



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 02:27 AM GMT

PDB ID : 5EL4  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA<sup>Lys</sup> in the A-site with a U-U mismatch in the first position  
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.  
Deposited on : 2015-11-04  
Resolution : 3.15 Å(reported)

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

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

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

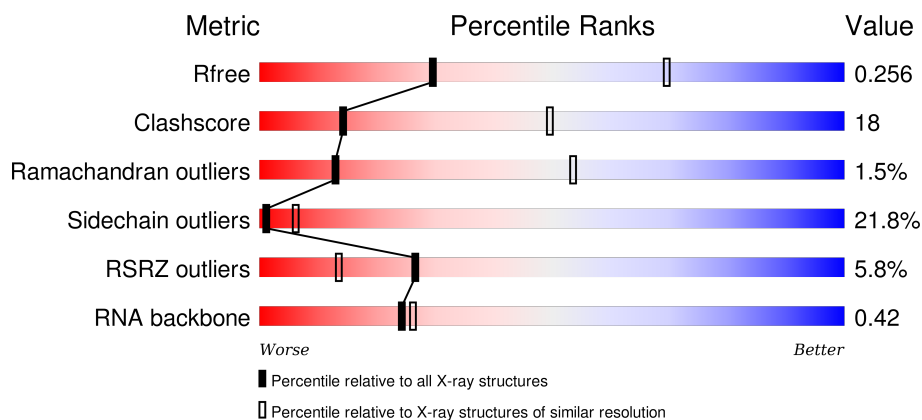
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

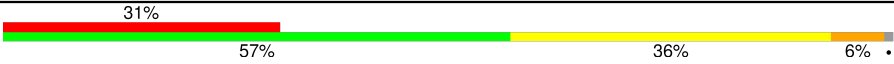


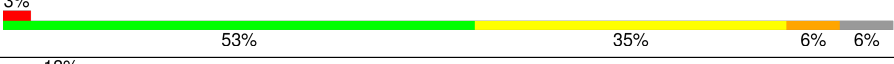
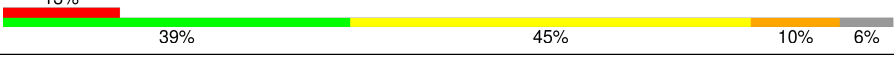
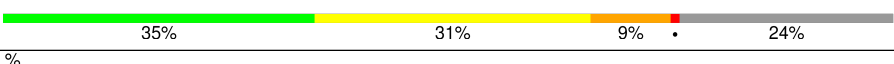
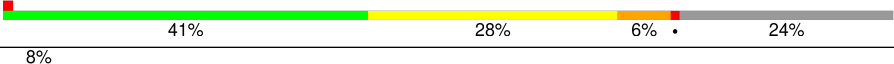
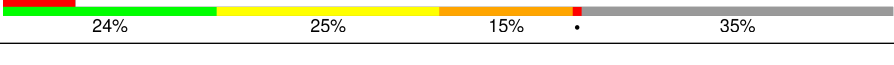
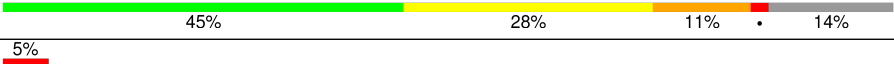


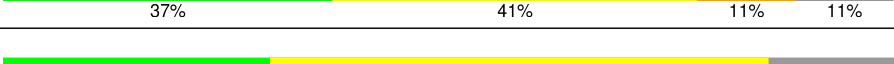
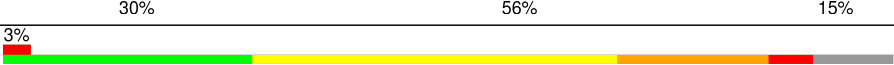
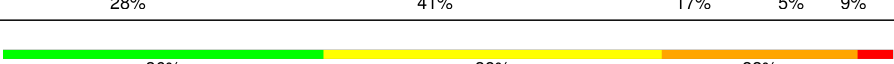
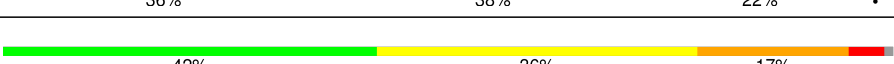
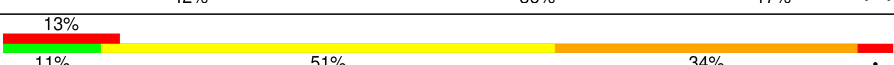

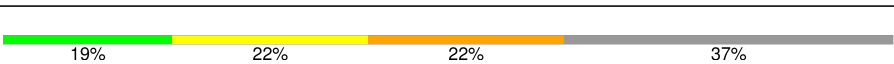
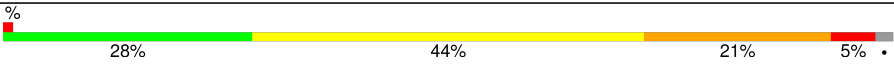


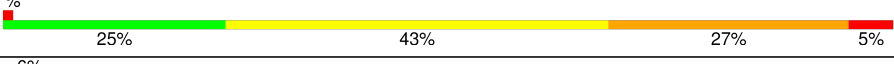
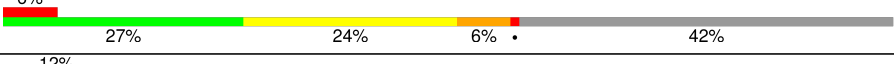


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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	
29	11	276	

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Mol	Chain	Length	Quality of chain
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	
41	75	146	
41	B8	146	

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Mol	Chain	Length	Quality of chain
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	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	

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Mol	Chain	Length	Quality of chain
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	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
58	MG	13	1604	-	-	-	X
58	MG	13	1608	-	-	-	X
58	MG	13	1613	-	-	-	X
58	MG	13	1621	-	-	-	X
58	MG	13	1622	-	-	-	X
58	MG	13	1638	-	-	-	X
58	MG	13	1639	-	-	-	X
58	MG	13	1645	-	-	-	X
58	MG	13	1646	-	-	-	X
58	MG	13	1654	-	-	-	X
58	MG	13	1655	-	-	-	X
58	MG	13	1664	-	-	-	X
58	MG	13	1672	-	-	-	X
58	MG	13	1677	-	-	-	X
58	MG	13	1686	-	-	-	X
58	MG	13	1694	-	-	-	X
58	MG	13	1697	-	-	-	X
58	MG	13	1699	-	-	-	X
58	MG	13	1741	-	-	-	X
58	MG	14	3003	-	-	-	X
58	MG	14	3004	-	-	-	X
58	MG	14	3006	-	-	-	X
58	MG	14	3007	-	-	-	X
58	MG	14	3009	-	-	-	X
58	MG	14	3015	-	-	-	X
58	MG	14	3016	-	-	-	X
58	MG	14	3024	-	-	-	X
58	MG	14	3029	-	-	-	X
58	MG	14	3030	-	-	-	X
58	MG	14	3035	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3037	-	-	-	X
58	MG	14	3038	-	-	-	X
58	MG	14	3049	-	-	-	X
58	MG	14	3050	-	-	-	X
58	MG	14	3054	-	-	-	X
58	MG	14	3056	-	-	-	X
58	MG	14	3057	-	-	-	X
58	MG	14	3063	-	-	-	X
58	MG	14	3067	-	-	-	X
58	MG	14	3073	-	-	-	X
58	MG	14	3074	-	-	-	X
58	MG	14	3075	-	-	-	X
58	MG	14	3078	-	-	-	X
58	MG	14	3079	-	-	-	X
58	MG	14	3083	-	-	-	X
58	MG	14	3085	-	-	-	X
58	MG	14	3095	-	-	-	X
58	MG	14	3097	-	-	-	X
58	MG	14	3099	-	-	-	X
58	MG	14	3117	-	-	-	X
58	MG	14	3123	-	-	-	X
58	MG	14	3143	-	-	-	X
58	MG	14	3149	-	-	-	X
58	MG	14	3157	-	-	-	X
58	MG	14	3158	-	-	-	X
58	MG	14	3160	-	-	-	X
58	MG	14	3164	-	-	-	X
58	MG	14	3165	-	-	-	X
58	MG	14	3176	-	-	-	X
58	MG	14	3177	-	-	-	X
58	MG	14	3178	-	-	-	X
58	MG	14	3179	-	-	-	X
58	MG	14	3185	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3190	-	-	-	X
58	MG	14	3192	-	-	-	X
58	MG	14	3193	-	-	-	X
58	MG	14	3194	-	-	-	X
58	MG	14	3198	-	-	-	X
58	MG	14	3205	-	-	-	X
58	MG	14	3206	-	-	-	X
58	MG	14	3212	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3213	-	-	-	X
58	MG	14	3215	-	-	-	X
58	MG	14	3216	-	-	-	X
58	MG	14	3224	-	-	-	X
58	MG	14	3233	-	-	-	X
58	MG	14	3242	-	-	-	X
58	MG	14	3249	-	-	-	X
58	MG	14	3252	-	-	-	X
58	MG	14	3253	-	-	-	X
58	MG	14	3255	-	-	-	X
58	MG	14	3258	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3277	-	-	-	X
58	MG	14	3287	-	-	-	X
58	MG	16	204	-	-	-	X
58	MG	16	205	-	-	-	X
58	MG	1G	1601	-	-	-	X
58	MG	1G	1602	-	-	-	X
58	MG	1G	1608	-	-	-	X
58	MG	1G	1614	-	-	-	X
58	MG	1G	1624	-	-	-	X
58	MG	1G	1626	-	-	-	X
58	MG	1G	1632	-	-	-	X
58	MG	1G	1644	-	-	-	X
58	MG	1G	1649	-	-	-	X
58	MG	1G	1653	-	-	-	X
58	MG	1G	1678	-	-	-	X
58	MG	1H	3001	-	-	-	X
58	MG	1H	3010	-	-	-	X
58	MG	1H	3012	-	-	-	X
58	MG	1H	3014	-	-	-	X
58	MG	1H	3016	-	-	-	X
58	MG	1H	3017	-	-	-	X
58	MG	1H	3019	-	-	-	X
58	MG	1H	3028	-	-	-	X
58	MG	1H	3029	-	-	-	X
58	MG	1H	3036	-	-	-	X
58	MG	1H	3042	-	-	-	X
58	MG	1H	3046	-	-	-	X
58	MG	1H	3051	-	-	-	X
58	MG	1H	3053	-	-	-	X
58	MG	1H	3054	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3061	-	-	-	X
58	MG	1H	3062	-	-	-	X
58	MG	1H	3065	-	-	-	X
58	MG	1H	3070	-	-	-	X
58	MG	1H	3071	-	-	-	X
58	MG	1H	3074	-	-	-	X
58	MG	1H	3079	-	-	-	X
58	MG	1H	3080	-	-	-	X
58	MG	1H	3082	-	-	-	X
58	MG	1H	3084	-	-	-	X
58	MG	1H	3085	-	-	-	X
58	MG	1H	3086	-	-	-	X
58	MG	1H	3088	-	-	-	X
58	MG	1H	3089	-	-	-	X
58	MG	1H	3094	-	-	-	X
58	MG	1H	3097	-	-	-	X
58	MG	1H	3099	-	-	-	X
58	MG	1H	3100	-	-	-	X
58	MG	1H	3115	-	-	-	X
58	MG	1H	3116	-	-	-	X
58	MG	1H	3124	-	-	-	X
58	MG	1H	3131	-	-	-	X
58	MG	1H	3134	-	-	-	X
58	MG	1H	3137	-	-	-	X
58	MG	1H	3142	-	-	-	X
58	MG	1H	3154	-	-	-	X
58	MG	1H	3155	-	-	-	X
58	MG	1H	3167	-	-	-	X
58	MG	1H	3168	-	-	-	X
58	MG	1H	3174	-	-	-	X
58	MG	1H	3179	-	-	-	X
58	MG	1H	3180	-	-	-	X
58	MG	1H	3186	-	-	-	X
58	MG	1H	3191	-	-	-	X
58	MG	1H	3195	-	-	-	X
58	MG	1H	3225	-	-	-	X
58	MG	1H	3226	-	-	-	X
58	MG	1H	3236	-	-	-	X
58	MG	1H	3237	-	-	-	X
58	MG	1H	3240	-	-	-	X
58	MG	1H	3243	-	-	-	X
58	MG	1H	3245	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3246	-	-	-	X
58	MG	1H	3253	-	-	-	X
58	MG	1H	3258	-	-	-	X
58	MG	1H	3260	-	-	-	X
58	MG	1H	3270	-	-	-	X
58	MG	1H	3273	-	-	-	X
58	MG	1H	3285	-	-	-	X
58	MG	1H	3291	-	-	-	X
58	MG	1H	3303	-	-	-	X
58	MG	1H	3309	-	-	-	X
58	MG	1H	3333	-	-	-	X
58	MG	1H	3343	-	-	-	X
58	MG	1H	3344	-	-	-	X
58	MG	1H	3347	-	-	-	X
58	MG	1H	3348	-	-	-	X
58	MG	1H	3443	-	-	-	X
58	MG	1H	3479	-	-	-	X
58	MG	1K	101	-	-	-	X
58	MG	29	302	-	-	-	X
58	MG	2K	101	-	-	-	X
58	MG	2L	101	-	-	-	X
58	MG	39	301	-	-	-	X
58	MG	5I	101	-	-	-	X
58	MG	N8	101	-	-	-	X

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 294304 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	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	insertion	GB 55771382
13	1543	C	-	insertion	GB 55771382
13	1544	U	-	insertion	GB 55771382
1G	1542	G	-	insertion	GB 55771382
1G	1543	C	-	insertion	GB 55771382
1G	1544	U	-	insertion	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	208	Total	C	N	O	S	0	0	0
			1711	1094	307	306	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	194	Total	C	N	O	S	0	0	0
			1529	967	296	265	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	147	Total	C	N	O	S	0	0	0
			1123	709	214	196	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	149	Total	C	N	O	S	0	0	0
			1214	754	244	210	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1005	637	197	171				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	124	Total	C	N	O	0	0	0
			983	624	190	169			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			
10	1A	78	Total	C	N	O		0	0	0
			626	388	126	112				

- 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	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	110	Total	C	N	O	S	0	0	0
			888	549	182	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			496	315	105	72	4			
14	5A	57	Total	C	N	O	S	0	0	0
			466	297	97	68	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			
15	6A	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	80	Total	C	N	O	S	0	0	0
			671	427	132	111	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	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	67	Total	C	N	O	0	0	0
			544	349	104	91			
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	80	Total	C	N	O	S	0	0	0
			643	411	118	112	2			
19	AA	60	Total	C	N	O	S	0	0	0
			471	300	83	86	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			
20	BA	98	Total	C	N	O	S	0	0	0
			757	467	161	127	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	24	Total	C	N	O		0	0	0
			208	128	50	30				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	295	528	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total 61028	C 27159	N 11418	O 19618	P 2833	0	0	0
26	14	2861	Total 61630	C 27429	N 11535	O 19806	P 2860	0	0	0

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 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total 1033	C 651	N 194	O 187	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
71	19	ILE	VAL	conflict	UNP Q5SLP7
71	27	HIS	ARG	conflict	UNP Q5SLP7

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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	205	Total	C	N	O	S	0	0	0
			1606	1024	300	280	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	180	Total	C	N	O	S	0	0	0
			1464	936	266	258	4			
32	49	180	Total	C	N	O	S	0	0	0
			1464	936	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	173	Total	C	N	O	S	0	0	0
			1327	842	249	235	1			
33	59	69	Total	C	N	O		0	0	0
			539	339	109	91				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- 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	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	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
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	134	Total	C	N	O	S	0	0	0
			1118	696	229	192	1			
41	75	136	Total	C	N	O	S	0	0	0
			1132	704	232	195	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	99	Total	C	N	O	S	0	0	0
			763	493	137	132	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	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	96	Total	C	N	O		0	0	0
			751	489	135	127				
45	B5	94	Total	C	N	O	S	0	0	0
			738	479	133	125	1			

- 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
			783	504	148	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	148	Total	C	N	O	S	0	0	0
			1222	781	221	217	3			
47	D5	126	Total	C	N	O	S	0	0	0
			1034	667	187	178	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	78	Total	C	N	O	S	0	0	0
			616	381	130	104	1			
48	E5	78	Total	C	N	O	S	0	0	0
			616	381	130	104	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
			571	355	115	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			573	355	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	S	0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O	S	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	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	49	Total	C	N	O	S	0	0	0
			381	238	76	62	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 tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	74	Total	C	N	O	P	0	0	0
			1570	702	271	523	74			

- Molecule 57 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	74	Total	C	N	O	P	0	0	0
			1571	703	277	518	73			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	45	3	Total	Mg	0	0
			3	3		
58	P8	1	Total	Mg	0	0
			1	1		
58	2I	1	Total	Mg	0	0
			1	1		
58	13	142	Total	Mg	0	0
			142	142		
58	1J	6	Total	Mg	0	0
			6	6		
58	5I	1	Total	Mg	0	0
			1	1		
58	16	11	Total	Mg	0	0
			11	11		
58	25	1	Total	Mg	0	0
			1	1		
58	21	2	Total	Mg	0	0
			2	2		
58	2K	2	Total	Mg	0	0
			2	2		
58	Q8	1	Total	Mg	0	0
			1	1		
58	4I	1	Total	Mg	0	0
			1	1		
58	3I	1	Total	Mg	0	0
			1	1		
58	I8	1	Total	Mg	0	0
			1	1		
58	1I	1	Total	Mg	0	0
			1	1		

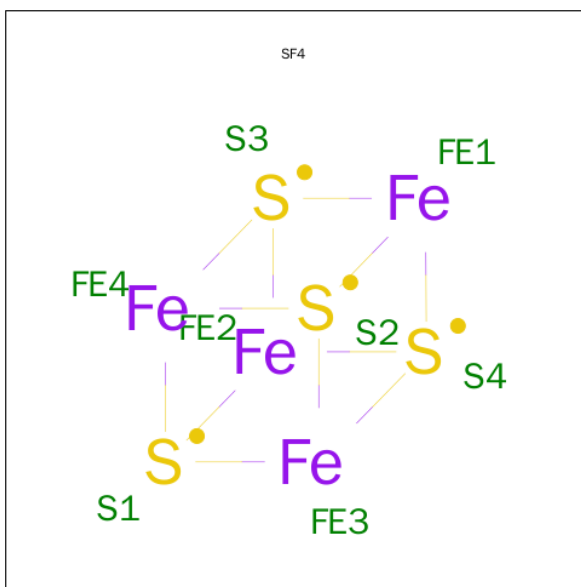
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	3	Total 3	Mg 3	0	0
58	78	1	Total 1	Mg 1	0	0
58	J8	1	Total 1	Mg 1	0	0
58	39	2	Total 2	Mg 2	0	0
58	1G	95	Total 95	Mg 95	0	0
58	11	1	Total 1	Mg 1	0	0
58	1H	495	Total 495	Mg 495	0	0
58	7I	1	Total 1	Mg 1	0	0
58	E5	1	Total 1	Mg 1	0	0
58	88	3	Total 3	Mg 3	0	0
58	N8	1	Total 1	Mg 1	0	0
58	14	421	Total 421	Mg 421	0	0
58	19	1	Total 1	Mg 1	0	0
58	3L	1	Total 1	Mg 1	0	0
58	4K	1	Total 1	Mg 1	0	0
58	1K	1	Total 1	Mg 1	0	0
58	41	1	Total 1	Mg 1	0	0
58	2L	2	Total 2	Mg 2	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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	207	Total	O	0	0
			207	207		
61	3E	2	Total	O	0	0
			2	2		
61	4E	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	8E	1	Total 1	O 1	0	0
61	1I	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	6I	1	Total 1	O 1	0	0
61	4K	4	Total 4	O 4	0	0
61	1H	819	Total 819	O 819	0	0
61	16	22	Total 22	O 22	0	0
61	11	9	Total 9	O 9	0	0
61	21	6	Total 6	O 6	0	0
61	31	4	Total 4	O 4	0	0
61	78	1	Total 1	O 1	0	0
61	B8	1	Total 1	O 1	0	0
61	C8	3	Total 3	O 3	0	0
61	F8	1	Total 1	O 1	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	2	Total 2	O 2	0	0
61	L8	3	Total 3	O 3	0	0
61	1G	117	Total 117	O 117	0	0
61	32	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0

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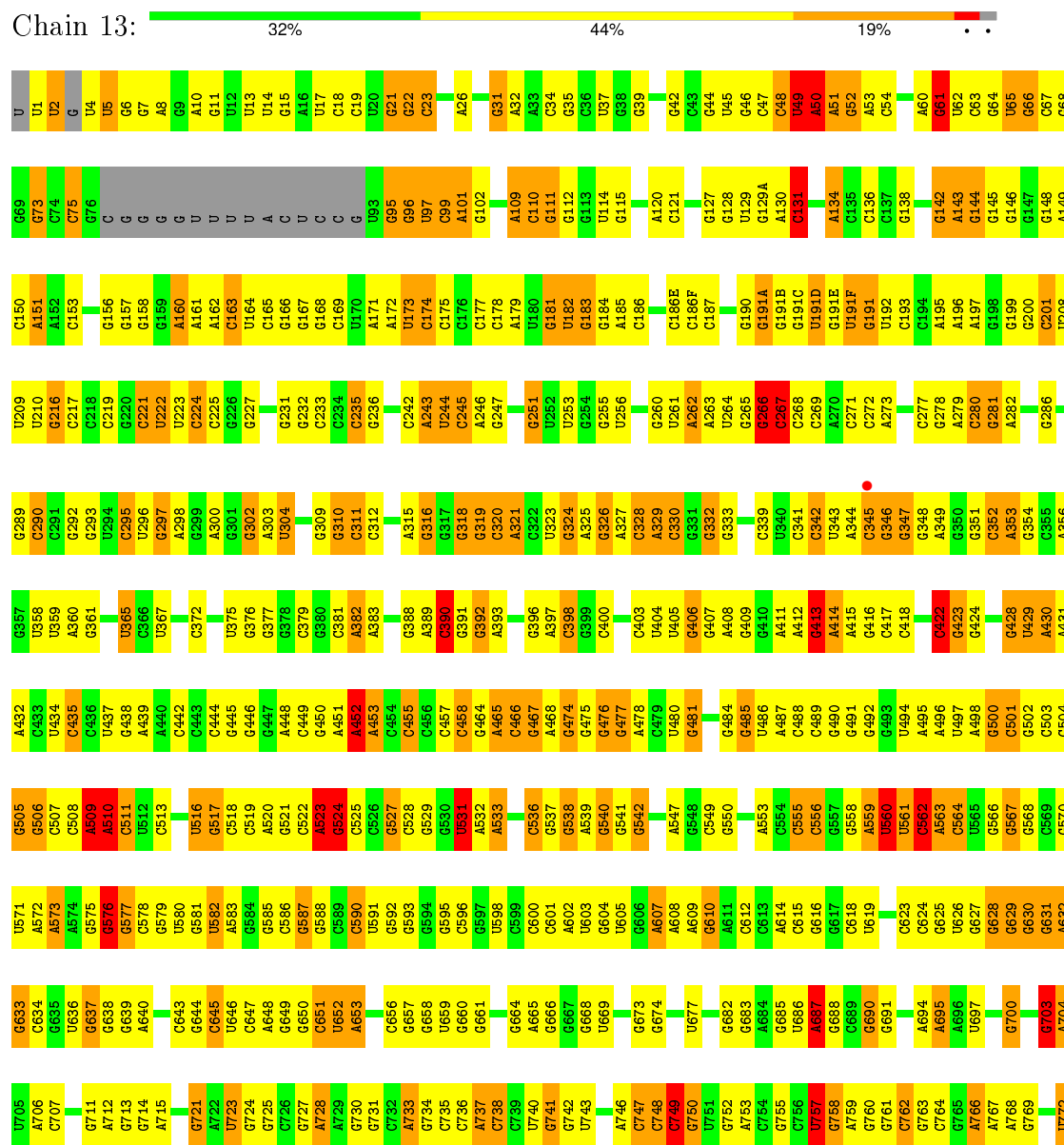
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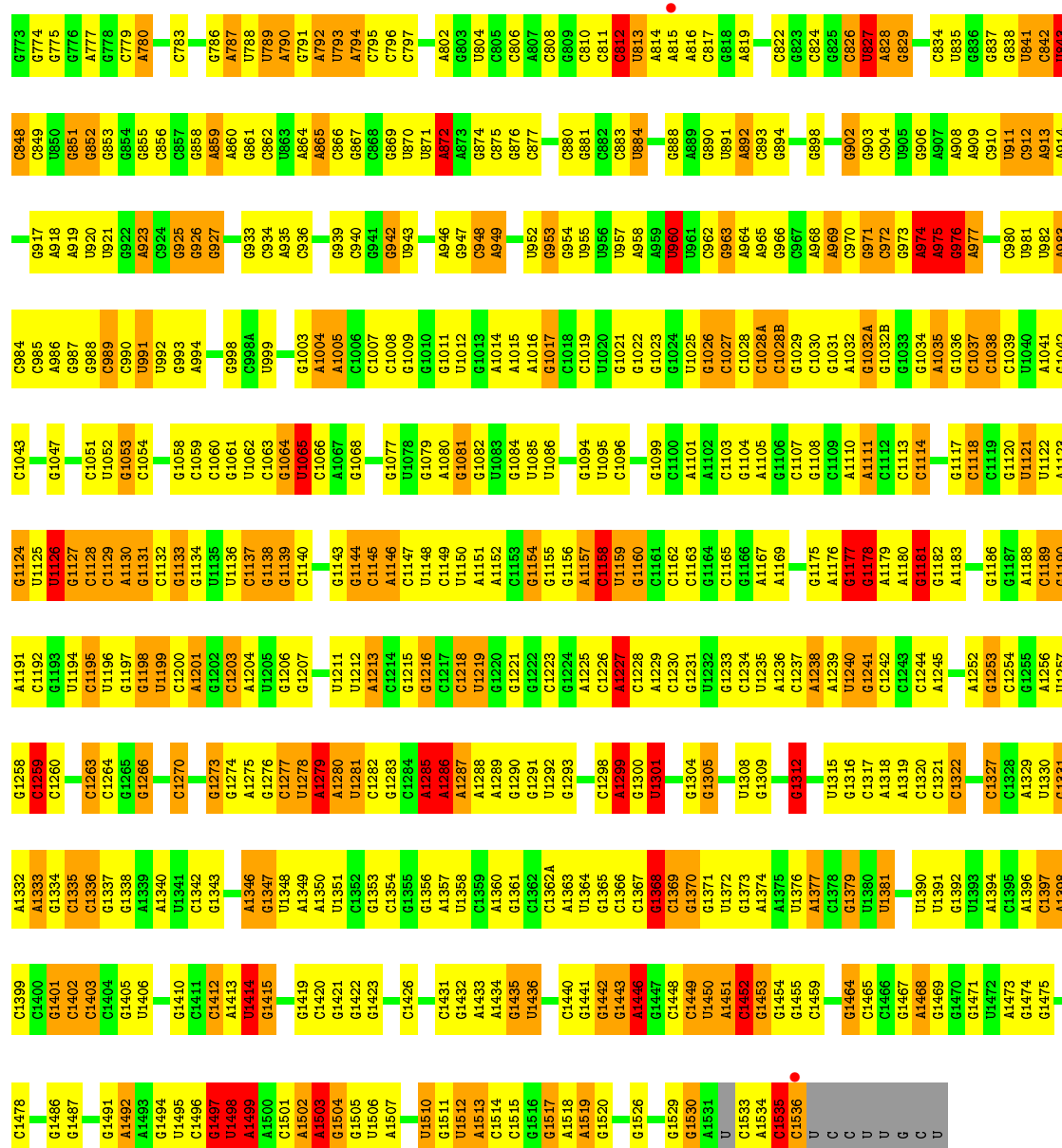
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	6A	2	Total 2	O 2	0	0
61	7A	1	Total 1	O 1	0	0
61	BA	1	Total 1	O 1	0	0
61	14	717	Total 717	O 717	0	0
61	1J	6	Total 6	O 6	0	0
61	19	10	Total 10	O 10	0	0
61	29	3	Total 3	O 3	0	0
61	39	3	Total 3	O 3	0	0
61	15	1	Total 1	O 1	0	0
61	35	3	Total 3	O 3	0	0
61	75	2	Total 2	O 2	0	0
61	85	3	Total 3	O 3	0	0
61	M5	3	Total 3	O 3	0	0

### 3 Residue-property plots

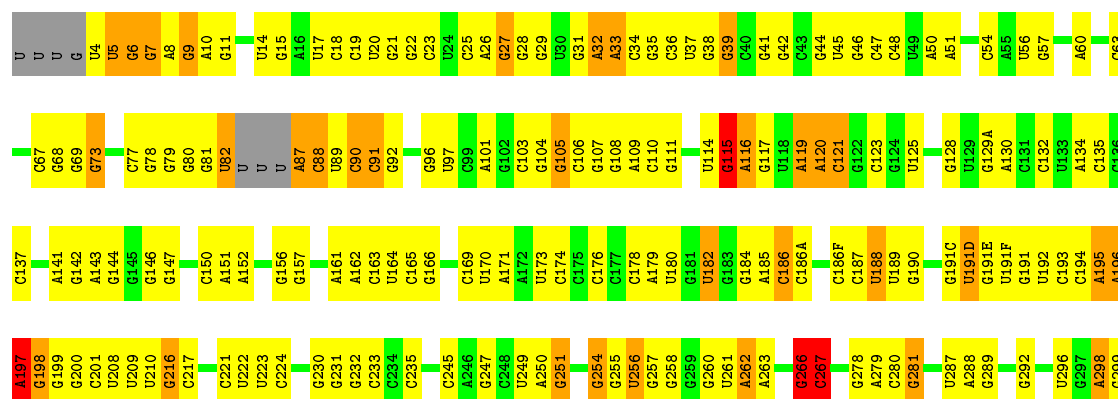
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

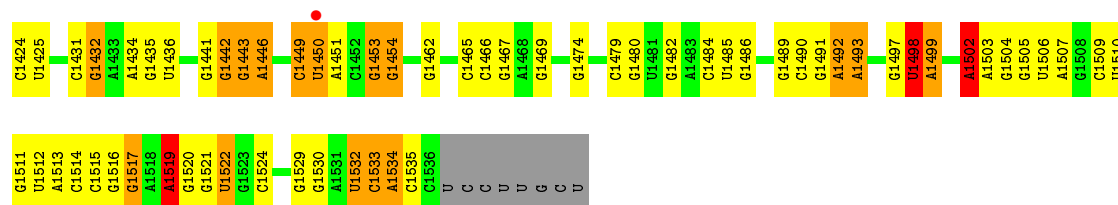




Chain 1G: 33% 47% 18%

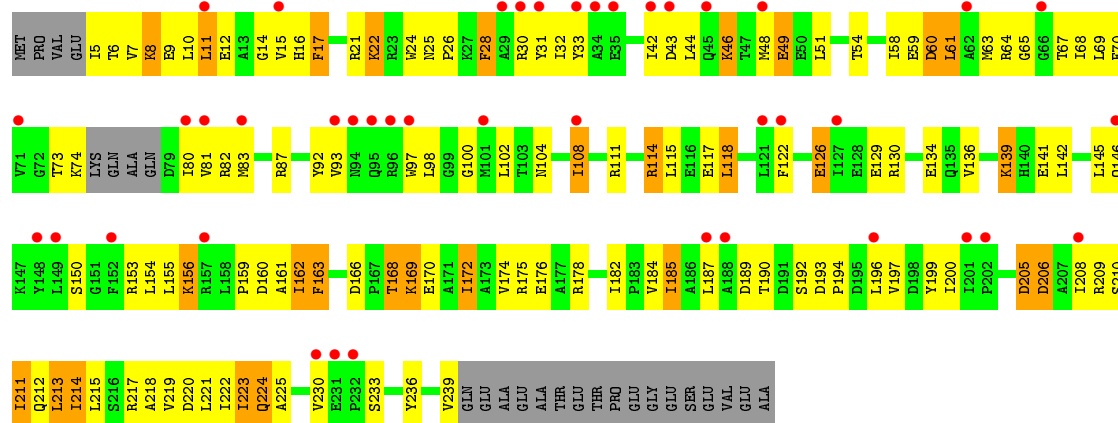


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G1353	G1291	A1227	G1160	C1097	G1029	C967	G894	U813	A741	G661	G584	C518	C443	A373	G301
C1354	U1292	C1228	C1355	C1098	C1030	A988	G895	A814	G741	G662	C586	C519	C444	A374	G302
G1355	G1293	A1229	C1165	G1099	G1031	A989	C896	A815	C745	A665	C587	C522	G446	U375	G305
G1356	G1294	G1230	A1166	C1100	A1032	G971	C897	A816	C746	G666	G588	A523	G447	G377	G308
A1357	G1295	G1231	A1167	A1101	G1032A	C972	A900	C817	A746	G667	G589	C526	A448	A382	G309
C1296	C1296	C1234	A1169	A1102	G1032B	C973	G906	C818	C747	U672	U591	G527	C449	A383	G310
C1297	G1297	U1235	G1171	G1104	G1034	A974	G906	U820	C748	G673	G592	C528	A452	A386	C311
A1360	C1298	U1235	C1172	A1105	A1035	A975	G906	C822	C749	G674	G593	C529	A453	C386	C312
C1362A	A1299	A1238	C1176	G1107	G1037	A977	A909	C826	U751	A675	C596	U531	C455	U387	A313
A1363	U1301	A1239	A1176	C1108	C1038	A978	G911	U827	A753	U677	C599	A532	C456	C390	A316
U1364	U1240	U1240	G1177	G1108	C1039	C979	C912	U827	C754	U678	C600	A533	C457	G391	G317
G1365	G1241	G1241	G1178	C1109	C1039	C980	A913	G829	C755	C679	C601	U534	C458	G392	G318
C1366	C1242	C1242	A1179	A1110	U1040	U981	A914	U829	C756	C680	A602	A535	G465	A393	G319
C1367	G1304	C1243	A1180	A1111	A1041	U982	G915	G836	C757	C681	U603	C536	G464	G394	G320
G1368	G1368	A1244	G1181	C1112	G1042	A983	G916	G837	U757	G682	G604	G537	G467	C395	C321
G1369	U1307	C1245	A1182	C1113	C1043	C984	G917	G837	C758	G683	U605	G538	G467	G396	A321
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U1376	G1253	G1254	A1188	U1123	U1052	C990	A923	C849	C769	G689	C613	C546	G481	U405	A329
A1377	G1255	G1255	G1189	G1124	G1053	U991	C924	U850	G769	G690	A614	A547	G481	G406	C330
C1378	C1256	A1256	A1191	U1125	C1054	U992	G925	G851	U772	G691	G615	C555	G489	A413	G340
G1379	C1192	U1257	C1192	U1126	A1055	G993	G926	G852	G773	G692	C615	C556	G490	A414	C341
C1382	G1193	G1193	G1193	G1127	U1056	C995	G927	G853	G774	G693	G616	C557	G491	A415	C342
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G1392	G1202	G1265	G1134	U1065	U1065	G1003	A938	C862	C784	C707	C622	C557	G496	A415	C342
C1326	C1203	C1266	U1135	C1066	C1066	A1004	G939	U863	G785	C708	C623	C558	G497	G416	G342
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C1328	U1205	A1268	C1137	A1067	G1068	C1006	G941	A865	C787	A712	C625	U560	G499	U421	C345
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C1332	U1207	G1271	C1140	U1070	U1070	C1008	U943	U870	U789	G714	C629	C563	A497	G423	G351
C1333	C1208	G1272	C1141	G1071	C1071	G1009	U943	U871	A790	A715	G630	C564	U497	G424	G352
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C1343	U1216	U1281	G1216	G1081	G1081	U1020	U957	C882	U801	G725	C647	A573	A504	A432	G361
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U1345	G1218	G1282	A1151	U1083	U1083	G1022	A959	C884	G803	C727	A649	C577	A506	C433	A363
C1346	U1219	G1283	A1152	U1084	U1084	G1023	U960	U884	U804	G731	C651	C578	A507	U434	A364
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U1348	G1222	A1286	G1155	U1090	U1090	G1026	G963	G887	A807	G734	A654	U580	A510	G438	U367
C1349	G1223	A1287	A1156	U1091	U1091	C1027	A964	G890	C808	C735	C656	C581	A511	A439	C368
C1400	C1224	A1288	G1157	G1094	G1094	C1028	A965	U891	C809	G736	C657	U582	A512	A440	G371
C1402	C1336	G1275	G1158	U1095	U1095	C1028A	A965	A892	G800	G724	U646	A572	A503	A431	A360
U1406	U1406	U1278	A1339	C1342	C1342	U1020	U957	C882	U801	G725	C647	A573	A504	A432	G361
C1411	C1343	U1281	G1216	U1150	U1082	G1021	A958	C883	A802	C726	A648	G576	A505	C432	G362
C1412	U1344	C1282	C1218	A1151	U1083	G1022	A959	C884	G803	C727	A649	C577	A506	U434	A363
C1413	G1345	G1283	U1219	A1152	U1084	G1023	U960	U884	U804	G731	C651	C578	A507	U437	C366
C1414	C1346	C1284	G1220	C1153	U1085	U1024	U961	G885	C805	C732	U652	C579	A508	G438	U367
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C1416	U1348	A1286	G1222	G1155	U1090	G1026	G963	G887	A807	G734	A654	U580	A510	A440	G371
C1417	C1349	A1287	A1156	U1091	U1091	C1027	A964	U891	C808	C735	C656	C581	A511	A440	G371
C1418	C1350	C1224	G1157	G1094	G1094	C1028	A965	A892	G800	G724	U646	A572	A503	A431	A360
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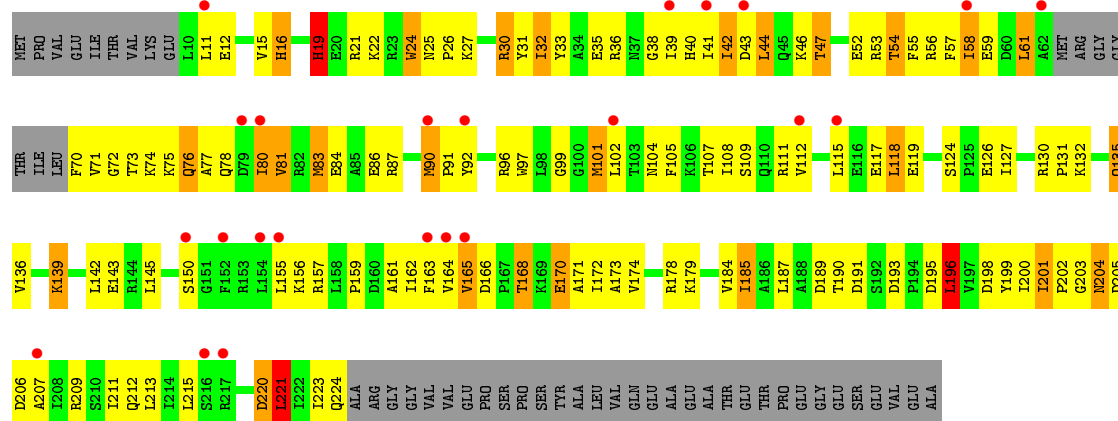
• Molecule 2: 30S ribosomal protein S2

Chain 1E: 16% 41% 39% 11% 10%



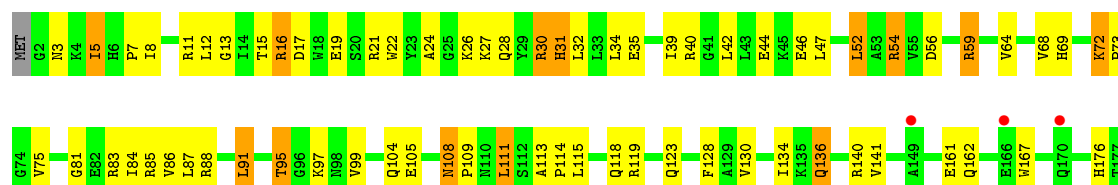
• Molecule 2: 30S ribosomal protein S2

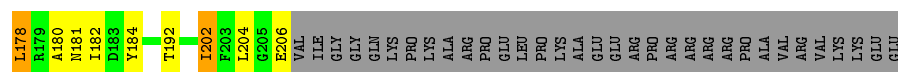
Chain 12: 9% 31% 39% 10% 19%



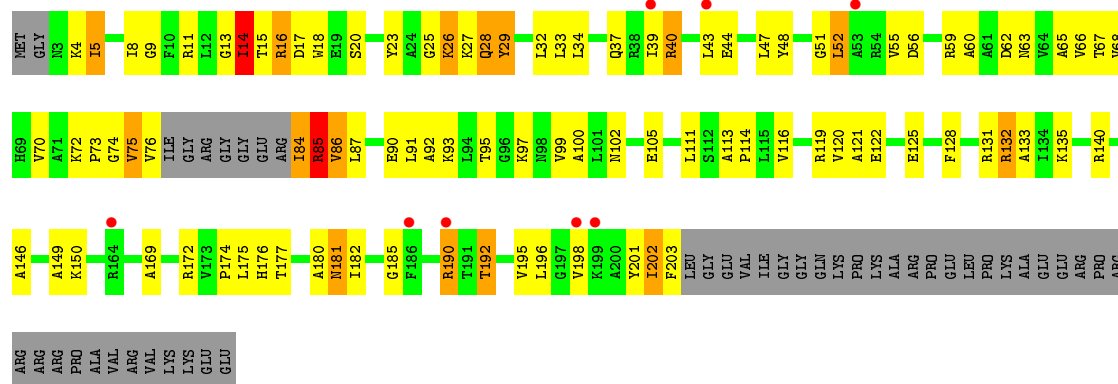
• Molecule 3: 30S ribosomal protein S3

Chain 2E: % 53% 27% 6% 14%

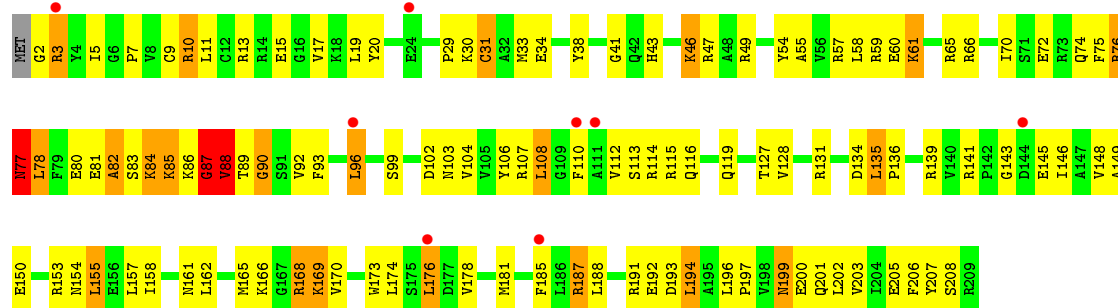
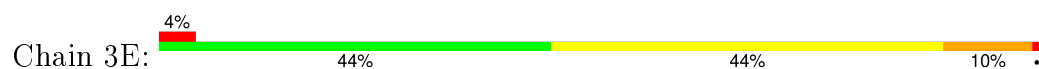




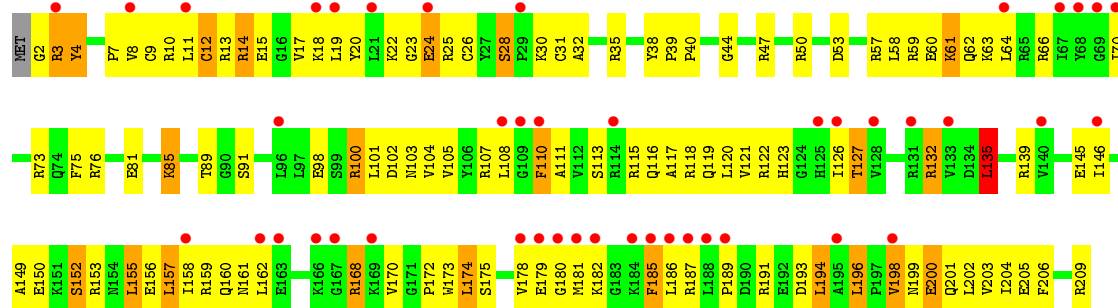
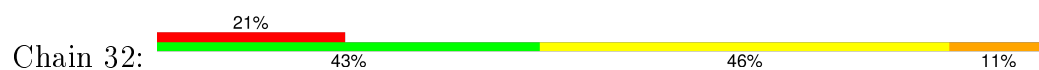
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



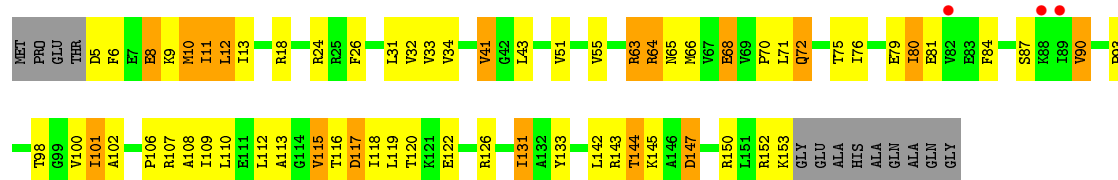
• Molecule 4: 30S ribosomal protein S4



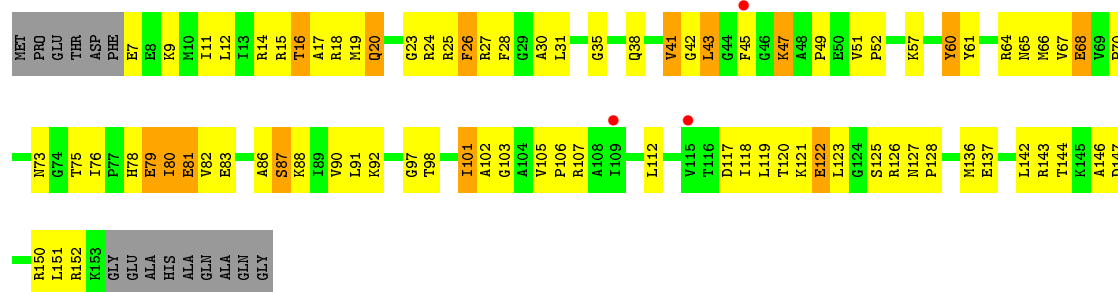
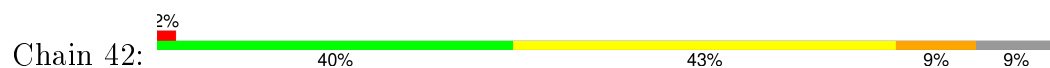
• Molecule 5: 30S ribosomal protein S5







• Molecule 5: 30S ribosomal protein S5



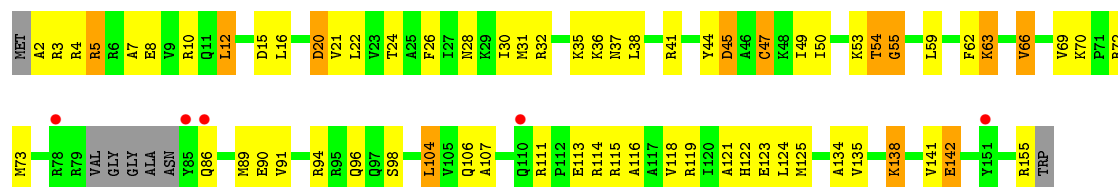
• Molecule 6: 30S ribosomal protein S6



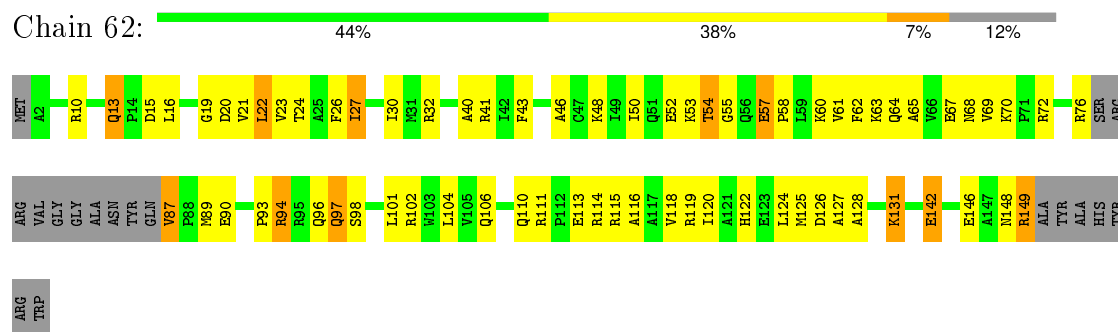
• Molecule 6: 30S ribosomal protein S6



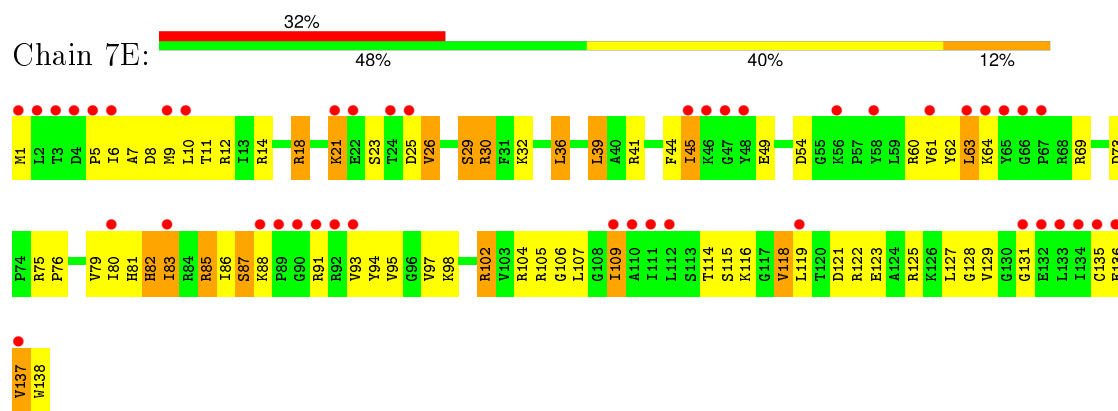
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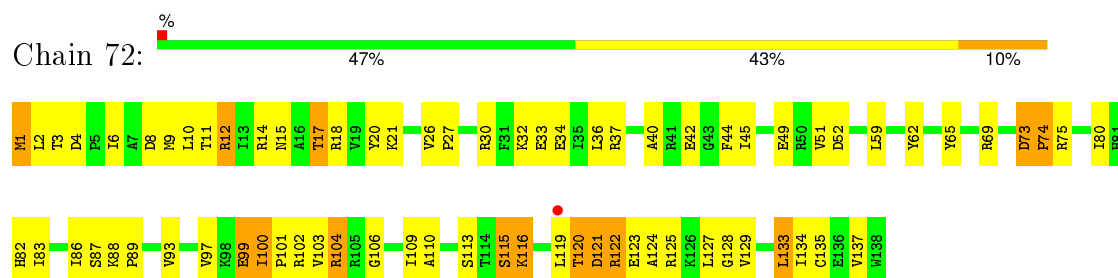
- Molecule 7: 30S ribosomal protein S7



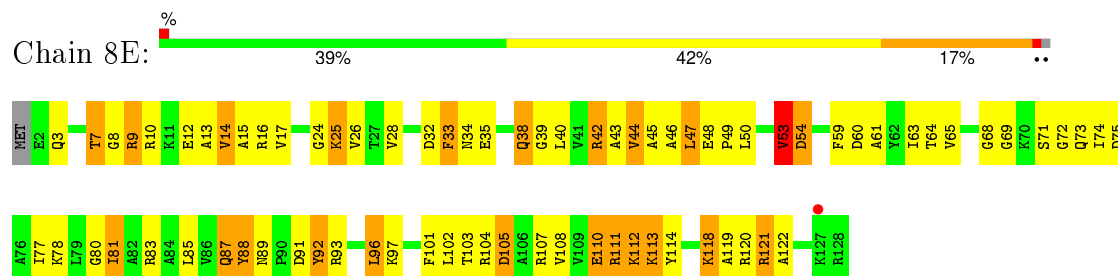
- Molecule 8: 30S ribosomal protein S8



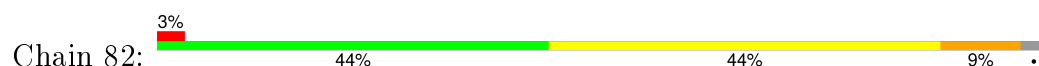
- Molecule 8: 30S ribosomal protein S8

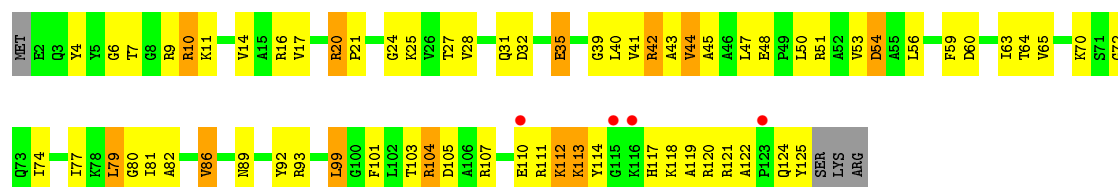


- Molecule 9: 30S ribosomal protein S9

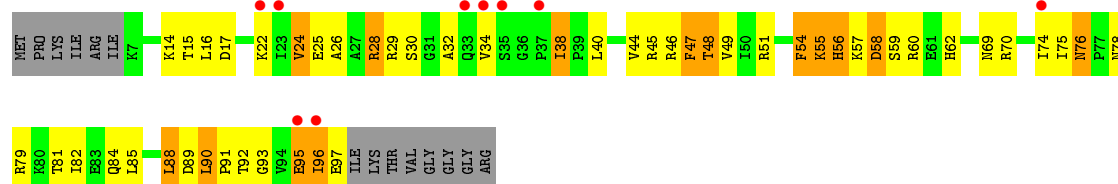
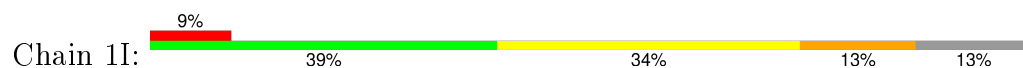


- Molecule 9: 30S ribosomal protein S9

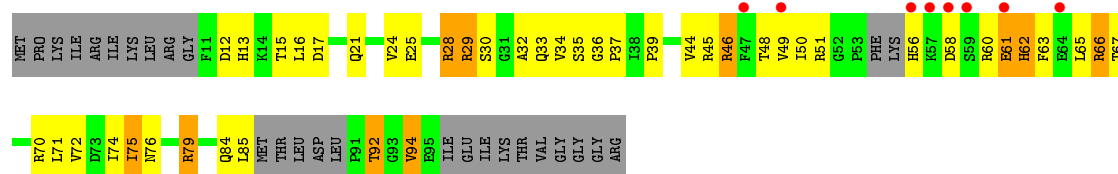




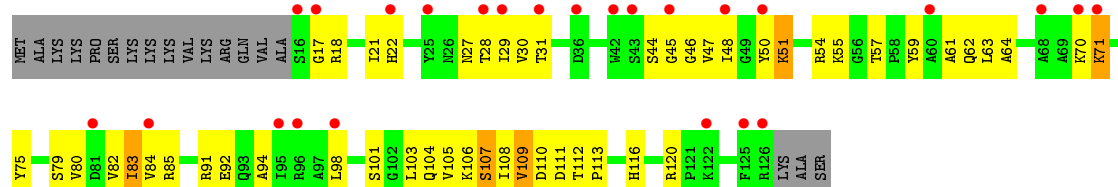
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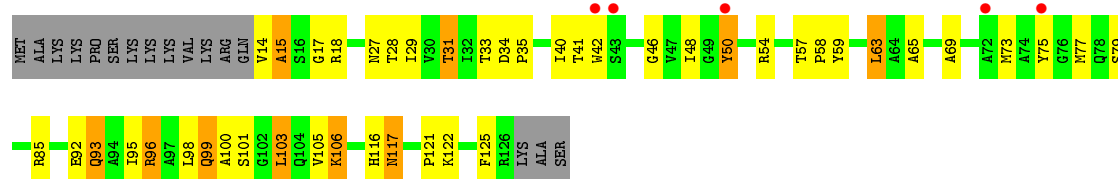
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

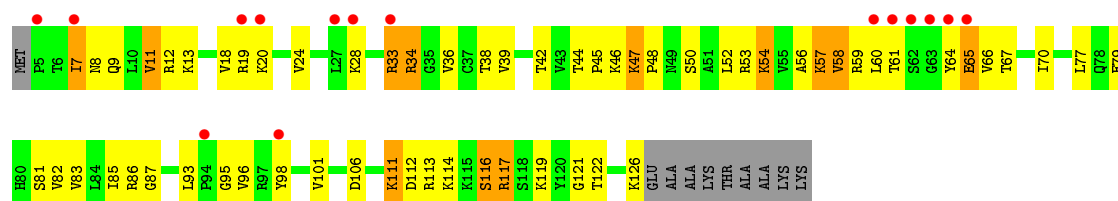


• Molecule 11: 30S ribosomal protein S11

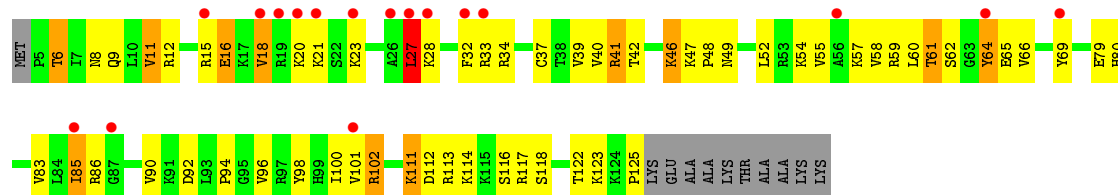


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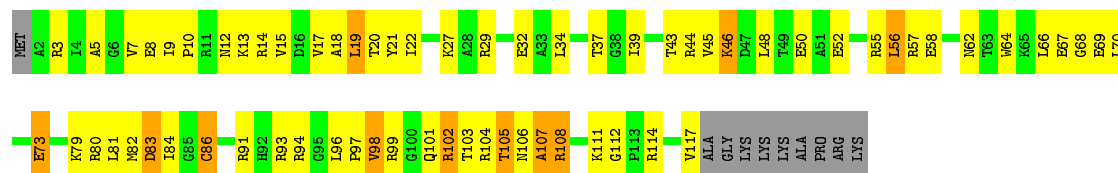




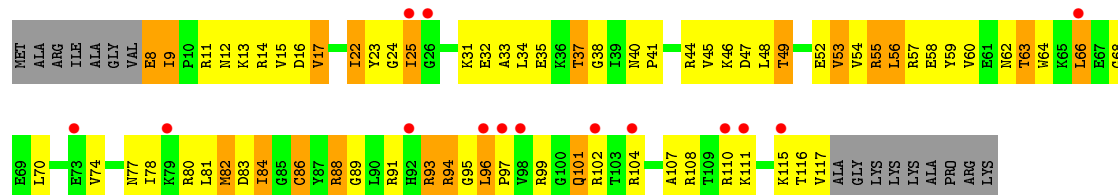
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



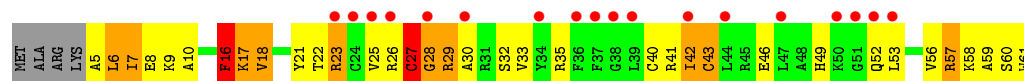
• Molecule 13: 30S ribosomal protein S13



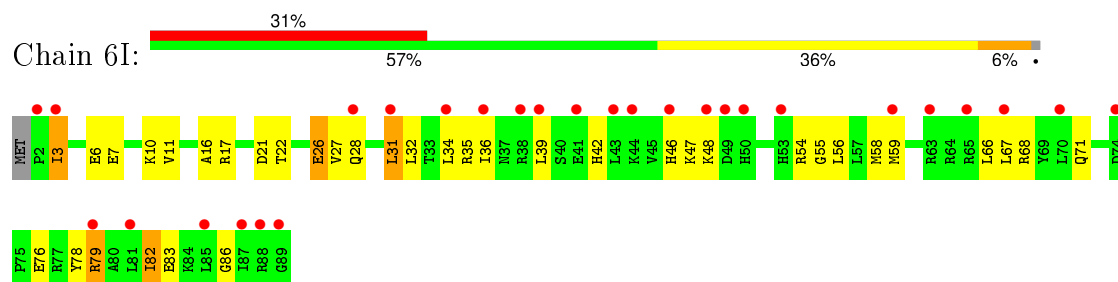
• Molecule 14: 30S ribosomal protein S14 type Z



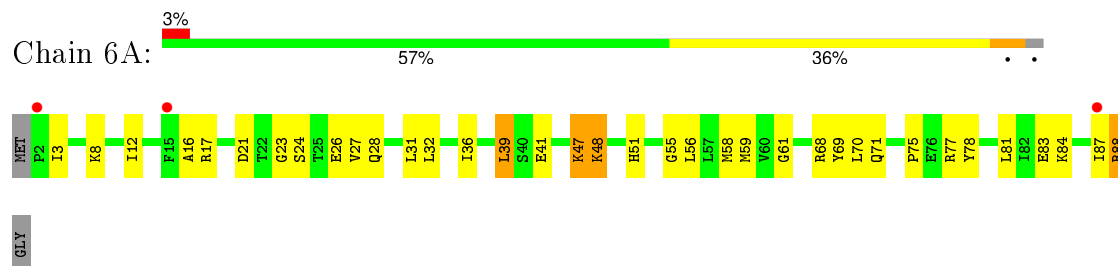
• Molecule 14: 30S ribosomal protein S14 type Z



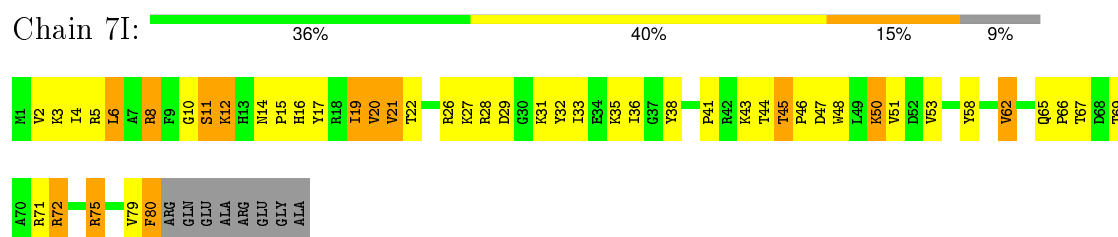
- Molecule 15: 30S ribosomal protein S15



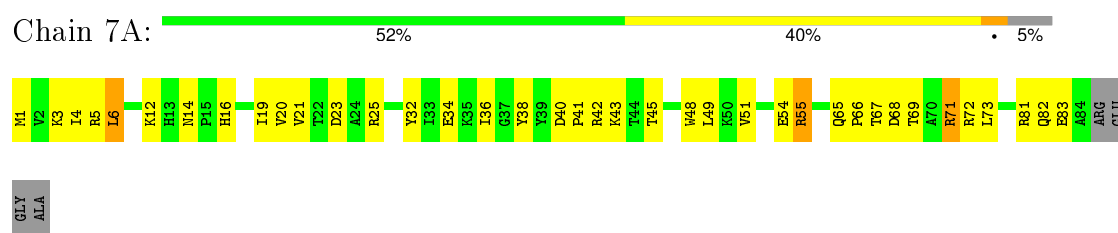
- Molecule 15: 30S ribosomal protein S15



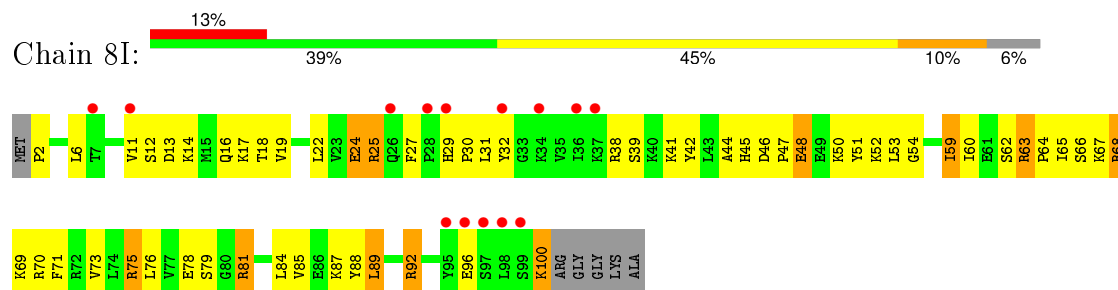
- Molecule 16: 30S ribosomal protein S16



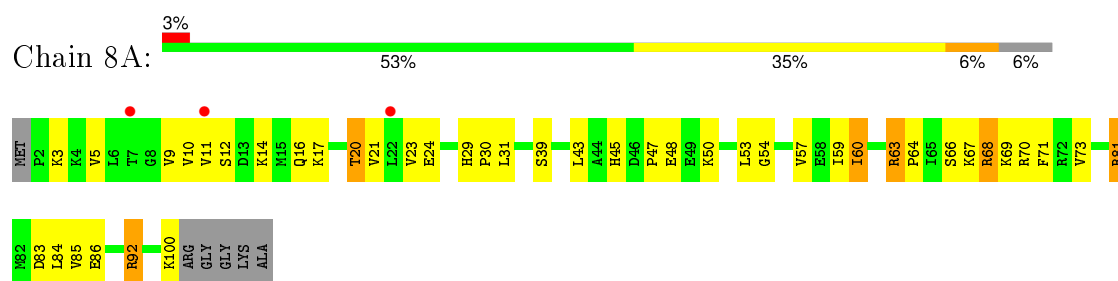
- Molecule 16: 30S ribosomal protein S16



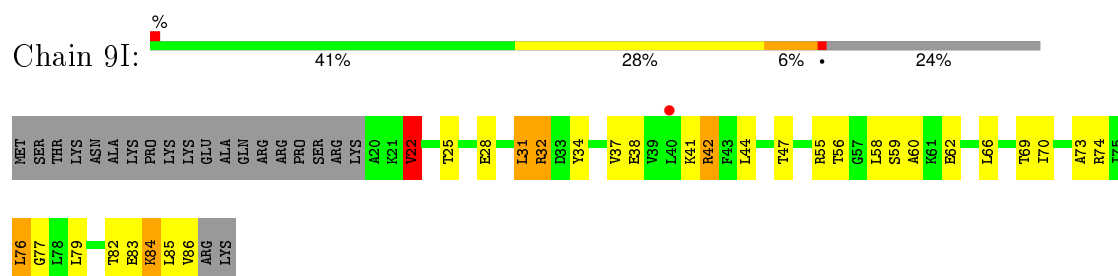
- Molecule 17: 30S ribosomal protein S17



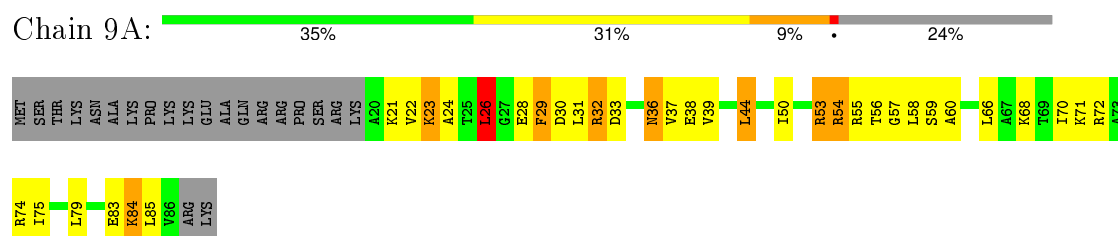
- Molecule 17: 30S ribosomal protein S17



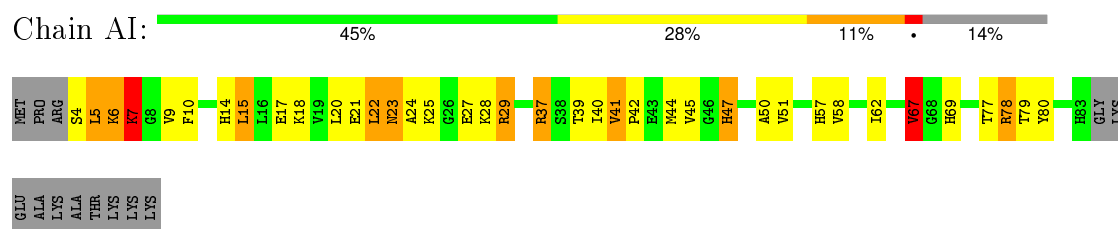
- Molecule 18: 30S ribosomal protein S18



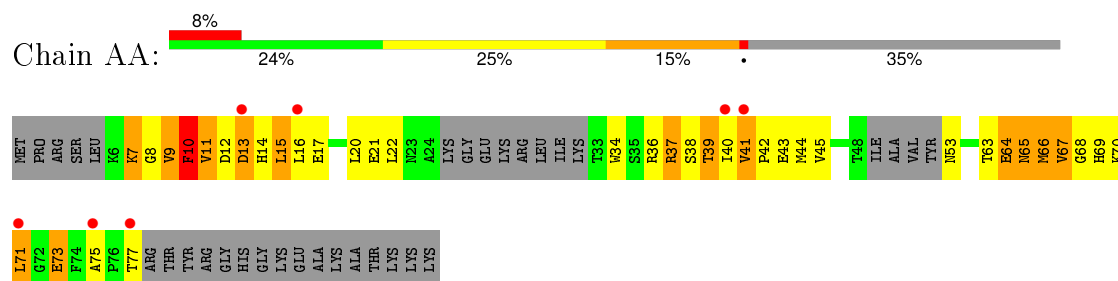
- Molecule 18: 30S ribosomal protein S18



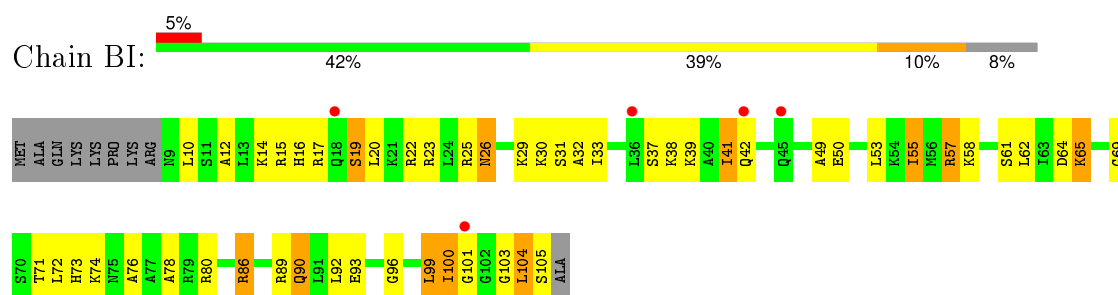
- Molecule 19: 30S ribosomal protein S19



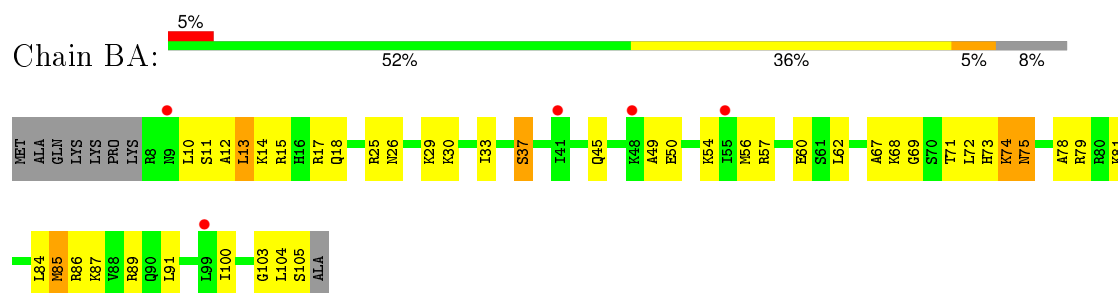
- Molecule 19: 30S ribosomal protein S19



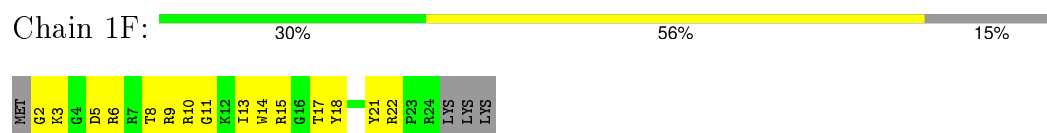
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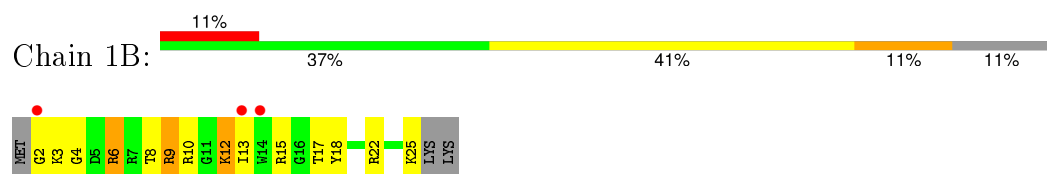
- Molecule 20: 30S ribosomal protein S20



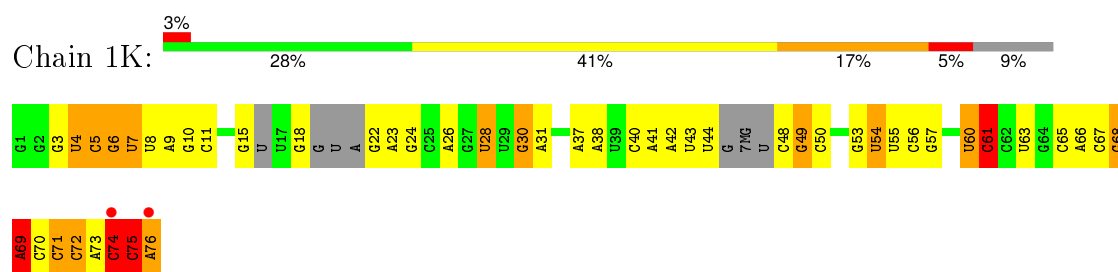
- Molecule 21: 30S ribosomal protein Thx



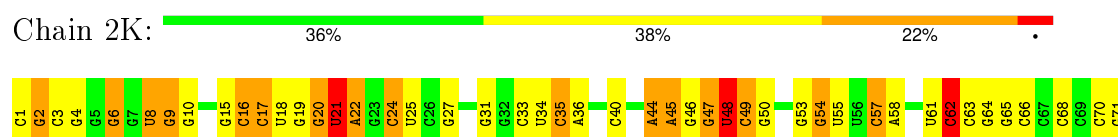
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA-Lys



- Molecule 23: tRNA-fMet





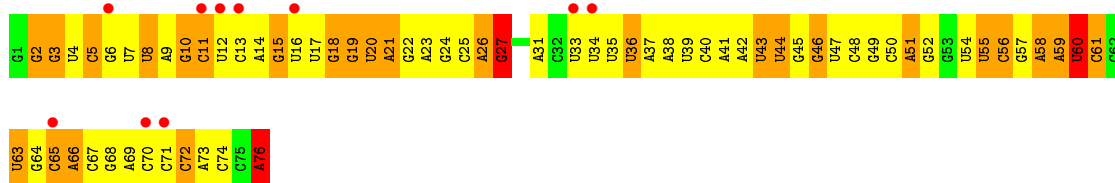
- Molecule 23: tRNA-fMet

Chain 2L: 42% 36% 17% . .



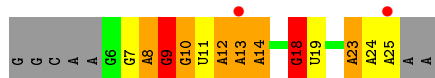
- Molecule 24: tRNA-Lys

Chain 3K: 13% 11% 51% 34% .



- Molecule 25: mRNA

Chain 4K: 7% 26% 19% 22% 7% 26%



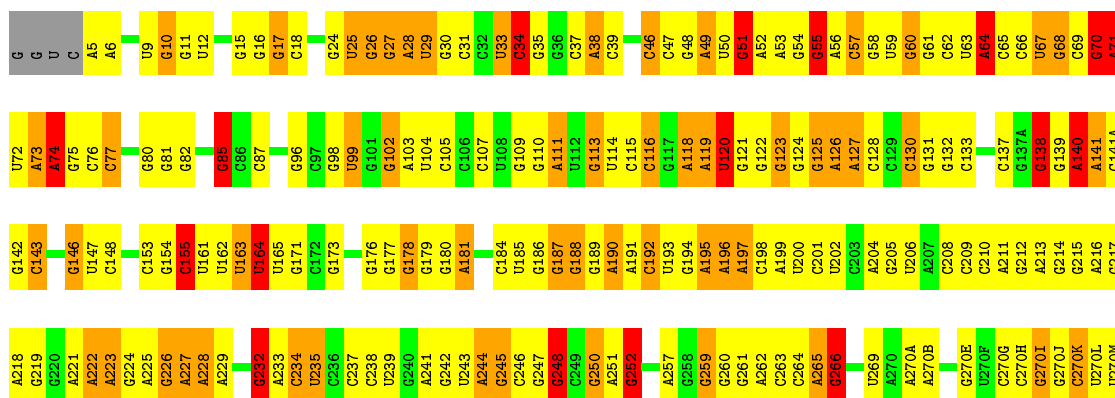
- Molecule 25: mRNA

Chain 4L: 19% 22% 22% 37%



- Molecule 26: 23S ribosomal RNA

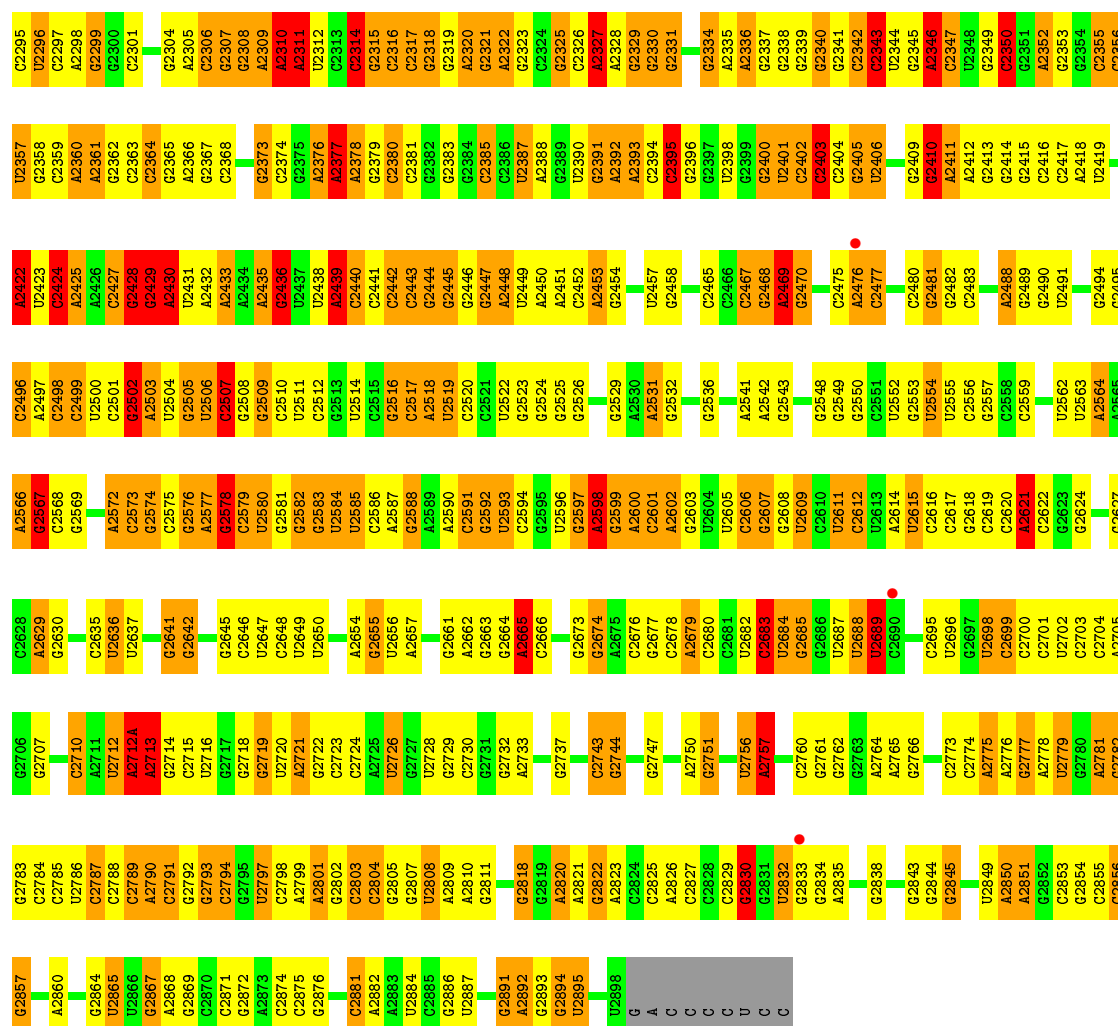
Chain 1H: 25% 40% 25% 6% .



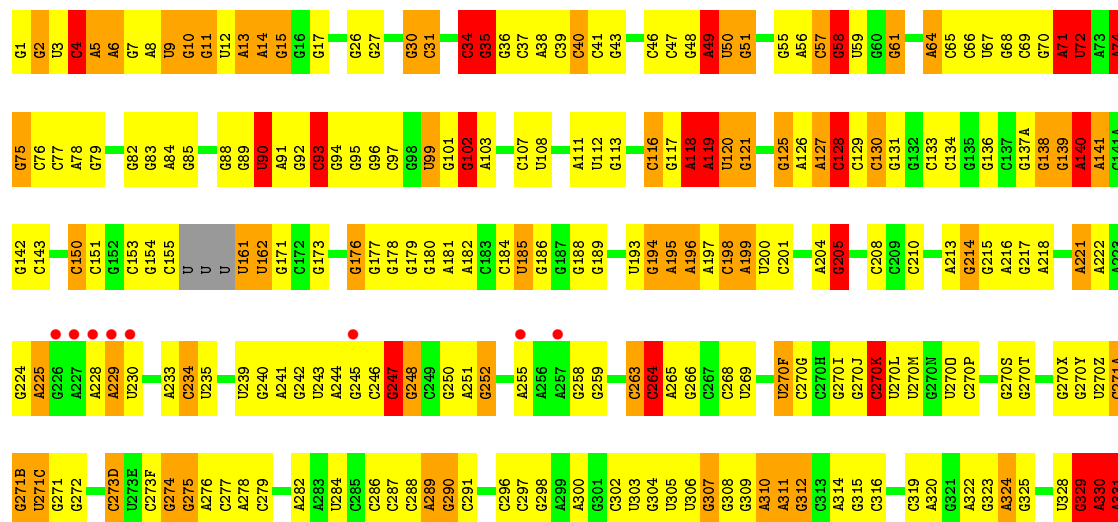






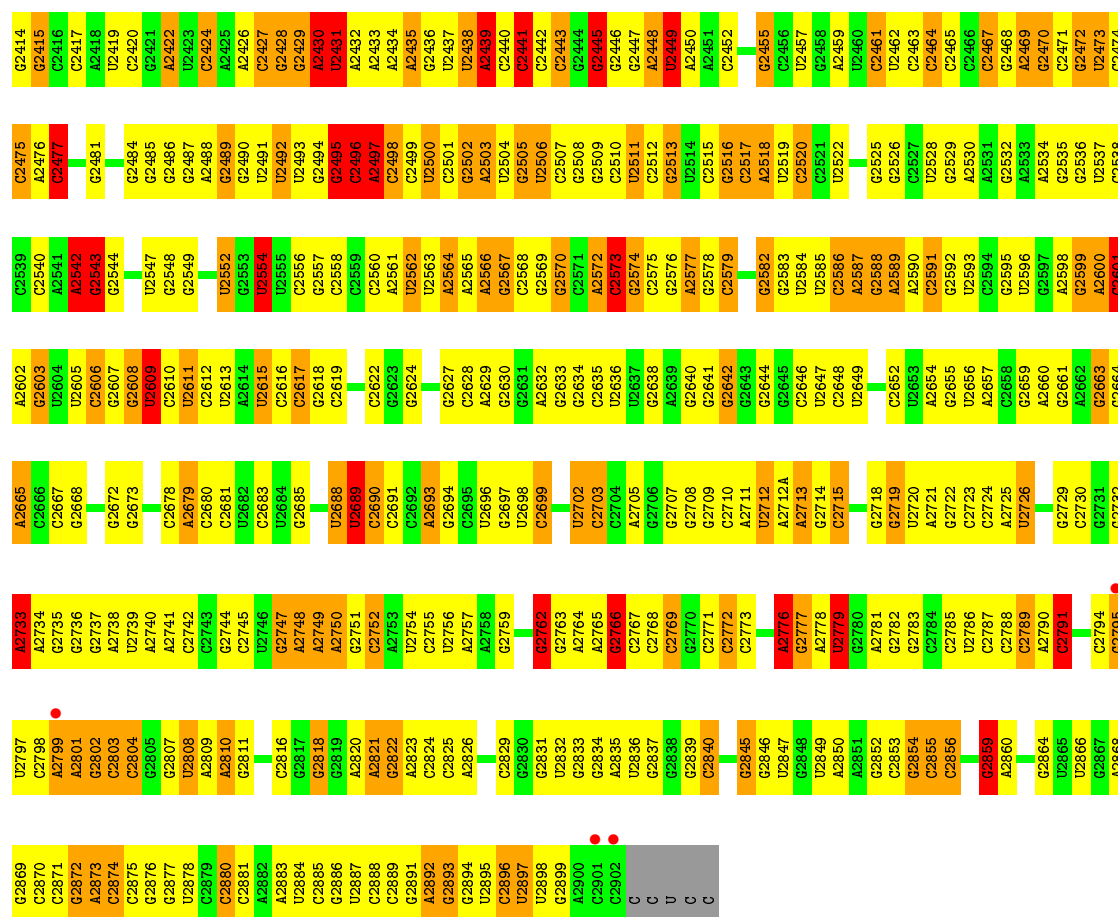


• Molecule 26: 23S ribosomal RNA

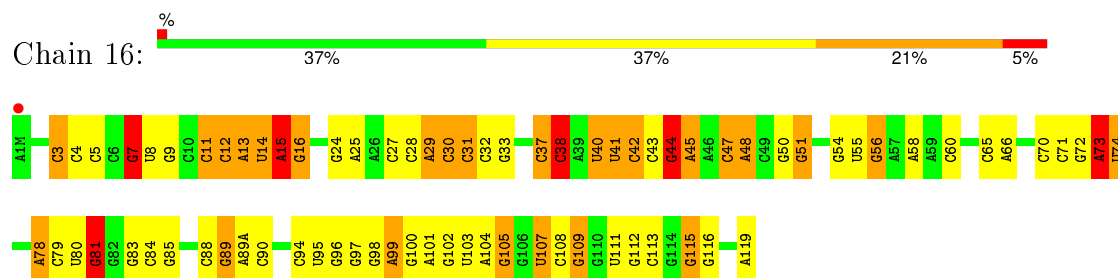


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G1324	C1258	G1192	A	A1000	C936	G873	U811	C749	C679	U639	U568	A492	U421	G333
G1325	G1259	G1193	G	A1001	U937	C876	U812	A750	G680	C540	U569	A493	U422	C336
U1326	G1260	G1194	A1069	G1002	U938	C877	U813	A751	G681	C541	G492	G493	A421	C366
G1327	C1261	U1195	A1070	C1006	G939	U877	C814	A752	G682	G542	A571	G494	A423	C343
G1328	A1262	U1196	G1071	C1007	G940	U878	C815	C753	G683	C543	G573	A495	G425	A347
U1329	U1263	G1197	C1072	C1008	A941	G879	C816	C754	G684	A546	C574	A496	C426	A347
C1330	G1264	G1198	A1073	G1009	G942	G880	C817	C755	G685	U647	C575	U499	C427	G352
A1331	A1265	G1199	G1074	A1010	U943	G	U818	C756	G686	G648	U576	A501	A428	G352
G1332	C1266	G1200	C1075	G1011	G944	G	A819	U757	G687	G649	U577	A502	A432	U358
C1333	U1267	G1201	C1076	A1012	A945	C	A820	G760	G688	C650	A578	A503	A433	G361
G1334	A1268	U1202	A	C1013	G946	C	U821	A761	G689	C651	G579	A504	U434	U362
U1335	A1269	U1203	U	C1014	G947	C	U822	G762	G690	C652	C580	U505	U435	G363
A1336	C1270	G1204	C	U1014	G948	C	G823	A764	G692	A653	G582	A505	C435	G363
G1337	G1271	A1142	A	G1015	C949	A	A824	G765	G693	A654	G583	G508	U441	U363E
G1338	A1272	A1143	U	G1016	G950	C	U827	C766	G694	A654B	G585	G509	G442	U363F
G1339	U1273	G1144	U	G1017	C951	A	U828	U767	G695	G654C	A586	C510	A443	A363F
U1340	A1274	C1145	U	C1018	G952	C	A829	G768	G696	G654D	A587	U511	C444	G370
U1341	A1275	C1146	A	U1019	A953	C	G830	G769	G700	C	C588	G512	C445	A371
A1342	G1276	G1147	A1085	A1020	G954	C	U831	G770	G701	C	C589	A514	A449	U372
G1343	G1277	A1148	A1086	A1021	C955	U	G832	G771	G702	C	G592	A515	G450	U373
C1344	A1278	G1149	G1087	U1022	G956	A	U833	C772	G703	G	G593	C516	A451	A374
C1345	U1279	C1150	A1088	G1023	A957	C	U834	U773	U704	C	G598	C517	G452	C375
G1346	G1281	G1151	G1089	G1024	U958	C	A835	A774	G705	A	G599	U524	A453	C376
G1347	U1282	G1152	U1090	G1025	A959	C	G836	G775	A706	C	G600	U525	C454	C377
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C1350	G1285	A1155	G1093	A1028	G968	C	U839	G778	C708	C	A603	A528	G458	G382
C1351	A1286	A1156	U	C1029	U969	C	G840	U779	G713	C	G604	A529	U459	U383
U1352	U1287	U1159	U	G1030	C970	U	G843	G780	G717	C	U605	G530	A460	U384
G1356	C1289	G1160	A1098	A1032	G971	A	C844	A782	G717	C	U606	G531	C461	C385
U1357	G1290	G1162	G1099	U1033	G972	C	G845	A783	A722	C654R	U607	A532	C462	G386
A1359	U1291	G1163	C1100	G1036	A973	C	U846	G784	A723	G654S	U608	A533	G463	U387
C1293	G1292	U1165	U1101	G1037	C974A	C	G847	G785	G724	A654T	U609	U534	U464	G388
G1298	G1293	C1166	G1102	C1041	G975	C	U848	C786	U724	A655	U613	C535	U465	G389
G1299	U1294	U1167	A1103	G1042	C976	C	A849	U787	G725	G656	U614	A536	A466	A390
U1300	G1295	G1168	C1104	C1043	G977	C	C850	A788	A726	G657	G615	G537	G467	G391
A1301	G1296	G1169	U1105	G1044	G978	C	U851	A789	A727	U657	A616	G539	G468	U395
A1302	G1297	G1170	G1106	A	G979	C	G852	C790	G728	C658	G617	G540	A469	G396
G1303	U1298	G1171	U1107	A	A980	C	G853	C791	G729	C659	G618	G541	A470	G397
C1304	G1299	G1172	U1108	G1047	A981	C	G854	G792	C730	G660	G619	C543	A471	G397
G1308	U1299	A1174	G1109	A1048	C982	C	G855	A793	C731	C661	G620	C544	A472	G400
G1309	C1300	G1175	G1110	C1049	A983	C	C856	G794	G732	G662	A621	C546	G473	A401
G1310	U1301	G1176	A1111	A1050	A984	C	U857	C795	G733	G663	G622	A547	U475	A402
U1312	G1311	A1177	G1112	C1043	C985	C	U858	C796	A734	C664	G623	A548	G476	U403
U1313	C1312	C1178	U1113	G1044	C986	C	G859	C797	A735	C665	C624	G549	G477	U404
U1314	G1313	G1179	G1114	A1054	G987	C	U860	G798	G736	G666	G627	G556	A479	U405
U1315	U1314	C1180	G1115	G1055	A988	C	A861	C799	C737	U667	G628	G557	A480	G406
C1316	U1315	C1181	C1116	G1056	G989	C	G862	A800	G738	G668	A627	G558	A481	G407
A1317	G1316	A1182	G1117	A1057	A990	C	A863	G801	G739	G669	G630	G559	A482	C409
U1318	C1317	G1183	C1118	U1058	C991	C	G864	A802	U740	A670	A631	G560	A483	G410
C1319	U1318	G1184	C1119	G1059	C992	C	C865	U803	G741	C671	G632	C561	C484	G411
G1320	G1319	C1185	G1120	U1060	G993	C	A866	A804	G742	G672	A633	C562	C485	A412
A1255	A1256	G1186	G1121	U1061	C994	C	C867	G805	G743	C673	G634	C563	C486	G412
G1322	C1320	G1187	C1122	G1062	C995	C	U868	C806	G744	G674	C635	C564	C487	G412
C1323	U1257	U1188	A1125	G1063	A996	C	G869	U807	G745	A675	G636	C565	C488	G412
A1324	G1258	A1189	G1126	C	A997	C	A870	G808	A746	A676	C	C566	C489	G412
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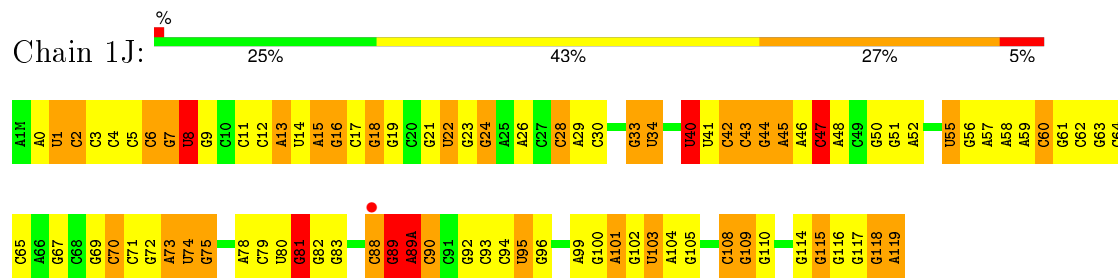




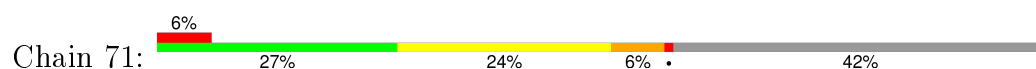
### • Molecule 27: 5S ribosomal RNA



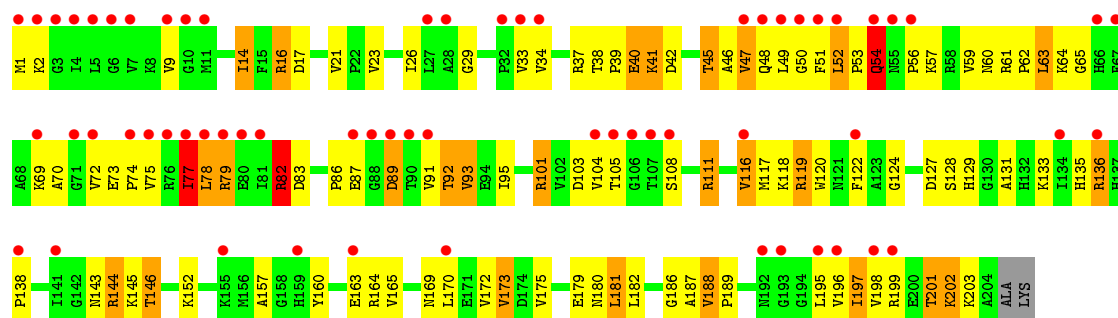
### • Molecule 27: 5S ribosomal RNA



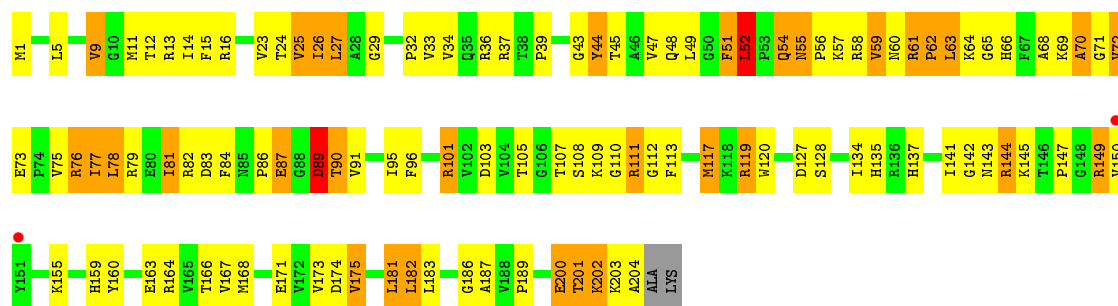
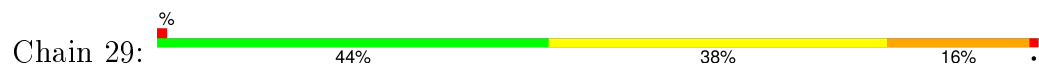
### • Molecule 28: 50S ribosomal protein L1



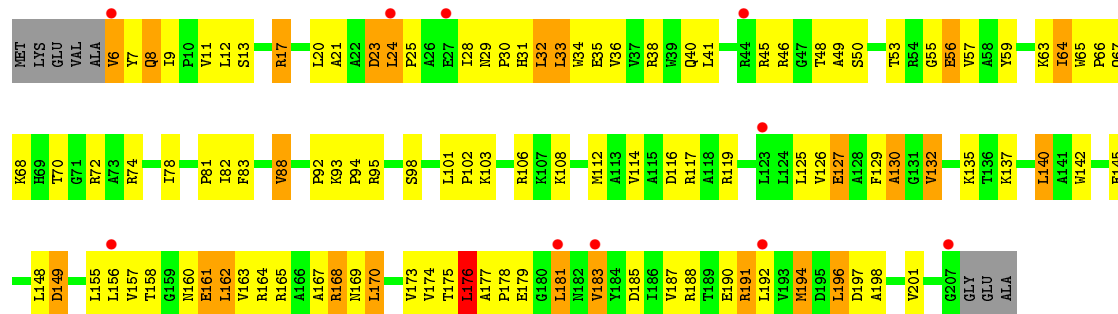
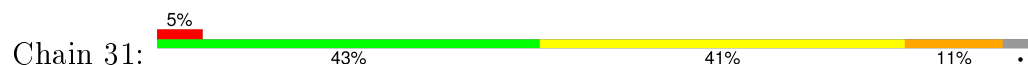




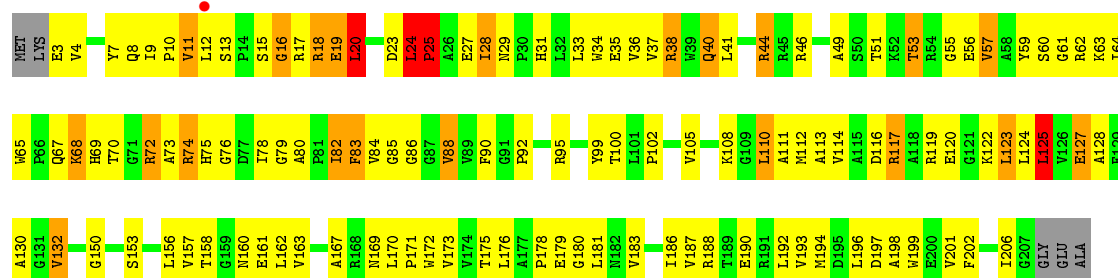
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4





Chain 41:

Item	Category	Percentage	
MET	Grey	2%	
P2	Green	43%	
L3	Green		
D4	Green		
V5	Green		
A6	Green		
L7	Green		
K8	Green		
R9	Green		
K10	Green		
Y11	Green		
Y12	Green		
E13	Green		
E14	Green		
V15	Green		
R16	Green		
P17	Green		
E18	Green		
L19	Green		
L20	Green		
R21	Green		
R22	Green		
P23	Green		
G24	Green		
V25	Green		
Q26	Green		
P27	Green		
V28	Green		
V31	Yellow		46%
P32	Yellow		
R33	Yellow		
L34	Yellow		
E35	Yellow		
K36	Yellow		
V37	Yellow		
V38	Yellow		
L43	Yellow		
Q44	Yellow		
E45	Yellow		
A46	Yellow		
K47	Yellow		
E48	Yellow		
R51	Yellow		
L52	Yellow		
L53	Yellow		
A56	Yellow		
A57	Yellow		
L60	Yellow		
A61	Yellow		
L62	Yellow		
L63	Yellow		
T64	Yellow		
A65	Yellow		
O66	Yellow		
V67	Yellow		
P68	Yellow		
A69	Yellow		
V70	Yellow		
S76	Yellow		
L77	Yellow		
S78	Yellow		
R79	Yellow		
R80	Yellow		
K81	Yellow		
L82	Yellow		
R83	Yellow		
R84	Yellow		
G85	Yellow		
M86	Yellow		
P87	Yellow		
E88	Yellow		
E89	Yellow		
L90	Yellow		
R91	Yellow		
V92	Yellow		
T93	Yellow		
R94	Yellow		
R95	Yellow		
R96	Yellow		
D97	Yellow		
R98	Yellow		
R99	Yellow		
V100	Yellow		
L101	Yellow		
F102	Yellow		
L103	Yellow		
E104	Yellow		
K105	Yellow		
L106	Yellow		
L107	Yellow		
R108	Yellow		
V109	Yellow		
A110	Yellow		
L111	Yellow		
P112	Yellow		
A113	Yellow		
L114	Yellow		
R115	Yellow		
D116	Yellow		
F117	Yellow		
R118	Yellow		
M121	Yellow		
P122	Yellow		
M123	Yellow		
S124	Yellow		
R128	Yellow		
Y131	Yellow		
L135	Yellow		
O136	Yellow		
R137	Yellow		
R138	Yellow		

Chain 49:

26% 39% 52% 8%

MET L62 L63 T64 L67 P68 A69 V70 T71 R72 K75 S76 I77 F80 K81 L82 K83 A84 G85 M86 P87 I88 G89 L90 R91 V92 T93 L94 R95 A96 D97 R98 N99 W100 I101 F102 L103 E104 K105 L106 L107 L111 I114 R115 D116 F117 R118 G119 L120 N123 S124 F125 N130 Y131

P2 L3 D4 V5 A6 L7 R8 K9 K10 Y11 Y12 E13 V15 R16 P17 E18 I19 I20 R21 R22 P23 G24 Y25 Q26 N27 V28 W29 P32 R33 L34 E35 K36 V37 V38 I39 N40 Q41 G42 L43 G44 E45 A46 K47 E48 D49 R51 I52 L53 E54 K55 A56 A57 Q58 E59 L60 A61

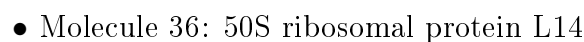
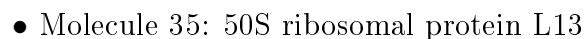
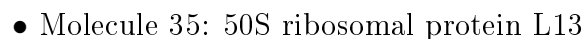
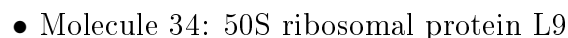
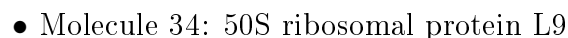
Chain 51:

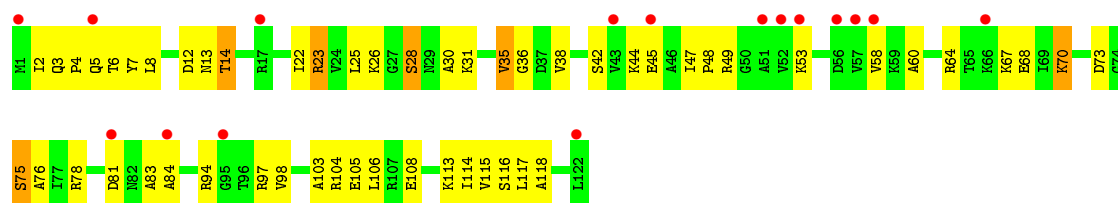
6% 46% 38% 12%

• •

MET S2 R3 I4 G5 R6 L7 P8 I9 P10 V11 P12 S16 V17 E18 V19 A20 P21 G22 P23 R24 V25 K26 D27 G28 P29 K30 G31 E32 L33 E34 V35 P36 V37 S38 P39 E40 M41 V42 V43 V44 V45 E46 V50 R51 V52 E53 R54 R59 R60 H61 R62 S63 L64 H65 L74

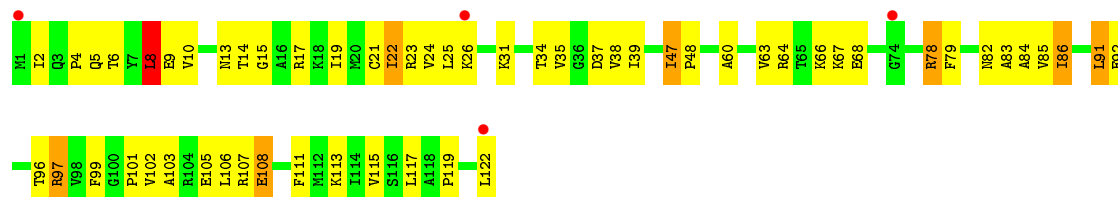
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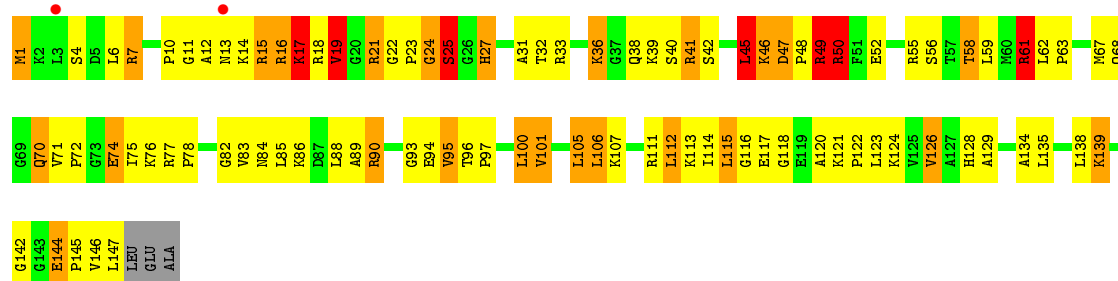
• Molecule 36: 50S ribosomal protein L14

Chain 25: 3% 53% 40% 6%



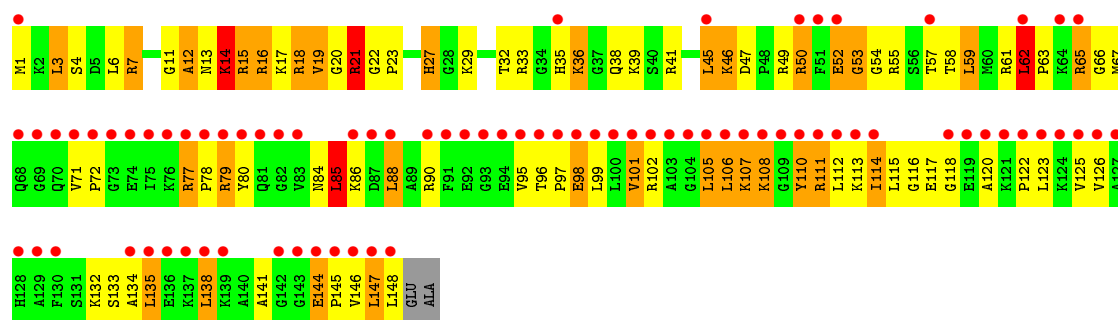
• Molecule 37: 50S ribosomal protein L15

Chain 78: 34% 43% 17% 5%



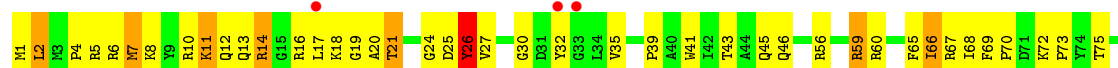
• Molecule 37: 50S ribosomal protein L15

Chain 35: 53% 37% 37% 21%



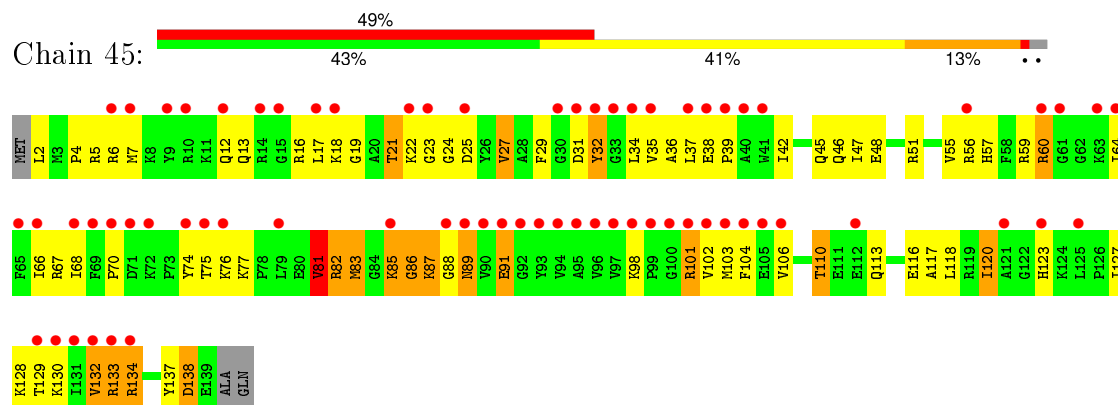
• Molecule 38: 50S ribosomal protein L16

Chain 88: 3% 50% 38% 11%

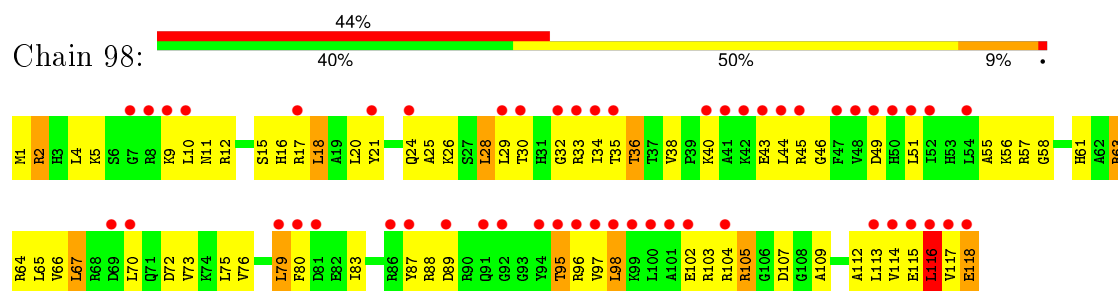




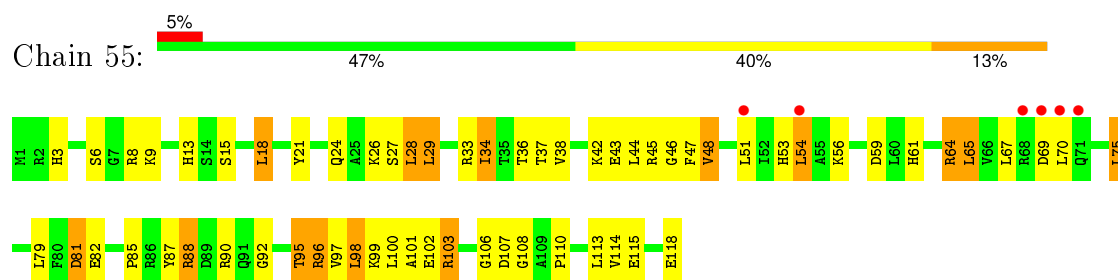
• Molecule 38: 50S ribosomal protein L16



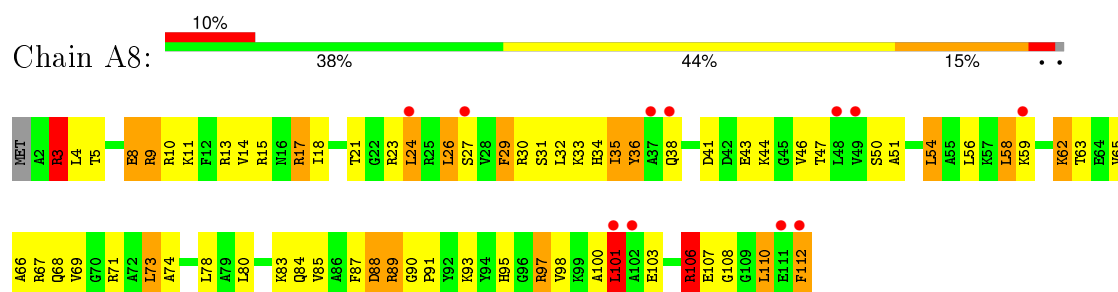
• Molecule 39: 50S ribosomal protein L17



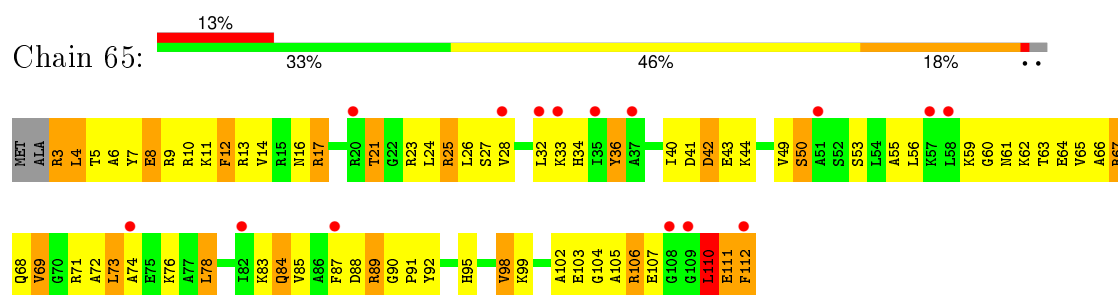
• Molecule 39: 50S ribosomal protein L17



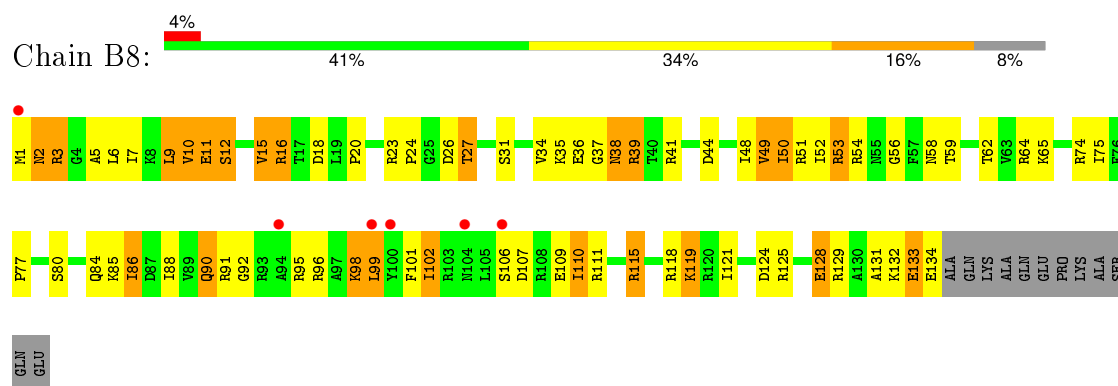
• Molecule 40: 50S ribosomal protein L18



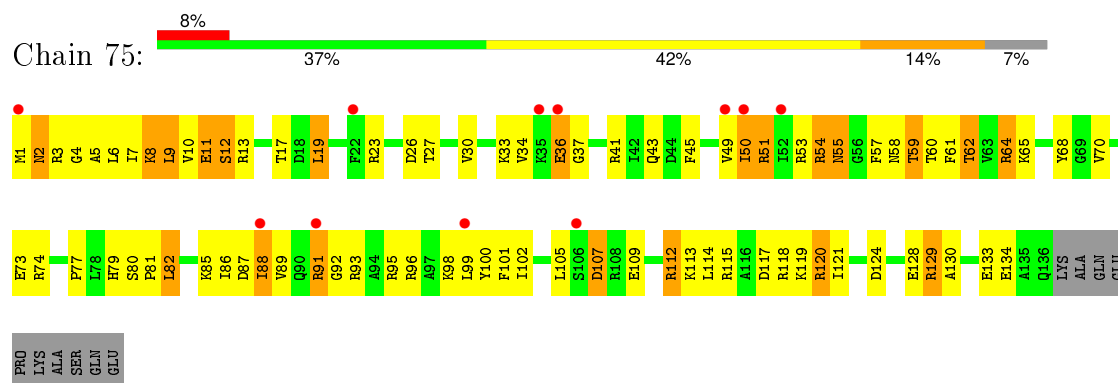
• Molecule 40: 50S ribosomal protein L18



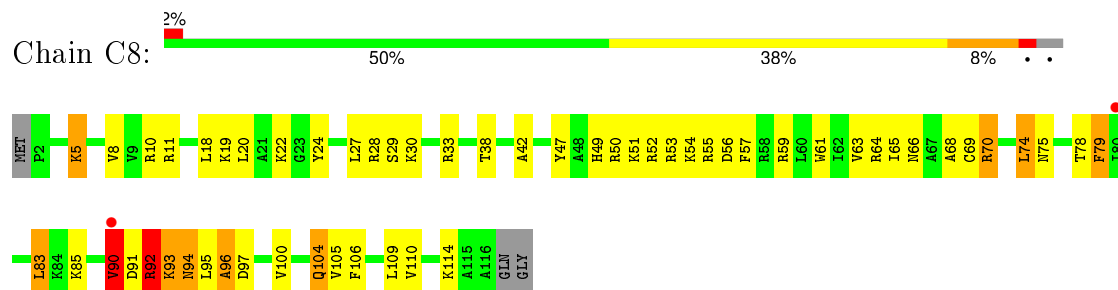
• Molecule 41: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L19



• Molecule 42: 50S ribosomal protein L20



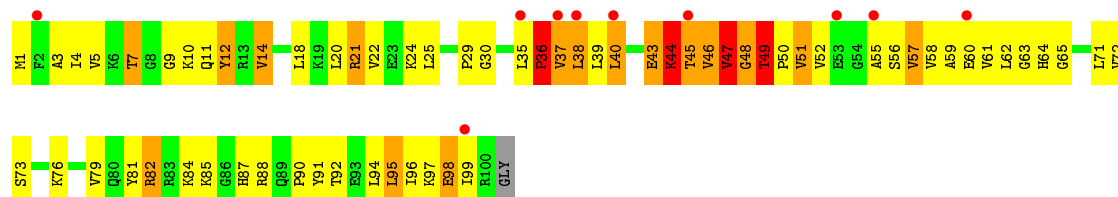
• Molecule 42: 50S ribosomal protein L20





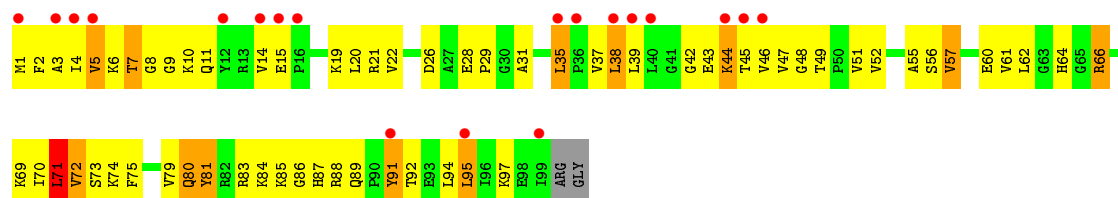
- Molecule 43: 50S ribosomal protein L21

Chain D8: 10% 35% 45% 16%



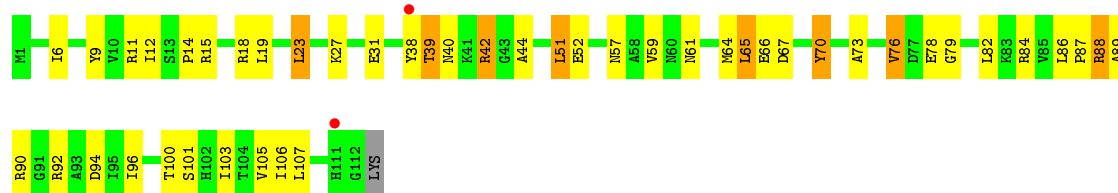
- Molecule 43: 50S ribosomal protein L21

Chain 95: 19% 34% 51% 12%



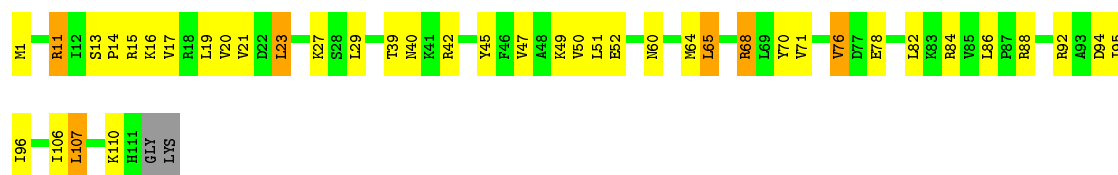
- Molecule 44: 50S ribosomal protein L22

Chain E8: 2% 58% 34% 7%



- Molecule 44: 50S ribosomal protein L22

Chain A5: 62% 31% 5%

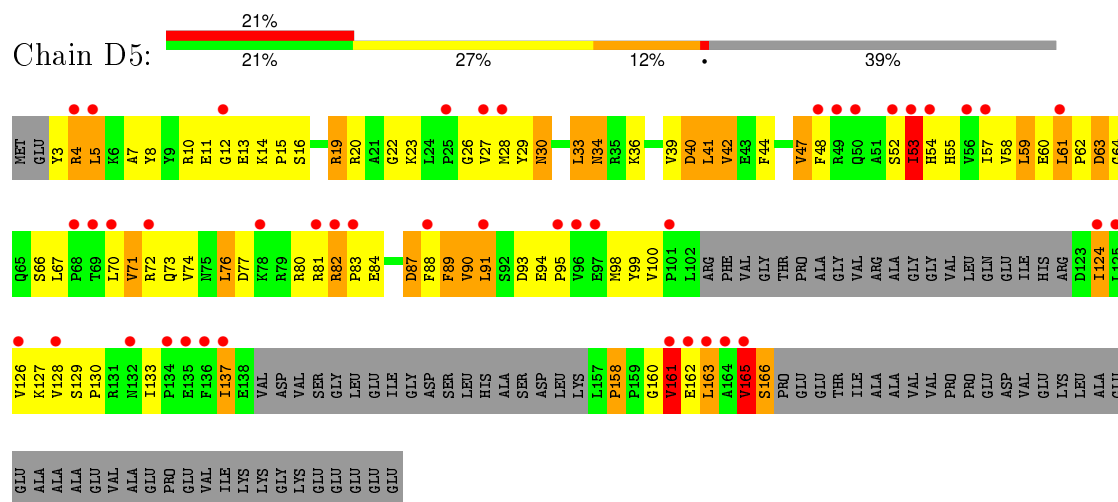


- Molecule 45: 50S ribosomal protein L23

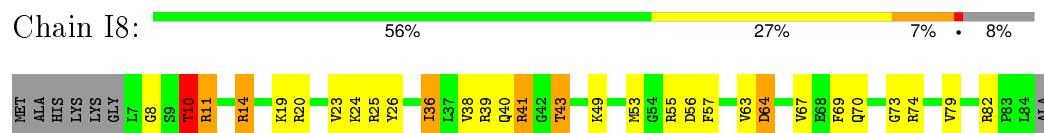


GLU  
GLU  
GLU

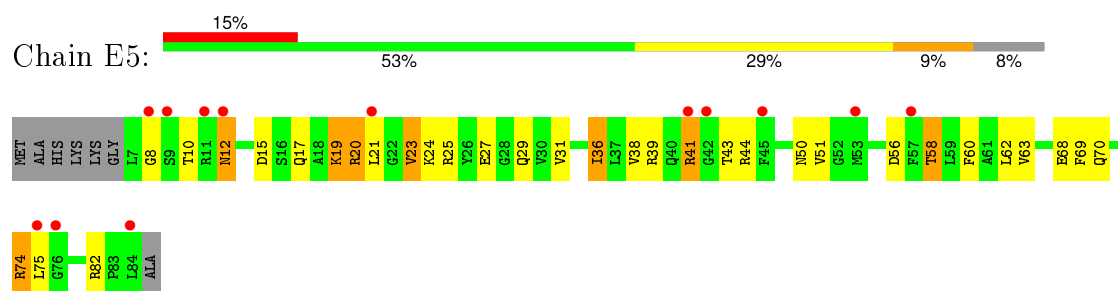
• Molecule 47: 50S ribosomal protein L25



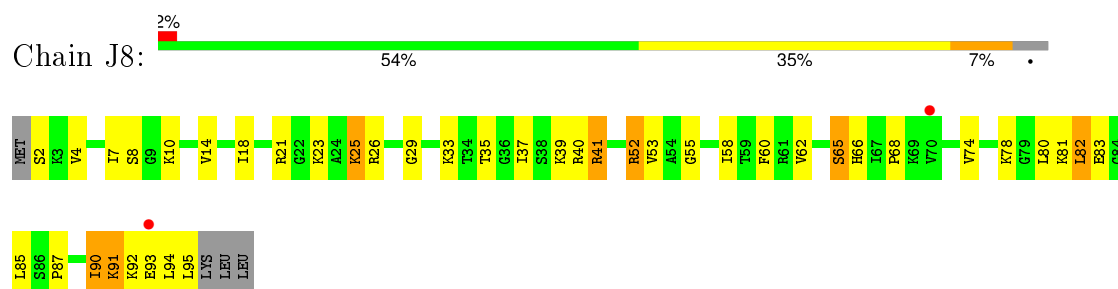
• Molecule 48: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L27



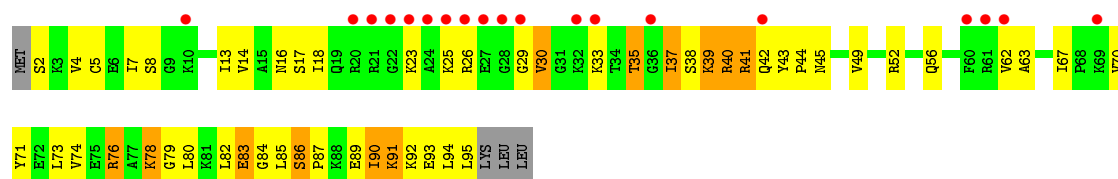
• Molecule 49: 50S ribosomal protein L28



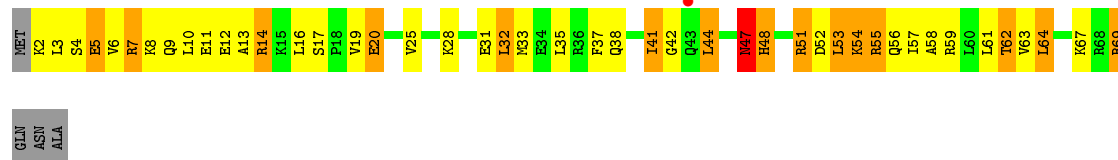
• Molecule 49: 50S ribosomal protein L28



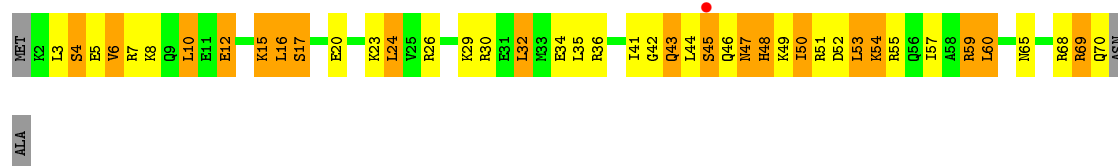




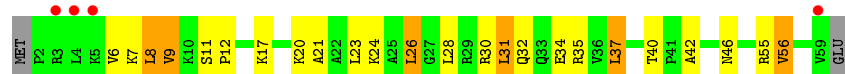
- Molecule 50: 50S ribosomal protein L29



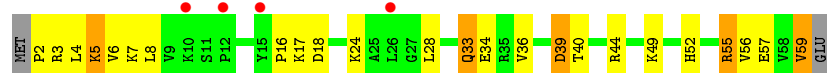
- Molecule 50: 50S ribosomal protein L29



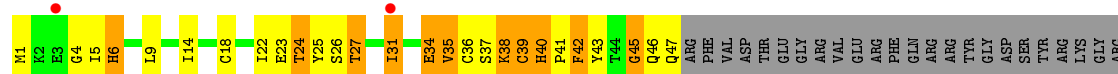
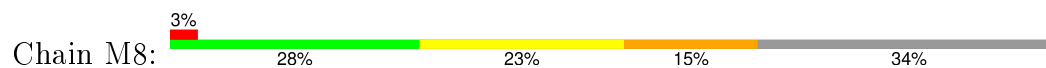
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32

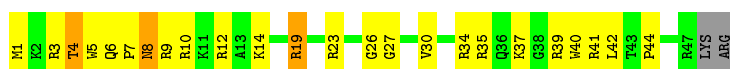




- Molecule 53: 50S ribosomal protein L32



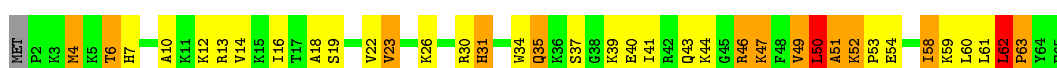
- Molecule 54: 50S ribosomal protein L34



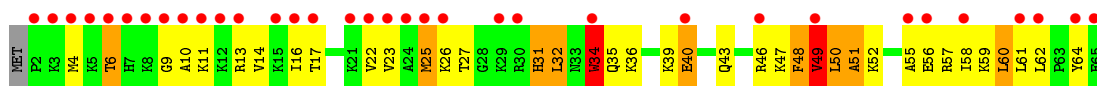
- Molecule 54: 50S ribosomal protein L34



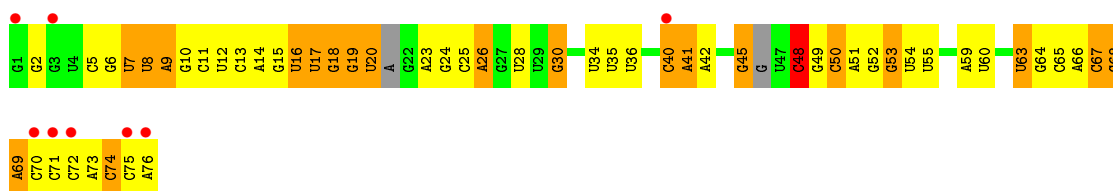
- Molecule 55: 50S ribosomal protein L35



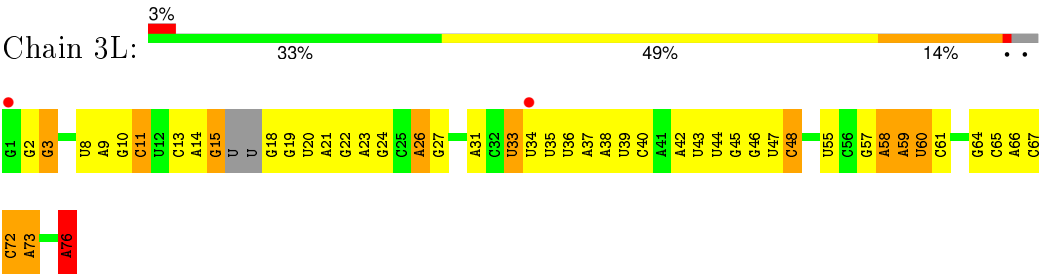
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA-Lys



- Molecule 57: tRNA-Lys



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.90Å 447.80Å 617.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.53 – 3.15 161.39 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.53-3.15) 93.3 (161.39-3.15)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.193 , 0.251 0.198 , 0.256	Depositor DCC
$R_{free}$ test set	2000 reflections (0.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 69.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 987283 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	294304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, U8U, 7MG, SF4, MG, 4SU, T6A, 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	0.78	5/35994 (0.0%)	1.45	459/56171 (0.8%)
1	1G	0.66	0/36258	1.30	243/56589 (0.4%)
2	12	0.49	0/1742	0.74	1/2346 (0.0%)
2	1E	0.46	0/1908	0.69	0/2573
3	22	0.43	0/1552	0.70	2/2093 (0.1%)
3	2E	0.53	0/1629	0.72	0/2195
4	32	0.47	0/1732	0.72	2/2318 (0.1%)
4	3E	0.61	0/1732	0.79	2/2318 (0.1%)
5	42	0.52	0/1138	0.73	1/1532 (0.1%)
5	4E	0.57	0/1158	0.75	0/1559
6	52	0.52	0/855	0.69	1/1154 (0.1%)
6	5E	0.53	0/850	0.70	0/1147
7	62	0.45	0/1122	0.68	0/1500
7	6E	0.47	0/1230	0.65	0/1645
8	72	0.42	0/1135	0.61	0/1527
8	7E	0.51	0/1135	0.74	0/1527
9	82	0.44	0/1002	0.65	0/1346
9	8E	0.48	0/1024	0.70	1/1374 (0.1%)
10	1A	0.43	0/636	0.65	0/855
10	1I	0.47	0/747	0.71	2/1006 (0.2%)
11	2A	0.47	0/850	0.67	0/1150
11	2I	0.54	0/838	0.73	0/1133
12	3A	0.54	0/963	0.76	1/1290 (0.1%)
12	3I	0.74	0/972	0.92	0/1301
13	4A	0.47	0/898	0.69	1/1204 (0.1%)
13	4I	0.54	0/938	0.76	1/1258 (0.1%)
14	5A	0.46	0/475	0.76	1/632 (0.2%)
14	5I	0.58	0/505	0.76	0/671
15	6A	0.46	0/740	0.65	1/987 (0.1%)
15	6I	0.51	0/744	0.69	0/992
16	7A	0.49	0/721	0.69	0/970
16	7I	0.48	0/687	0.74	0/925

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.49	0/836	0.63	0/1117
17	8I	0.64	2/836 (0.2%)	0.77	0/1117
18	9A	0.51	0/549	0.72	1/732 (0.1%)
18	9I	0.54	0/549	0.74	0/732
19	AA	0.45	0/480	0.76	0/648
19	AI	0.58	0/657	0.86	0/885
20	BA	0.46	0/759	0.69	0/1000
20	BI	0.44	0/748	0.63	0/986
21	1B	0.43	0/212	0.60	0/277
21	1F	0.44	0/203	0.67	0/266
22	1K	0.64	0/1516	1.28	12/2350 (0.5%)
23	2K	0.83	0/1721	1.52	28/2682 (1.0%)
23	2L	0.68	0/1698	1.29	10/2644 (0.4%)
24	3K	0.62	0/1799	1.27	16/2801 (0.6%)
25	4K	0.90	0/495	1.40	4/771 (0.5%)
25	4L	0.70	0/420	1.09	0/654
26	14	0.94	73/69023 (0.1%)	1.67	1714/107740 (1.6%)
26	1H	1.08	148/68351 (0.2%)	1.86	2473/106700 (2.3%)
27	16	0.83	0/2928	1.65	60/4568 (1.3%)
27	1J	0.74	1/2928 (0.0%)	1.45	28/4568 (0.6%)
28	71	0.56	1/1055 (0.1%)	0.80	3/1425 (0.2%)
29	11	0.83	2/2175 (0.1%)	1.03	7/2933 (0.2%)
29	19	0.83	1/2170 (0.0%)	0.97	4/2926 (0.1%)
30	21	0.70	0/1596	0.93	3/2153 (0.1%)
30	29	0.66	0/1596	0.93	1/2153 (0.0%)
31	31	0.76	0/1620	0.93	3/2194 (0.1%)
31	39	0.65	0/1641	0.90	1/2223 (0.0%)
32	41	0.55	0/1489	0.74	0/2005
32	49	0.43	0/1489	0.71	0/2005
33	51	0.60	0/1353	0.89	3/1830 (0.2%)
33	59	0.51	0/548	0.78	0/738
34	61	0.51	0/1146	0.74	1/1551 (0.1%)
34	69	0.50	0/1146	0.78	2/1551 (0.1%)
35	15	0.47	0/1123	0.72	0/1515
35	58	0.62	0/1131	0.84	1/1525 (0.1%)
36	25	0.61	0/942	0.79	1/1269 (0.1%)
36	68	0.67	0/942	0.82	1/1269 (0.1%)
37	35	0.69	0/1147	1.06	4/1525 (0.3%)
37	78	0.76	0/1139	1.14	8/1514 (0.5%)
38	45	0.66	0/1120	0.90	2/1498 (0.1%)
38	88	0.79	0/1134	0.95	2/1519 (0.1%)
39	55	0.65	0/981	0.83	0/1312
39	98	0.61	0/981	0.85	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	65	0.55	0/886	0.83	2/1180 (0.2%)
40	A8	0.67	0/891	0.94	3/1187 (0.3%)
41	75	0.64	0/1146	0.88	0/1531
41	B8	0.70	0/1132	0.88	0/1512
42	85	0.59	0/977	0.75	0/1301
42	C8	0.71	0/968	0.84	1/1289 (0.1%)
43	95	0.74	0/774	0.91	2/1038 (0.2%)
43	D8	0.69	0/785	0.88	3/1052 (0.3%)
44	A5	0.63	0/897	0.82	0/1204
44	E8	0.75	0/901	0.91	0/1209
45	B5	0.76	0/752	0.87	1/1010 (0.1%)
45	F8	0.83	0/765	0.91	2/1029 (0.2%)
46	C5	0.65	0/807	0.88	1/1076 (0.1%)
46	G8	0.82	0/796	1.08	2/1062 (0.2%)
47	D5	0.49	0/1057	0.76	0/1430
47	H8	0.51	0/1248	0.78	1/1687 (0.1%)
48	E5	0.61	0/624	0.83	0/832
48	I8	0.78	0/624	0.94	1/832 (0.1%)
49	F5	0.67	0/744	0.83	0/989
49	J8	0.73	0/744	0.97	1/989 (0.1%)
50	G5	0.61	0/575	0.81	0/762
50	K8	0.87	2/573 (0.3%)	0.84	0/759
51	H5	0.51	0/464	0.69	0/623
51	L8	0.59	0/464	0.80	0/623
52	M8	0.52	0/375	0.86	1/507 (0.2%)
53	J5	0.65	1/448 (0.2%)	0.83	0/606
53	N8	0.74	0/394	0.92	0/534
54	L5	0.71	0/409	0.93	1/540 (0.2%)
54	P8	0.88	0/409	1.05	0/540
55	M5	0.85	1/524 (0.2%)	0.92	1/691 (0.1%)
55	Q8	0.80	0/524	1.05	3/691 (0.4%)
56	1L	0.62	0/1705	1.20	6/2649 (0.2%)
57	3L	0.60	0/1732	1.14	8/2695 (0.3%)
All	All	0.84	237/316396 (0.1%)	1.46	5154/474130 (1.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	32	0	2
4	3E	0	4
7	62	0	1
7	6E	0	1
10	1A	0	1
12	3A	0	2
12	3I	0	2
13	4I	0	2
14	5A	0	1
19	AA	0	1
19	AI	0	3
28	71	0	1
29	11	0	4
29	19	0	2
30	21	0	2
30	29	0	6
31	31	0	2
31	39	0	6
32	41	0	1
32	49	0	2
33	51	0	3
33	59	0	1
34	61	0	3
34	69	0	1
35	58	0	1
37	35	0	10
37	78	0	7
38	45	0	4
38	88	0	1
40	65	0	1
40	A8	0	1
41	75	0	3
41	B8	0	4
42	85	0	2
42	C8	0	3
43	D8	0	3
45	B5	0	3
45	F8	0	1
46	C5	0	4
46	G8	0	2
47	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	H8	0	2
50	G5	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	2
All	All	0	119

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-13.80	1.29	1.37
26	1H	676	A	N9-C4	-13.67	1.29	1.37
26	14	783	A	N9-C4	-10.88	1.31	1.37
26	1H	472	A	N3-C4	-10.55	1.28	1.34
26	1H	783	A	N3-C4	-10.35	1.28	1.34

The worst 5 of 5154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-22.91	112.25	126.00
26	1H	676	A	C2-N3-C4	-20.00	100.60	110.60
26	1H	945	A	N1-C6-N6	19.59	130.36	118.60
26	1H	945	A	C6-C5-N7	-18.66	119.24	132.30
26	1H	1332	G	C2-N3-C4	-18.37	102.72	111.90

There are no chirality outliers.

5 of 119 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
4	3E	77	ASN	Peptide
4	3E	82	ALA	Peptide
4	3E	87	GLY	Peptide
4	3E	88	VAL	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	16233	797	0
1	1G	32391	0	16352	818	1
2	12	1711	0	1751	90	0
2	1E	1874	0	1926	86	0
3	22	1529	0	1592	72	0
3	2E	1605	0	1668	50	0
4	32	1702	0	1766	96	0
4	3E	1702	0	1762	103	0
5	42	1123	0	1191	56	0
5	4E	1142	0	1204	44	0
6	52	842	0	857	31	0
6	5E	837	0	852	47	0
7	62	1110	0	1163	53	0
7	6E	1214	0	1259	41	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	53	0
9	82	983	0	1006	57	0
9	8E	1005	0	1033	76	0
10	1A	626	0	639	34	0
10	1I	734	0	761	51	0
11	2A	835	0	847	38	0
11	2I	823	0	833	33	0
12	3A	947	0	1033	50	0
12	3I	956	0	1046	43	0
13	4A	888	0	941	64	0
13	4I	928	0	987	50	0
14	5A	466	0	499	38	0
14	5I	496	0	535	25	0
15	6A	729	0	768	29	0
15	6I	733	0	771	23	0
16	7A	705	0	725	31	0
16	7I	671	0	693	40	0
17	8A	823	0	891	34	0
17	8I	823	0	891	48	0
18	9A	544	0	605	30	0
18	9I	544	0	605	28	0
19	AA	471	0	464	35	0
19	AI	643	0	662	36	0
20	BA	757	0	856	34	0
20	BI	746	0	843	42	0
21	1B	208	0	221	26	0
21	1F	199	0	208	7	0
22	1K	1477	0	758	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	844	30	0
23	2L	1626	0	835	30	0
24	3K	1611	0	817	57	0
25	4K	439	0	218	14	0
25	4L	373	0	185	9	0
26	14	61630	0	31070	1393	1
26	1H	61028	0	30763	1409	0
27	16	2617	0	1328	71	0
27	1J	2617	0	1328	87	0
28	71	1033	0	1048	54	0
29	11	2125	0	2199	118	0
29	19	2120	0	2197	118	0
30	21	1563	0	1629	92	0
30	29	1563	0	1629	110	0
31	31	1585	0	1632	101	0
31	39	1606	0	1652	93	0
32	41	1464	0	1522	74	0
32	49	1464	0	1522	73	0
33	51	1327	0	1405	62	0
33	59	539	0	563	34	0
34	61	1131	0	1218	51	0
34	69	1131	0	1218	55	0
35	15	1096	0	1168	61	0
35	58	1104	0	1180	69	0
36	25	932	0	996	42	0
36	68	932	0	996	41	0
37	35	1130	0	1217	98	0
37	78	1122	0	1206	91	0
38	45	1099	0	1154	67	0
38	88	1113	0	1157	54	0
39	55	967	0	1033	46	0
39	98	967	0	1033	48	0
40	65	876	0	938	81	0
40	A8	881	0	943	61	0
41	75	1132	0	1189	75	0
41	B8	1118	0	1176	62	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	54	0
43	95	763	0	836	71	0
43	D8	774	0	849	52	0
44	A5	886	0	948	23	0
44	E8	890	0	951	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B5	738	0	792	36	0
45	F8	751	0	807	40	0
46	C5	794	0	886	53	0
46	G8	783	0	873	67	0
47	D5	1034	0	1061	68	0
47	H8	1222	0	1247	80	0
48	E5	616	0	633	38	0
48	I8	616	0	633	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	39	0
50	G5	573	0	616	33	0
50	K8	571	0	623	37	0
51	H5	459	0	512	17	0
51	L8	459	0	512	18	0
52	M8	366	0	370	31	0
53	J5	434	0	454	18	0
53	N8	381	0	397	27	0
54	L5	401	0	436	18	0
54	P8	401	0	436	21	0
55	M5	516	0	582	36	0
55	Q8	516	0	582	34	0
56	1L	1570	0	798	34	0
57	3L	1571	0	798	34	0
58	11	1	0	0	0	0
58	13	142	0	0	0	0
58	14	421	0	0	0	0
58	16	11	0	0	0	0
58	19	1	0	0	0	0
58	1G	95	0	0	0	0
58	1H	495	0	0	0	0
58	1I	1	0	0	0	0
58	1J	6	0	0	0	0
58	1K	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	3	0	0	0	0
58	2I	1	0	0	0	0
58	2K	2	0	0	0	0
58	2L	2	0	0	0	0
58	39	2	0	0	0	0
58	3I	1	0	0	0	0
58	3L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	4I	1	0	0	0	0
58	45	3	0	0	0	0
58	4I	1	0	0	0	0
58	4K	1	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7I	1	0	0	0	0
58	88	3	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	1	0	0	0	0
58	N8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	0	0
59	3E	8	0	0	0	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	9	0	0	2	0
61	13	207	0	0	37	0
61	14	717	0	0	118	0
61	15	1	0	0	0	0
61	16	22	0	0	3	0
61	19	10	0	0	4	0
61	1G	117	0	0	23	0
61	1H	819	0	0	163	0
61	1I	1	0	0	0	0
61	1J	6	0	0	0	0
61	21	6	0	0	3	0
61	29	3	0	0	0	0
61	2A	1	0	0	0	0
61	31	4	0	0	1	0
61	32	2	0	0	0	0
61	35	3	0	0	0	0
61	39	3	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	4E	2	0	0	0	0
61	4K	4	0	0	0	0
61	5I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	6A	2	0	0	1	0
61	6I	1	0	0	0	0
61	75	2	0	0	0	0
61	78	1	0	0	0	0
61	7A	1	0	0	0	0
61	85	3	0	0	1	0
61	8E	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	C8	3	0	0	1	0
61	F8	1	0	0	0	0
61	I8	5	0	0	0	0
61	J8	2	0	0	0	0
61	L8	3	0	0	0	0
61	M5	3	0	0	0	0
All	All	294304	0	195547	8554	1

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

The worst 5 of 8554 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)
30:21:135:HIS:NE2	61:21:401:HOH:O	1.87	1.06
1:13:788:U:H2'	1:13:789:U:H5'	1.29	1.06
26:1H:511:U:OP2	61:1H:3501:HOH:O	1.72	1.05
47:H8:5:LEU:HD11	47:H8:44:PHE:HA	1.40	1.02
26:14:1899:G:H21	26:14:1902:C:N4	1.56	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	204/256 (80%)	170 (83%)	32 (16%)	2 (1%)	19	63
2	1E	227/256 (89%)	191 (84%)	34 (15%)	2 (1%)	21	65
3	22	190/239 (80%)	173 (91%)	15 (8%)	2 (1%)	17	61
3	2E	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	34	76
4	3E	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	7	41
5	42	145/162 (90%)	136 (94%)	8 (6%)	1 (1%)	26	71
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	26	71
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	62	134/156 (86%)	126 (94%)	8 (6%)	0	100	100
7	6E	145/156 (93%)	136 (94%)	9 (6%)	0	100	100
8	72	136/138 (99%)	126 (93%)	8 (6%)	2 (2%)	13	53
8	7E	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	82	122/128 (95%)	111 (91%)	11 (9%)	0	100	100
9	8E	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	24	67
10	1A	72/105 (69%)	64 (89%)	8 (11%)	0	100	100
10	1I	89/105 (85%)	81 (91%)	7 (8%)	1 (1%)	17	61
11	2A	111/129 (86%)	99 (89%)	11 (10%)	1 (1%)	21	65
11	2I	109/129 (84%)	99 (91%)	8 (7%)	2 (2%)	11	49
12	3A	119/132 (90%)	99 (83%)	19 (16%)	1 (1%)	24	67
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	24	67
13	4A	108/126 (86%)	87 (81%)	20 (18%)	1 (1%)	21	65
13	4I	114/126 (90%)	93 (82%)	19 (17%)	2 (2%)	11	49
14	5A	55/61 (90%)	46 (84%)	8 (14%)	1 (2%)	11	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	59/61 (97%)	51 (86%)	8 (14%)	0	100	100
15	6A	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
15	6I	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	16	58
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	78/88 (89%)	76 (97%)	2 (3%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	13	53
19	AA	54/93 (58%)	45 (83%)	5 (9%)	4 (7%)	1	8
19	AI	78/93 (84%)	68 (87%)	6 (8%)	4 (5%)	2	19
20	BA	96/106 (91%)	88 (92%)	8 (8%)	0	100	100
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
29	11	272/276 (99%)	247 (91%)	16 (6%)	9 (3%)	5	30
29	19	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	11	49
30	21	202/206 (98%)	173 (86%)	25 (12%)	4 (2%)	9	46
30	29	202/206 (98%)	153 (76%)	36 (18%)	13 (6%)	2	12
31	31	200/210 (95%)	179 (90%)	19 (10%)	2 (1%)	19	63
31	39	203/210 (97%)	174 (86%)	24 (12%)	5 (2%)	7	39
32	41	178/182 (98%)	152 (85%)	23 (13%)	3 (2%)	11	50
32	49	178/182 (98%)	158 (89%)	18 (10%)	2 (1%)	17	61
33	51	171/180 (95%)	132 (77%)	35 (20%)	4 (2%)	8	42
33	59	63/180 (35%)	45 (71%)	17 (27%)	1 (2%)	12	52
34	61	143/148 (97%)	116 (81%)	25 (18%)	2 (1%)	14	55
34	69	143/148 (97%)	116 (81%)	27 (19%)	0	100	100
35	15	135/140 (96%)	123 (91%)	11 (8%)	1 (1%)	26	71
35	58	136/140 (97%)	116 (85%)	17 (12%)	3 (2%)	8	43
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
37	35	146/150 (97%)	112 (77%)	27 (18%)	7 (5%)	3	20
37	78	145/150 (97%)	118 (81%)	20 (14%)	7 (5%)	3	20
38	45	136/141 (96%)	111 (82%)	22 (16%)	3 (2%)	8	43
38	88	139/141 (99%)	114 (82%)	19 (14%)	6 (4%)	3	23
39	55	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
39	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
40	65	108/112 (96%)	92 (85%)	14 (13%)	2 (2%)	10	48
40	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	11	49
41	75	134/146 (92%)	115 (86%)	18 (13%)	1 (1%)	26	71
41	B8	132/146 (90%)	118 (89%)	14 (11%)	0	100	100
42	85	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	21	65
42	C8	113/118 (96%)	105 (93%)	6 (5%)	2 (2%)	11	49
43	95	97/101 (96%)	78 (80%)	15 (16%)	4 (4%)	3	25
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	32
44	A5	109/113 (96%)	99 (91%)	10 (9%)	0	100	100
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	6 (6%)	1 (1%)	17	61
45	F8	94/96 (98%)	83 (88%)	8 (8%)	3 (3%)	5	31
46	C5	102/110 (93%)	69 (68%)	26 (26%)	7 (7%)	1	10
46	G8	101/110 (92%)	90 (89%)	9 (9%)	2 (2%)	9	46
47	D5	120/206 (58%)	92 (77%)	24 (20%)	4 (3%)	5	30
47	H8	142/206 (69%)	120 (84%)	15 (11%)	7 (5%)	3	20
48	E5	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
48	I8	76/85 (89%)	67 (88%)	8 (10%)	1 (1%)	15	57
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	8	43
49	J8	92/98 (94%)	88 (96%)	3 (3%)	1 (1%)	17	61
50	G5	67/72 (93%)	60 (90%)	5 (8%)	2 (3%)	5	34
50	K8	66/72 (92%)	62 (94%)	3 (4%)	1 (2%)	13	53
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	M8	45/71 (63%)	26 (58%)	18 (40%)	1 (2%)	8	43
53	J5	54/60 (90%)	47 (87%)	7 (13%)	0	100	100
53	N8	47/60 (78%)	43 (92%)	4 (8%)	0	100	100
54	L5	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
54	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	3	20
55	Q8	62/65 (95%)	54 (87%)	4 (6%)	4 (6%)	1	12
All	All	10880/12104 (90%)	9578 (88%)	1134 (10%)	168 (2%)	13	53

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3E	88	VAL
18	9I	22	VAL
29	11	40	THR
29	11	237	GLU
37	78	16	ARG

### 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	182/220 (83%)	138 (76%)	44 (24%)	1	3
2	1E	200/220 (91%)	152 (76%)	48 (24%)	1	3
3	22	153/188 (81%)	126 (82%)	27 (18%)	2	11
3	2E	159/188 (85%)	129 (81%)	30 (19%)	2	10
4	32	180/181 (99%)	145 (81%)	35 (19%)	2	9
4	3E	180/181 (99%)	149 (83%)	31 (17%)	2	12
5	42	113/123 (92%)	85 (75%)	28 (25%)	1	3
5	4E	115/123 (94%)	91 (79%)	24 (21%)	1	7
6	52	90/90 (100%)	80 (89%)	10 (11%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5E	90/90 (100%)	80 (89%)	10 (11%)	8	31
7	62	114/127 (90%)	94 (82%)	20 (18%)	2	11
7	6E	123/127 (97%)	91 (74%)	32 (26%)	0	2
8	72	119/119 (100%)	98 (82%)	21 (18%)	2	11
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	7
9	82	95/99 (96%)	75 (79%)	20 (21%)	1	7
9	8E	97/99 (98%)	70 (72%)	27 (28%)	0	2
10	1A	69/92 (75%)	53 (77%)	16 (23%)	1	4
10	1I	81/92 (88%)	62 (76%)	19 (24%)	1	4
11	2A	85/99 (86%)	73 (86%)	12 (14%)	4	19
11	2I	84/99 (85%)	68 (81%)	16 (19%)	2	10
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	9
12	3I	103/109 (94%)	81 (79%)	22 (21%)	1	6
13	4A	91/101 (90%)	65 (71%)	26 (29%)	0	1
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	6
14	5A	47/50 (94%)	31 (66%)	16 (34%)	0	0
14	5I	49/50 (98%)	40 (82%)	9 (18%)	2	10
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9	35
15	6I	79/80 (99%)	68 (86%)	11 (14%)	4	20
16	7A	72/74 (97%)	62 (86%)	10 (14%)	4	20
16	7I	69/74 (93%)	50 (72%)	19 (28%)	0	2
17	8A	94/97 (97%)	82 (87%)	12 (13%)	5	24
17	8I	94/97 (97%)	73 (78%)	21 (22%)	1	5
18	9A	58/77 (75%)	45 (78%)	13 (22%)	1	5
18	9I	58/77 (75%)	48 (83%)	10 (17%)	2	12
19	AA	52/80 (65%)	34 (65%)	18 (35%)	0	0
19	AI	70/80 (88%)	57 (81%)	13 (19%)	2	10
20	BA	76/82 (93%)	65 (86%)	11 (14%)	4	18
20	BI	75/82 (92%)	62 (83%)	13 (17%)	2	12
21	1B	19/22 (86%)	16 (84%)	3 (16%)	3	14
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	71	109/181 (60%)	76 (70%)	33 (30%)	0	1
29	11	214/218 (98%)	169 (79%)	45 (21%)	1	7
29	19	214/218 (98%)	164 (77%)	50 (23%)	1	4
30	21	165/166 (99%)	128 (78%)	37 (22%)	1	5
30	29	165/166 (99%)	134 (81%)	31 (19%)	2	10
31	31	161/166 (97%)	126 (78%)	35 (22%)	1	6
31	39	163/166 (98%)	128 (78%)	35 (22%)	1	6
32	41	154/156 (99%)	118 (77%)	36 (23%)	1	4
32	49	154/156 (99%)	123 (80%)	31 (20%)	1	8
33	51	144/148 (97%)	113 (78%)	31 (22%)	1	6
33	59	56/148 (38%)	41 (73%)	15 (27%)	0	2
34	61	122/124 (98%)	93 (76%)	29 (24%)	1	4
34	69	122/124 (98%)	90 (74%)	32 (26%)	0	2
35	15	116/119 (98%)	92 (79%)	24 (21%)	1	7
35	58	117/119 (98%)	91 (78%)	26 (22%)	1	5
36	25	100/100 (100%)	85 (85%)	15 (15%)	3	17
36	68	100/100 (100%)	82 (82%)	18 (18%)	2	11
37	35	115/116 (99%)	82 (71%)	33 (29%)	0	1
37	78	114/116 (98%)	79 (69%)	35 (31%)	0	1
38	45	109/111 (98%)	85 (78%)	24 (22%)	1	6
38	88	109/111 (98%)	89 (82%)	20 (18%)	2	10
39	55	101/101 (100%)	81 (80%)	20 (20%)	1	8
39	98	101/101 (100%)	76 (75%)	25 (25%)	1	3
40	65	87/88 (99%)	66 (76%)	21 (24%)	1	3
40	A8	87/88 (99%)	60 (69%)	27 (31%)	0	1
41	75	119/127 (94%)	88 (74%)	31 (26%)	0	2
41	B8	118/127 (93%)	87 (74%)	31 (26%)	0	2
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	12
42	C8	92/94 (98%)	77 (84%)	15 (16%)	3	13
43	95	81/82 (99%)	61 (75%)	20 (25%)	1	3
43	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	A5	91/92 (99%)	74 (81%)	17 (19%)	2	10
44	E8	91/92 (99%)	71 (78%)	20 (22%)	1	6
45	B5	75/78 (96%)	60 (80%)	15 (20%)	1	8
45	F8	76/78 (97%)	63 (83%)	13 (17%)	2	12
46	C5	85/91 (93%)	62 (73%)	23 (27%)	0	2
46	G8	84/91 (92%)	59 (70%)	25 (30%)	0	1
47	D5	115/179 (64%)	82 (71%)	33 (29%)	0	1
47	H8	137/179 (76%)	103 (75%)	34 (25%)	1	3
48	E5	62/67 (92%)	51 (82%)	11 (18%)	2	11
48	I8	62/67 (92%)	50 (81%)	12 (19%)	2	9
49	F5	79/83 (95%)	56 (71%)	23 (29%)	0	1
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	11
50	G5	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	K8	63/67 (94%)	43 (68%)	20 (32%)	0	1
51	H5	50/52 (96%)	42 (84%)	8 (16%)	3	14
51	L8	50/52 (96%)	42 (84%)	8 (16%)	3	14
52	M8	42/63 (67%)	34 (81%)	8 (19%)	2	10
53	J5	48/52 (92%)	39 (81%)	9 (19%)	2	10
53	N8	44/52 (85%)	32 (73%)	12 (27%)	0	2
54	L5	38/42 (90%)	32 (84%)	6 (16%)	3	14
54	P8	38/42 (90%)	31 (82%)	7 (18%)	2	10
55	M5	54/55 (98%)	37 (68%)	17 (32%)	0	1
55	Q8	54/55 (98%)	40 (74%)	14 (26%)	0	2
All	All	9210/10012 (92%)	7199 (78%)	2011 (22%)	1	6

5 of 2011 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	G8	33	LYS
3	22	181	ASN
46	C5	11	ASP
47	H8	19	ARG
52	M8	34	GLU

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

Mol	Chain	Res	Type
2	12	135	GLN
3	22	181	ASN
32	49	79	ASN
2	12	19	HIS
40	65	95	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	374 (25%)	34 (2%)
1	1G	1505/1522 (98%)	376 (24%)	30 (1%)
22	1K	64/76 (84%)	31 (48%)	3 (4%)
23	2K	76/77 (98%)	22 (28%)	3 (3%)
23	2L	74/77 (96%)	19 (25%)	3 (4%)
24	3K	75/76 (98%)	43 (57%)	2 (2%)
25	4K	19/27 (70%)	9 (47%)	2 (10%)
25	4L	16/27 (59%)	7 (43%)	0
26	14	2852/2917 (97%)	732 (25%)	47 (1%)
26	1H	2828/2917 (96%)	709 (25%)	52 (1%)
27	16	121/122 (99%)	25 (20%)	2 (1%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	31 (43%)	4 (5%)
57	3L	72/76 (94%)	21 (29%)	2 (2%)
All	All	9387/9634 (97%)	2440 (25%)	186 (1%)

5 of 2440 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	11	G
1	13	31	G

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2060	A
1	1G	266	G
26	14	2135	A

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Mol	Chain	Res	Type
26	1H	2210	G
26	1H	2598	A

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

18 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	U8U	1K	34	25,22	15,24,25	2.55	3 (20%)	17,34,37	2.10	3 (17%)
22	T6A	1K	37	22	23,34,35	2.50	4 (17%)	26,49,52	3.83	9 (34%)
22	PSU	1K	39	22	15,21,22	0.97	1 (6%)	16,30,33	1.97	4 (25%)
22	5MU	1K	54	22	13,22,23	1.64	2 (15%)	16,32,35	1.49	1 (6%)
22	PSU	1K	55	22	15,21,22	1.11	1 (6%)	16,30,33	2.40	3 (18%)
56	5MU	1L	54	56	13,22,23	1.70	2 (15%)	16,32,35	1.56	1 (6%)
56	PSU	1L	55	56	15,21,22	0.97	1 (6%)	16,30,33	2.06	3 (18%)
23	OMC	2K	33	23	15,22,23	2.16	4 (26%)	20,31,34	1.55	3 (15%)
23	7MG	2K	47	23	20,26,27	3.36	6 (30%)	23,39,42	2.25	7 (30%)
23	5MU	2K	55	23	13,22,23	1.69	2 (15%)	16,32,35	1.42	1 (6%)
23	PSU	2K	56	23	15,21,22	1.12	1 (6%)	16,30,33	2.12	2 (12%)
23	4SU	2K	8	23	12,21,22	3.31	2 (16%)	15,30,33	0.90	1 (6%)
23	OMC	2L	33	23	15,22,23	2.40	4 (26%)	20,31,34	1.31	2 (10%)
23	7MG	2L	47	23	20,26,27	3.34	7 (35%)	23,39,42	2.31	7 (30%)
23	5MU	2L	55	23	13,22,23	1.68	2 (15%)	16,32,35	1.46	1 (6%)
23	PSU	2L	56	23	15,21,22	1.15	1 (6%)	16,30,33	1.98	3 (18%)
23	4SU	2L	8	23	12,21,22	3.28	2 (16%)	15,30,33	1.04	1 (6%)
57	PSU	3L	39	57	15,21,22	1.06	1 (6%)	16,30,33	2.00	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
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	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
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C5-C4	-5.70	1.24	1.39
23	2K	47	7MG	C5-C4	-5.43	1.24	1.39
22	1K	37	T6A	C5-C4	-3.39	1.32	1.40
23	2L	55	5MU	C4-N3	-2.97	1.27	1.33
56	1L	54	5MU	C4-N3	-2.93	1.27	1.33

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	T6A	N3-C2-N1	-14.01	117.86	128.87
22	1K	34	U8U	C5-C4-N3	-6.61	119.26	125.19
22	1K	37	T6A	C6-N6-C10	-6.58	121.44	130.33
23	2L	47	7MG	C5-C4-N3	-6.20	120.43	126.74
22	1K	55	PSU	C5-C1'-C2'	-4.68	107.49	115.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	T6A	1	0
22	1K	54	5MU	3	0
22	1K	55	PSU	1	0
23	2K	33	OMC	1	0
23	2K	47	7MG	1	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	1	0
23	2L	47	7MG	1	0
23	2L	55	5MU	1	0
23	2L	8	4SU	2	0
57	3L	39	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	SF4	32	301	-	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
59	SF4	32	301	-	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1496/1522 (98%)	-0.52	3 (0%) 95 94	61, 106, 170, 196	0
1	1G	1507/1522 (99%)	-0.57	2 (0%) 95 95	74, 126, 175, 200	0
2	12	208/256 (81%)	0.59	23 (11%) 7 3	134, 156, 168, 176	0
2	1E	231/256 (90%)	1.07	42 (18%) 2 1	116, 144, 162, 166	0
3	22	194/239 (81%)	0.03	8 (4%) 41 25	129, 148, 164, 167	0
3	2E	205/239 (85%)	-0.25	3 (1%) 76 62	89, 111, 139, 148	0
4	32	208/209 (99%)	1.11	44 (21%) 1 1	105, 125, 146, 151	0
4	3E	208/209 (99%)	0.18	8 (3%) 44 27	85, 106, 126, 135	0
5	42	147/162 (90%)	0.04	3 (2%) 68 52	112, 126, 138, 145	0
5	4E	149/162 (91%)	0.22	3 (2%) 68 52	81, 103, 122, 131	0
6	52	101/101 (100%)	0.14	2 (1%) 68 52	92, 111, 128, 134	0
6	5E	100/101 (99%)	1.07	21 (21%) 1 1	90, 109, 127, 132	0
7	62	138/156 (88%)	-0.15	0 100 100	122, 133, 142, 148	0
7	6E	149/156 (95%)	0.04	5 (3%) 49 32	107, 124, 143, 149	0
8	72	138/138 (100%)	-0.22	1 (0%) 89 82	112, 131, 141, 149	0
8	7E	138/138 (100%)	1.36	44 (31%) 1 0	92, 115, 130, 139	0
9	82	124/128 (96%)	-0.06	4 (3%) 51 34	121, 153, 162, 166	0
9	8E	127/128 (99%)	-0.38	1 (0%) 87 79	91, 137, 154, 159	0
10	1A	78/105 (74%)	-0.26	8 (10%) 9 4	119, 148, 159, 161	0
10	1I	91/105 (86%)	0.39	9 (9%) 9 4	87, 128, 157, 163	0
11	2A	113/129 (87%)	0.46	5 (4%) 38 22	89, 115, 135, 141	0
11	2I	111/129 (86%)	1.18	25 (22%) 1 1	82, 110, 127, 140	0
12	3A	121/132 (91%)	0.62	17 (14%) 4 2	93, 113, 129, 148	0
12	3I	122/132 (92%)	0.91	15 (12%) 5 3	72, 80, 103, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	110/126 (87%)	0.35	14 (12%) 5 2	135, 149, 160, 164	0
13	4I	116/126 (92%)	-0.26	0 100 100	94, 127, 141, 150	0
14	5A	57/61 (93%)	1.33	18 (31%) 1 0	134, 146, 155, 158	0
14	5I	61/61 (100%)	-0.57	0 100 100	86, 100, 118, 123	0
15	6A	87/89 (97%)	0.27	3 (3%) 49 32	93, 119, 139, 144	0
15	6I	88/89 (98%)	1.54	28 (31%) 1 0	81, 104, 125, 134	0
16	7A	84/88 (95%)	0.03	0 100 100	95, 114, 137, 148	0
16	7I	80/88 (90%)	-0.18	0 100 100	101, 115, 133, 142	0
17	8A	99/105 (94%)	0.39	3 (3%) 54 37	102, 119, 130, 135	0
17	8I	99/105 (94%)	0.86	14 (14%) 4 2	93, 109, 125, 130	0
18	9A	67/88 (76%)	-0.19	0 100 100	101, 118, 136, 139	0
18	9I	67/88 (76%)	0.18	1 (1%) 76 62	94, 112, 132, 136	0
19	AA	60/93 (64%)	0.57	7 (11%) 6 3	133, 161, 167, 171	0
19	AI	80/93 (86%)	-0.85	0 100 100	105, 121, 143, 150	0
20	BA	98/106 (92%)	0.52	5 (5%) 32 17	87, 115, 141, 154	0
20	BI	97/106 (91%)	0.33	5 (5%) 31 16	114, 126, 152, 156	0
21	1B	24/27 (88%)	0.66	3 (12%) 5 3	128, 144, 156, 160	0
21	1F	23/27 (85%)	-0.07	0 100 100	106, 114, 122, 128	0
22	1K	64/76 (84%)	0.02	2 (3%) 52 36	96, 170, 182, 184	0
23	2K	72/77 (93%)	-0.29	0 100 100	74, 103, 134, 154	0
23	2L	71/77 (92%)	-0.16	0 100 100	84, 121, 153, 157	0
24	3K	76/76 (100%)	0.35	10 (13%) 4 2	79, 183, 195, 202	0
25	4K	20/27 (74%)	0.37	2 (10%) 9 4	78, 145, 186, 186	0
25	4L	17/27 (62%)	0.47	0 100 100	104, 160, 189, 189	0
26	14	2861/2917 (98%)	-0.28	16 (0%) 90 84	54, 88, 183, 207	0
26	1H	2833/2917 (97%)	-0.36	7 (0%) 95 94	45, 77, 169, 200	0
27	16	122/122 (100%)	-0.63	1 (0%) 87 79	70, 97, 122, 187	0
27	1J	122/122 (100%)	-0.55	1 (0%) 87 79	94, 131, 151, 186	0
28	7I	133/229 (58%)	0.49	13 (9%) 10 5	126, 158, 171, 177	0
29	11	274/276 (99%)	1.01	34 (12%) 5 3	47, 69, 89, 99	0
29	19	273/276 (98%)	0.53	10 (3%) 45 28	51, 76, 92, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	21	204/206 (99%)	1.44	63 (30%) 1 0	52, 92, 133, 150	0
30	29	204/206 (99%)	0.09	2 (0%) 84 74	59, 96, 131, 135	0
31	31	202/210 (96%)	0.48	10 (4%) 32 17	51, 81, 113, 135	0
31	39	205/210 (97%)	0.10	1 (0%) 91 87	61, 104, 144, 171	0
32	41	180/182 (98%)	0.11	4 (2%) 65 49	90, 110, 144, 155	0
32	49	180/182 (98%)	1.40	47 (26%) 1 0	124, 143, 162, 169	0
33	51	173/180 (96%)	0.31	11 (6%) 23 11	87, 109, 124, 137	0
33	59	69/180 (38%)	0.41	15 (21%) 1 1	136, 158, 168, 170	0
34	61	145/148 (97%)	-0.18	3 (2%) 67 50	84, 133, 147, 158	0
34	69	145/148 (97%)	0.69	25 (17%) 2 1	87, 127, 146, 152	0
35	15	137/140 (97%)	0.45	4 (2%) 55 39	78, 109, 138, 155	0
35	58	138/140 (98%)	1.14	31 (22%) 1 1	69, 92, 132, 145	0
36	25	122/122 (100%)	0.53	4 (3%) 50 33	70, 92, 109, 116	0
36	68	122/122 (100%)	0.86	16 (13%) 5 2	60, 81, 99, 113	0
37	35	148/150 (98%)	2.27	80 (54%) 0 0	59, 105, 140, 156	0
37	78	147/150 (98%)	-0.09	2 (1%) 78 64	52, 84, 108, 119	0
38	45	138/141 (97%)	2.25	69 (50%) 0 0	75, 110, 134, 149	0
38	88	141/141 (100%)	0.13	4 (2%) 56 40	58, 85, 105, 122	0
39	55	118/118 (100%)	0.49	6 (5%) 32 17	64, 84, 102, 119	0
39	98	118/118 (100%)	1.89	52 (44%) 0 0	66, 87, 108, 130	0
40	65	110/112 (98%)	0.80	15 (13%) 4 2	92, 120, 137, 143	0
40	A8	111/112 (99%)	0.64	11 (9%) 9 4	75, 93, 115, 135	0
41	75	136/146 (93%)	0.71	11 (8%) 15 7	80, 100, 138, 155	0
41	B8	134/146 (91%)	0.17	6 (4%) 37 21	74, 95, 137, 155	0
42	85	116/118 (98%)	0.47	8 (6%) 20 10	68, 97, 129, 138	0
42	C8	115/118 (97%)	-0.11	2 (1%) 73 59	57, 83, 110, 117	0
43	95	99/101 (98%)	1.11	19 (19%) 2 1	65, 123, 136, 145	0
43	D8	100/101 (99%)	0.69	10 (10%) 9 4	59, 102, 124, 139	0
44	A5	111/113 (98%)	0.10	0 100 100	65, 77, 107, 135	0
44	E8	112/113 (99%)	0.15	2 (1%) 71 56	61, 75, 105, 140	0
45	B5	94/96 (97%)	0.29	2 (2%) 67 50	69, 90, 111, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	F8	96/96 (100%)	0.25	0 100 100	53, 74, 112, 125	0
46	C5	104/110 (94%)	0.62	13 (12%) 5 3	91, 119, 148, 157	0
46	G8	103/110 (93%)	0.37	3 (2%) 55 39	74, 93, 127, 130	0
47	D5	126/206 (61%)	1.43	43 (34%) 0 0	117, 137, 159, 164	0
47	H8	148/206 (71%)	0.08	1 (0%) 89 82	86, 121, 154, 160	0
48	E5	78/85 (91%)	0.89	13 (16%) 2 1	73, 93, 110, 138	0
48	I8	78/85 (91%)	-0.07	0 100 100	62, 77, 98, 110	0
49	F5	94/98 (95%)	1.07	19 (20%) 1 1	65, 86, 123, 133	0
49	J8	94/98 (95%)	0.18	2 (2%) 67 50	57, 79, 115, 126	0
50	G5	69/72 (95%)	-0.20	1 (1%) 78 64	89, 109, 131, 150	0
50	K8	68/72 (94%)	0.11	1 (1%) 76 62	64, 81, 98, 126	0
51	H5	58/60 (96%)	0.74	4 (6%) 20 10	77, 103, 128, 137	0
51	L8	58/60 (96%)	0.49	4 (6%) 20 10	66, 81, 110, 129	0
52	M8	47/71 (66%)	0.51	2 (4%) 39 23	114, 147, 163, 171	0
53	J5	56/60 (93%)	-0.01	0 100 100	61, 87, 134, 143	0
53	N8	49/60 (81%)	0.96	10 (20%) 1 1	55, 82, 140, 150	0
54	L5	47/49 (95%)	-0.05	0 100 100	57, 62, 79, 91	0
54	P8	47/49 (95%)	-0.17	0 100 100	49, 55, 78, 89	0
55	M5	64/65 (98%)	2.11	34 (53%) 0 0	72, 82, 97, 124	0
55	Q8	64/65 (98%)	0.28	0 100 100	56, 73, 86, 101	0
56	1L	72/76 (94%)	0.39	8 (11%) 7 3	127, 184, 195, 204	0
57	3L	73/76 (96%)	-0.16	2 (2%) 58 42	84, 172, 185, 193	0
All	All	20506/21738 (94%)	0.10	1188 (5%) 26 13	45, 104, 163, 207	0

The worst 5 of 1188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	35	110	TYR	11.7
43	95	1	MET	9.4
43	95	45	THR	9.3
37	35	148	LEU	8.7
38	45	91	GLU	8.0

## 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
56	PSU	1L	55	20/21	0.88	0.12	-	137,155,161,162	0
22	5MU	1K	54	21/22	0.91	0.14	-	118,129,141,147	0
22	PSU	1K	39	20/21	0.93	0.14	-	104,124,130,132	0
23	PSU	2L	56	20/21	0.91	0.15	-	133,136,141,142	0
56	5MU	1L	54	21/22	0.92	0.11	-	143,156,161,162	0
22	T6A	1K	37	32/33	0.91	0.18	-	89,102,123,128	0
57	PSU	3L	39	20/21	0.91	0.13	-	147,156,160,160	0
22	U8U	1K	34	23/24	0.96	0.14	-	88,99,103,104	0
23	5MU	2K	55	21/22	0.94	0.15	-	117,123,131,135	0
23	7MG	2L	47	24/25	0.96	0.13	-	133,141,147,149	0
23	7MG	2K	47	24/25	0.94	0.16	-	103,111,119,127	0
23	5MU	2L	55	21/22	0.94	0.12	-	131,139,146,151	0
23	4SU	2K	8	20/21	0.93	0.18	-	90,100,108,111	0
23	PSU	2K	56	20/21	0.91	0.12	-	103,115,124,125	0
23	OMC	2K	33	21/22	0.96	0.20	-	80,86,90,95	0
23	4SU	2L	8	20/21	0.90	0.16	-	110,128,130,136	0
23	OMC	2L	33	21/22	0.93	0.17	-	106,117,118,119	0
22	PSU	1K	55	20/21	0.86	0.12	-	121,129,137,142	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
58	MG	14	3242	1/1	0.87	1.24	61.06	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1644	1/1	0.92	0.47	48.91	93,93,93,93	0
58	MG	14	3277	1/1	0.72	0.65	38.22	98,98,98,98	0
58	MG	1H	3070	1/1	0.88	0.36	32.15	68,68,68,68	0
58	MG	14	3252	1/1	0.88	0.90	30.88	82,82,82,82	0
58	MG	1H	3137	1/1	0.95	0.46	30.62	56,56,56,56	0
58	MG	1H	3028	1/1	0.92	0.45	29.59	63,63,63,63	0
58	MG	1H	3333	1/1	0.83	0.63	28.77	88,88,88,88	0
58	MG	1H	3014	1/1	0.95	0.35	28.19	80,80,80,80	0
58	MG	13	1699	1/1	0.92	0.31	26.78	88,88,88,88	0
58	MG	14	3216	1/1	0.73	0.55	26.36	58,58,58,58	0
58	MG	1H	3258	1/1	0.90	0.58	26.34	66,66,66,66	0
58	MG	14	3075	1/1	0.98	0.41	26.16	60,60,60,60	0
58	MG	14	3164	1/1	0.83	0.52	26.13	70,70,70,70	0
58	MG	1H	3344	1/1	0.90	0.47	23.65	57,57,57,57	0
58	MG	14	3255	1/1	0.90	0.52	23.62	79,79,79,79	0
58	MG	1H	3089	1/1	0.96	0.36	22.86	50,50,50,50	0
58	MG	1H	3131	1/1	0.92	0.52	21.42	59,59,59,59	0
58	MG	14	3224	1/1	0.92	0.55	20.92	59,59,59,59	0
58	MG	13	1686	1/1	0.41	0.36	20.87	94,94,94,94	0
58	MG	14	3178	1/1	0.97	0.41	20.11	65,65,65,65	0
58	MG	13	1638	1/1	0.96	0.33	19.28	80,80,80,80	0
58	MG	1H	3042	1/1	0.88	0.47	19.24	67,67,67,67	0
58	MG	1H	3053	1/1	0.99	0.31	18.49	54,54,54,54	0
58	MG	14	3179	1/1	0.93	0.31	18.45	91,91,91,91	0
58	MG	1H	3012	1/1	0.91	0.29	18.36	57,57,57,57	0
58	MG	1H	3347	1/1	0.75	0.36	17.62	66,66,66,66	0
58	MG	1H	3237	1/1	0.98	0.32	17.52	72,72,72,72	0
58	MG	14	3249	1/1	0.67	0.35	17.15	93,93,93,93	0
58	MG	13	1645	1/1	0.88	0.38	16.40	75,75,75,75	0
58	MG	14	3143	1/1	0.95	0.33	16.17	60,60,60,60	0
58	MG	1H	3001	1/1	0.98	0.39	16.09	52,52,52,52	0
58	MG	14	3186	1/1	0.74	0.47	16.06	63,63,63,63	0
58	MG	1H	3099	1/1	0.72	0.40	15.67	57,57,57,57	0
58	MG	14	3057	1/1	0.95	0.42	15.12	64,64,64,64	0
58	MG	1H	3036	1/1	0.97	0.35	14.74	126,126,126,126	0
58	MG	14	3097	1/1	0.98	0.35	14.37	49,49,49,49	0
58	MG	1H	3154	1/1	0.94	0.34	14.27	42,42,42,42	0
58	MG	1H	3253	1/1	0.95	0.28	14.09	62,62,62,62	0
58	MG	14	3054	1/1	0.91	0.40	14.07	54,54,54,54	0
58	MG	1H	3195	1/1	0.93	0.40	13.80	85,85,85,85	0
58	MG	1H	3309	1/1	0.63	0.33	13.73	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
58	MG	1H	3186	1/1	0.90	0.24	13.26	58,58,58,58	0
58	MG	1H	3191	1/1	0.83	0.40	12.79	67,67,67,67	0
58	MG	14	3206	1/1	0.93	0.47	12.74	71,71,71,71	0
58	MG	1H	3054	1/1	0.97	0.38	12.71	45,45,45,45	0
58	MG	14	3009	1/1	0.90	0.57	12.67	73,73,73,73	0
58	MG	1H	3179	1/1	0.97	0.32	12.61	76,76,76,76	0
58	MG	1H	3088	1/1	0.98	0.28	12.40	58,58,58,58	0
58	MG	1H	3074	1/1	0.92	0.41	12.25	44,44,44,44	0
58	MG	1G	1602	1/1	0.91	0.43	12.16	79,79,79,79	0
58	MG	1H	3094	1/1	0.88	0.30	12.15	62,62,62,62	0
58	MG	1H	3168	1/1	0.77	0.33	12.10	70,70,70,70	0
58	MG	1K	101	1/1	0.56	0.45	12.01	147,147,147,147	0
58	MG	14	3205	1/1	0.86	0.40	11.86	63,63,63,63	0
58	MG	1H	3124	1/1	0.75	0.31	11.85	56,56,56,56	0
58	MG	1H	3479	1/1	0.74	0.20	11.50	102,102,102,102	0
58	MG	14	3258	1/1	0.94	0.25	11.45	100,100,100,100	0
58	MG	14	3004	1/1	0.98	0.42	11.43	57,57,57,57	0
58	MG	14	3038	1/1	0.98	0.41	11.24	59,59,59,59	0
58	MG	1H	3285	1/1	0.82	0.33	11.01	61,61,61,61	0
58	MG	13	1677	1/1	0.98	0.28	10.86	71,71,71,71	0
58	MG	14	3160	1/1	0.90	0.30	10.73	76,76,76,76	0
58	MG	2K	101	1/1	0.97	0.37	10.57	72,72,72,72	0
58	MG	14	3067	1/1	0.98	0.35	10.53	60,60,60,60	0
58	MG	1H	3029	1/1	0.95	0.54	10.52	67,67,67,67	0
58	MG	14	3253	1/1	0.71	0.33	10.51	84,84,84,84	0
58	MG	1H	3016	1/1	0.98	0.28	10.49	52,52,52,52	0
58	MG	14	3073	1/1	0.96	0.46	10.31	57,57,57,57	0
58	MG	14	3212	1/1	0.84	0.32	10.15	63,63,63,63	0
58	MG	2L	101	1/1	0.94	0.46	10.14	81,81,81,81	0
58	MG	1H	3343	1/1	0.94	0.28	9.93	77,77,77,77	0
58	MG	13	1697	1/1	0.93	0.34	9.85	95,95,95,95	0
58	MG	14	3194	1/1	0.55	0.31	9.81	74,74,74,74	0
58	MG	13	1694	1/1	0.64	0.48	9.79	88,88,88,88	0
58	MG	13	1608	1/1	0.81	0.27	9.59	86,86,86,86	0
58	MG	14	3015	1/1	0.97	0.40	9.42	67,67,67,67	0
58	MG	1H	3240	1/1	0.95	0.26	9.40	49,49,49,49	0
58	MG	1H	3079	1/1	0.86	0.34	9.21	51,51,51,51	0
58	MG	14	3198	1/1	0.93	0.37	9.16	69,69,69,69	0
58	MG	1H	3225	1/1	0.89	0.32	9.12	56,56,56,56	0
58	MG	1H	3100	1/1	0.98	0.35	8.98	38,38,38,38	0
58	MG	1H	3061	1/1	0.94	0.28	8.86	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3074	1/1	0.96	0.49	8.73	48,48,48,48	0
58	MG	1H	3071	1/1	0.89	0.29	8.72	80,80,80,80	0
58	MG	1H	3291	1/1	0.97	0.34	8.71	64,64,64,64	0
58	MG	14	3029	1/1	0.96	0.38	8.51	49,49,49,49	0
58	MG	1H	3019	1/1	0.87	0.35	8.47	64,64,64,64	0
58	MG	1H	3142	1/1	0.95	0.28	8.45	62,62,62,62	0
58	MG	14	3190	1/1	0.75	0.27	8.33	106,106,106,106	0
58	MG	14	3007	1/1	0.98	0.29	8.30	52,52,52,52	0
58	MG	14	3157	1/1	0.95	0.43	8.30	67,67,67,67	0
58	MG	1H	3082	1/1	0.96	0.30	8.27	80,80,80,80	0
58	MG	14	3006	1/1	0.97	0.38	8.08	47,47,47,47	0
58	MG	14	3176	1/1	0.90	0.42	8.04	92,92,92,92	0
58	MG	1G	1614	1/1	0.91	0.24	7.90	120,120,120,120	0
58	MG	1H	3246	1/1	0.64	0.21	7.83	75,75,75,75	0
58	MG	14	3185	1/1	0.93	0.24	7.79	87,87,87,87	0
58	MG	13	1613	1/1	0.97	0.23	7.79	76,76,76,76	0
58	MG	14	3287	1/1	0.83	0.42	7.76	83,83,83,83	0
58	MG	14	3149	1/1	0.75	0.20	7.62	83,83,83,83	0
58	MG	1H	3085	1/1	0.83	0.29	7.39	59,59,59,59	0
58	MG	1H	3226	1/1	0.86	0.26	7.03	74,74,74,74	0
58	MG	1H	3155	1/1	0.84	0.25	7.00	71,71,71,71	0
58	MG	1H	3115	1/1	0.97	0.37	7.00	62,62,62,62	0
58	MG	1H	3273	1/1	0.94	0.31	6.88	80,80,80,80	0
58	MG	14	3213	1/1	0.82	0.25	6.74	72,72,72,72	0
58	MG	14	3050	1/1	0.96	0.43	6.73	71,71,71,71	0
58	MG	13	1622	1/1	0.85	0.17	6.61	109,109,109,109	0
58	MG	13	1654	1/1	0.91	0.27	6.47	76,76,76,76	0
58	MG	1G	1653	1/1	0.98	0.34	6.47	86,86,86,86	0
58	MG	14	3085	1/1	0.90	0.27	6.37	54,54,54,54	0
58	MG	14	3158	1/1	0.68	0.30	6.33	69,69,69,69	0
58	MG	14	3003	1/1	0.95	0.31	6.29	74,74,74,74	0
58	MG	N8	101	1/1	0.96	0.32	5.93	67,67,67,67	0
58	MG	14	3192	1/1	0.92	0.32	5.85	69,69,69,69	0
58	MG	14	3233	1/1	0.96	0.30	5.82	79,79,79,79	0
58	MG	1H	3236	1/1	0.71	0.24	5.74	76,76,76,76	0
58	MG	14	3083	1/1	0.98	0.30	5.69	67,67,67,67	0
58	MG	14	3095	1/1	0.96	0.30	5.61	83,83,83,83	0
58	MG	14	3024	1/1	0.97	0.26	5.57	58,58,58,58	0
58	MG	14	3079	1/1	0.98	0.30	5.43	63,63,63,63	0
58	MG	1H	3174	1/1	0.87	0.31	5.34	93,93,93,93	0
58	MG	14	3215	1/1	0.94	0.26	5.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3117	1/1	0.98	0.29	5.29	62,62,62,62	0
58	MG	1H	3010	1/1	0.94	0.29	5.27	57,57,57,57	0
58	MG	1H	3080	1/1	0.89	0.20	5.24	65,65,65,65	0
58	MG	14	3037	1/1	0.94	0.23	5.14	55,55,55,55	0
58	MG	14	3030	1/1	0.98	0.26	5.10	65,65,65,65	0
58	MG	1H	3097	1/1	0.99	0.27	4.91	56,56,56,56	0
58	MG	1G	1678	1/1	0.57	0.20	4.72	120,120,120,120	0
58	MG	14	3260	1/1	0.89	0.23	4.63	65,65,65,65	0
58	MG	13	1639	1/1	0.98	0.33	4.59	80,80,80,80	0
58	MG	14	3193	1/1	0.92	0.24	4.55	69,69,69,69	0
58	MG	1H	3046	1/1	0.98	0.29	4.53	55,55,55,55	0
58	MG	14	3099	1/1	0.96	0.27	4.53	69,69,69,69	0
58	MG	1G	1632	1/1	0.86	0.34	4.49	106,106,106,106	0
58	MG	13	1664	1/1	0.94	0.25	4.48	82,82,82,82	0
58	MG	14	3123	1/1	0.52	0.34	4.43	79,79,79,79	0
58	MG	1H	3051	1/1	0.97	0.32	4.42	45,45,45,45	0
58	MG	1G	1649	1/1	0.95	0.25	4.38	97,97,97,97	0
58	MG	13	1646	1/1	0.85	0.19	4.30	93,93,93,93	0
58	MG	14	3063	1/1	0.96	0.23	4.20	73,73,73,73	0
58	MG	16	204	1/1	0.79	0.29	4.20	80,80,80,80	0
58	MG	14	3177	1/1	0.87	0.28	4.19	75,75,75,75	0
58	MG	29	302	1/1	0.70	0.49	4.14	74,74,74,74	0
58	MG	13	1672	1/1	0.92	0.20	3.91	112,112,112,112	0
58	MG	14	3078	1/1	0.94	0.39	3.90	76,76,76,76	0
58	MG	1H	3134	1/1	0.76	0.24	3.88	58,58,58,58	0
58	MG	1H	3180	1/1	0.89	0.23	3.87	71,71,71,71	0
58	MG	1H	3167	1/1	0.90	0.24	3.82	78,78,78,78	0
58	MG	1H	3270	1/1	0.96	0.24	3.78	43,43,43,43	0
58	MG	1H	3017	1/1	0.94	0.28	3.71	54,54,54,54	0
58	MG	14	3165	1/1	0.85	0.26	3.57	47,47,47,47	0
58	MG	1H	3443	1/1	0.83	0.23	3.47	86,86,86,86	0
58	MG	1G	1626	1/1	0.99	0.20	3.46	93,93,93,93	0
58	MG	14	3035	1/1	0.96	0.20	3.37	72,72,72,72	0
58	MG	1H	3348	1/1	0.82	0.27	3.26	63,63,63,63	0
58	MG	1H	3065	1/1	0.89	0.20	3.20	64,64,64,64	0
58	MG	1H	3116	1/1	0.96	0.29	3.08	71,71,71,71	0
58	MG	39	301	1/1	0.88	0.33	3.05	66,66,66,66	0
58	MG	1H	3303	1/1	0.81	0.53	2.95	99,99,99,99	0
58	MG	13	1741	1/1	0.87	0.43	2.94	103,103,103,103	0
58	MG	1H	3062	1/1	0.82	0.17	2.93	88,88,88,88	0
58	MG	5I	101	1/1	0.93	0.18	2.93	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
58	MG	14	3056	1/1	0.98	0.33	2.85	50,50,50,50	0
58	MG	1H	3243	1/1	0.94	0.20	2.77	65,65,65,65	0
58	MG	1H	3245	1/1	0.71	0.21	2.66	72,72,72,72	0
58	MG	1H	3260	1/1	0.82	0.22	2.56	60,60,60,60	0
58	MG	1G	1624	1/1	0.94	0.29	2.56	100,100,100,100	0
58	MG	13	1604	1/1	0.94	0.21	2.40	86,86,86,86	0
58	MG	1H	3086	1/1	0.70	0.32	2.36	59,59,59,59	0
58	MG	14	3016	1/1	0.77	0.21	2.31	61,61,61,61	0
58	MG	1H	3084	1/1	0.82	0.25	2.28	49,49,49,49	0
58	MG	16	205	1/1	0.85	0.15	2.23	88,88,88,88	0
58	MG	1G	1601	1/1	0.97	0.23	2.13	85,85,85,85	0
58	MG	13	1655	1/1	0.94	0.28	2.09	72,72,72,72	0
58	MG	13	1621	1/1	0.95	0.24	2.06	101,101,101,101	0
58	MG	1G	1608	1/1	0.92	0.18	2.06	97,97,97,97	0
58	MG	14	3049	1/1	0.95	0.22	2.04	63,63,63,63	0
58	MG	1H	3118	1/1	0.95	0.26	1.90	54,54,54,54	0
58	MG	1G	1606	1/1	0.94	0.24	1.81	88,88,88,88	0
58	MG	1H	3058	1/1	0.98	0.27	1.75	54,54,54,54	0
58	MG	14	3291	1/1	0.97	0.23	1.72	55,55,55,55	0
58	MG	1H	3173	1/1	0.94	0.22	1.72	66,66,66,66	0
58	MG	1H	3363	1/1	0.94	0.20	1.65	53,53,53,53	0
58	MG	13	1618	1/1	0.93	0.15	1.62	107,107,107,107	0
58	MG	1G	1661	1/1	0.62	0.11	1.59	96,96,96,96	0
58	MG	1H	3044	1/1	0.97	0.21	1.59	41,41,41,41	0
58	MG	1G	1664	1/1	0.90	0.35	1.58	122,122,122,122	0
58	MG	14	3236	1/1	0.80	0.15	1.55	74,74,74,74	0
58	MG	1H	3215	1/1	0.86	0.28	1.55	67,67,67,67	0
58	MG	1H	3176	1/1	0.71	0.14	1.43	76,76,76,76	0
58	MG	14	3031	1/1	0.99	0.22	1.38	75,75,75,75	0
58	MG	39	302	1/1	0.97	0.25	1.32	96,96,96,96	0
58	MG	1H	3076	1/1	0.96	0.22	1.29	56,56,56,56	0
58	MG	14	3039	1/1	0.86	0.33	1.28	72,72,72,72	0
58	MG	16	202	1/1	0.94	0.17	1.26	90,90,90,90	0
58	MG	Q8	101	1/1	0.91	0.32	1.20	72,72,72,72	0
58	MG	14	3091	1/1	0.96	0.21	1.15	66,66,66,66	0
58	MG	13	1648	1/1	0.98	0.17	1.13	76,76,76,76	0
58	MG	13	1676	1/1	0.90	0.19	1.12	94,94,94,94	0
58	MG	1G	1613	1/1	0.96	0.17	1.11	89,89,89,89	0
58	MG	1G	1634	1/1	0.95	0.24	1.09	85,85,85,85	0
58	MG	13	1634	1/1	0.84	0.19	1.08	81,81,81,81	0
58	MG	13	1727	1/1	0.93	0.20	0.99	79,79,79,79	0
58	MG	1G	1656	1/1	0.93	0.17	0.95	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1637	1/1	0.95	0.33	0.94	82,82,82,82	0
58	MG	1H	3129	1/1	0.95	0.14	0.88	68,68,68,68	0
58	MG	1G	1647	1/1	0.90	0.23	0.85	105,105,105,105	0
58	MG	14	3145	1/1	0.89	0.13	0.82	87,87,87,87	0
58	MG	14	3171	1/1	0.94	0.30	0.80	65,65,65,65	0
58	MG	1H	3113	1/1	0.95	0.20	0.80	52,52,52,52	0
58	MG	1G	1666	1/1	0.95	0.24	0.75	125,125,125,125	0
58	MG	1H	3106	1/1	0.94	0.21	0.75	46,46,46,46	0
58	MG	14	3168	1/1	0.90	0.25	0.71	64,64,64,64	0
58	MG	14	3137	1/1	0.93	0.21	0.69	55,55,55,55	0
58	MG	14	3181	1/1	0.96	0.20	0.65	57,57,57,57	0
58	MG	14	3338	1/1	0.96	0.17	0.51	64,64,64,64	0
58	MG	13	1681	1/1	0.97	0.18	0.48	66,66,66,66	0
58	MG	1H	3289	1/1	0.69	0.17	0.45	91,91,91,91	0
58	MG	1H	3222	1/1	0.86	0.16	0.42	74,74,74,74	0
58	MG	3I	201	1/1	0.93	0.18	0.39	62,62,62,62	0
58	MG	14	3100	1/1	0.96	0.23	0.38	67,67,67,67	0
58	MG	1H	3101	1/1	0.95	0.21	0.35	47,47,47,47	0
58	MG	14	3419	1/1	0.96	0.27	0.35	62,62,62,62	0
58	MG	14	3293	1/1	0.97	0.19	0.34	67,67,67,67	0
60	ZN	5I	102	1/1	0.98	0.16	0.28	92,92,92,92	0
58	MG	13	1640	1/1	0.96	0.20	0.21	63,63,63,63	0
58	MG	14	3244	1/1	0.92	0.20	0.14	78,78,78,78	0
58	MG	14	3128	1/1	0.89	0.15	0.14	65,65,65,65	0
58	MG	14	3175	1/1	0.97	0.24	0.12	88,88,88,88	0
58	MG	1H	3217	1/1	0.92	0.18	-0.01	67,67,67,67	0
58	MG	14	3289	1/1	0.74	0.12	-0.05	99,99,99,99	0
58	MG	1G	1618	1/1	0.97	0.19	-0.05	85,85,85,85	0
58	MG	16	207	1/1	0.93	0.14	-0.07	84,84,84,84	0
58	MG	1G	1676	1/1	0.93	0.13	-0.10	91,91,91,91	0
58	MG	13	1635	1/1	0.97	0.13	-0.13	97,97,97,97	0
58	MG	4I	201	1/1	0.92	0.15	-0.18	84,84,84,84	0
58	MG	14	3336	1/1	0.91	0.20	-0.25	107,107,107,107	0
58	MG	13	1612	1/1	0.98	0.18	-0.30	75,75,75,75	0
58	MG	1G	1610	1/1	0.93	0.18	-0.32	92,92,92,92	0
58	MG	14	3412	1/1	0.85	0.13	-0.37	113,113,113,113	0
58	MG	1H	3192	1/1	0.89	0.14	-0.38	86,86,86,86	0
58	MG	14	3012	1/1	0.90	0.20	-0.43	58,58,58,58	0
58	MG	14	3305	1/1	0.96	0.18	-0.45	51,51,51,51	0
58	MG	13	1658	1/1	0.98	0.15	-0.48	74,74,74,74	0
58	MG	14	3110	1/1	0.91	0.15	-0.49	66,66,66,66	0
58	MG	1H	3227	1/1	0.89	0.23	-0.51	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
58	MG	41	201	1/1	0.92	0.16	-0.51	86,86,86,86	0
58	MG	13	1615	1/1	0.89	0.14	-0.52	85,85,85,85	0
58	MG	14	3367	1/1	0.95	0.17	-0.53	67,67,67,67	0
58	MG	14	3319	1/1	0.98	0.18	-0.56	50,50,50,50	0
59	SF4	3E	301	8/8	0.99	0.20	-0.57	78,90,95,100	0
58	MG	1H	3023	1/1	0.85	0.15	-0.62	78,78,78,78	0
58	MG	1H	3379	1/1	0.78	0.12	-0.63	92,92,92,92	0
58	MG	13	1626	1/1	0.93	0.21	-0.64	62,62,62,62	0
58	MG	1H	3005	1/1	0.91	0.17	-0.68	52,52,52,52	0
58	MG	13	1601	1/1	0.94	0.20	-0.70	72,72,72,72	0
58	MG	1H	3064	1/1	0.92	0.20	-0.75	57,57,57,57	0
58	MG	14	3329	1/1	0.99	0.16	-0.78	75,75,75,75	0
58	MG	1H	3256	1/1	0.93	0.18	-0.79	70,70,70,70	0
59	SF4	32	301	8/8	0.99	0.18	-0.80	119,123,130,133	0
58	MG	13	1630	1/1	0.91	0.21	-0.84	62,62,62,62	0
58	MG	1H	3230	1/1	0.87	0.11	-0.85	85,85,85,85	0
58	MG	14	3320	1/1	0.98	0.14	-0.86	78,78,78,78	0
58	MG	13	1717	1/1	0.92	0.13	-0.88	97,97,97,97	0
58	MG	13	1656	1/1	0.77	0.13	-0.91	83,83,83,83	0
58	MG	1H	3296	1/1	0.86	0.14	-0.96	66,66,66,66	0
58	MG	1G	1663	1/1	0.88	0.09	-0.97	99,99,99,99	0
58	MG	1H	3448	1/1	0.97	0.13	-0.99	67,67,67,67	0
58	MG	1H	3373	1/1	0.97	0.12	-1.02	76,76,76,76	0
58	MG	1H	3378	1/1	0.97	0.12	-1.02	85,85,85,85	0
58	MG	14	3345	1/1	0.86	0.12	-1.05	90,90,90,90	0
58	MG	1H	3007	1/1	0.97	0.11	-1.07	83,83,83,83	0
58	MG	1G	1685	1/1	0.97	0.10	-1.11	109,109,109,109	0
58	MG	1H	3221	1/1	0.83	0.13	-1.11	63,63,63,63	0
58	MG	1H	3361	1/1	0.94	0.17	-1.12	47,47,47,47	0
58	MG	14	3251	1/1	0.95	0.12	-1.12	66,66,66,66	0
60	ZN	G8	201	1/1	0.97	0.16	-1.13	147,147,147,147	0
58	MG	1H	3140	1/1	0.99	0.16	-1.14	61,61,61,61	0
58	MG	14	3415	1/1	0.92	0.17	-1.14	97,97,97,97	0
58	MG	J8	101	1/1	0.95	0.14	-1.15	77,77,77,77	0
60	ZN	5A	101	1/1	0.97	0.11	-1.16	128,128,128,128	0
58	MG	13	1631	1/1	0.93	0.21	-1.16	55,55,55,55	0
58	MG	1H	3238	1/1	0.95	0.14	-1.20	63,63,63,63	0
58	MG	1H	3157	1/1	0.89	0.13	-1.20	67,67,67,67	0
58	MG	88	201	1/1	0.98	0.16	-1.23	75,75,75,75	0
58	MG	14	3360	1/1	0.98	0.12	-1.31	48,48,48,48	0
58	MG	13	1742	1/1	0.88	0.10	-1.32	85,85,85,85	0
58	MG	14	3088	1/1	0.87	0.11	-1.34	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	ZN	C5	201	1/1	0.65	0.08	-1.34	153,153,153,153	0
58	MG	13	1685	1/1	0.84	0.05	-1.36	101,101,101,101	0
58	MG	1H	3073	1/1	0.97	0.17	-1.37	67,67,67,67	0
58	MG	14	3203	1/1	0.98	0.11	-1.39	71,71,71,71	0
58	MG	1H	3419	1/1	0.94	0.10	-1.41	51,51,51,51	0
58	MG	1H	3117	1/1	0.98	0.18	-1.44	68,68,68,68	0
58	MG	1H	3213	1/1	0.97	0.18	-1.45	49,49,49,49	0
58	MG	1H	3390	1/1	0.96	0.10	-1.45	58,58,58,58	0
58	MG	1H	3441	1/1	0.96	0.17	-1.46	78,78,78,78	0
58	MG	1H	3135	1/1	0.94	0.15	-1.47	55,55,55,55	0
58	MG	1H	3111	1/1	0.90	0.17	-1.50	39,39,39,39	0
58	MG	45	202	1/1	0.94	0.11	-1.53	102,102,102,102	0
58	MG	14	3334	1/1	0.78	0.13	-1.54	89,89,89,89	0
58	MG	1H	3424	1/1	0.98	0.13	-1.55	66,66,66,66	0
58	MG	14	3418	1/1	0.97	0.17	-1.60	52,52,52,52	0
58	MG	1G	1691	1/1	0.89	0.07	-1.60	123,123,123,123	0
58	MG	14	3196	1/1	0.98	0.09	-1.60	87,87,87,87	0
58	MG	1H	3139	1/1	0.91	0.15	-1.62	58,58,58,58	0
58	MG	14	3214	1/1	0.96	0.10	-1.64	82,82,82,82	0
58	MG	1H	3350	1/1	0.84	0.15	-1.66	49,49,49,49	0
58	MG	1H	3457	1/1	0.99	0.11	-1.78	75,75,75,75	0
58	MG	1G	1619	1/1	0.92	0.16	-1.78	78,78,78,78	0
58	MG	14	3400	1/1	0.93	0.12	-1.79	82,82,82,82	0
58	MG	14	3033	1/1	0.90	0.16	-1.83	68,68,68,68	0
58	MG	14	3045	1/1	0.93	0.12	-1.83	83,83,83,83	0
58	MG	1G	1672	1/1	0.94	0.09	-1.88	110,110,110,110	0
58	MG	88	202	1/1	0.98	0.07	-1.94	81,81,81,81	0
58	MG	1J	204	1/1	0.88	0.10	-1.95	99,99,99,99	0
58	MG	14	3108	1/1	0.99	0.13	-1.99	77,77,77,77	0
58	MG	1H	3366	1/1	0.97	0.12	-1.99	53,53,53,53	0
58	MG	13	1711	1/1	0.83	0.09	-2.02	102,102,102,102	0
58	MG	14	3349	1/1	0.97	0.13	-2.03	47,47,47,47	0
58	MG	1H	3389	1/1	0.99	0.11	-2.06	50,50,50,50	0
58	MG	14	3046	1/1	0.97	0.11	-2.10	74,74,74,74	0
58	MG	14	3420	1/1	0.94	0.10	-2.15	72,72,72,72	0
58	MG	14	3340	1/1	0.94	0.10	-2.19	72,72,72,72	0
58	MG	1H	3476	1/1	0.94	0.12	-2.22	72,72,72,72	0
58	MG	1H	3432	1/1	0.97	0.12	-2.23	78,78,78,78	0
58	MG	1H	3494	1/1	0.97	0.12	-2.25	44,44,44,44	0
58	MG	14	3169	1/1	0.90	0.10	-2.26	63,63,63,63	0
58	MG	14	3087	1/1	0.96	0.14	-2.27	56,56,56,56	0
58	MG	14	3403	1/1	0.86	0.07	-2.28	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3125	1/1	0.94	0.12	-2.29	60,60,60,60	0
58	MG	14	3308	1/1	0.97	0.15	-2.30	75,75,75,75	0
58	MG	1G	1658	1/1	0.72	0.11	-2.31	99,99,99,99	0
58	MG	14	3174	1/1	0.94	0.15	-2.31	53,53,53,53	0
58	MG	1H	3402	1/1	0.98	0.07	-2.32	60,60,60,60	0
58	MG	1H	3152	1/1	0.97	0.12	-2.34	64,64,64,64	0
58	MG	13	1667	1/1	0.85	0.14	-2.42	90,90,90,90	0
58	MG	14	3180	1/1	0.91	0.10	-2.45	83,83,83,83	0
58	MG	1H	3254	1/1	0.88	0.11	-2.46	58,58,58,58	0
58	MG	1H	3380	1/1	0.98	0.09	-2.47	56,56,56,56	0
58	MG	1H	3121	1/1	0.94	0.12	-2.47	60,60,60,60	0
58	MG	13	1722	1/1	0.98	0.15	-2.47	70,70,70,70	0
58	MG	1H	3278	1/1	0.83	0.15	-2.55	61,61,61,61	0
58	MG	13	1705	1/1	0.88	0.07	-2.58	99,99,99,99	0
58	MG	14	3294	1/1	0.95	0.11	-2.61	65,65,65,65	0
58	MG	1H	3242	1/1	0.95	0.11	-2.70	66,66,66,66	0
58	MG	13	1706	1/1	0.97	0.07	-2.72	80,80,80,80	0
58	MG	1H	3395	1/1	0.97	0.10	-2.75	72,72,72,72	0
58	MG	1H	3374	1/1	0.97	0.12	-2.76	63,63,63,63	0
58	MG	13	1712	1/1	0.98	0.07	-2.79	66,66,66,66	0
58	MG	1H	3444	1/1	0.94	0.14	-2.82	50,50,50,50	0
58	MG	1H	3369	1/1	0.97	0.13	-2.84	49,49,49,49	0
58	MG	13	1703	1/1	0.97	0.12	-2.87	64,64,64,64	0
58	MG	14	3220	1/1	0.85	0.12	-2.89	64,64,64,64	0
58	MG	14	3310	1/1	0.95	0.13	-2.97	59,59,59,59	0
58	MG	1H	3063	1/1	0.91	0.12	-2.97	58,58,58,58	0
58	MG	1G	1675	1/1	0.95	0.13	-2.99	78,78,78,78	0
58	MG	1H	3358	1/1	0.95	0.14	-3.01	54,54,54,54	0
58	MG	1H	3353	1/1	0.97	0.12	-3.09	54,54,54,54	0
58	MG	14	3311	1/1	0.97	0.14	-3.09	62,62,62,62	0
58	MG	14	3421	1/1	0.96	0.05	-3.22	79,79,79,79	0
58	MG	1H	3387	1/1	0.95	0.11	-3.31	51,51,51,51	0
58	MG	1H	3422	1/1	0.82	0.09	-3.33	83,83,83,83	0
58	MG	1H	3434	1/1	0.99	0.11	-3.33	45,45,45,45	0
58	MG	1H	3412	1/1	0.96	0.10	-3.38	55,55,55,55	0
58	MG	1H	3362	1/1	0.99	0.09	-3.40	42,42,42,42	0
58	MG	14	3298	1/1	0.98	0.14	-3.50	69,69,69,69	0
58	MG	14	3048	1/1	0.96	0.08	-3.51	79,79,79,79	0
58	MG	14	3348	1/1	0.98	0.09	-3.52	86,86,86,86	0
58	MG	1H	3368	1/1	0.95	0.07	-3.56	53,53,53,53	0
58	MG	1H	3355	1/1	0.97	0.13	-3.58	60,60,60,60	0
58	MG	1H	3049	1/1	0.98	0.14	-3.59	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
58	MG	1H	3145	1/1	0.87	0.11	-3.62	53,53,53,53	0
58	MG	1H	3445	1/1	0.96	0.12	-3.66	49,49,49,49	0
58	MG	1H	3403	1/1	0.99	0.14	-3.67	45,45,45,45	0
58	MG	1H	3411	1/1	0.98	0.08	-3.75	63,63,63,63	0
58	MG	1H	3392	1/1	0.99	0.10	-3.82	50,50,50,50	0
58	MG	13	1661	1/1	0.98	0.07	-3.92	86,86,86,86	0
58	MG	14	3304	1/1	0.91	0.12	-4.18	62,62,62,62	0
58	MG	1H	3364	1/1	0.95	0.12	-4.18	48,48,48,48	0
58	MG	1H	3292	1/1	0.95	0.06	-4.18	68,68,68,68	0
58	MG	1H	3442	1/1	0.94	0.06	-4.32	64,64,64,64	0
58	MG	1H	3354	1/1	0.96	0.12	-4.37	49,49,49,49	0
58	MG	1H	3356	1/1	0.94	0.10	-4.37	56,56,56,56	0
58	MG	1H	3398	1/1	0.94	0.11	-4.55	48,48,48,48	0
58	MG	14	3369	1/1	0.99	0.13	-4.56	49,49,49,49	0
58	MG	1H	3472	1/1	0.95	0.09	-4.62	60,60,60,60	0
58	MG	14	3314	1/1	0.90	0.13	-4.63	63,63,63,63	0
58	MG	1H	3120	1/1	0.94	0.09	-4.78	47,47,47,47	0
58	MG	1H	3391	1/1	0.98	0.10	-4.78	61,61,61,61	0
58	MG	14	3217	1/1	0.94	0.14	-4.85	91,91,91,91	0
58	MG	14	3207	1/1	0.72	0.12	-4.88	66,66,66,66	0
58	MG	1H	3415	1/1	0.91	0.07	-5.20	69,69,69,69	0
58	MG	14	3318	1/1	0.93	0.08	-5.39	65,65,65,65	0
58	MG	1H	3375	1/1	0.97	0.09	-5.59	50,50,50,50	0
58	MG	1H	3446	1/1	0.92	0.07	-5.64	77,77,77,77	0
58	MG	14	3323	1/1	0.95	0.10	-5.71	61,61,61,61	0
58	MG	1H	3066	1/1	0.92	0.11	-5.83	60,60,60,60	0
58	MG	14	3363	1/1	0.93	0.09	-6.07	63,63,63,63	0
58	MG	1H	3488	1/1	0.84	0.05	-6.08	92,92,92,92	0
58	MG	1H	3218	1/1	0.97	0.11	-6.29	48,48,48,48	0
58	MG	14	3322	1/1	0.99	0.06	-6.32	69,69,69,69	0
58	MG	1H	3351	1/1	0.97	0.05	-6.40	49,49,49,49	0
58	MG	14	3366	1/1	0.90	0.10	-6.44	68,68,68,68	0
58	MG	14	3414	1/1	0.90	0.12	-6.50	104,104,104,104	0
58	MG	14	3296	1/1	0.95	0.08	-6.52	67,67,67,67	0
58	MG	1H	3384	1/1	0.97	0.11	-6.82	45,45,45,45	0
58	MG	1H	3418	1/1	0.90	0.06	-7.20	74,74,74,74	0
58	MG	1G	1681	1/1	0.89	0.10	-7.22	88,88,88,88	0
58	MG	14	3316	1/1	0.99	0.06	-7.56	59,59,59,59	0
58	MG	14	3327	1/1	0.86	0.06	-7.60	102,102,102,102	0
58	MG	14	3380	1/1	0.97	0.08	-7.93	85,85,85,85	0
58	MG	1H	3438	1/1	0.93	0.06	-8.07	79,79,79,79	0
58	MG	14	3365	1/1	0.94	0.07	-8.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3356	1/1	0.97	0.09	-8.96	61,61,61,61	0
58	MG	1H	3473	1/1	0.91	0.05	-9.03	89,89,89,89	0
58	MG	1H	3414	1/1	0.95	0.08	-9.78	59,59,59,59	0
58	MG	14	3300	1/1	0.97	0.12	-9.95	57,57,57,57	0
58	MG	1H	3393	1/1	0.99	0.06	-10.39	51,51,51,51	0
58	MG	14	3295	1/1	0.93	0.08	-11.35	61,61,61,61	0
58	MG	14	3303	1/1	0.84	0.06	-12.20	72,72,72,72	0
58	MG	14	3183	1/1	0.95	0.29	-	59,59,59,59	0
58	MG	14	3280	1/1	0.90	0.45	-	49,49,49,49	0
58	MG	14	3247	1/1	0.89	0.36	-	75,75,75,75	0
58	MG	1G	1694	1/1	0.93	0.09	-	129,129,129,129	0
58	MG	1H	3043	1/1	0.92	0.45	-	86,86,86,86	0
58	MG	1H	3177	1/1	0.94	0.17	-	86,86,86,86	0
58	MG	14	3262	1/1	0.68	0.28	-	78,78,78,78	0
58	MG	1H	3482	1/1	0.89	0.08	-	95,95,95,95	0
58	MG	14	3081	1/1	0.95	0.28	-	56,56,56,56	0
58	MG	1H	3057	1/1	0.99	0.32	-	51,51,51,51	0
58	MG	1H	3209	1/1	0.83	0.45	-	87,87,87,87	0
58	MG	14	3017	1/1	0.58	0.28	-	87,87,87,87	0
58	MG	1G	1623	1/1	0.94	0.42	-	80,80,80,80	0
58	MG	1H	3386	1/1	0.96	0.10	-	59,59,59,59	0
58	MG	14	3170	1/1	0.98	0.46	-	82,82,82,82	0
58	MG	14	3162	1/1	0.89	0.23	-	75,75,75,75	0
58	MG	1G	1654	1/1	0.81	0.28	-	132,132,132,132	0
58	MG	14	3210	1/1	0.85	0.23	-	58,58,58,58	0
58	MG	14	3109	1/1	0.94	0.20	-	66,66,66,66	0
58	MG	14	3272	1/1	0.99	0.10	-	71,71,71,71	0
58	MG	1H	3349	1/1	0.86	0.24	-	89,89,89,89	0
58	MG	1G	1622	1/1	0.96	0.46	-	84,84,84,84	0
58	MG	1H	3087	1/1	0.94	0.25	-	46,46,46,46	0
58	MG	14	3061	1/1	0.99	0.28	-	56,56,56,56	0
58	MG	1H	3231	1/1	0.98	0.41	-	75,75,75,75	0
58	MG	14	3325	1/1	0.97	0.06	-	75,75,75,75	0
58	MG	14	3208	1/1	0.85	0.78	-	76,76,76,76	0
58	MG	1H	3264	1/1	0.68	0.48	-	87,87,87,87	0
58	MG	14	3371	1/1	0.97	0.09	-	89,89,89,89	0
58	MG	1G	1657	1/1	0.73	0.59	-	84,84,84,84	0
58	MG	13	1663	1/1	0.98	0.46	-	77,77,77,77	0
58	MG	14	3275	1/1	0.91	0.50	-	71,71,71,71	0
58	MG	14	3342	1/1	0.91	0.04	-	129,129,129,129	0
58	MG	13	1683	1/1	0.49	0.21	-	97,97,97,97	0
58	MG	14	3018	1/1	0.94	0.55	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3271	1/1	0.77	0.35	-	77,77,77,77	0
58	MG	13	1698	1/1	0.90	0.28	-	104,104,104,104	0
58	MG	21	302	1/1	0.82	0.22	-	69,69,69,69	0
58	MG	1H	3011	1/1	0.90	0.50	-	62,62,62,62	0
58	MG	14	3324	1/1	0.69	0.11	-	93,93,93,93	0
58	MG	14	3034	1/1	0.97	0.38	-	53,53,53,53	0
58	MG	13	1607	1/1	0.66	0.66	-	84,84,84,84	0
58	MG	1G	1668	1/1	0.95	0.45	-	141,141,141,141	0
58	MG	1H	3495	1/1	0.93	0.06	-	70,70,70,70	0
58	MG	14	3307	1/1	0.95	0.09	-	67,67,67,67	0
58	MG	14	3406	1/1	0.94	0.06	-	100,100,100,100	0
58	MG	1G	1628	1/1	0.63	0.49	-	102,102,102,102	0
58	MG	13	1623	1/1	0.94	0.18	-	81,81,81,81	0
58	MG	14	3355	1/1	0.99	0.08	-	91,91,91,91	0
58	MG	1H	3416	1/1	0.93	0.18	-	108,108,108,108	0
58	MG	13	1614	1/1	0.95	0.06	-	81,81,81,81	0
58	MG	1H	3466	1/1	0.93	0.08	-	77,77,77,77	0
58	MG	1H	3267	1/1	0.79	0.15	-	97,97,97,97	0
58	MG	14	3254	1/1	0.74	0.52	-	90,90,90,90	0
58	MG	1H	3006	1/1	0.96	0.19	-	56,56,56,56	0
58	MG	1H	3311	1/1	0.89	0.19	-	127,127,127,127	0
58	MG	14	3072	1/1	0.99	0.37	-	43,43,43,43	0
58	MG	1G	1684	1/1	0.98	0.08	-	82,82,82,82	0
58	MG	1H	3204	1/1	0.83	0.66	-	81,81,81,81	0
58	MG	1H	3320	1/1	0.90	0.29	-	84,84,84,84	0
58	MG	14	3390	1/1	0.90	0.13	-	118,118,118,118	0
58	MG	14	3066	1/1	0.96	0.44	-	47,47,47,47	0
58	MG	14	3153	1/1	0.78	0.66	-	77,77,77,77	0
58	MG	13	1619	1/1	0.95	0.22	-	72,72,72,72	0
58	MG	1H	3463	1/1	0.89	0.31	-	99,99,99,99	0
58	MG	14	3391	1/1	0.94	0.15	-	85,85,85,85	0
58	MG	1H	3341	1/1	0.87	0.24	-	81,81,81,81	0
58	MG	14	3014	1/1	0.53	0.65	-	78,78,78,78	0
58	MG	1H	3055	1/1	0.98	0.26	-	50,50,50,50	0
58	MG	13	1724	1/1	0.88	0.16	-	85,85,85,85	0
58	MG	14	3301	1/1	0.97	0.10	-	49,49,49,49	0
58	MG	1H	3469	1/1	0.86	0.12	-	81,81,81,81	0
58	MG	1H	3426	1/1	0.83	0.11	-	103,103,103,103	0
58	MG	1H	3301	1/1	0.69	0.45	-	80,80,80,80	0
58	MG	1H	3382	1/1	0.95	0.07	-	58,58,58,58	0
58	MG	14	3154	1/1	0.95	0.33	-	66,66,66,66	0
58	MG	14	3135	1/1	0.97	0.83	-	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
58	MG	14	3288	1/1	0.90	0.34	-	56,56,56,56	0
58	MG	13	1738	1/1	0.94	0.13	-	105,105,105,105	0
58	MG	1H	3455	1/1	0.98	0.06	-	65,65,65,65	0
58	MG	1H	3200	1/1	0.94	0.41	-	72,72,72,72	0
58	MG	14	3010	1/1	0.97	0.29	-	76,76,76,76	0
58	MG	14	3126	1/1	0.77	0.57	-	78,78,78,78	0
58	MG	1H	3069	1/1	0.94	0.24	-	62,62,62,62	0
58	MG	1H	3144	1/1	0.91	0.14	-	48,48,48,48	0
58	MG	1H	3026	1/1	0.90	0.24	-	60,60,60,60	0
58	MG	1H	3477	1/1	0.89	0.07	-	96,96,96,96	0
58	MG	1H	3286	1/1	0.55	0.26	-	100,100,100,100	0
58	MG	13	1715	1/1	0.93	0.06	-	106,106,106,106	0
58	MG	1H	3091	1/1	0.99	0.23	-	70,70,70,70	0
58	MG	1H	3171	1/1	0.95	0.14	-	62,62,62,62	0
58	MG	14	3146	1/1	0.81	0.39	-	71,71,71,71	0
58	MG	1H	3308	1/1	0.88	0.35	-	76,76,76,76	0
58	MG	14	3201	1/1	0.44	0.27	-	91,91,91,91	0
58	MG	14	3184	1/1	0.92	0.40	-	85,85,85,85	0
58	MG	1H	3030	1/1	0.88	0.26	-	82,82,82,82	0
58	MG	1H	3406	1/1	0.92	0.09	-	91,91,91,91	0
58	MG	14	3274	1/1	0.59	0.27	-	91,91,91,91	0
58	MG	1H	3377	1/1	0.98	0.14	-	68,68,68,68	0
58	MG	1H	3127	1/1	0.91	0.30	-	64,64,64,64	0
58	MG	1G	1639	1/1	0.90	0.36	-	68,68,68,68	0
58	MG	14	3200	1/1	0.90	0.22	-	84,84,84,84	0
58	MG	1G	1646	1/1	0.89	0.51	-	70,70,70,70	0
58	MG	14	3256	1/1	0.97	0.52	-	77,77,77,77	0
58	MG	14	3141	1/1	0.83	0.41	-	80,80,80,80	0
58	MG	14	3111	1/1	0.98	0.28	-	48,48,48,48	0
58	MG	1G	1633	1/1	0.90	0.15	-	102,102,102,102	0
58	MG	1H	3409	1/1	0.93	0.09	-	58,58,58,58	0
58	MG	1G	1611	1/1	0.94	0.39	-	105,105,105,105	0
58	MG	1G	1631	1/1	0.84	0.53	-	104,104,104,104	0
58	MG	1H	3288	1/1	0.72	0.28	-	77,77,77,77	0
58	MG	14	3350	1/1	0.78	0.10	-	89,89,89,89	0
58	MG	1G	1659	1/1	0.81	0.11	-	107,107,107,107	0
58	MG	14	3002	1/1	0.98	0.38	-	53,53,53,53	0
58	MG	14	3405	1/1	0.84	0.09	-	107,107,107,107	0
58	MG	1G	1662	1/1	0.73	0.15	-	84,84,84,84	0
58	MG	13	1734	1/1	0.78	0.07	-	130,130,130,130	0
58	MG	1G	1683	1/1	0.96	0.05	-	106,106,106,106	0
58	MG	1H	3468	1/1	0.79	0.19	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3081	1/1	0.95	0.26	-	83,83,83,83	0
58	MG	13	1735	1/1	0.64	0.09	-	124,124,124,124	0
58	MG	1H	3193	1/1	0.79	0.39	-	89,89,89,89	0
58	MG	1G	1604	1/1	0.97	0.31	-	91,91,91,91	0
58	MG	1H	3266	1/1	0.77	0.22	-	82,82,82,82	0
58	MG	1H	3188	1/1	0.75	0.57	-	90,90,90,90	0
58	MG	1H	3040	1/1	0.96	0.12	-	89,89,89,89	0
58	MG	1H	3388	1/1	0.96	0.15	-	78,78,78,78	0
58	MG	13	1690	1/1	0.91	0.27	-	105,105,105,105	0
58	MG	14	3221	1/1	0.74	0.56	-	86,86,86,86	0
58	MG	1H	3133	1/1	0.98	0.21	-	60,60,60,60	0
58	MG	13	1659	1/1	0.87	0.25	-	87,87,87,87	0
58	MG	1H	3126	1/1	0.90	0.60	-	77,77,77,77	0
58	MG	13	1669	1/1	0.69	0.52	-	81,81,81,81	0
58	MG	1H	3464	1/1	0.88	0.07	-	97,97,97,97	0
58	MG	14	3156	1/1	0.96	0.39	-	66,66,66,66	0
58	MG	1H	3325	1/1	0.95	0.12	-	82,82,82,82	0
58	MG	1G	1674	1/1	0.71	0.33	-	110,110,110,110	0
58	MG	1H	3033	1/1	0.91	0.39	-	66,66,66,66	0
58	MG	1H	3160	1/1	0.86	0.31	-	93,93,93,93	0
58	MG	1H	3261	1/1	0.98	0.07	-	85,85,85,85	0
58	MG	1G	1641	1/1	0.57	0.19	-	102,102,102,102	0
58	MG	1H	3430	1/1	0.83	0.28	-	112,112,112,112	0
58	MG	1H	3052	1/1	0.98	0.18	-	57,57,57,57	0
58	MG	14	3112	1/1	0.87	0.39	-	83,83,83,83	0
58	MG	1H	3294	1/1	0.88	0.42	-	141,141,141,141	0
58	MG	1H	3252	1/1	0.78	0.30	-	77,77,77,77	0
58	MG	1G	1687	1/1	0.91	0.14	-	116,116,116,116	0
58	MG	14	3107	1/1	0.87	0.08	-	92,92,92,92	0
58	MG	1H	3239	1/1	0.85	0.26	-	58,58,58,58	0
58	MG	1H	3095	1/1	0.95	0.50	-	66,66,66,66	0
58	MG	1H	3297	1/1	0.81	0.32	-	78,78,78,78	0
58	MG	1H	3219	1/1	0.93	0.23	-	96,96,96,96	0
58	MG	13	1700	1/1	0.95	0.24	-	93,93,93,93	0
58	MG	1H	3214	1/1	0.97	0.14	-	50,50,50,50	0
58	MG	14	3279	1/1	0.83	0.25	-	77,77,77,77	0
58	MG	1H	3481	1/1	0.94	0.05	-	100,100,100,100	0
58	MG	1G	1607	1/1	0.97	0.21	-	92,92,92,92	0
58	MG	1H	3279	1/1	0.74	0.40	-	71,71,71,71	0
58	MG	13	1625	1/1	0.86	0.35	-	69,69,69,69	0
58	MG	1H	3164	1/1	0.83	0.39	-	70,70,70,70	0
58	MG	14	3386	1/1	0.98	0.05	-	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
58	MG	14	3361	1/1	0.91	0.14	-	70,70,70,70	0
58	MG	1H	3212	1/1	0.96	0.27	-	42,42,42,42	0
58	MG	14	3166	1/1	0.99	0.21	-	60,60,60,60	0
58	MG	14	3071	1/1	0.97	0.28	-	75,75,75,75	0
58	MG	14	3121	1/1	0.89	0.47	-	83,83,83,83	0
58	MG	1H	3271	1/1	0.91	0.44	-	72,72,72,72	0
58	MG	13	1736	1/1	0.88	0.10	-	116,116,116,116	0
58	MG	1H	3268	1/1	0.70	0.29	-	72,72,72,72	0
58	MG	1H	3068	1/1	0.94	0.44	-	92,92,92,92	0
58	MG	1H	3471	1/1	0.98	0.21	-	92,92,92,92	0
58	MG	13	1718	1/1	0.88	0.10	-	100,100,100,100	0
58	MG	1H	3326	1/1	0.98	0.45	-	119,119,119,119	0
58	MG	14	3333	1/1	0.97	0.11	-	98,98,98,98	0
58	MG	14	3358	1/1	0.98	0.05	-	83,83,83,83	0
58	MG	14	3257	1/1	0.41	0.71	-	92,92,92,92	0
58	MG	1H	3202	1/1	0.88	0.28	-	84,84,84,84	0
58	MG	1H	3427	1/1	0.87	0.15	-	84,84,84,84	0
58	MG	1H	3281	1/1	0.89	0.51	-	85,85,85,85	0
58	MG	1H	3385	1/1	0.92	0.12	-	60,60,60,60	0
58	MG	13	1651	1/1	0.79	0.38	-	105,105,105,105	0
58	MG	13	1723	1/1	0.98	0.05	-	80,80,80,80	0
58	MG	14	3381	1/1	0.92	0.24	-	95,95,95,95	0
58	MG	14	3267	1/1	0.88	0.31	-	94,94,94,94	0
58	MG	1H	3420	1/1	0.93	0.13	-	80,80,80,80	0
58	MG	14	3387	1/1	0.91	0.24	-	89,89,89,89	0
58	MG	14	3389	1/1	0.92	0.08	-	94,94,94,94	0
58	MG	1G	1635	1/1	0.77	0.51	-	82,82,82,82	0
58	MG	1H	3277	1/1	0.90	0.45	-	96,96,96,96	0
58	MG	13	1684	1/1	0.83	0.16	-	101,101,101,101	0
58	MG	14	3409	1/1	0.82	0.08	-	106,106,106,106	0
58	MG	14	3144	1/1	0.96	0.20	-	82,82,82,82	0
58	MG	1H	3316	1/1	0.87	0.65	-	79,79,79,79	0
58	MG	14	3115	1/1	0.88	0.17	-	104,104,104,104	0
58	MG	1H	3312	1/1	0.90	0.21	-	80,80,80,80	0
58	MG	13	1678	1/1	0.82	0.36	-	89,89,89,89	0
58	MG	1H	3431	1/1	0.99	0.04	-	74,74,74,74	0
58	MG	1H	3323	1/1	0.96	0.06	-	77,77,77,77	0
58	MG	14	3092	1/1	0.95	0.15	-	74,74,74,74	0
58	MG	1H	3159	1/1	0.72	0.26	-	70,70,70,70	0
58	MG	13	1611	1/1	0.92	0.22	-	85,85,85,85	0
58	MG	1H	3450	1/1	0.98	0.13	-	77,77,77,77	0
58	MG	1H	3334	1/1	0.77	0.38	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3060	1/1	0.94	0.27	-	67,67,67,67	0
58	MG	14	3264	1/1	0.94	0.15	-	86,86,86,86	0
58	MG	14	3312	1/1	0.98	0.17	-	56,56,56,56	0
58	MG	14	3393	1/1	0.96	0.12	-	140,140,140,140	0
58	MG	13	1602	1/1	0.98	0.32	-	74,74,74,74	0
58	MG	1G	1689	1/1	0.97	0.07	-	98,98,98,98	0
58	MG	14	3362	1/1	0.97	0.11	-	81,81,81,81	0
58	MG	14	3230	1/1	0.78	0.29	-	87,87,87,87	0
58	MG	1H	3211	1/1	0.62	0.37	-	83,83,83,83	0
58	MG	14	3401	1/1	0.97	0.06	-	83,83,83,83	0
58	MG	14	3028	1/1	0.99	0.23	-	53,53,53,53	0
58	MG	4K	101	1/1	0.89	0.23	-	85,85,85,85	0
58	MG	14	3239	1/1	0.90	0.53	-	102,102,102,102	0
58	MG	14	3223	1/1	0.66	0.23	-	92,92,92,92	0
58	MG	14	3359	1/1	0.99	0.08	-	70,70,70,70	0
58	MG	14	3268	1/1	0.80	0.33	-	79,79,79,79	0
58	MG	29	301	1/1	0.97	0.26	-	58,58,58,58	0
58	MG	13	1714	1/1	0.92	0.06	-	106,106,106,106	0
58	MG	14	3118	1/1	0.86	0.21	-	53,53,53,53	0
58	MG	1H	3050	1/1	0.98	0.31	-	53,53,53,53	0
58	MG	1H	3175	1/1	0.67	0.43	-	84,84,84,84	0
58	MG	1H	3487	1/1	0.88	0.21	-	117,117,117,117	0
58	MG	1H	3150	1/1	0.81	0.38	-	62,62,62,62	0
58	MG	14	3283	1/1	0.93	0.56	-	78,78,78,78	0
58	MG	13	1688	1/1	0.95	0.35	-	85,85,85,85	0
58	MG	1G	1621	1/1	0.83	0.75	-	79,79,79,79	0
58	MG	1H	3206	1/1	0.97	0.47	-	69,69,69,69	0
58	MG	1G	1680	1/1	0.82	0.07	-	127,127,127,127	0
58	MG	1H	3305	1/1	0.90	0.35	-	90,90,90,90	0
58	MG	1H	3022	1/1	0.98	0.33	-	60,60,60,60	0
58	MG	1H	3404	1/1	0.92	0.06	-	78,78,78,78	0
58	MG	14	3090	1/1	0.96	0.26	-	64,64,64,64	0
58	MG	14	3023	1/1	0.99	0.26	-	42,42,42,42	0
58	MG	13	1728	1/1	0.96	0.07	-	76,76,76,76	0
58	MG	14	3269	1/1	0.80	0.12	-	86,86,86,86	0
58	MG	14	3191	1/1	0.85	0.54	-	81,81,81,81	0
58	MG	13	1710	1/1	0.96	0.07	-	74,74,74,74	0
58	MG	14	3152	1/1	0.79	0.41	-	91,91,91,91	0
58	MG	14	3344	1/1	0.82	0.10	-	96,96,96,96	0
58	MG	14	3104	1/1	0.93	0.43	-	85,85,85,85	0
58	MG	1H	3437	1/1	0.93	0.16	-	82,82,82,82	0
58	MG	1H	3223	1/1	0.96	0.15	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3194	1/1	0.85	0.42	-	79,79,79,79	0
58	MG	1H	3047	1/1	0.96	0.33	-	43,43,43,43	0
58	MG	13	1702	1/1	0.93	0.21	-	157,157,157,157	0
58	MG	2L	102	1/1	0.61	0.45	-	94,94,94,94	0
58	MG	1H	3037	1/1	0.95	0.29	-	99,99,99,99	0
58	MG	14	3234	1/1	0.90	0.24	-	81,81,81,81	0
58	MG	14	3103	1/1	0.91	0.54	-	75,75,75,75	0
58	MG	1H	3317	1/1	0.94	0.77	-	81,81,81,81	0
58	MG	14	3106	1/1	0.96	0.24	-	66,66,66,66	0
58	MG	1H	3034	1/1	0.67	0.22	-	91,91,91,91	0
58	MG	14	3139	1/1	0.80	0.49	-	55,55,55,55	0
58	MG	16	208	1/1	0.92	0.49	-	82,82,82,82	0
58	MG	1H	3229	1/1	0.85	0.44	-	59,59,59,59	0
58	MG	14	3020	1/1	0.91	0.46	-	78,78,78,78	0
58	MG	1H	3183	1/1	0.96	0.50	-	67,67,67,67	0
58	MG	14	3021	1/1	0.67	0.35	-	77,77,77,77	0
58	MG	14	3070	1/1	0.93	0.40	-	72,72,72,72	0
58	MG	1G	1636	1/1	0.91	0.46	-	90,90,90,90	0
58	MG	1H	3287	1/1	0.93	0.21	-	77,77,77,77	0
58	MG	16	211	1/1	0.89	0.08	-	88,88,88,88	0
58	MG	1H	3002	1/1	0.99	0.26	-	48,48,48,48	0
58	MG	1H	3275	1/1	0.92	0.36	-	69,69,69,69	0
58	MG	14	3098	1/1	0.93	0.82	-	57,57,57,57	0
58	MG	14	3372	1/1	0.95	0.05	-	119,119,119,119	0
58	MG	14	3408	1/1	0.91	0.17	-	108,108,108,108	0
58	MG	1G	1693	1/1	0.92	0.10	-	123,123,123,123	0
58	MG	1G	1616	1/1	0.90	0.35	-	116,116,116,116	0
58	MG	14	3008	1/1	0.83	0.39	-	85,85,85,85	0
58	MG	14	3129	1/1	0.97	0.47	-	53,53,53,53	0
58	MG	1H	3337	1/1	0.92	0.23	-	53,53,53,53	0
58	MG	1G	1629	1/1	0.98	0.37	-	98,98,98,98	0
58	MG	14	3297	1/1	0.93	0.10	-	55,55,55,55	0
58	MG	14	3231	1/1	0.90	0.20	-	90,90,90,90	0
58	MG	13	1721	1/1	0.97	0.19	-	63,63,63,63	0
58	MG	1H	3447	1/1	0.64	0.28	-	87,87,87,87	0
58	MG	P8	101	1/1	0.83	0.26	-	68,68,68,68	0
58	MG	14	3343	1/1	0.93	0.18	-	72,72,72,72	0
58	MG	1H	3284	1/1	0.85	0.38	-	92,92,92,92	0
58	MG	13	1695	1/1	0.92	0.24	-	80,80,80,80	0
58	MG	1H	3331	1/1	0.90	0.23	-	84,84,84,84	0
58	MG	14	3151	1/1	0.97	0.53	-	65,65,65,65	0
58	MG	1G	1603	1/1	0.55	0.63	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3299	1/1	0.88	0.16	-	98,98,98,98	0
58	MG	1H	3208	1/1	0.92	0.56	-	71,71,71,71	0
58	MG	1H	3093	1/1	0.92	0.47	-	45,45,45,45	0
58	MG	1H	3321	1/1	0.94	0.18	-	78,78,78,78	0
58	MG	14	3378	1/1	0.96	0.09	-	90,90,90,90	0
58	MG	13	1610	1/1	0.98	0.12	-	66,66,66,66	0
58	MG	14	3243	1/1	0.73	0.40	-	118,118,118,118	0
58	MG	1H	3440	1/1	0.80	0.13	-	102,102,102,102	0
58	MG	1H	3060	1/1	0.95	0.19	-	47,47,47,47	0
58	MG	1H	3396	1/1	0.97	0.07	-	75,75,75,75	0
58	MG	14	3105	1/1	0.90	0.43	-	91,91,91,91	0
58	MG	1H	3161	1/1	0.85	0.36	-	71,71,71,71	0
58	MG	13	1665	1/1	0.93	0.14	-	85,85,85,85	0
58	MG	14	3347	1/1	0.97	0.11	-	83,83,83,83	0
58	MG	1G	1638	1/1	0.90	0.38	-	131,131,131,131	0
58	MG	14	3069	1/1	0.97	0.43	-	64,64,64,64	0
58	MG	14	3084	1/1	0.95	0.42	-	71,71,71,71	0
58	MG	14	3065	1/1	0.85	0.44	-	67,67,67,67	0
58	MG	1H	3013	1/1	0.98	0.39	-	67,67,67,67	0
58	MG	1H	3078	1/1	0.96	0.39	-	56,56,56,56	0
58	MG	14	3261	1/1	0.95	0.23	-	74,74,74,74	0
58	MG	14	3375	1/1	0.96	0.16	-	49,49,49,49	0
58	MG	1G	1686	1/1	0.88	0.09	-	126,126,126,126	0
58	MG	1H	3008	1/1	0.96	0.17	-	90,90,90,90	0
58	MG	14	3273	1/1	0.69	1.01	-	87,87,87,87	0
58	MG	1H	3371	1/1	0.93	0.15	-	66,66,66,66	0
58	MG	1H	3449	1/1	0.88	0.07	-	76,76,76,76	0
58	MG	1H	3338	1/1	0.91	0.44	-	66,66,66,66	0
58	MG	1H	3400	1/1	0.88	0.12	-	71,71,71,71	0
58	MG	14	3025	1/1	0.97	0.27	-	52,52,52,52	0
58	MG	13	1679	1/1	0.87	0.21	-	117,117,117,117	0
58	MG	1H	3247	1/1	0.97	0.45	-	76,76,76,76	0
58	MG	1H	3489	1/1	0.91	0.20	-	83,83,83,83	0
58	MG	13	1680	1/1	0.68	0.18	-	149,149,149,149	0
58	MG	14	3064	1/1	0.92	0.43	-	62,62,62,62	0
58	MG	14	3395	1/1	0.93	0.07	-	69,69,69,69	0
58	MG	1H	3156	1/1	0.77	0.27	-	76,76,76,76	0
58	MG	1H	3335	1/1	0.90	0.12	-	79,79,79,79	0
58	MG	1H	3257	1/1	0.91	0.24	-	75,75,75,75	0
58	MG	14	3062	1/1	0.93	0.29	-	72,72,72,72	0
58	MG	13	1652	1/1	0.92	0.28	-	93,93,93,93	0
58	MG	1H	3189	1/1	0.84	0.56	-	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
58	MG	13	1627	1/1	0.96	0.21	-	97,97,97,97	0
58	MG	1H	3302	1/1	0.14	0.30	-	94,94,94,94	0
58	MG	1H	3421	1/1	0.85	0.15	-	118,118,118,118	0
58	MG	14	3047	1/1	0.95	0.23	-	56,56,56,56	0
58	MG	1H	3439	1/1	0.94	0.13	-	80,80,80,80	0
58	MG	14	3309	1/1	0.98	0.18	-	51,51,51,51	0
58	MG	1H	3365	1/1	0.98	0.07	-	60,60,60,60	0
58	MG	1H	3123	1/1	0.90	0.22	-	63,63,63,63	0
58	MG	14	3382	1/1	0.78	0.07	-	75,75,75,75	0
58	MG	14	3019	1/1	0.92	0.30	-	83,83,83,83	0
58	MG	13	1649	1/1	0.71	0.37	-	92,92,92,92	0
58	MG	13	1636	1/1	0.97	0.29	-	76,76,76,76	0
58	MG	1H	3461	1/1	0.96	0.07	-	80,80,80,80	0
58	MG	14	3416	1/1	0.97	0.31	-	83,83,83,83	0
58	MG	13	1620	1/1	0.92	0.11	-	87,87,87,87	0
58	MG	1G	1625	1/1	0.94	0.36	-	87,87,87,87	0
58	MG	1H	3128	1/1	0.79	0.38	-	83,83,83,83	0
58	MG	1H	3077	1/1	0.92	0.56	-	62,62,62,62	0
58	MG	1H	3307	1/1	0.75	0.33	-	68,68,68,68	0
58	MG	1H	3339	1/1	0.76	0.20	-	84,84,84,84	0
58	MG	1H	3196	1/1	0.81	0.30	-	72,72,72,72	0
58	MG	14	3011	1/1	0.99	0.43	-	66,66,66,66	0
58	MG	1H	3459	1/1	0.95	0.11	-	85,85,85,85	0
58	MG	1G	1642	1/1	0.92	0.41	-	78,78,78,78	0
58	MG	14	3101	1/1	0.97	0.32	-	61,61,61,61	0
58	MG	1H	3357	1/1	0.98	0.09	-	56,56,56,56	0
58	MG	1H	3399	1/1	0.97	0.09	-	40,40,40,40	0
58	MG	1H	3342	1/1	0.90	0.28	-	82,82,82,82	0
58	MG	1H	3405	1/1	0.97	0.09	-	70,70,70,70	0
58	MG	14	3140	1/1	0.73	0.30	-	90,90,90,90	0
58	MG	1H	3107	1/1	0.88	0.31	-	69,69,69,69	0
58	MG	14	3417	1/1	0.89	0.07	-	113,113,113,113	0
58	MG	13	1737	1/1	0.82	0.13	-	111,111,111,111	0
58	MG	14	3240	1/1	0.74	0.58	-	82,82,82,82	0
58	MG	14	3385	1/1	0.92	0.20	-	86,86,86,86	0
58	MG	14	3379	1/1	0.95	0.37	-	93,93,93,93	0
58	MG	14	3132	1/1	0.91	0.38	-	81,81,81,81	0
58	MG	1H	3198	1/1	0.88	0.33	-	72,72,72,72	0
58	MG	1H	3090	1/1	0.97	0.29	-	48,48,48,48	0
58	MG	14	3326	1/1	0.98	0.12	-	77,77,77,77	0
58	MG	16	201	1/1	0.89	0.06	-	99,99,99,99	0
58	MG	14	3114	1/1	0.99	0.26	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3155	1/1	0.94	0.47	-	69,69,69,69	0
58	MG	1H	3184	1/1	0.69	0.40	-	81,81,81,81	0
58	MG	1H	3141	1/1	0.95	0.16	-	47,47,47,47	0
58	MG	1H	3234	1/1	0.72	0.42	-	78,78,78,78	0
58	MG	1J	203	1/1	0.75	0.29	-	88,88,88,88	0
58	MG	14	3354	1/1	0.89	0.07	-	92,92,92,92	0
58	MG	1H	3429	1/1	0.93	0.09	-	105,105,105,105	0
58	MG	14	3232	1/1	0.85	0.25	-	84,84,84,84	0
58	MG	14	3292	1/1	0.89	0.12	-	68,68,68,68	0
58	MG	13	1713	1/1	0.93	0.09	-	84,84,84,84	0
58	MG	14	3096	1/1	0.99	0.36	-	65,65,65,65	0
58	MG	1H	3138	1/1	0.87	0.32	-	83,83,83,83	0
58	MG	1H	3146	1/1	0.92	0.49	-	72,72,72,72	0
58	MG	1H	3417	1/1	0.96	0.08	-	83,83,83,83	0
58	MG	1H	3454	1/1	0.96	0.17	-	102,102,102,102	0
58	MG	14	3027	1/1	1.00	0.27	-	49,49,49,49	0
58	MG	1H	3110	1/1	0.96	0.29	-	60,60,60,60	0
58	MG	11	301	1/1	0.94	0.18	-	50,50,50,50	0
58	MG	1H	3336	1/1	0.95	0.21	-	76,76,76,76	0
58	MG	1H	3345	1/1	0.85	0.23	-	68,68,68,68	0
58	MG	1G	1630	1/1	0.69	0.40	-	79,79,79,79	0
58	MG	1H	3163	1/1	0.93	0.24	-	76,76,76,76	0
58	MG	13	1674	1/1	0.91	0.14	-	102,102,102,102	0
58	MG	14	3328	1/1	0.94	0.13	-	105,105,105,105	0
58	MG	1G	1650	1/1	0.68	0.38	-	102,102,102,102	0
58	MG	13	1641	1/1	0.88	0.34	-	86,86,86,86	0
58	MG	1H	3045	1/1	0.91	0.25	-	52,52,52,52	0
58	MG	1H	3490	1/1	0.95	0.05	-	95,95,95,95	0
58	MG	1H	3143	1/1	0.96	0.19	-	75,75,75,75	0
58	MG	14	3229	1/1	0.65	0.42	-	85,85,85,85	0
58	MG	13	1729	1/1	0.97	0.08	-	80,80,80,80	0
58	MG	14	3055	1/1	0.90	0.48	-	71,71,71,71	0
58	MG	1H	3280	1/1	0.90	0.17	-	90,90,90,90	0
58	MG	1H	3038	1/1	0.94	0.30	-	72,72,72,72	0
58	MG	1H	3453	1/1	0.95	0.06	-	98,98,98,98	0
58	MG	16	203	1/1	0.87	0.39	-	84,84,84,84	0
58	MG	1H	3172	1/1	0.90	0.16	-	76,76,76,76	0
58	MG	1H	3372	1/1	0.97	0.09	-	73,73,73,73	0
58	MG	13	1671	1/1	0.92	0.17	-	121,121,121,121	0
58	MG	1H	3460	1/1	0.91	0.17	-	87,87,87,87	0
58	MG	14	3182	1/1	0.98	0.50	-	89,89,89,89	0
58	MG	1H	3251	1/1	0.97	0.82	-	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
58	MG	14	3082	1/1	0.97	0.34	-	85,85,85,85	0
58	MG	14	3041	1/1	0.99	0.20	-	81,81,81,81	0
58	MG	1H	3332	1/1	0.75	0.17	-	72,72,72,72	0
58	MG	1H	3470	1/1	0.97	0.04	-	96,96,96,96	0
58	MG	13	1739	1/1	0.77	0.05	-	110,110,110,110	0
58	MG	14	3068	1/1	0.66	0.83	-	86,86,86,86	0
58	MG	1H	3021	1/1	0.96	0.28	-	64,64,64,64	0
58	MG	1H	3295	1/1	0.87	0.53	-	88,88,88,88	0
58	MG	13	1732	1/1	0.93	0.13	-	120,120,120,120	0
58	MG	14	3398	1/1	0.99	0.08	-	67,67,67,67	0
58	MG	14	3187	1/1	0.88	0.24	-	72,72,72,72	0
58	MG	1H	3109	1/1	0.98	0.32	-	47,47,47,47	0
58	MG	14	3346	1/1	0.48	0.09	-	144,144,144,144	0
58	MG	1H	3072	1/1	0.84	0.27	-	80,80,80,80	0
58	MG	1H	3300	1/1	0.92	0.38	-	85,85,85,85	0
58	MG	13	1605	1/1	0.93	0.24	-	79,79,79,79	0
58	MG	1H	3436	1/1	0.96	0.07	-	73,73,73,73	0
58	MG	13	1730	1/1	0.93	0.07	-	95,95,95,95	0
58	MG	13	1682	1/1	0.81	0.30	-	151,151,151,151	0
58	MG	1H	3367	1/1	0.95	0.06	-	59,59,59,59	0
58	MG	1H	3319	1/1	0.85	0.26	-	80,80,80,80	0
58	MG	14	3276	1/1	0.83	0.60	-	87,87,87,87	0
58	MG	14	3285	1/1	0.79	0.22	-	70,70,70,70	0
58	MG	14	3331	1/1	0.90	0.10	-	102,102,102,102	0
58	MG	1H	3003	1/1	0.99	0.29	-	38,38,38,38	0
58	MG	13	1716	1/1	0.97	0.14	-	75,75,75,75	0
58	MG	14	3235	1/1	0.84	0.25	-	76,76,76,76	0
58	MG	1G	1673	1/1	0.78	0.22	-	93,93,93,93	0
58	MG	14	3394	1/1	0.95	0.09	-	101,101,101,101	0
58	MG	1H	3485	1/1	0.73	0.10	-	116,116,116,116	0
58	MG	1H	3224	1/1	0.97	0.41	-	50,50,50,50	0
58	MG	14	3248	1/1	0.88	0.72	-	85,85,85,85	0
58	MG	1H	3474	1/1	0.91	0.11	-	97,97,97,97	0
58	MG	1H	3185	1/1	0.96	0.33	-	63,63,63,63	0
58	MG	14	3133	1/1	0.93	0.41	-	66,66,66,66	0
58	MG	1H	3324	1/1	0.50	0.38	-	65,65,65,65	0
58	MG	1H	3048	1/1	0.96	0.33	-	43,43,43,43	0
58	MG	13	1633	1/1	0.87	0.37	-	91,91,91,91	0
58	MG	1G	1640	1/1	0.89	0.57	-	75,75,75,75	0
58	MG	1H	3114	1/1	0.95	0.60	-	64,64,64,64	0
58	MG	1H	3310	1/1	0.66	0.16	-	126,126,126,126	0
58	MG	1H	3032	1/1	0.93	0.54	-	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
58	MG	1G	1609	1/1	0.95	0.20	-	98,98,98,98	0
58	MG	13	1720	1/1	0.87	0.06	-	111,111,111,111	0
58	MG	14	3131	1/1	0.93	0.50	-	70,70,70,70	0
58	MG	1H	3232	1/1	0.92	0.50	-	75,75,75,75	0
58	MG	14	3284	1/1	0.85	0.41	-	81,81,81,81	0
58	MG	1H	3352	1/1	0.93	0.11	-	70,70,70,70	0
58	MG	3L	101	1/1	0.17	0.24	-	160,160,160,160	0
58	MG	13	1709	1/1	0.94	0.07	-	96,96,96,96	0
58	MG	13	1740	1/1	0.95	0.28	-	93,93,93,93	0
58	MG	1G	1695	1/1	0.87	0.06	-	136,136,136,136	0
58	MG	1I	201	1/1	0.65	0.26	-	79,79,79,79	0
58	MG	1G	1648	1/1	0.84	0.35	-	90,90,90,90	0
58	MG	14	3052	1/1	0.85	0.36	-	75,75,75,75	0
58	MG	13	1653	1/1	0.90	0.12	-	86,86,86,86	0
58	MG	13	1691	1/1	0.92	0.23	-	89,89,89,89	0
58	MG	13	1704	1/1	0.82	0.19	-	72,72,72,72	0
58	MG	1H	3024	1/1	0.90	0.21	-	74,74,74,74	0
58	MG	13	1719	1/1	0.96	0.07	-	95,95,95,95	0
58	MG	1H	3056	1/1	0.92	0.36	-	50,50,50,50	0
58	MG	1G	1665	1/1	0.77	0.21	-	85,85,85,85	0
58	MG	14	3172	1/1	0.94	0.33	-	75,75,75,75	0
58	MG	25	201	1/1	0.82	0.22	-	85,85,85,85	0
58	MG	1H	3475	1/1	0.96	0.09	-	80,80,80,80	0
58	MG	1H	3182	1/1	0.76	0.24	-	76,76,76,76	0
58	MG	1H	3158	1/1	0.83	0.42	-	78,78,78,78	0
58	MG	1G	1677	1/1	0.84	0.11	-	130,130,130,130	0
58	MG	14	3352	1/1	0.95	0.06	-	69,69,69,69	0
58	MG	14	3199	1/1	0.92	0.41	-	91,91,91,91	0
58	MG	1H	3492	1/1	0.95	0.11	-	95,95,95,95	0
58	MG	1H	3329	1/1	0.69	0.27	-	91,91,91,91	0
58	MG	1G	1692	1/1	0.91	0.13	-	130,130,130,130	0
58	MG	14	3163	1/1	0.85	0.68	-	65,65,65,65	0
58	MG	1J	206	1/1	0.68	0.08	-	115,115,115,115	0
58	MG	1H	3125	1/1	0.95	0.16	-	79,79,79,79	0
58	MG	1H	3265	1/1	0.46	0.26	-	115,115,115,115	0
58	MG	13	1693	1/1	0.87	0.62	-	77,77,77,77	0
58	MG	1H	3216	1/1	0.94	0.11	-	57,57,57,57	0
58	MG	1H	3132	1/1	0.83	0.32	-	74,74,74,74	0
58	MG	1G	1651	1/1	0.82	0.37	-	100,100,100,100	0
58	MG	13	1662	1/1	0.76	0.13	-	81,81,81,81	0
58	MG	I8	101	1/1	0.85	0.15	-	90,90,90,90	0
58	MG	1H	3105	1/1	0.82	0.36	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3313	1/1	0.68	0.38	-	96,96,96,96	0
58	MG	14	3374	1/1	0.97	0.14	-	95,95,95,95	0
58	MG	14	3080	1/1	0.99	0.26	-	62,62,62,62	0
58	MG	1H	3228	1/1	0.94	0.56	-	68,68,68,68	0
58	MG	45	203	1/1	0.75	0.46	-	70,70,70,70	0
58	MG	1H	3151	1/1	0.74	0.37	-	76,76,76,76	0
58	MG	14	3411	1/1	0.94	0.04	-	113,113,113,113	0
58	MG	1H	3119	1/1	0.82	0.28	-	72,72,72,72	0
58	MG	1H	3248	1/1	0.95	0.30	-	77,77,77,77	0
58	MG	1H	3027	1/1	0.72	0.56	-	83,83,83,83	0
58	MG	13	1707	1/1	0.89	0.13	-	87,87,87,87	0
58	MG	1H	3098	1/1	0.83	0.29	-	65,65,65,65	0
58	MG	1H	3314	1/1	0.90	0.30	-	76,76,76,76	0
58	MG	1H	3401	1/1	0.94	0.10	-	71,71,71,71	0
58	MG	E5	101	1/1	0.92	0.25	-	53,53,53,53	0
58	MG	14	3226	1/1	0.91	0.50	-	99,99,99,99	0
58	MG	13	1603	1/1	0.80	0.39	-	76,76,76,76	0
58	MG	14	3032	1/1	0.98	0.33	-	62,62,62,62	0
58	MG	1H	3306	1/1	0.97	0.24	-	63,63,63,63	0
58	MG	1H	3283	1/1	0.90	0.44	-	84,84,84,84	0
58	MG	14	3150	1/1	0.87	0.27	-	78,78,78,78	0
58	MG	78	201	1/1	0.90	0.36	-	76,76,76,76	0
58	MG	29	303	1/1	0.93	0.28	-	74,74,74,74	0
58	MG	14	3330	1/1	0.98	0.06	-	73,73,73,73	0
58	MG	14	3353	1/1	0.96	0.11	-	80,80,80,80	0
58	MG	14	3167	1/1	0.90	0.24	-	50,50,50,50	0
58	MG	14	3127	1/1	0.89	0.37	-	69,69,69,69	0
58	MG	1H	3467	1/1	0.93	0.16	-	101,101,101,101	0
58	MG	14	3058	1/1	0.97	0.23	-	55,55,55,55	0
58	MG	1H	3067	1/1	0.96	0.34	-	88,88,88,88	0
58	MG	14	3197	1/1	0.71	0.30	-	146,146,146,146	0
58	MG	13	1731	1/1	0.95	0.08	-	78,78,78,78	0
58	MG	14	3218	1/1	0.71	0.12	-	84,84,84,84	0
58	MG	1H	3018	1/1	0.99	0.44	-	51,51,51,51	0
58	MG	1H	3263	1/1	0.88	0.51	-	106,106,106,106	0
58	MG	1H	3408	1/1	0.96	0.10	-	61,61,61,61	0
58	MG	1H	3346	1/1	0.87	0.24	-	80,80,80,80	0
58	MG	1H	3483	1/1	0.95	0.05	-	99,99,99,99	0
58	MG	1G	1652	1/1	0.88	0.11	-	81,81,81,81	0
58	MG	14	3159	1/1	0.77	0.25	-	75,75,75,75	0
58	MG	13	1708	1/1	0.89	0.12	-	76,76,76,76	0
58	MG	13	1660	1/1	0.93	0.38	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3484	1/1	0.83	0.08	-	104,104,104,104	0
58	MG	1H	3480	1/1	0.93	0.09	-	98,98,98,98	0
58	MG	14	3306	1/1	0.87	0.18	-	64,64,64,64	0
58	MG	14	3370	1/1	0.94	0.08	-	80,80,80,80	0
58	MG	14	3188	1/1	0.94	0.15	-	73,73,73,73	0
58	MG	14	3040	1/1	0.95	0.26	-	49,49,49,49	0
58	MG	1G	1671	1/1	0.81	0.28	-	102,102,102,102	0
58	MG	1H	3020	1/1	0.98	0.48	-	52,52,52,52	0
58	MG	14	3315	1/1	0.95	0.07	-	81,81,81,81	0
58	MG	1G	1620	1/1	0.95	0.36	-	74,74,74,74	0
58	MG	14	3263	1/1	0.32	0.45	-	86,86,86,86	0
58	MG	1H	3290	1/1	0.80	0.30	-	83,83,83,83	0
58	MG	1H	3096	1/1	0.99	0.25	-	51,51,51,51	0
58	MG	13	1632	1/1	0.98	0.14	-	57,57,57,57	0
58	MG	21	301	1/1	0.99	0.23	-	48,48,48,48	0
58	MG	13	1675	1/1	0.61	0.35	-	97,97,97,97	0
58	MG	14	3250	1/1	0.84	0.53	-	87,87,87,87	0
58	MG	1H	3259	1/1	0.96	0.48	-	82,82,82,82	0
58	MG	14	3265	1/1	0.82	0.55	-	83,83,83,83	0
58	MG	13	1696	1/1	0.23	0.41	-	105,105,105,105	0
58	MG	13	1701	1/1	0.71	0.30	-	92,92,92,92	0
58	MG	13	1692	1/1	0.77	0.36	-	101,101,101,101	0
58	MG	14	3402	1/1	0.94	0.07	-	110,110,110,110	0
58	MG	14	3299	1/1	0.77	0.06	-	99,99,99,99	0
58	MG	1H	3190	1/1	0.86	0.39	-	66,66,66,66	0
58	MG	1H	3244	1/1	0.87	0.21	-	100,100,100,100	0
58	MG	14	3302	1/1	0.91	0.11	-	67,67,67,67	0
58	MG	1G	1682	1/1	0.85	0.05	-	113,113,113,113	0
58	MG	1H	3201	1/1	0.91	0.12	-	67,67,67,67	0
58	MG	14	3351	1/1	0.92	0.17	-	79,79,79,79	0
58	MG	1H	3059	1/1	0.96	0.26	-	66,66,66,66	0
58	MG	14	3130	1/1	0.89	0.60	-	78,78,78,78	0
58	MG	1H	3102	1/1	0.94	0.31	-	64,64,64,64	0
58	MG	1H	3187	1/1	0.94	0.16	-	69,69,69,69	0
58	MG	14	3089	1/1	0.92	0.10	-	80,80,80,80	0
58	MG	1H	3394	1/1	0.90	0.25	-	104,104,104,104	0
58	MG	1G	1617	1/1	0.84	0.09	-	101,101,101,101	0
58	MG	1H	3340	1/1	0.94	0.29	-	72,72,72,72	0
58	MG	14	3093	1/1	0.94	0.41	-	52,52,52,52	0
58	MG	1H	3493	1/1	0.95	0.07	-	96,96,96,96	0
58	MG	1H	3407	1/1	0.92	0.16	-	59,59,59,59	0
58	MG	1G	1655	1/1	0.90	0.72	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3228	1/1	0.92	0.24	-	76,76,76,76	0
58	MG	1H	3428	1/1	0.99	0.08	-	64,64,64,64	0
58	MG	1G	1643	1/1	0.53	0.29	-	83,83,83,83	0
58	MG	13	1643	1/1	0.92	0.16	-	90,90,90,90	0
58	MG	1H	3370	1/1	0.98	0.12	-	72,72,72,72	0
58	MG	1H	3199	1/1	0.89	0.30	-	68,68,68,68	0
58	MG	14	3339	1/1	0.77	0.12	-	109,109,109,109	0
58	MG	14	3410	1/1	0.96	0.09	-	75,75,75,75	0
58	MG	14	3051	1/1	0.87	0.35	-	88,88,88,88	0
58	MG	1H	3376	1/1	0.95	0.11	-	71,71,71,71	0
58	MG	14	3392	1/1	0.95	0.05	-	88,88,88,88	0
58	MG	1H	3315	1/1	0.90	0.39	-	58,58,58,58	0
58	MG	1H	3330	1/1	0.72	0.25	-	87,87,87,87	0
58	MG	1H	3041	1/1	0.80	0.44	-	86,86,86,86	0
58	MG	1H	3304	1/1	0.81	0.40	-	94,94,94,94	0
58	MG	14	3136	1/1	0.88	0.31	-	79,79,79,79	0
58	MG	7I	101	1/1	0.59	0.19	-	95,95,95,95	0
58	MG	14	3281	1/1	0.85	0.20	-	93,93,93,93	0
58	MG	1J	205	1/1	0.87	0.18	-	89,89,89,89	0
58	MG	14	3399	1/1	0.92	0.09	-	80,80,80,80	0
58	MG	1H	3359	1/1	0.98	0.07	-	43,43,43,43	0
58	MG	1H	3255	1/1	0.54	0.45	-	68,68,68,68	0
58	MG	1H	3092	1/1	0.90	0.18	-	69,69,69,69	0
58	MG	14	3397	1/1	0.95	0.06	-	89,89,89,89	0
58	MG	14	3270	1/1	0.85	0.20	-	90,90,90,90	0
58	MG	14	3237	1/1	0.89	0.52	-	77,77,77,77	0
58	MG	1H	3452	1/1	0.90	0.10	-	85,85,85,85	0
58	MG	14	3076	1/1	0.93	0.23	-	88,88,88,88	0
58	MG	1H	3491	1/1	0.98	0.03	-	91,91,91,91	0
58	MG	1H	3298	1/1	0.92	0.42	-	84,84,84,84	0
58	MG	1H	3004	1/1	0.90	0.25	-	54,54,54,54	0
58	MG	1H	3465	1/1	0.84	0.07	-	97,97,97,97	0
58	MG	14	3134	1/1	0.86	0.48	-	83,83,83,83	0
58	MG	1H	3249	1/1	0.67	0.25	-	77,77,77,77	0
58	MG	1H	3327	1/1	0.93	0.34	-	134,134,134,134	0
58	MG	1H	3241	1/1	0.94	0.39	-	71,71,71,71	0
58	MG	1H	3262	1/1	0.94	0.74	-	78,78,78,78	0
58	MG	14	3337	1/1	0.86	0.07	-	78,78,78,78	0
58	MG	2K	102	1/1	0.76	0.45	-	79,79,79,79	0
58	MG	1H	3425	1/1	0.87	0.06	-	110,110,110,110	0
58	MG	1H	3397	1/1	0.91	0.10	-	79,79,79,79	0
58	MG	13	1725	1/1	0.97	0.06	-	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
58	MG	14	3026	1/1	0.99	0.33	-	51,51,51,51	0
58	MG	1H	3322	1/1	0.84	0.34	-	78,78,78,78	0
58	MG	14	3376	1/1	0.84	0.11	-	117,117,117,117	0
58	MG	13	1666	1/1	0.65	0.28	-	97,97,97,97	0
58	MG	1H	3136	1/1	0.95	0.25	-	63,63,63,63	0
58	MG	1H	3293	1/1	0.77	0.32	-	92,92,92,92	0
58	MG	1H	3423	1/1	0.93	0.06	-	71,71,71,71	0
58	MG	1H	3456	1/1	0.97	0.08	-	93,93,93,93	0
58	MG	13	1624	1/1	0.94	0.18	-	75,75,75,75	0
58	MG	13	1647	1/1	0.78	0.33	-	107,107,107,107	0
58	MG	19	301	1/1	0.94	0.40	-	70,70,70,70	0
58	MG	14	3377	1/1	0.89	0.11	-	105,105,105,105	0
58	MG	1H	3274	1/1	0.78	0.38	-	75,75,75,75	0
58	MG	14	3209	1/1	0.90	0.24	-	70,70,70,70	0
58	MG	14	3022	1/1	0.99	0.38	-	63,63,63,63	0
58	MG	1H	3269	1/1	0.85	0.52	-	71,71,71,71	0
58	MG	1H	3148	1/1	0.88	0.58	-	77,77,77,77	0
58	MG	14	3368	1/1	0.94	0.06	-	79,79,79,79	0
58	MG	1H	3075	1/1	0.97	0.47	-	70,70,70,70	0
58	MG	1H	3233	1/1	0.90	0.29	-	77,77,77,77	0
58	MG	16	209	1/1	0.96	0.11	-	64,64,64,64	0
58	MG	14	3147	1/1	0.82	0.49	-	91,91,91,91	0
58	MG	1H	3112	1/1	0.95	0.42	-	52,52,52,52	0
58	MG	14	3094	1/1	0.96	0.37	-	67,67,67,67	0
58	MG	1G	1645	1/1	0.96	0.19	-	96,96,96,96	0
58	MG	14	3286	1/1	0.93	0.08	-	103,103,103,103	0
58	MG	1H	3009	1/1	0.97	0.32	-	69,69,69,69	0
58	MG	88	203	1/1	0.79	0.35	-	75,75,75,75	0
58	MG	14	3148	1/1	0.91	0.47	-	84,84,84,84	0
58	MG	1H	3318	1/1	0.92	0.53	-	71,71,71,71	0
58	MG	14	3225	1/1	0.64	0.73	-	84,84,84,84	0
58	MG	1H	3108	1/1	0.90	0.25	-	51,51,51,51	0
58	MG	1H	3149	1/1	0.73	0.47	-	79,79,79,79	0
58	MG	1H	3203	1/1	0.95	0.16	-	76,76,76,76	0
58	MG	1H	3039	1/1	0.91	0.35	-	64,64,64,64	0
58	MG	1H	3381	1/1	0.90	0.15	-	47,47,47,47	0
58	MG	14	3189	1/1	0.98	0.29	-	90,90,90,90	0
58	MG	1J	201	1/1	0.96	0.17	-	76,76,76,76	0
58	MG	1H	3207	1/1	0.62	0.56	-	84,84,84,84	0
58	MG	14	3278	1/1	0.87	0.23	-	63,63,63,63	0
58	MG	1H	3478	1/1	0.89	0.18	-	64,64,64,64	0
58	MG	14	3204	1/1	0.96	0.36	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3104	1/1	0.97	0.36	-	66,66,66,66	0
58	MG	1H	3031	1/1	0.90	0.34	-	70,70,70,70	0
58	MG	13	1617	1/1	0.94	0.27	-	74,74,74,74	0
58	MG	1H	3015	1/1	0.73	0.26	-	70,70,70,70	0
58	MG	1G	1612	1/1	0.82	0.41	-	100,100,100,100	0
58	MG	1H	3433	1/1	0.98	0.19	-	45,45,45,45	0
58	MG	14	3113	1/1	0.68	0.18	-	84,84,84,84	0
58	MG	14	3005	1/1	0.98	0.22	-	51,51,51,51	0
58	MG	16	206	1/1	0.95	0.32	-	77,77,77,77	0
58	MG	1H	3235	1/1	0.88	0.52	-	64,64,64,64	0
58	MG	1H	3025	1/1	0.98	0.29	-	41,41,41,41	0
58	MG	1H	3122	1/1	0.97	0.29	-	65,65,65,65	0
58	MG	2I	201	1/1	0.55	0.28	-	98,98,98,98	0
58	MG	14	3219	1/1	0.77	0.35	-	107,107,107,107	0
58	MG	13	1650	1/1	0.97	0.14	-	100,100,100,100	0
58	MG	14	3266	1/1	0.90	0.42	-	72,72,72,72	0
58	MG	1H	3162	1/1	0.60	0.39	-	74,74,74,74	0
58	MG	1H	3435	1/1	0.93	0.10	-	70,70,70,70	0
58	MG	14	3396	1/1	0.89	0.17	-	67,67,67,67	0
58	MG	14	3335	1/1	0.82	0.10	-	120,120,120,120	0
58	MG	1H	3035	1/1	0.72	0.52	-	87,87,87,87	0
58	MG	14	3195	1/1	0.92	0.28	-	75,75,75,75	0
58	MG	14	3222	1/1	0.79	0.41	-	73,73,73,73	0
58	MG	1H	3181	1/1	0.86	0.41	-	74,74,74,74	0
58	MG	14	3013	1/1	0.76	0.48	-	83,83,83,83	0
58	MG	1H	3272	1/1	0.90	0.08	-	80,80,80,80	0
58	MG	14	3053	1/1	0.97	0.30	-	74,74,74,74	0
58	MG	14	3043	1/1	0.85	0.16	-	85,85,85,85	0
58	MG	1H	3083	1/1	0.96	0.17	-	99,99,99,99	0
58	MG	1H	3197	1/1	0.73	0.46	-	91,91,91,91	0
58	MG	1G	1688	1/1	0.92	0.07	-	122,122,122,122	0
58	MG	1H	3169	1/1	0.89	0.30	-	84,84,84,84	0
58	MG	14	3373	1/1	0.96	0.16	-	96,96,96,96	0
58	MG	1H	3170	1/1	0.87	0.37	-	70,70,70,70	0
58	MG	13	1657	1/1	0.81	0.15	-	72,72,72,72	0
58	MG	14	3321	1/1	0.85	0.14	-	87,87,87,87	0
58	MG	14	3388	1/1	0.96	0.08	-	83,83,83,83	0
58	MG	14	3407	1/1	0.90	0.10	-	98,98,98,98	0
58	MG	14	3241	1/1	0.83	0.18	-	115,115,115,115	0
58	MG	14	3384	1/1	0.97	0.08	-	93,93,93,93	0
58	MG	14	3044	1/1	0.73	0.33	-	85,85,85,85	0
58	MG	1H	3220	1/1	0.97	0.25	-	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
58	MG	14	3290	1/1	0.80	0.12	-	89,89,89,89	0
58	MG	13	1673	1/1	0.75	0.34	-	99,99,99,99	0
58	MG	14	3142	1/1	0.94	0.07	-	89,89,89,89	0
58	MG	1H	3451	1/1	0.96	0.08	-	68,68,68,68	0
58	MG	1G	1605	1/1	0.97	0.40	-	102,102,102,102	0
58	MG	1H	3130	1/1	0.91	0.18	-	67,67,67,67	0
58	MG	1G	1679	1/1	0.94	0.09	-	103,103,103,103	0
58	MG	1H	3103	1/1	0.84	0.31	-	75,75,75,75	0
58	MG	13	1642	1/1	0.89	0.24	-	92,92,92,92	0
58	MG	1G	1690	1/1	0.96	0.08	-	105,105,105,105	0
58	MG	1G	1669	1/1	0.68	0.19	-	93,93,93,93	0
58	MG	13	1609	1/1	0.98	0.28	-	79,79,79,79	0
58	MG	14	3122	1/1	0.78	0.46	-	71,71,71,71	0
58	MG	14	3042	1/1	0.93	0.21	-	95,95,95,95	0
58	MG	14	3124	1/1	0.94	0.42	-	86,86,86,86	0
58	MG	13	1733	1/1	0.97	0.24	-	83,83,83,83	0
58	MG	1G	1660	1/1	0.85	0.41	-	107,107,107,107	0
58	MG	14	3001	1/1	0.94	0.19	-	46,46,46,46	0
58	MG	14	3332	1/1	0.80	0.07	-	103,103,103,103	0
58	MG	14	3227	1/1	0.84	0.24	-	91,91,91,91	0
58	MG	1H	3462	1/1	0.92	0.07	-	91,91,91,91	0
58	MG	13	1668	1/1	0.67	0.15	-	105,105,105,105	0
58	MG	14	3138	1/1	0.91	0.39	-	91,91,91,91	0
58	MG	14	3259	1/1	0.84	0.43	-	81,81,81,81	0
58	MG	14	3341	1/1	0.94	0.05	-	92,92,92,92	0
58	MG	14	3413	1/1	0.89	0.10	-	102,102,102,102	0
58	MG	14	3282	1/1	0.81	0.33	-	82,82,82,82	0
58	MG	1H	3486	1/1	0.64	0.22	-	98,98,98,98	0
58	MG	14	3119	1/1	0.84	0.08	-	80,80,80,80	0
58	MG	14	3238	1/1	0.88	0.46	-	82,82,82,82	0
58	MG	1H	3360	1/1	0.98	0.11	-	70,70,70,70	0
58	MG	1H	3282	1/1	0.80	0.17	-	67,67,67,67	0
58	MG	14	3404	1/1	0.96	0.04	-	85,85,85,85	0
58	MG	1H	3250	1/1	0.84	0.27	-	69,69,69,69	0
58	MG	13	1606	1/1	0.91	0.15	-	124,124,124,124	0
58	MG	13	1644	1/1	0.94	0.22	-	85,85,85,85	0
58	MG	1G	1615	1/1	0.92	0.13	-	132,132,132,132	0
58	MG	16	210	1/1	0.96	0.08	-	80,80,80,80	0
58	MG	14	3161	1/1	0.97	0.14	-	99,99,99,99	0
58	MG	1G	1670	1/1	0.94	0.44	-	110,110,110,110	0
58	MG	14	3059	1/1	0.93	0.39	-	63,63,63,63	0
58	MG	1G	1637	1/1	0.97	0.42	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3317	1/1	0.98	0.11	-	52,52,52,52	0
58	MG	13	1616	1/1	0.76	0.30	-	62,62,62,62	0
58	MG	14	3116	1/1	0.96	0.50	-	48,48,48,48	0
58	MG	13	1689	1/1	0.91	0.78	-	80,80,80,80	0
58	MG	1G	1667	1/1	0.93	0.28	-	81,81,81,81	0
58	MG	14	3246	1/1	0.71	0.40	-	90,90,90,90	0
58	MG	13	1629	1/1	0.95	0.24	-	58,58,58,58	0
58	MG	14	3245	1/1	0.64	0.30	-	90,90,90,90	0
58	MG	1H	3413	1/1	0.93	0.11	-	72,72,72,72	0
58	MG	13	1670	1/1	0.81	0.20	-	103,103,103,103	0
58	MG	1J	202	1/1	0.87	0.34	-	84,84,84,84	0
58	MG	1H	3153	1/1	0.92	0.49	-	80,80,80,80	0
58	MG	14	3086	1/1	0.91	0.53	-	74,74,74,74	0
58	MG	1H	3276	1/1	0.78	0.41	-	67,67,67,67	0
58	MG	1H	3166	1/1	0.93	0.27	-	77,77,77,77	0
58	MG	14	3364	1/1	0.98	0.09	-	98,98,98,98	0
58	MG	1H	3458	1/1	0.76	0.10	-	99,99,99,99	0
58	MG	14	3173	1/1	0.95	0.22	-	92,92,92,92	0
58	MG	1H	3210	1/1	0.98	0.49	-	67,67,67,67	0
58	MG	1H	3165	1/1	0.96	0.24	-	76,76,76,76	0
58	MG	1H	3328	1/1	0.82	0.36	-	65,65,65,65	0
58	MG	14	3313	1/1	0.95	0.13	-	84,84,84,84	0
58	MG	14	3077	1/1	0.93	0.64	-	84,84,84,84	0
58	MG	14	3211	1/1	0.94	0.09	-	85,85,85,85	0
58	MG	13	1687	1/1	0.88	0.15	-	96,96,96,96	0
58	MG	14	3357	1/1	0.92	0.11	-	83,83,83,83	0
58	MG	45	201	1/1	0.90	0.12	-	69,69,69,69	0
58	MG	14	3036	1/1	0.81	0.38	-	115,115,115,115	0
58	MG	14	3202	1/1	0.91	0.25	-	77,77,77,77	0
58	MG	1H	3205	1/1	0.58	0.43	-	101,101,101,101	0
58	MG	1H	3147	1/1	0.79	0.28	-	90,90,90,90	0
58	MG	1H	3178	1/1	0.87	0.30	-	76,76,76,76	0
58	MG	1G	1627	1/1	0.80	0.54	-	103,103,103,103	0
58	MG	13	1628	1/1	0.69	0.51	-	82,82,82,82	0
58	MG	1H	3383	1/1	0.97	0.13	-	49,49,49,49	0
58	MG	14	3383	1/1	0.96	0.16	-	93,93,93,93	0
58	MG	14	3120	1/1	0.80	0.23	-	70,70,70,70	0
58	MG	1H	3410	1/1	0.97	0.07	-	76,76,76,76	0
58	MG	13	1726	1/1	0.92	0.09	-	122,122,122,122	0
58	MG	14	3102	1/1	0.78	0.80	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.