,102	0
57	MG	1H	3279	1/1	0.74	0.47	-	76,76,76,76	0
57	MG	1H	3523	1/1	0.84	0.20	-	91,91,91,91	0
57	MG	14	3372	1/1	0.75	0.24	-	87,87,87,87	0
57	MG	1G	1719	1/1	0.93	0.11	-	91,91,91,91	0
57	MG	1H	3399	1/1	0.98	0.16	-	61,61,61,61	0
57	MG	13	1659	1/1	0.92	0.49	-	75,75,75,75	0
57	MG	14	3420	1/1	0.90	0.09	-	101,101,101,101	0
57	MG	1H	3218	1/1	0.67	0.20	-	81,81,81,81	0
57	MG	13	1613	1/1	0.91	0.18	-	81,81,81,81	0
57	MG	1H	3445	1/1	0.86	0.10	-	73,73,73,73	0
57	MG	1H	3244	1/1	0.94	0.32	-	77,77,77,77	0
57	MG	1H	3074	1/1	0.93	0.41	-	73,73,73,73	0
57	MG	1H	3037	1/1	0.90	0.35	-	71,71,71,71	0
57	MG	14	3045	1/1	0.97	0.32	-	61,61,61,61	0
57	MG	1H	3138	1/1	0.95	0.47	-	41,41,41,41	0
57	MG	1G	1658	1/1	0.73	0.21	-	82,82,82,82	0
57	MG	14	3355	1/1	0.86	0.11	-	90,90,90,90	0
57	MG	14	3441	1/1	0.91	0.14	-	99,99,99,99	0
57	MG	14	3260	1/1	0.97	0.09	-	71,71,71,71	0
57	MG	1H	3238	1/1	0.60	0.36	-	87,87,87,87	0
57	MG	14	3356	1/1	0.97	0.09	-	73,73,73,73	0
57	MG	1G	1643	1/1	0.61	0.34	-	83,83,83,83	0
57	MG	1H	3076	1/1	0.95	0.17	-	39,39,39,39	0
57	MG	1H	3118	1/1	0.46	0.33	-	83,83,83,83	0
57	MG	14	3443	1/1	0.91	0.26	-	102,102,102,102	0
57	MG	1H	3512	1/1	0.85	0.05	-	92,92,92,92	0
57	MG	14	3195	1/1	0.90	0.70	-	87,87,87,87	0
57	MG	14	3197	1/1	0.91	0.46	-	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
57	MG	1I	301	1/1	0.89	0.66	-	60,60,60,60	0
57	MG	1H	3506	1/1	0.96	0.06	-	79,79,79,79	0
57	MG	1G	1617	1/1	0.92	0.36	-	86,86,86,86	0
57	MG	1H	3112	1/1	0.93	0.32	-	79,79,79,79	0
57	MG	13	1684	1/1	0.83	0.28	-	85,85,85,85	0
57	MG	14	3134	1/1	0.72	0.43	-	71,71,71,71	0
57	MG	14	3095	1/1	0.96	0.35	-	74,74,74,74	0
57	MG	13	1717	1/1	0.92	0.13	-	114,114,114,114	0
57	MG	1H	3306	1/1	0.91	0.30	-	70,70,70,70	0
57	MG	1G	1636	1/1	0.90	0.07	-	91,91,91,91	0
57	MG	14	3187	1/1	0.93	0.17	-	74,74,74,74	0
57	MG	1G	1650	1/1	0.72	0.16	-	114,114,114,114	0
57	MG	14	3022	1/1	0.92	0.35	-	44,44,44,44	0
57	MG	14	3054	1/1	0.93	0.27	-	49,49,49,49	0
57	MG	1G	1707	1/1	0.97	0.07	-	79,79,79,79	0
57	MG	14	3439	1/1	0.76	0.07	-	107,107,107,107	0
57	MG	14	3278	1/1	0.85	0.07	-	95,95,95,95	0
57	MG	14	3359	1/1	0.87	0.09	-	96,96,96,96	0
57	MG	14	3202	1/1	0.85	0.29	-	98,98,98,98	0
57	MG	14	3189	1/1	0.95	0.52	-	76,76,76,76	0
57	MG	14	3066	1/1	0.85	0.37	-	59,59,59,59	0
57	MG	1H	3514	1/1	0.86	0.11	-	80,80,80,80	0
57	MG	1H	3298	1/1	0.92	0.14	-	83,83,83,83	0
57	MG	1H	3260	1/1	0.70	0.43	-	98,98,98,98	0
57	MG	14	3432	1/1	0.95	0.13	-	88,88,88,88	0
57	MG	14	3064	1/1	0.92	0.30	-	62,62,62,62	0
57	MG	1G	1688	1/1	0.95	0.11	-	95,95,95,95	0
57	MG	14	3205	1/1	0.85	0.44	-	93,93,93,93	0
57	MG	14	3379	1/1	0.90	0.09	-	64,64,64,64	0
57	MG	13	1677	1/1	0.93	0.34	-	92,92,92,92	0
57	MG	1H	3069	1/1	0.92	0.28	-	60,60,60,60	0
57	MG	14	3136	1/1	0.68	0.12	-	127,127,127,127	0
57	MG	1H	3210	1/1	0.51	0.37	-	83,83,83,83	0
57	MG	1H	3215	1/1	0.95	0.41	-	69,69,69,69	0
57	MG	14	3062	1/1	0.82	0.88	-	71,71,71,71	0
57	MG	14	3254	1/1	0.85	0.25	-	62,62,62,62	0
57	MG	1H	3361	1/1	0.88	0.15	-	76,76,76,76	0
57	MG	1H	3492	1/1	0.95	0.16	-	62,62,62,62	0
57	MG	4K	101	1/1	0.95	0.07	-	93,93,93,93	0
57	MG	1H	3518	1/1	0.71	0.12	-	87,87,87,87	0
57	MG	1H	3213	1/1	0.92	0.27	-	77,77,77,77	0
57	MG	1H	3177	1/1	0.87	0.62	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3068	1/1	0.95	0.37	-	64,64,64,64	0
57	MG	1H	3205	1/1	0.50	0.32	-	90,90,90,90	0
57	MG	14	3317	1/1	0.96	0.10	-	86,86,86,86	0
57	MG	14	3138	1/1	0.83	0.34	-	86,86,86,86	0
57	MG	1H	3454	1/1	0.94	0.19	-	58,58,58,58	0
57	MG	1H	3511	1/1	0.94	0.07	-	70,70,70,70	0
57	MG	1G	1665	1/1	0.81	0.19	-	73,73,73,73	0
57	MG	14	3353	1/1	0.77	0.18	-	104,104,104,104	0
57	MG	1H	3419	1/1	0.84	0.09	-	86,86,86,86	0
57	MG	1H	3286	1/1	0.88	0.29	-	87,87,87,87	0
57	MG	14	3198	1/1	0.95	0.12	-	85,85,85,85	0
57	MG	14	3446	1/1	0.91	0.27	-	85,85,85,85	0
57	MG	13	1673	1/1	0.83	0.84	-	86,86,86,86	0
57	MG	14	3294	1/1	0.85	0.11	-	85,85,85,85	0
57	MG	1G	1720	1/1	0.70	0.06	-	119,119,119,119	0
57	MG	14	3392	1/1	0.64	0.18	-	108,108,108,108	0
57	MG	13	1664	1/1	0.74	0.25	-	90,90,90,90	0
57	MG	14	3040	1/1	0.90	0.40	-	72,72,72,72	0
57	MG	1H	3012	1/1	0.91	0.22	-	84,84,84,84	0
57	MG	14	3252	1/1	0.93	0.15	-	76,76,76,76	0
57	MG	13	1675	1/1	0.85	0.39	-	92,92,92,92	0
57	MG	1H	3394	1/1	0.95	0.10	-	69,69,69,69	0
57	MG	1H	3197	1/1	0.84	0.36	-	80,80,80,80	0
57	MG	14	3185	1/1	0.94	0.26	-	72,72,72,72	0
57	MG	14	3111	1/1	0.67	0.48	-	86,86,86,86	0
57	MG	1G	1654	1/1	0.90	0.37	-	94,94,94,94	0
57	MG	1H	3307	1/1	0.84	0.64	-	72,72,72,72	0
57	MG	1G	1685	1/1	0.62	0.07	-	120,120,120,120	0
57	MG	1G	1653	1/1	0.77	0.28	-	103,103,103,103	0
57	MG	13	1745	1/1	0.64	0.13	-	153,153,153,153	0
57	MG	14	3143	1/1	0.94	0.43	-	54,54,54,54	0
57	MG	14	3090	1/1	0.97	0.49	-	65,65,65,65	0
57	MG	88	203	1/1	0.88	0.20	-	76,76,76,76	0
57	MG	14	3093	1/1	0.87	0.24	-	79,79,79,79	0
57	MG	14	3132	1/1	0.95	0.31	-	78,78,78,78	0
57	MG	1H	3233	1/1	0.86	0.19	-	110,110,110,110	0
57	MG	13	1742	1/1	0.82	0.05	-	132,132,132,132	0
57	MG	1H	3322	1/1	0.75	0.33	-	100,100,100,100	0
57	MG	1H	3146	1/1	0.95	0.66	-	58,58,58,58	0
57	MG	1H	3178	1/1	0.92	0.24	-	57,57,57,57	0
57	MG	1H	3292	1/1	0.87	0.23	-	84,84,84,84	0
57	MG	14	3108	1/1	0.94	0.85	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3155	1/1	0.88	0.30	-	80,80,80,80	0
57	MG	13	1621	1/1	0.96	0.21	-	56,56,56,56	0
57	MG	1H	3435	1/1	0.74	0.19	-	68,68,68,68	0
57	MG	1H	3482	1/1	0.94	0.08	-	80,80,80,80	0
60	ZN	C5	202	1/1	0.94	0.12	-	151,151,151,151	0
57	MG	16	202	1/1	0.96	0.32	-	78,78,78,78	0
57	MG	1H	3491	1/1	0.96	0.11	-	65,65,65,65	0
57	MG	1H	3160	1/1	0.96	0.44	-	68,68,68,68	0
57	MG	14	3299	1/1	0.93	0.19	-	66,66,66,66	0
57	MG	1H	3362	1/1	0.97	0.04	-	74,74,74,74	0
57	MG	1H	3525	1/1	0.60	0.17	-	96,96,96,96	0
57	MG	1H	3539	1/1	0.98	0.06	-	58,58,58,58	0
57	MG	1H	3471	1/1	0.93	0.07	-	73,73,73,73	0
57	MG	1H	3488	1/1	0.96	0.10	-	72,72,72,72	0
57	MG	14	3159	1/1	0.90	0.40	-	93,93,93,93	0
57	MG	13	1682	1/1	0.94	0.36	-	84,84,84,84	0
57	MG	14	3103	1/1	0.92	0.82	-	75,75,75,75	0
57	MG	1H	3328	1/1	0.95	0.19	-	46,46,46,46	0
57	MG	1G	1728	1/1	0.87	0.09	-	93,93,93,93	0
57	MG	14	3389	1/1	0.80	0.12	-	89,89,89,89	0
57	MG	1G	1638	1/1	0.77	0.12	-	93,93,93,93	0
57	MG	1H	3272	1/1	0.92	0.31	-	80,80,80,80	0
57	MG	1H	3134	1/1	0.87	0.23	-	44,44,44,44	0
57	MG	1H	3433	1/1	0.96	0.24	-	56,56,56,56	0
57	MG	1G	1682	1/1	0.77	0.11	-	96,96,96,96	0
57	MG	14	3276	1/1	0.83	0.14	-	81,81,81,81	0
57	MG	1G	1709	1/1	0.94	0.04	-	140,140,140,140	0
57	MG	14	3329	1/1	0.41	0.12	-	100,100,100,100	0
57	MG	14	3224	1/1	0.85	0.58	-	88,88,88,88	0
57	MG	14	3041	1/1	0.85	0.64	-	76,76,76,76	0
57	MG	13	1735	1/1	0.67	0.10	-	106,106,106,106	0
57	MG	1H	3470	1/1	0.89	0.09	-	93,93,93,93	0
57	MG	1H	3529	1/1	0.74	0.11	-	96,96,96,96	0
57	MG	14	3178	1/1	0.89	0.51	-	92,92,92,92	0
57	MG	1H	3234	1/1	0.86	0.75	-	76,76,76,76	0
57	MG	14	3413	1/1	0.82	0.26	-	93,93,93,93	0
57	MG	1H	3022	1/1	0.94	0.33	-	41,41,41,41	0
57	MG	1H	3005	1/1	0.75	0.73	-	74,74,74,74	0
57	MG	13	1692	1/1	0.80	0.43	-	100,100,100,100	0
57	MG	14	3048	1/1	0.98	0.28	-	67,67,67,67	0
57	MG	14	3003	1/1	0.94	0.49	-	54,54,54,54	0
57	MG	14	3042	1/1	0.97	0.45	-	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
57	MG	14	3098	1/1	0.93	0.68	-	62,62,62,62	0
57	MG	13	1728	1/1	0.51	0.20	-	103,103,103,103	0
57	MG	1H	3175	1/1	0.91	0.15	-	64,64,64,64	0
57	MG	1H	3084	1/1	0.82	0.61	-	68,68,68,68	0
57	MG	14	3297	1/1	0.66	0.29	-	90,90,90,90	0
57	MG	14	3218	1/1	0.53	0.14	-	106,106,106,106	0
57	MG	14	3404	1/1	0.73	0.14	-	118,118,118,118	0
57	MG	14	3378	1/1	0.71	0.12	-	78,78,78,78	0
57	MG	1H	3301	1/1	0.88	0.27	-	70,70,70,70	0
57	MG	14	3194	1/1	0.87	0.39	-	95,95,95,95	0
57	MG	1H	3388	1/1	0.94	0.13	-	53,53,53,53	0
57	MG	14	3397	1/1	0.82	0.10	-	91,91,91,91	0
57	MG	14	3352	1/1	0.95	0.10	-	61,61,61,61	0
57	MG	1H	3221	1/1	0.75	0.28	-	64,64,64,64	0
57	MG	1H	3126	1/1	0.90	0.22	-	75,75,75,75	0
57	MG	14	3403	1/1	0.90	0.29	-	85,85,85,85	0
57	MG	1H	3255	1/1	0.90	0.24	-	73,73,73,73	0
57	MG	14	3208	1/1	0.95	0.26	-	101,101,101,101	0
57	MG	1H	3285	1/1	0.89	0.42	-	96,96,96,96	0
57	MG	1H	3370	1/1	0.92	0.26	-	54,54,54,54	0
57	MG	1H	3337	1/1	0.95	0.19	-	44,44,44,44	0
57	MG	1H	3004	1/1	0.94	0.72	-	79,79,79,79	0
57	MG	1H	3498	1/1	0.96	0.06	-	79,79,79,79	0
57	MG	14	3165	1/1	0.82	0.45	-	74,74,74,74	0
57	MG	14	3281	1/1	0.93	0.26	-	83,83,83,83	0
57	MG	1H	3282	1/1	0.70	0.43	-	89,89,89,89	0
57	MG	1H	3226	1/1	0.95	0.55	-	60,60,60,60	0
57	MG	14	3236	1/1	0.93	0.11	-	56,56,56,56	0
57	MG	1H	3360	1/1	0.97	0.11	-	60,60,60,60	0
57	MG	14	3216	1/1	0.47	0.78	-	93,93,93,93	0
57	MG	13	1623	1/1	0.84	0.40	-	80,80,80,80	0
57	MG	4L	101	1/1	0.46	0.09	-	110,110,110,110	0
57	MG	1H	3447	1/1	0.96	0.07	-	60,60,60,60	0
57	MG	13	1722	1/1	0.92	0.04	-	100,100,100,100	0
57	MG	1H	3407	1/1	0.87	0.16	-	46,46,46,46	0
57	MG	16	204	1/1	0.89	0.27	-	70,70,70,70	0
57	MG	14	3336	1/1	0.87	0.07	-	94,94,94,94	0
57	MG	1H	3396	1/1	0.88	0.10	-	84,84,84,84	0
57	MG	1H	3321	1/1	0.70	0.37	-	90,90,90,90	0
57	MG	14	3015	1/1	0.92	0.24	-	73,73,73,73	0
57	MG	14	3368	1/1	0.88	0.12	-	98,98,98,98	0
57	MG	1H	3350	1/1	0.85	0.20	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3521	1/1	0.61	0.11	-	97,97,97,97	0
57	MG	1G	1651	1/1	0.73	0.14	-	105,105,105,105	0
57	MG	1G	1698	1/1	0.81	0.07	-	110,110,110,110	0
57	MG	1H	3153	1/1	0.92	0.23	-	82,82,82,82	0
57	MG	13	1610	1/1	0.96	0.36	-	73,73,73,73	0
57	MG	1H	3425	1/1	0.86	0.05	-	100,100,100,100	0
57	MG	14	3172	1/1	0.76	0.50	-	82,82,82,82	0
57	MG	14	3145	1/1	0.94	0.12	-	85,85,85,85	0
57	MG	1H	3021	1/1	0.96	0.34	-	63,63,63,63	0
57	MG	1H	3262	1/1	0.91	0.25	-	71,71,71,71	0
57	MG	1H	3294	1/1	0.76	0.15	-	90,90,90,90	0
57	MG	14	3364	1/1	0.84	0.09	-	97,97,97,97	0
57	MG	14	3193	1/1	0.95	0.39	-	82,82,82,82	0
57	MG	14	3339	1/1	0.95	0.11	-	57,57,57,57	0
57	MG	14	3002	1/1	0.91	0.70	-	68,68,68,68	0
57	MG	1H	3417	1/1	0.79	0.06	-	89,89,89,89	0
57	MG	1G	1605	1/1	0.88	0.31	-	82,82,82,82	0
57	MG	1H	3039	1/1	0.98	0.29	-	40,40,40,40	0
57	MG	14	3380	1/1	0.81	0.11	-	86,86,86,86	0
57	MG	1H	3497	1/1	0.64	0.12	-	98,98,98,98	0
57	MG	14	3128	1/1	0.98	0.34	-	88,88,88,88	0
57	MG	1G	1641	1/1	0.93	0.11	-	88,88,88,88	0
57	MG	14	3074	1/1	0.93	0.27	-	81,81,81,81	0
57	MG	1H	3130	1/1	0.89	0.73	-	87,87,87,87	0
57	MG	1G	1616	1/1	0.77	0.33	-	88,88,88,88	0
57	MG	1H	3412	1/1	0.99	0.09	-	80,80,80,80	0
57	MG	14	3351	1/1	0.49	0.07	-	105,105,105,105	0
57	MG	1G	1714	1/1	0.90	0.13	-	113,113,113,113	0
57	MG	13	1710	1/1	0.83	0.09	-	95,95,95,95	0
57	MG	1H	3008	1/1	0.80	0.47	-	75,75,75,75	0
57	MG	1G	1604	1/1	0.94	0.30	-	103,103,103,103	0
57	MG	1H	3147	1/1	0.88	0.44	-	64,64,64,64	0
57	MG	14	3049	1/1	0.92	0.32	-	57,57,57,57	0
57	MG	14	3006	1/1	0.92	0.25	-	79,79,79,79	0
57	MG	13	1602	1/1	0.91	0.27	-	78,78,78,78	0
57	MG	14	3328	1/1	0.98	0.09	-	60,60,60,60	0
57	MG	4L	102	1/1	0.89	0.11	-	108,108,108,108	0
57	MG	14	3221	1/1	0.95	0.44	-	54,54,54,54	0
57	MG	13	1658	1/1	0.81	0.41	-	80,80,80,80	0
57	MG	1H	3003	1/1	0.80	0.48	-	65,65,65,65	0
57	MG	1H	3031	1/1	0.95	0.43	-	74,74,74,74	0
57	MG	1H	3142	1/1	0.98	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3204	1/1	0.67	0.42	-	81,81,81,81	0
57	MG	13	1678	1/1	0.69	0.28	-	86,86,86,86	0
57	MG	14	3289	1/1	0.90	0.07	-	73,73,73,73	0
57	MG	1H	3501	1/1	0.66	0.09	-	93,93,93,93	0
57	MG	1H	3509	1/1	0.66	0.08	-	84,84,84,84	0
57	MG	35	201	1/1	0.82	0.16	-	86,86,86,86	0
57	MG	14	3391	1/1	0.90	0.17	-	94,94,94,94	0
57	MG	1H	3098	1/1	0.84	0.54	-	78,78,78,78	0
57	MG	1G	1680	1/1	0.96	0.07	-	93,93,93,93	0
57	MG	14	3174	1/1	0.46	0.45	-	83,83,83,83	0
57	MG	14	3277	1/1	0.89	0.07	-	74,74,74,74	0
57	MG	1H	3216	1/1	0.45	0.55	-	89,89,89,89	0
57	MG	1H	3087	1/1	0.83	0.39	-	79,79,79,79	0
57	MG	14	3303	1/1	0.83	0.07	-	117,117,117,117	0
57	MG	16	206	1/1	0.56	0.38	-	77,77,77,77	0
57	MG	1G	1727	1/1	0.90	0.06	-	113,113,113,113	0
57	MG	1H	3143	1/1	0.96	0.15	-	66,66,66,66	0
57	MG	1H	3269	1/1	0.74	0.37	-	86,86,86,86	0
57	MG	1H	3228	1/1	0.83	0.35	-	70,70,70,70	0
57	MG	14	3349	1/1	0.96	0.07	-	101,101,101,101	0
57	MG	14	3179	1/1	0.78	0.43	-	75,75,75,75	0
57	MG	1H	3386	1/1	0.90	0.08	-	77,77,77,77	0
57	MG	I8	101	1/1	0.96	0.05	-	69,69,69,69	0
57	MG	13	1647	1/1	0.88	0.27	-	91,91,91,91	0
57	MG	16	211	1/1	0.74	0.12	-	99,99,99,99	0
57	MG	1H	3423	1/1	0.73	0.14	-	101,101,101,101	0
57	MG	1H	3200	1/1	0.86	0.34	-	73,73,73,73	0
57	MG	1J	207	1/1	0.85	0.10	-	92,92,92,92	0
57	MG	1H	3202	1/1	0.86	1.00	-	82,82,82,82	0
57	MG	1H	3314	1/1	0.93	0.19	-	88,88,88,88	0
57	MG	1H	3398	1/1	0.78	0.17	-	58,58,58,58	0
57	MG	14	3401	1/1	0.90	0.14	-	95,95,95,95	0
57	MG	14	3188	1/1	0.83	0.34	-	90,90,90,90	0
57	MG	13	1718	1/1	0.94	0.09	-	55,55,55,55	0
57	MG	14	3105	1/1	0.96	0.35	-	73,73,73,73	0
57	MG	1H	3502	1/1	0.98	0.15	-	75,75,75,75	0
57	MG	14	3332	1/1	0.91	0.14	-	64,64,64,64	0
57	MG	45	201	1/1	0.96	0.12	-	74,74,74,74	0
57	MG	1G	1706	1/1	0.92	0.11	-	124,124,124,124	0
57	MG	1H	3163	1/1	0.91	0.19	-	74,74,74,74	0
57	MG	14	3077	1/1	0.74	0.20	-	84,84,84,84	0
57	MG	1H	3452	1/1	0.95	0.12	-	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
57	MG	1H	3505	1/1	0.70	0.19	-	93,93,93,93	0
57	MG	14	3388	1/1	0.27	0.15	-	93,93,93,93	0
57	MG	1H	3431	1/1	0.97	0.14	-	61,61,61,61	0
57	MG	1H	3047	1/1	0.94	0.27	-	55,55,55,55	0
57	MG	13	1712	1/1	0.89	0.10	-	82,82,82,82	0
57	MG	14	3382	1/1	0.70	0.17	-	85,85,85,85	0
57	MG	14	3017	1/1	0.97	0.48	-	60,60,60,60	0
57	MG	1H	3207	1/1	0.79	0.72	-	87,87,87,87	0
57	MG	14	3139	1/1	0.95	0.48	-	84,84,84,84	0
57	MG	1H	3211	1/1	0.68	0.50	-	79,79,79,79	0
57	MG	1H	3093	1/1	0.94	0.33	-	71,71,71,71	0
57	MG	21	302	1/1	0.98	0.14	-	46,46,46,46	0
57	MG	1H	3401	1/1	0.98	0.13	-	59,59,59,59	0
57	MG	14	3152	1/1	0.78	0.66	-	86,86,86,86	0
57	MG	14	3211	1/1	0.86	0.33	-	65,65,65,65	0
57	MG	14	3287	1/1	0.94	0.09	-	79,79,79,79	0
57	MG	14	3056	1/1	0.88	0.33	-	80,80,80,80	0
57	MG	1H	3330	1/1	0.81	0.17	-	47,47,47,47	0
57	MG	1H	3258	1/1	0.73	0.40	-	84,84,84,84	0
57	MG	14	3182	1/1	0.84	0.34	-	81,81,81,81	0
57	MG	1H	3051	1/1	0.86	0.48	-	76,76,76,76	0
57	MG	1G	1634	1/1	0.94	0.18	-	93,93,93,93	0
57	MG	14	3361	1/1	0.86	0.06	-	86,86,86,86	0
57	MG	1H	3182	1/1	0.62	0.26	-	90,90,90,90	0
57	MG	14	3311	1/1	0.97	0.06	-	71,71,71,71	0
57	MG	1H	3192	1/1	0.91	0.28	-	76,76,76,76	0
57	MG	1G	1725	1/1	0.77	0.08	-	94,94,94,94	0
57	MG	1H	3173	1/1	0.93	0.75	-	89,89,89,89	0
57	MG	1H	3397	1/1	0.96	0.14	-	64,64,64,64	0
57	MG	1H	3019	1/1	0.88	0.30	-	61,61,61,61	0
57	MG	1H	3027	1/1	0.91	0.35	-	84,84,84,84	0
57	MG	1H	3424	1/1	0.90	0.08	-	66,66,66,66	0
57	MG	14	3191	1/1	0.84	0.34	-	79,79,79,79	0
57	MG	1H	3103	1/1	0.70	0.30	-	82,82,82,82	0
57	MG	1H	3067	1/1	0.80	0.18	-	62,62,62,62	0
57	MG	1H	3527	1/1	0.78	0.11	-	113,113,113,113	0
57	MG	1G	1718	1/1	0.49	0.10	-	99,99,99,99	0
57	MG	1H	3248	1/1	0.84	0.39	-	96,96,96,96	0
57	MG	1H	3122	1/1	0.82	0.27	-	67,67,67,67	0
57	MG	14	3057	1/1	0.94	0.45	-	84,84,84,84	0
57	MG	14	3013	1/1	0.94	0.44	-	63,63,63,63	0
57	MG	14	3241	1/1	0.84	0.17	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3189	1/1	0.74	0.44	-	78,78,78,78	0
57	MG	1H	3099	1/1	0.86	0.37	-	84,84,84,84	0
57	MG	1H	3347	1/1	0.97	0.20	-	56,56,56,56	0
57	MG	14	3343	1/1	0.87	0.08	-	91,91,91,91	0
57	MG	1H	3259	1/1	0.85	0.43	-	92,92,92,92	0
57	MG	25	201	1/1	0.64	0.09	-	118,118,118,118	0
57	MG	1H	3171	1/1	0.79	0.30	-	90,90,90,90	0
57	MG	1H	3318	1/1	0.97	0.20	-	54,54,54,54	0
57	MG	1H	3168	1/1	0.58	0.16	-	80,80,80,80	0
57	MG	14	3106	1/1	0.94	0.80	-	94,94,94,94	0
57	MG	14	3092	1/1	0.65	0.50	-	81,81,81,81	0
57	MG	14	3417	1/1	0.87	0.10	-	101,101,101,101	0
57	MG	1H	3121	1/1	0.74	0.95	-	80,80,80,80	0
57	MG	14	3175	1/1	0.96	0.08	-	107,107,107,107	0
57	MG	14	3360	1/1	0.88	0.10	-	88,88,88,88	0
57	MG	14	3423	1/1	0.84	0.19	-	98,98,98,98	0
57	MG	14	3164	1/1	0.95	0.32	-	80,80,80,80	0
57	MG	1G	1619	1/1	0.77	0.30	-	86,86,86,86	0
57	MG	14	3177	1/1	0.81	0.31	-	82,82,82,82	0
57	MG	14	3226	1/1	0.81	0.16	-	113,113,113,113	0
57	MG	1H	3517	1/1	0.83	0.09	-	79,79,79,79	0
57	MG	1H	3083	1/1	0.92	0.49	-	71,71,71,71	0
57	MG	1G	1729	1/1	0.70	0.05	-	114,114,114,114	0
57	MG	1G	1721	1/1	0.84	0.05	-	106,106,106,106	0
57	MG	1H	3044	1/1	0.90	0.67	-	81,81,81,81	0
57	MG	1H	3339	1/1	0.95	0.22	-	43,43,43,43	0
57	MG	1G	1601	1/1	0.95	0.19	-	70,70,70,70	0
57	MG	L8	101	1/1	0.81	0.35	-	86,86,86,86	0
57	MG	14	3436	1/1	0.81	0.14	-	115,115,115,115	0
57	MG	1G	1710	1/1	0.82	0.14	-	87,87,87,87	0
57	MG	13	1646	1/1	0.91	0.32	-	97,97,97,97	0
57	MG	1H	3064	1/1	0.96	0.36	-	63,63,63,63	0
57	MG	1H	3013	1/1	0.94	0.32	-	37,37,37,37	0
57	MG	1H	3091	1/1	0.97	0.40	-	77,77,77,77	0
57	MG	13	1732	1/1	0.90	0.08	-	81,81,81,81	0
57	MG	13	1605	1/1	0.96	0.25	-	70,70,70,70	0
57	MG	1H	3268	1/1	0.93	0.67	-	92,92,92,92	0
57	MG	13	1739	1/1	0.87	0.10	-	98,98,98,98	0
57	MG	1H	3374	1/1	0.70	0.15	-	89,89,89,89	0
57	MG	1H	3246	1/1	0.23	0.49	-	72,72,72,72	0
57	MG	1H	3274	1/1	0.54	0.47	-	83,83,83,83	0
57	MG	14	3032	1/1	0.85	0.46	-	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
57	MG	14	3063	1/1	0.90	0.37	-	52,52,52,52	0
57	MG	1H	3352	1/1	0.86	0.08	-	84,84,84,84	0
57	MG	1H	3089	1/1	0.88	0.28	-	66,66,66,66	0
57	MG	1G	1687	1/1	0.47	0.10	-	107,107,107,107	0
57	MG	1H	3188	1/1	0.58	0.68	-	95,95,95,95	0
57	MG	14	3400	1/1	0.78	0.07	-	99,99,99,99	0
57	MG	14	3162	1/1	0.64	0.61	-	67,67,67,67	0
57	MG	1H	3162	1/1	0.90	0.32	-	68,68,68,68	0
57	MG	1H	3436	1/1	0.92	0.10	-	60,60,60,60	0
57	MG	1H	3356	1/1	0.98	0.13	-	67,67,67,67	0
57	MG	1H	3041	1/1	0.98	0.25	-	51,51,51,51	0
57	MG	13	1690	1/1	0.81	0.53	-	72,72,72,72	0
57	MG	1H	3280	1/1	0.89	0.55	-	68,68,68,68	0
57	MG	13	1653	1/1	0.84	0.53	-	94,94,94,94	0
57	MG	P8	101	1/1	0.89	0.35	-	71,71,71,71	0
57	MG	14	3233	1/1	0.92	0.68	-	80,80,80,80	0
57	MG	1H	3090	1/1	0.92	0.74	-	77,77,77,77	0
57	MG	14	3367	1/1	0.89	0.17	-	96,96,96,96	0
57	MG	1H	3530	1/1	0.92	0.43	-	78,78,78,78	0
57	MG	14	3371	1/1	0.87	0.11	-	92,92,92,92	0
57	MG	13	1651	1/1	0.78	0.30	-	97,97,97,97	0
57	MG	1H	3181	1/1	0.91	0.16	-	94,94,94,94	0
57	MG	1H	3296	1/1	0.83	0.30	-	81,81,81,81	0
57	MG	1G	1676	1/1	0.53	0.12	-	107,107,107,107	0
57	MG	1G	1695	1/1	0.81	0.10	-	94,94,94,94	0
57	MG	1H	3030	1/1	0.98	0.34	-	75,75,75,75	0
57	MG	14	3309	1/1	0.89	0.15	-	72,72,72,72	0
57	MG	1H	3536	1/1	0.66	0.24	-	93,93,93,93	0
57	MG	14	3358	1/1	0.90	0.10	-	67,67,67,67	0
57	MG	68	201	1/1	0.79	0.23	-	78,78,78,78	0
57	MG	14	3051	1/1	0.97	0.31	-	72,72,72,72	0
57	MG	14	3412	1/1	0.84	0.07	-	116,116,116,116	0
57	MG	14	3035	1/1	0.90	0.86	-	79,79,79,79	0
57	MG	1H	3120	1/1	0.70	0.46	-	96,96,96,96	0
57	MG	14	3402	1/1	0.89	0.09	-	76,76,76,76	0
57	MG	13	1698	1/1	0.96	0.15	-	83,83,83,83	0
57	MG	1H	3453	1/1	0.89	0.09	-	75,75,75,75	0
57	MG	14	3157	1/1	0.62	0.69	-	89,89,89,89	0
57	MG	1H	3375	1/1	0.79	0.11	-	86,86,86,86	0
57	MG	1H	3219	1/1	0.96	0.54	-	82,82,82,82	0
57	MG	1H	3403	1/1	0.52	0.10	-	79,79,79,79	0
57	MG	1H	3485	1/1	0.79	0.15	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3180	1/1	0.88	0.23	-	71,71,71,71	0
57	MG	1H	3206	1/1	0.78	0.25	-	91,91,91,91	0
57	MG	1H	3507	1/1	0.98	0.09	-	61,61,61,61	0
57	MG	1H	3422	1/1	0.77	0.14	-	99,99,99,99	0
57	MG	1H	3496	1/1	0.89	0.06	-	94,94,94,94	0
57	MG	1G	1689	1/1	0.94	0.11	-	89,89,89,89	0
57	MG	1H	3449	1/1	0.67	0.19	-	86,86,86,86	0
57	MG	1H	3276	1/1	0.85	0.36	-	90,90,90,90	0
57	MG	1H	3354	1/1	0.94	0.10	-	73,73,73,73	0
57	MG	1H	3128	1/1	0.88	0.14	-	79,79,79,79	0
57	MG	1H	3190	1/1	0.83	0.41	-	75,75,75,75	0
57	MG	14	3094	1/1	0.75	0.96	-	70,70,70,70	0
57	MG	1H	3193	1/1	0.89	0.52	-	93,93,93,93	0
57	MG	1H	3212	1/1	0.64	0.20	-	65,65,65,65	0
57	MG	1H	3335	1/1	0.97	0.12	-	53,53,53,53	0
57	MG	14	3199	1/1	1.00	0.20	-	78,78,78,78	0
57	MG	1H	3462	1/1	0.93	0.15	-	48,48,48,48	0
57	MG	1H	3389	1/1	0.86	0.18	-	58,58,58,58	0
57	MG	14	3445	1/1	0.53	0.14	-	92,92,92,92	0
57	MG	2L	102	1/1	0.69	0.64	-	90,90,90,90	0
57	MG	1G	1670	1/1	0.89	0.11	-	99,99,99,99	0
57	MG	1H	3158	1/1	0.84	0.48	-	71,71,71,71	0
57	MG	1H	3460	1/1	0.95	0.15	-	64,64,64,64	0
57	MG	1G	1732	1/1	0.74	0.08	-	114,114,114,114	0
57	MG	14	3024	1/1	0.90	0.13	-	77,77,77,77	0
57	MG	1H	3245	1/1	0.88	0.53	-	78,78,78,78	0
57	MG	13	1643	1/1	0.75	0.42	-	86,86,86,86	0
57	MG	1H	3543	1/1	0.79	0.33	-	90,90,90,90	0
57	MG	13	1740	1/1	0.90	0.10	-	70,70,70,70	0
57	MG	1H	3265	1/1	0.73	0.15	-	77,77,77,77	0
57	MG	1H	3532	1/1	0.90	0.21	-	76,76,76,76	0
57	MG	1H	3541	1/1	0.92	0.10	-	81,81,81,81	0
57	MG	13	1744	1/1	0.79	0.10	-	98,98,98,98	0
57	MG	1H	3300	1/1	0.95	0.24	-	87,87,87,87	0
57	MG	1H	3429	1/1	0.92	0.16	-	68,68,68,68	0
57	MG	1H	3077	1/1	0.65	0.26	-	56,56,56,56	0
57	MG	14	3230	1/1	0.96	1.18	-	86,86,86,86	0
57	MG	1G	1731	1/1	0.93	0.06	-	94,94,94,94	0
57	MG	1G	1712	1/1	0.80	0.13	-	108,108,108,108	0
57	MG	1H	3421	1/1	0.79	0.06	-	102,102,102,102	0
57	MG	14	3288	1/1	0.85	0.06	-	93,93,93,93	0
57	MG	1G	1703	1/1	0.54	0.13	-	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
57	MG	1H	3390	1/1	0.95	0.12	-	68,68,68,68	0
57	MG	1H	3155	1/1	0.72	0.22	-	91,91,91,91	0
57	MG	1H	3420	1/1	0.92	0.07	-	78,78,78,78	0
57	MG	14	3243	1/1	0.91	0.09	-	100,100,100,100	0
57	MG	1H	3426	1/1	0.88	0.17	-	74,74,74,74	0
57	MG	1H	3438	1/1	0.95	0.17	-	46,46,46,46	0
57	MG	14	3362	1/1	0.96	0.07	-	94,94,94,94	0
57	MG	14	3325	1/1	0.88	0.12	-	83,83,83,83	0
57	MG	14	3426	1/1	0.87	0.13	-	94,94,94,94	0
57	MG	14	3442	1/1	0.90	0.10	-	98,98,98,98	0
57	MG	14	3052	1/1	0.86	0.47	-	79,79,79,79	0
57	MG	1G	1697	1/1	0.74	0.13	-	91,91,91,91	0
57	MG	31	301	1/1	0.93	0.26	-	63,63,63,63	0
57	MG	1H	3467	1/1	0.86	0.03	-	89,89,89,89	0
57	MG	14	3430	1/1	0.43	0.16	-	109,109,109,109	0
57	MG	14	3081	1/1	0.79	0.36	-	81,81,81,81	0
57	MG	13	1737	1/1	0.89	0.08	-	111,111,111,111	0
57	MG	1H	3546	1/1	0.85	0.07	-	116,116,116,116	0
57	MG	16	208	1/1	0.85	0.37	-	79,79,79,79	0
57	MG	1H	3302	1/1	0.93	0.52	-	81,81,81,81	0
57	MG	Q8	101	1/1	0.90	0.26	-	81,81,81,81	0
57	MG	14	3229	1/1	0.88	0.28	-	76,76,76,76	0
57	MG	1H	3316	1/1	0.70	0.48	-	89,89,89,89	0
57	MG	14	3342	1/1	0.96	0.07	-	69,69,69,69	0
57	MG	14	3190	1/1	0.70	0.67	-	85,85,85,85	0
57	MG	1G	1683	1/1	0.83	0.08	-	105,105,105,105	0
57	MG	1G	1690	1/1	0.87	0.16	-	89,89,89,89	0
57	MG	2K	103	1/1	0.84	0.38	-	89,89,89,89	0
57	MG	14	3047	1/1	0.97	0.26	-	81,81,81,81	0
57	MG	1H	3247	1/1	0.92	0.39	-	101,101,101,101	0
57	MG	1H	3428	1/1	0.96	0.07	-	66,66,66,66	0
57	MG	1H	3430	1/1	0.85	0.18	-	56,56,56,56	0
57	MG	13	1618	1/1	0.93	0.59	-	60,60,60,60	0
57	MG	1H	3304	1/1	0.89	0.43	-	85,85,85,85	0
57	MG	1H	3020	1/1	0.93	0.26	-	47,47,47,47	0
57	MG	1H	3201	1/1	0.76	0.37	-	88,88,88,88	0
57	MG	1H	3261	1/1	0.56	0.41	-	77,77,77,77	0
57	MG	1H	3114	1/1	0.89	0.68	-	67,67,67,67	0
57	MG	1H	3107	1/1	0.94	0.44	-	72,72,72,72	0
57	MG	F8	101	1/1	0.83	0.43	-	86,86,86,86	0
57	MG	1H	3408	1/1	0.93	0.04	-	77,77,77,77	0
57	MG	14	3176	1/1	0.87	0.35	-	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
57	MG	1H	3288	1/1	0.95	0.30	-	77,77,77,77	0
57	MG	14	3071	1/1	0.93	0.24	-	63,63,63,63	0
57	MG	1G	1633	1/1	0.88	0.17	-	89,89,89,89	0
57	MG	1H	3475	1/1	0.88	0.09	-	82,82,82,82	0
57	MG	1H	3537	1/1	0.91	0.18	-	60,60,60,60	0
57	MG	1G	1663	1/1	0.83	0.91	-	94,94,94,94	0
57	MG	14	3346	1/1	0.93	0.09	-	88,88,88,88	0
57	MG	1J	201	1/1	0.82	0.29	-	86,86,86,86	0
57	MG	1H	3149	1/1	0.83	0.29	-	86,86,86,86	0
57	MG	1H	3317	1/1	0.77	0.49	-	83,83,83,83	0
57	MG	14	3020	1/1	0.96	0.42	-	61,61,61,61	0
57	MG	14	3419	1/1	0.92	0.11	-	89,89,89,89	0
57	MG	1G	1696	1/1	0.57	0.07	-	112,112,112,112	0
57	MG	13	1615	1/1	0.86	0.23	-	73,73,73,73	0
57	MG	E5	101	1/1	0.89	0.08	-	100,100,100,100	0
57	MG	14	3200	1/1	0.80	0.20	-	86,86,86,86	0
57	MG	1H	3049	1/1	0.97	0.44	-	69,69,69,69	0
57	MG	1H	3229	1/1	0.93	0.38	-	64,64,64,64	0
57	MG	14	3284	1/1	0.57	0.15	-	105,105,105,105	0
57	MG	13	1741	1/1	0.88	0.05	-	92,92,92,92	0
57	MG	1H	3006	1/1	0.89	0.44	-	71,71,71,71	0
57	MG	1H	3287	1/1	0.89	0.39	-	78,78,78,78	0
57	MG	1H	3267	1/1	0.87	0.54	-	68,68,68,68	0
57	MG	1H	3214	1/1	0.89	0.26	-	86,86,86,86	0
57	MG	1H	3487	1/1	0.83	0.10	-	89,89,89,89	0
57	MG	1H	3477	1/1	0.95	0.12	-	68,68,68,68	0
57	MG	1H	3034	1/1	0.93	0.38	-	72,72,72,72	0
57	MG	1H	3208	1/1	0.91	0.45	-	78,78,78,78	0
57	MG	1G	1649	1/1	0.98	0.38	-	89,89,89,89	0
57	MG	14	3009	1/1	0.95	0.26	-	68,68,68,68	0
57	MG	14	3209	1/1	0.73	0.28	-	85,85,85,85	0
57	MG	14	3334	1/1	0.88	0.10	-	80,80,80,80	0
57	MG	14	3153	1/1	0.94	0.59	-	65,65,65,65	0
57	MG	14	3405	1/1	0.95	0.06	-	83,83,83,83	0
57	MG	14	3424	1/1	0.56	0.17	-	100,100,100,100	0
57	MG	13	1603	1/1	0.91	0.12	-	116,116,116,116	0
57	MG	1G	1648	1/1	0.81	0.39	-	79,79,79,79	0
57	MG	14	3415	1/1	0.89	0.27	-	81,81,81,81	0
57	MG	13	1686	1/1	0.81	0.31	-	74,74,74,74	0
57	MG	1H	3133	1/1	0.68	0.49	-	78,78,78,78	0
57	MG	13	1638	1/1	0.94	0.08	-	78,78,78,78	0
57	MG	14	3080	1/1	0.94	0.35	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3273	1/1	0.85	0.06	-	72,72,72,72	0
57	MG	1H	3061	1/1	0.59	0.45	-	76,76,76,76	0
57	MG	1H	3123	1/1	0.80	0.61	-	65,65,65,65	0
57	MG	14	3406	1/1	0.72	0.15	-	100,100,100,100	0
57	MG	1G	1716	1/1	0.56	0.13	-	119,119,119,119	0
57	MG	1J	206	1/1	0.44	0.16	-	109,109,109,109	0
57	MG	14	3173	1/1	0.46	0.16	-	98,98,98,98	0
57	MG	14	3008	1/1	0.67	0.40	-	90,90,90,90	0
57	MG	14	3370	1/1	0.85	0.12	-	74,74,74,74	0
57	MG	1H	3319	1/1	0.95	0.17	-	56,56,56,56	0
57	MG	1H	3080	1/1	0.87	0.53	-	103,103,103,103	0
57	MG	13	1680	1/1	0.65	0.60	-	94,94,94,94	0
57	MG	1H	3336	1/1	0.90	0.16	-	50,50,50,50	0
57	MG	14	3171	1/1	0.90	0.17	-	57,57,57,57	0
57	MG	1G	1624	1/1	0.86	0.44	-	76,76,76,76	0
57	MG	88	202	1/1	0.82	0.33	-	72,72,72,72	0
57	MG	14	3387	1/1	0.89	0.13	-	80,80,80,80	0
57	MG	14	3161	1/1	0.84	0.89	-	79,79,79,79	0
57	MG	1H	3185	1/1	0.77	0.35	-	90,90,90,90	0
57	MG	1H	3513	1/1	0.92	0.16	-	97,97,97,97	0
57	MG	14	3069	1/1	0.95	0.13	-	93,93,93,93	0
57	MG	1G	1669	1/1	0.89	0.06	-	95,95,95,95	0
57	MG	1H	3380	1/1	0.89	0.17	-	58,58,58,58	0
57	MG	1H	3079	1/1	0.90	0.28	-	45,45,45,45	0
57	MG	1H	3459	1/1	0.86	0.14	-	82,82,82,82	0
57	MG	1H	3309	1/1	0.87	0.74	-	74,74,74,74	0
57	MG	13	1721	1/1	0.90	0.10	-	71,71,71,71	0
57	MG	1G	1705	1/1	0.83	0.07	-	107,107,107,107	0
57	MG	1G	1657	1/1	0.96	0.23	-	66,66,66,66	0
57	MG	1H	3320	1/1	0.79	0.41	-	80,80,80,80	0
57	MG	14	3099	1/1	0.89	0.35	-	77,77,77,77	0
57	MG	1H	3366	1/1	0.92	0.15	-	62,62,62,62	0
57	MG	1H	3082	1/1	0.84	0.39	-	76,76,76,76	0
57	MG	1G	1618	1/1	0.88	0.24	-	89,89,89,89	0
57	MG	1G	1620	1/1	0.81	0.27	-	79,79,79,79	0
57	MG	1H	3127	1/1	0.84	0.38	-	84,84,84,84	0
57	MG	14	3067	1/1	0.95	0.35	-	69,69,69,69	0
57	MG	1G	1630	1/1	0.47	0.49	-	106,106,106,106	0
57	MG	14	3082	1/1	0.77	0.34	-	90,90,90,90	0
57	MG	1H	3150	1/1	0.94	0.30	-	67,67,67,67	0
57	MG	14	3001	1/1	0.93	0.16	-	52,52,52,52	0
57	MG	13	1709	1/1	0.50	0.17	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3313	1/1	0.99	0.10	-	68,68,68,68	0
57	MG	1H	3531	1/1	0.83	0.09	-	98,98,98,98	0
57	MG	1H	3450	1/1	0.84	0.41	-	80,80,80,80	0
57	MG	1H	3068	1/1	0.97	0.58	-	71,71,71,71	0
57	MG	13	1733	1/1	0.78	0.05	-	90,90,90,90	0
57	MG	1H	3371	1/1	0.84	0.17	-	59,59,59,59	0
57	MG	1G	1659	1/1	0.93	0.26	-	84,84,84,84	0
57	MG	1H	3186	1/1	0.64	0.43	-	94,94,94,94	0
57	MG	C5	201	1/1	0.89	0.08	-	103,103,103,103	0
57	MG	1H	3293	1/1	0.97	0.45	-	46,46,46,46	0
57	MG	2K	102	1/1	0.76	0.32	-	92,92,92,92	0
57	MG	14	3220	1/1	0.67	0.28	-	84,84,84,84	0
57	MG	13	1626	1/1	0.89	0.28	-	67,67,67,67	0
57	MG	1H	3312	1/1	0.87	0.23	-	94,94,94,94	0
57	MG	13	1631	1/1	0.93	0.24	-	78,78,78,78	0
57	MG	1H	3499	1/1	0.79	0.16	-	85,85,85,85	0
57	MG	1H	3100	1/1	0.79	0.16	-	62,62,62,62	0
57	MG	13	1604	1/1	0.98	0.32	-	77,77,77,77	0
57	MG	2K	104	1/1	0.96	0.06	-	89,89,89,89	0
57	MG	14	3151	1/1	0.76	0.20	-	87,87,87,87	0
57	MG	1H	3159	1/1	0.98	0.30	-	74,74,74,74	0
57	MG	13	1663	1/1	0.82	0.19	-	76,76,76,76	0
57	MG	14	3340	1/1	0.91	0.08	-	81,81,81,81	0
57	MG	1H	3277	1/1	0.86	0.55	-	82,82,82,82	0
57	MG	14	3115	1/1	0.92	0.41	-	48,48,48,48	0
57	MG	1H	3011	1/1	0.94	0.24	-	73,73,73,73	0
57	MG	1H	3406	1/1	0.96	0.16	-	46,46,46,46	0
57	MG	29	303	1/1	0.98	0.13	-	52,52,52,52	0
57	MG	14	3037	1/1	0.96	0.34	-	57,57,57,57	0
57	MG	14	3384	1/1	0.94	0.10	-	72,72,72,72	0
57	MG	14	3337	1/1	0.85	0.14	-	63,63,63,63	0
57	MG	14	3431	1/1	0.86	0.09	-	99,99,99,99	0
57	MG	13	1668	1/1	0.89	0.86	-	96,96,96,96	0
57	MG	14	3059	1/1	0.97	0.26	-	70,70,70,70	0
57	MG	1H	3400	1/1	0.93	0.20	-	54,54,54,54	0
57	MG	14	3030	1/1	0.94	0.45	-	89,89,89,89	0
57	MG	1H	3239	1/1	0.90	0.52	-	92,92,92,92	0
57	MG	1H	3007	1/1	0.95	0.16	-	58,58,58,58	0
57	MG	14	3207	1/1	0.75	0.44	-	79,79,79,79	0
57	MG	1H	3105	1/1	0.88	0.44	-	79,79,79,79	0
57	MG	14	3084	1/1	0.95	0.31	-	87,87,87,87	0
57	MG	14	3196	1/1	0.90	0.27	-	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
57	MG	14	3043	1/1	0.93	0.39	-	83,83,83,83	0
57	MG	14	3028	1/1	0.93	0.32	-	61,61,61,61	0
57	MG	13	1749	1/1	0.92	0.11	-	110,110,110,110	0
57	MG	1H	3169	1/1	0.91	0.94	-	82,82,82,82	0
57	MG	14	3018	1/1	0.93	0.34	-	78,78,78,78	0
57	MG	14	3097	1/1	0.73	0.44	-	90,90,90,90	0
57	MG	13	1730	1/1	0.82	0.14	-	112,112,112,112	0
57	MG	14	3347	1/1	0.98	0.09	-	83,83,83,83	0
57	MG	13	1657	1/1	0.90	0.26	-	87,87,87,87	0
57	MG	1H	3148	1/1	0.90	0.22	-	80,80,80,80	0
57	MG	1H	3237	1/1	0.88	0.17	-	73,73,73,73	0
57	MG	14	3206	1/1	0.88	0.80	-	80,80,80,80	0
57	MG	1G	1691	1/1	0.94	0.08	-	114,114,114,114	0
57	MG	1H	3180	1/1	0.67	0.38	-	88,88,88,88	0
57	MG	1H	3484	1/1	0.71	0.08	-	103,103,103,103	0
57	MG	13	1608	1/1	0.91	0.13	-	71,71,71,71	0
57	MG	14	3107	1/1	0.92	0.24	-	65,65,65,65	0
57	MG	1H	3373	1/1	0.78	0.11	-	76,76,76,76	0
57	MG	14	3398	1/1	0.74	0.14	-	109,109,109,109	0
57	MG	1H	3432	1/1	0.93	0.09	-	60,60,60,60	0
57	MG	1H	3297	1/1	0.87	0.17	-	78,78,78,78	0
57	MG	16	210	1/1	0.95	0.06	-	78,78,78,78	0
57	MG	1H	3345	1/1	0.99	0.12	-	51,51,51,51	0
57	MG	14	3350	1/1	0.79	0.10	-	101,101,101,101	0
57	MG	14	3120	1/1	0.96	0.28	-	75,75,75,75	0
57	MG	13	1674	1/1	0.78	0.37	-	80,80,80,80	0
57	MG	1H	3053	1/1	0.92	0.78	-	66,66,66,66	0
57	MG	1H	3303	1/1	0.86	0.48	-	76,76,76,76	0
57	MG	14	3434	1/1	0.89	0.14	-	103,103,103,103	0
57	MG	1G	1613	1/1	0.97	0.35	-	83,83,83,83	0
57	MG	1G	1733	1/1	0.97	0.05	-	114,114,114,114	0
57	MG	14	3429	1/1	0.84	0.18	-	92,92,92,92	0
57	MG	1H	3455	1/1	0.97	0.13	-	48,48,48,48	0
57	MG	14	3262	1/1	0.93	0.12	-	55,55,55,55	0
57	MG	1H	3236	1/1	0.92	0.36	-	70,70,70,70	0
57	MG	13	1708	1/1	0.88	0.10	-	103,103,103,103	0
57	MG	13	1691	1/1	0.96	0.41	-	85,85,85,85	0
57	MG	14	3232	1/1	0.76	0.33	-	81,81,81,81	0
57	MG	14	3308	1/1	0.97	0.13	-	86,86,86,86	0
57	MG	1G	1715	1/1	0.46	0.19	-	99,99,99,99	0
57	MG	14	3345	1/1	0.82	0.08	-	87,87,87,87	0
57	MG	1H	3325	1/1	0.84	0.38	-	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
57	MG	13	1727	1/1	0.96	0.10	-	90,90,90,90	0
57	MG	13	1661	1/1	0.87	0.50	-	96,96,96,96	0
57	MG	14	3314	1/1	0.94	0.07	-	80,80,80,80	0
57	MG	1H	3495	1/1	0.90	0.09	-	98,98,98,98	0
57	MG	13	1622	1/1	0.92	0.35	-	74,74,74,74	0
57	MG	1G	1681	1/1	0.67	0.29	-	91,91,91,91	0
57	MG	1H	3117	1/1	0.77	0.37	-	54,54,54,54	0
57	MG	13	1662	1/1	0.93	0.20	-	92,92,92,92	0
57	MG	1H	3323	1/1	0.85	0.23	-	75,75,75,75	0
57	MG	14	3234	1/1	0.80	0.28	-	56,56,56,56	0
57	MG	13	1687	1/1	0.75	0.39	-	91,91,91,91	0
57	MG	14	3119	1/1	0.98	0.38	-	79,79,79,79	0
57	MG	13	1679	1/1	0.63	0.29	-	92,92,92,92	0
57	MG	14	3414	1/1	0.90	0.10	-	101,101,101,101	0
57	MG	1H	3516	1/1	0.52	0.16	-	98,98,98,98	0
57	MG	1H	3172	1/1	0.88	0.26	-	84,84,84,84	0
57	MG	1H	3493	1/1	0.95	0.07	-	83,83,83,83	0
57	MG	1H	3009	1/1	0.72	0.44	-	77,77,77,77	0
57	MG	13	1699	1/1	0.84	0.11	-	78,78,78,78	0
57	MG	1G	1693	1/1	0.79	0.09	-	105,105,105,105	0
57	MG	1H	3230	1/1	0.93	0.22	-	87,87,87,87	0
57	MG	68	202	1/1	0.93	0.22	-	83,83,83,83	0
57	MG	14	3130	1/1	0.92	0.39	-	70,70,70,70	0
57	MG	13	1706	1/1	0.93	0.10	-	77,77,77,77	0
57	MG	1H	3235	1/1	0.82	0.52	-	99,99,99,99	0
57	MG	1H	3111	1/1	0.83	0.50	-	73,73,73,73	0
57	MG	1H	3078	1/1	0.71	0.37	-	79,79,79,79	0
57	MG	1H	3015	1/1	0.94	0.40	-	65,65,65,65	0
57	MG	1H	3240	1/1	0.94	0.38	-	67,67,67,67	0
57	MG	13	1743	1/1	0.66	0.12	-	110,110,110,110	0
57	MG	1G	1722	1/1	0.87	0.07	-	107,107,107,107	0
57	MG	14	3246	1/1	0.74	0.22	-	58,58,58,58	0
57	MG	13	1736	1/1	0.83	0.07	-	100,100,100,100	0
57	MG	1H	3295	1/1	0.58	0.16	-	70,70,70,70	0
57	MG	1H	3224	1/1	0.87	0.45	-	90,90,90,90	0
57	MG	13	1700	1/1	0.98	0.04	-	94,94,94,94	0
57	MG	1G	1673	1/1	0.90	0.10	-	92,92,92,92	0
57	MG	14	3365	1/1	0.89	0.09	-	102,102,102,102	0
57	MG	1H	3241	1/1	0.89	0.13	-	64,64,64,64	0
57	MG	1H	3479	1/1	0.89	0.06	-	78,78,78,78	0
57	MG	1H	3473	1/1	0.95	0.16	-	62,62,62,62	0
57	MG	1H	3289	1/1	0.63	0.31	-	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
57	MG	14	3427	1/1	0.89	0.10	-	91,91,91,91	0
57	MG	1G	1603	1/1	0.96	0.26	-	79,79,79,79	0
57	MG	13	1748	1/1	0.78	0.12	-	119,119,119,119	0
57	MG	1H	3365	1/1	0.81	0.12	-	72,72,72,72	0
57	MG	14	3274	1/1	0.84	0.08	-	78,78,78,78	0
57	MG	14	3201	1/1	0.84	0.58	-	68,68,68,68	0
57	MG	14	3011	1/1	0.96	0.39	-	51,51,51,51	0
57	MG	13	1617	1/1	0.95	0.70	-	78,78,78,78	0
57	MG	14	3223	1/1	0.92	0.12	-	91,91,91,91	0
57	MG	13	1635	1/1	0.88	0.22	-	99,99,99,99	0
57	MG	14	3044	1/1	0.97	0.51	-	48,48,48,48	0
57	MG	1G	1644	1/1	0.75	0.37	-	107,107,107,107	0
57	MG	1J	203	1/1	0.93	0.23	-	91,91,91,91	0
57	MG	14	3192	1/1	0.75	0.31	-	82,82,82,82	0
57	MG	14	3369	1/1	0.85	0.08	-	99,99,99,99	0
57	MG	31	302	1/1	0.85	0.21	-	73,73,73,73	0
57	MG	1H	3232	1/1	0.64	0.50	-	85,85,85,85	0
57	MG	14	3440	1/1	0.31	0.12	-	101,101,101,101	0
57	MG	1H	3528	1/1	0.82	0.11	-	107,107,107,107	0
57	MG	1H	3369	1/1	0.94	0.20	-	59,59,59,59	0
57	MG	1H	3483	1/1	0.91	0.20	-	102,102,102,102	0
57	MG	14	3300	1/1	0.71	0.24	-	56,56,56,56	0
57	MG	1G	1700	1/1	0.93	0.08	-	93,93,93,93	0
57	MG	1H	3243	1/1	0.97	0.22	-	79,79,79,79	0
57	MG	1H	3544	1/1	0.93	0.10	-	70,70,70,70	0
57	MG	13	1701	1/1	0.84	0.09	-	102,102,102,102	0
57	MG	1G	1628	1/1	0.94	0.62	-	76,76,76,76	0
57	MG	1G	1713	1/1	0.14	0.13	-	142,142,142,142	0
57	MG	1G	1611	1/1	0.89	0.69	-	77,77,77,77	0
57	MG	1G	1726	1/1	0.86	0.11	-	113,113,113,113	0
57	MG	1H	3131	1/1	0.93	0.35	-	75,75,75,75	0
57	MG	1H	3001	1/1	0.95	0.30	-	61,61,61,61	0
57	MG	1G	1711	1/1	0.63	0.31	-	102,102,102,102	0
57	MG	14	3125	1/1	0.95	0.48	-	70,70,70,70	0
57	MG	13	1689	1/1	0.77	1.04	-	82,82,82,82	0
57	MG	14	3102	1/1	0.96	0.14	-	73,73,73,73	0
57	MG	1G	1723	1/1	0.83	0.12	-	101,101,101,101	0
57	MG	1H	3310	1/1	0.91	0.69	-	87,87,87,87	0
57	MG	1G	1701	1/1	0.60	0.11	-	109,109,109,109	0
57	MG	14	3348	1/1	0.91	0.07	-	92,92,92,92	0
57	MG	13	1648	1/1	0.96	0.17	-	77,77,77,77	0
57	MG	1H	3324	1/1	0.93	0.40	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1726	1/1	0.81	0.17	-	73,73,73,73	0
57	MG	1H	3203	1/1	0.88	0.36	-	74,74,74,74	0
57	MG	13	1667	1/1	0.95	0.14	-	78,78,78,78	0
57	MG	1H	3266	1/1	0.57	0.30	-	89,89,89,89	0
57	MG	13	1746	1/1	0.92	0.04	-	90,90,90,90	0
57	MG	1G	1642	1/1	0.95	0.23	-	82,82,82,82	0
57	MG	14	3363	1/1	0.97	0.04	-	80,80,80,80	0
57	MG	14	3065	1/1	0.97	0.36	-	60,60,60,60	0
57	MG	1H	3184	1/1	0.81	0.24	-	93,93,93,93	0
57	MG	13	1711	1/1	0.93	0.04	-	69,69,69,69	0
57	MG	1G	1694	1/1	0.88	0.06	-	84,84,84,84	0
57	MG	13	1731	1/1	0.97	0.07	-	73,73,73,73	0
57	MG	35	202	1/1	0.81	0.35	-	84,84,84,84	0
57	MG	1H	3315	1/1	0.81	0.36	-	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.