



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 09:20 AM GMT

PDB ID : 5EL7  
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 second position and antibiotic paromomycin  
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.

---

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

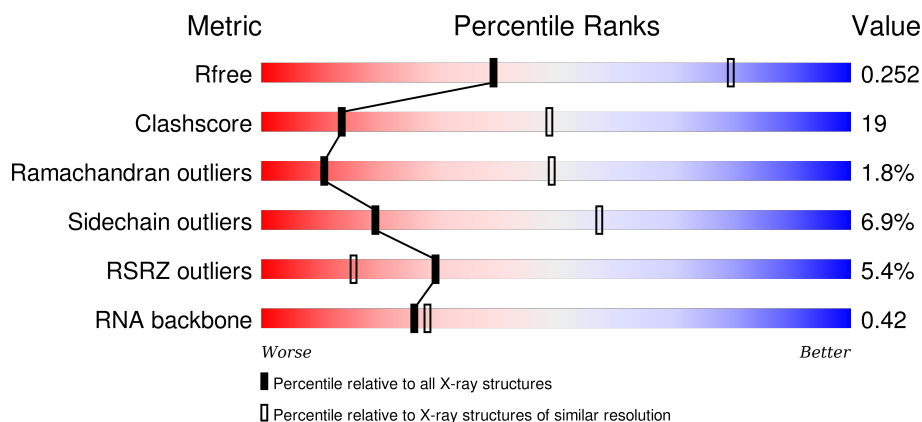
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

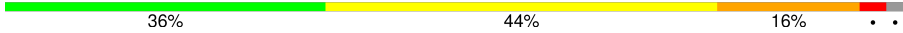

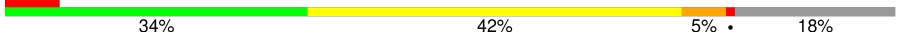

The reported resolution of this entry is 3.15 Å.

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.



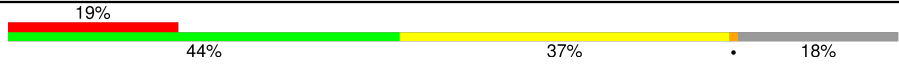

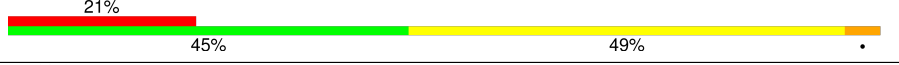

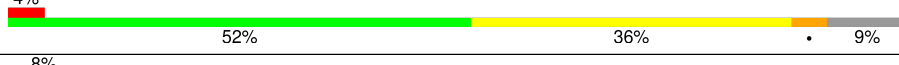
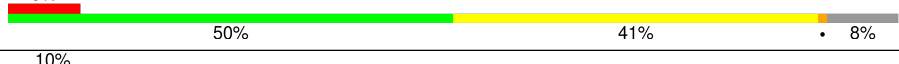
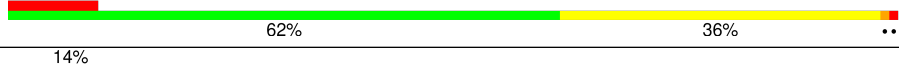

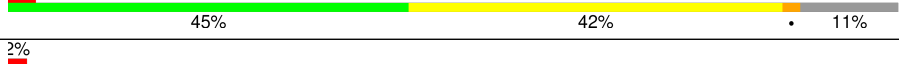


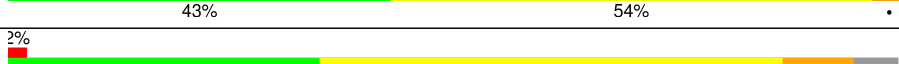
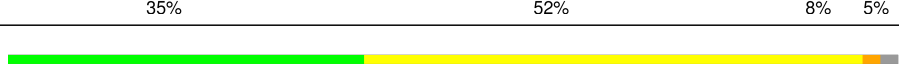
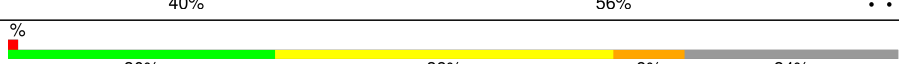
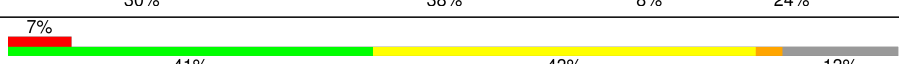



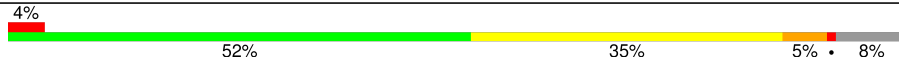






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (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	

*Continued on next page...*

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	
22	1L	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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	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
57	MG	13	1601	-	-	-	X
57	MG	13	1602	-	-	-	X
57	MG	13	1606	-	-	-	X
57	MG	13	1607	-	-	-	X
57	MG	13	1608	-	-	-	X
57	MG	13	1610	-	-	-	X
57	MG	13	1611	-	-	-	X
57	MG	13	1616	-	-	-	X
57	MG	13	1620	-	-	-	X
57	MG	13	1623	-	-	-	X
57	MG	13	1627	-	-	-	X
57	MG	13	1634	-	-	-	X
57	MG	13	1642	-	-	-	X
57	MG	13	1644	-	-	-	X
57	MG	13	1645	-	-	-	X
57	MG	13	1646	-	-	-	X
57	MG	13	1650	-	-	-	X
57	MG	13	1651	-	-	-	X
57	MG	13	1654	-	-	-	X
57	MG	13	1668	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1677	-	-	-	X
57	MG	13	1678	-	-	-	X
57	MG	13	1680	-	-	-	X
57	MG	13	1683	-	-	-	X
57	MG	13	1684	-	-	-	X
57	MG	13	1687	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3007	-	-	-	X
57	MG	14	3017	-	-	-	X
57	MG	14	3018	-	-	-	X
57	MG	14	3019	-	-	-	X
57	MG	14	3024	-	-	-	X
57	MG	14	3028	-	-	-	X
57	MG	14	3030	-	-	-	X
57	MG	14	3035	-	-	-	X
57	MG	14	3037	-	-	-	X
57	MG	14	3041	-	-	-	X
57	MG	14	3042	-	-	-	X
57	MG	14	3046	-	-	-	X
57	MG	14	3047	-	-	-	X
57	MG	14	3049	-	-	-	X
57	MG	14	3050	-	-	-	X
57	MG	14	3061	-	-	-	X
57	MG	14	3064	-	-	-	X
57	MG	14	3068	-	-	-	X
57	MG	14	3071	-	-	-	X
57	MG	14	3073	-	-	-	X
57	MG	14	3074	-	-	-	X
57	MG	14	3078	-	-	-	X
57	MG	14	3080	-	-	-	X
57	MG	14	3082	-	-	-	X
57	MG	14	3083	-	-	-	X
57	MG	14	3088	-	-	-	X
57	MG	14	3092	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3098	-	-	-	X
57	MG	14	3105	-	-	-	X
57	MG	14	3109	-	-	-	X
57	MG	14	3111	-	-	-	X
57	MG	14	3119	-	-	-	X
57	MG	14	3120	-	-	-	X
57	MG	14	3123	-	-	-	X
57	MG	14	3136	-	-	-	X
57	MG	14	3137	-	-	-	X
57	MG	14	3139	-	-	-	X
57	MG	14	3143	-	-	-	X
57	MG	14	3144	-	-	-	X
57	MG	14	3150	-	-	-	X
57	MG	14	3166	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3167	-	-	-	X
57	MG	14	3168	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	14	3172	-	-	-	X
57	MG	14	3174	-	-	-	X
57	MG	14	3175	-	-	-	X
57	MG	14	3186	-	-	-	X
57	MG	14	3191	-	-	-	X
57	MG	14	3205	-	-	-	X
57	MG	14	3212	-	-	-	X
57	MG	14	3219	-	-	-	X
57	MG	14	3222	-	-	-	X
57	MG	14	3223	-	-	-	X
57	MG	14	3229	-	-	-	X
57	MG	14	3231	-	-	-	X
57	MG	14	3238	-	-	-	X
57	MG	14	3243	-	-	-	X
57	MG	14	3254	-	-	-	X
57	MG	14	3259	-	-	-	X
57	MG	14	3260	-	-	-	X
57	MG	14	3268	-	-	-	X
57	MG	16	201	-	-	-	X
57	MG	16	205	-	-	-	X
57	MG	1G	1602	-	-	-	X
57	MG	1G	1604	-	-	-	X
57	MG	1G	1607	-	-	-	X
57	MG	1G	1609	-	-	-	X
57	MG	1G	1611	-	-	-	X
57	MG	1G	1613	-	-	-	X
57	MG	1G	1614	-	-	-	X
57	MG	1G	1615	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1625	-	-	-	X
57	MG	1G	1636	-	-	-	X
57	MG	1G	1640	-	-	-	X
57	MG	1G	1644	-	-	-	X
57	MG	1G	1645	-	-	-	X
57	MG	1G	1647	-	-	-	X
57	MG	1G	1650	-	-	-	X
57	MG	1H	3004	-	-	-	X
57	MG	1H	3005	-	-	-	X
57	MG	1H	3008	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3009	-	-	-	X
57	MG	1H	3014	-	-	-	X
57	MG	1H	3018	-	-	-	X
57	MG	1H	3024	-	-	-	X
57	MG	1H	3025	-	-	-	X
57	MG	1H	3029	-	-	-	X
57	MG	1H	3035	-	-	-	X
57	MG	1H	3036	-	-	-	X
57	MG	1H	3038	-	-	-	X
57	MG	1H	3041	-	-	-	X
57	MG	1H	3043	-	-	-	X
57	MG	1H	3045	-	-	-	X
57	MG	1H	3050	-	-	-	X
57	MG	1H	3053	-	-	-	X
57	MG	1H	3054	-	-	-	X
57	MG	1H	3056	-	-	-	X
57	MG	1H	3057	-	-	-	X
57	MG	1H	3061	-	-	-	X
57	MG	1H	3064	-	-	-	X
57	MG	1H	3066	-	-	-	X
57	MG	1H	3067	-	-	-	X
57	MG	1H	3070	-	-	-	X
57	MG	1H	3074	-	-	-	X
57	MG	1H	3078	-	-	-	X
57	MG	1H	3079	-	-	-	X
57	MG	1H	3082	-	-	-	X
57	MG	1H	3088	-	-	-	X
57	MG	1H	3090	-	-	-	X
57	MG	1H	3091	-	-	-	X
57	MG	1H	3098	-	-	-	X
57	MG	1H	3101	-	-	-	X
57	MG	1H	3105	-	-	-	X
57	MG	1H	3107	-	-	-	X
57	MG	1H	3109	-	-	-	X
57	MG	1H	3115	-	-	-	X
57	MG	1H	3116	-	-	-	X
57	MG	1H	3120	-	-	-	X
57	MG	1H	3123	-	-	-	X
57	MG	1H	3124	-	-	-	X
57	MG	1H	3128	-	-	-	X
57	MG	1H	3135	-	-	-	X
57	MG	1H	3139	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3146	-	-	-	X
57	MG	1H	3153	-	-	-	X
57	MG	1H	3154	-	-	-	X
57	MG	1H	3162	-	-	-	X
57	MG	1H	3164	-	-	-	X
57	MG	1H	3173	-	-	-	X
57	MG	1H	3174	-	-	-	X
57	MG	1H	3179	-	-	-	X
57	MG	1H	3180	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3221	-	-	-	X
57	MG	1H	3230	-	-	-	X
57	MG	1H	3232	-	-	-	X
57	MG	1H	3240	-	-	-	X
57	MG	1H	3247	-	-	-	X
57	MG	1H	3249	-	-	-	X
57	MG	1H	3259	-	-	-	X
57	MG	1H	3267	-	-	-	X
57	MG	1H	3268	-	-	-	X
57	MG	1H	3286	-	-	-	X
57	MG	1H	3287	-	-	-	X
57	MG	1H	3290	-	-	-	X
57	MG	1H	3375	-	-	-	X
57	MG	1H	3465	-	-	-	X
57	MG	1J	201	-	-	-	X
57	MG	29	301	-	-	-	X
57	MG	2K	103	-	-	-	X
57	MG	2L	101	-	-	-	X
59	SF4	32	301	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296184 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32368	14408	5999	10456	1505			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	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	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	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	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1690	1058	336	289	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	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	139	Total	C	N	O	S	0	0	0
			1115	692	222	195	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

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

- Molecule 22 is a RNA chain called tRNA<sup>Lys</sup>.

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			
22	1L	73	Total	C	N	O	P	S	0	0	0
			1563	700	271	518	73	1			

- Molecule 23 is a RNA chain called E. coli tRNA<sup>fMet</sup>.

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

- Molecule 24 is a RNA chain called tRNA<sup>Lys</sup>.

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	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			



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

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

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 rRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1458	931	266	257	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	74	Total	C	N	O		0	0	0
			573	359	117	97				

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			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			
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
			875	550	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	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			774	499	141	133	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	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	105	Total	C	N	O	S	0	0	0
			796	513	150	128	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	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
47	D5	132	Total	C	N	O	S	0	0	0
			1074	691	193	188	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			568	352	115	100	1			

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	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	48	Total	C	N	O	S	0	0	0
			369	229	75	60	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<sup>Lys</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	3L	75	Total	C	N	O	P	0	0	0
			1601	717	280	530	74			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	3	Total	Mg	0	0
			3	3		
57	P8	1	Total	Mg	0	0
			1	1		
57	85	1	Total	Mg	0	0
			1	1		
57	C5	1	Total	Mg	0	0
			1	1		
57	13	150	Total	Mg	0	0
			150	150		
57	1J	6	Total	Mg	0	0
			6	6		
57	5I	1	Total	Mg	0	0
			1	1		
57	35	2	Total	Mg	0	0
			2	2		
57	BI	1	Total	Mg	0	0
			1	1		
57	16	12	Total	Mg	0	0
			12	12		
57	M5	1	Total	Mg	0	0
			1	1		
57	21	3	Total	Mg	0	0
			3	3		
57	31	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		
57	L8	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		
57	I8	1	Total	Mg	0	0
			1	1		
57	5E	1	Total	Mg	0	0
			1	1		
57	29	4	Total	Mg	0	0
			4	4		

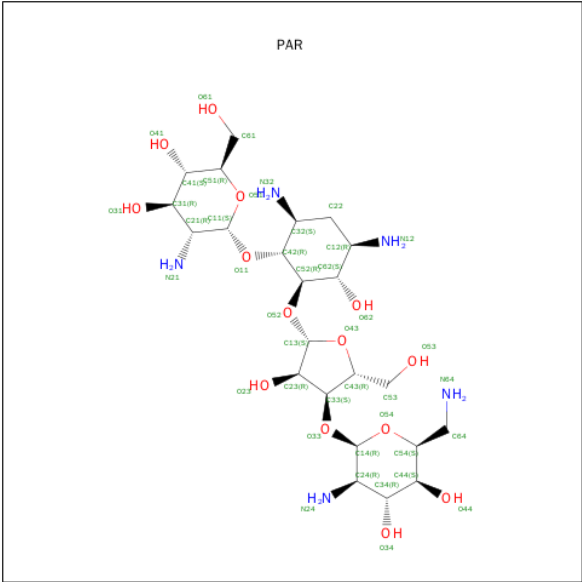
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7A	1	Total 1	Mg 1	0	0
57	2K	3	Total 3	Mg 3	0	0
57	39	2	Total 2	Mg 2	0	0
57	1G	93	Total 93	Mg 93	0	0
57	11	3	Total 3	Mg 3	0	0
57	1H	502	Total 502	Mg 502	0	0
57	E5	1	Total 1	Mg 1	0	0
57	88	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	14	454	Total 454	Mg 454	0	0
57	78	1	Total 1	Mg 1	0	0
57	55	1	Total 1	Mg 1	0	0
57	41	2	Total 2	Mg 2	0	0
57	2L	4	Total 4	Mg 4	0	0

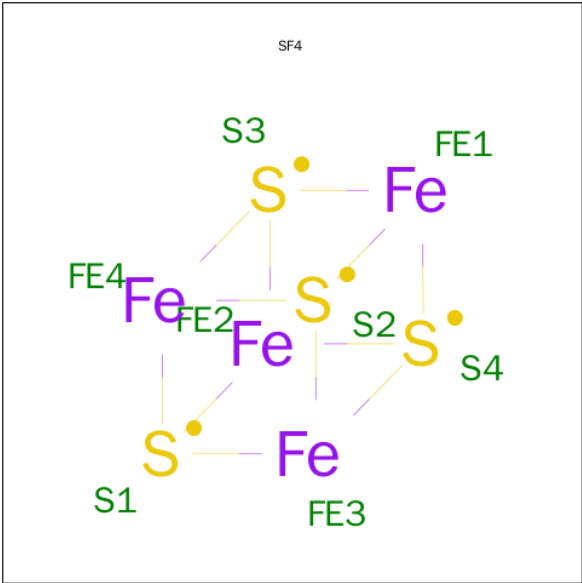
- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total	C	N	O	0	0
			42	23	5	14		
58	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- 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 1	Zn 1	0	0
60	5A	1	Total 1	Zn 1	0	0
60	G8	1	Total 1	Zn 1	0	0
60	5I	1	Total 1	Zn 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	319	Total 319	O 319	0	0
61	3E	3	Total 3	O 3	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	3I	3	Total 3	O 3	0	0
61	5I	1	Total 1	O 1	0	0
61	6I	2	Total 2	O 2	0	0
61	8I	2	Total 2	O 2	0	0
61	BI	5	Total 5	O 5	0	0
61	1F	1	Total 1	O 1	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	7	Total 7	O 7	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	1158	Total 1158	O 1158	0	0
61	16	26	Total 26	O 26	0	0
61	11	12	Total 12	O 12	0	0
61	21	6	Total 6	O 6	0	0
61	31	9	Total 9	O 9	0	0
61	58	1	Total 1	O 1	0	0
61	78	6	Total 6	O 6	0	0
61	88	2	Total 2	O 2	0	0
61	C8	2	Total 2	O 2	0	0
61	E8	3	Total 3	O 3	0	0
61	F8	2	Total 2	O 2	0	0
61	G8	2	Total 2	O 2	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	3	Total 3	O 3	0	0
61	K8	2	Total 2	O 2	0	0
61	L8	2	Total 2	O 2	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	9	Total 9	O 9	0	0
61	1G	226	Total 226	O 226	0	0
61	32	3	Total 3	O 3	0	0
61	42	1	Total 1	O 1	0	0

*Continued on next page...*

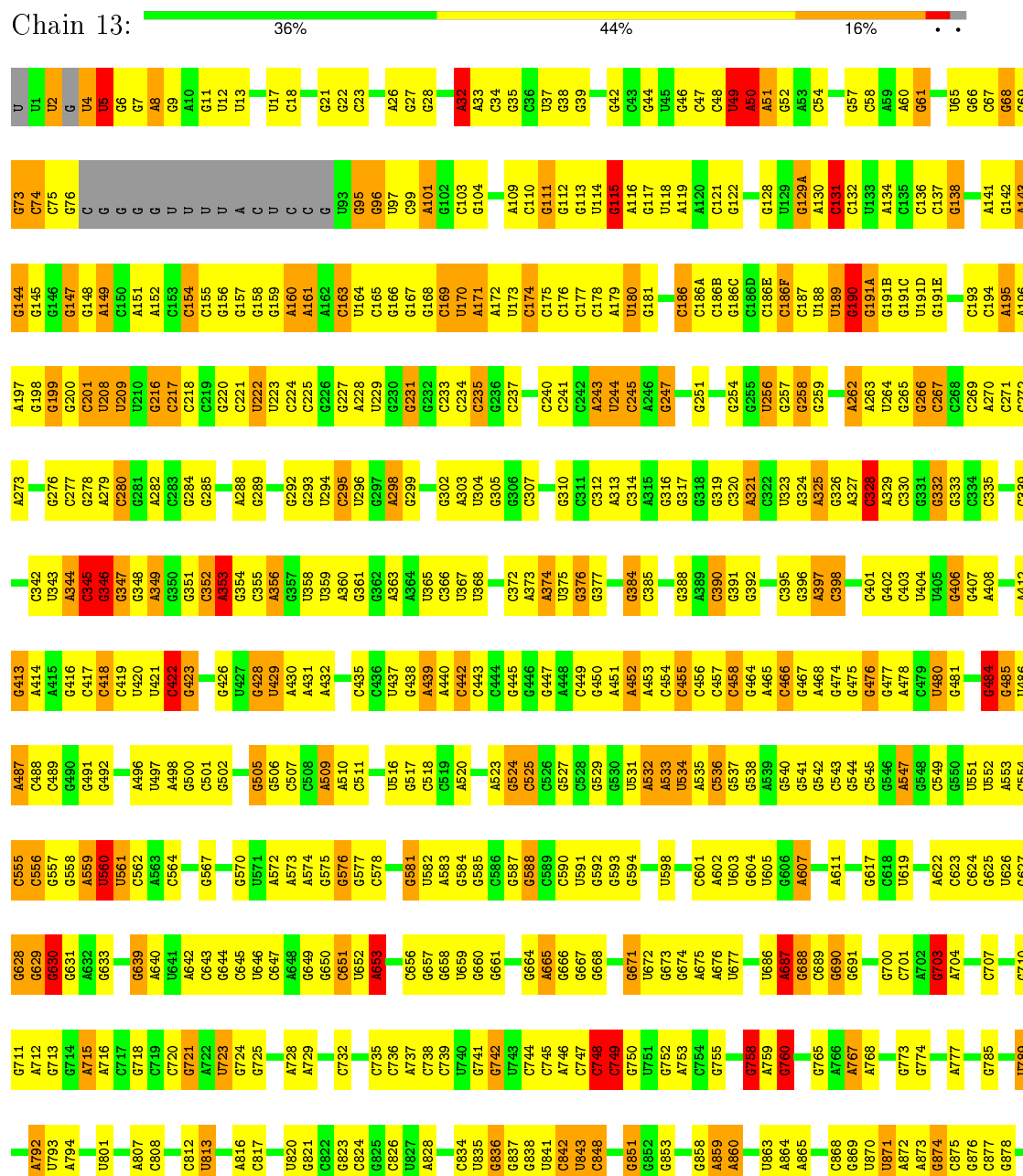
*Continued from previous page...*

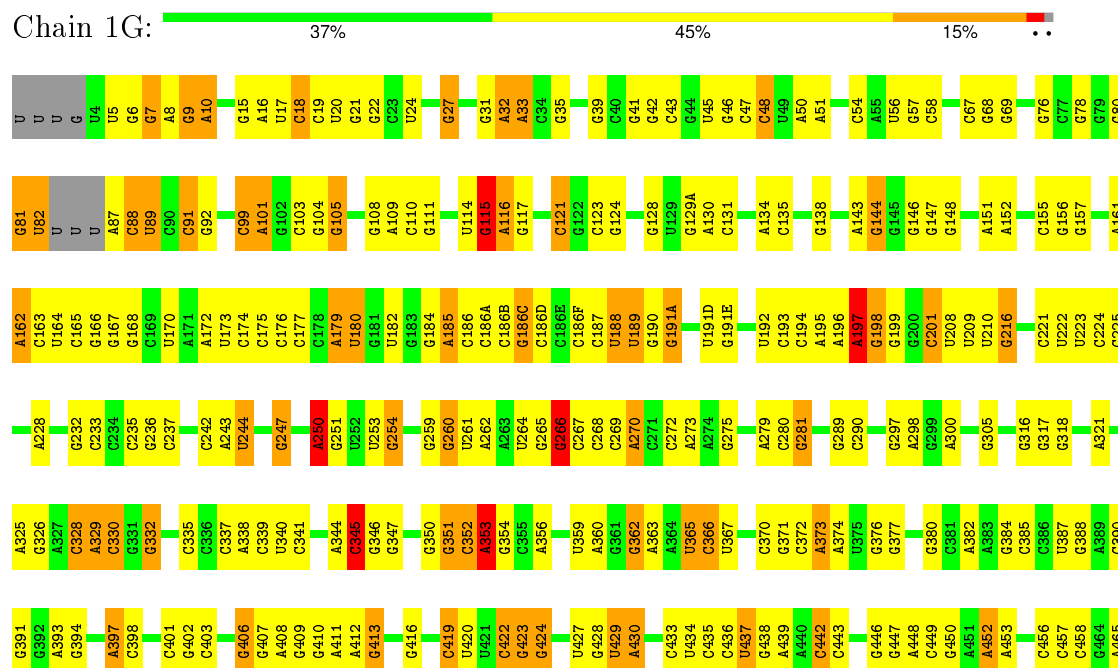
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3A	1	Total 1	O 1	0	0
61	6A	3	Total 3	O 3	0	0
61	8A	1	Total 1	O 1	0	0
61	BA	3	Total 3	O 3	0	0
61	2L	1	Total 1	O 1	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1015	Total 1015	O 1015	0	0
61	1J	18	Total 18	O 18	0	0
61	19	12	Total 12	O 12	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	35	5	Total 5	O 5	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	2	Total 2	O 2	0	0
61	A5	2	Total 2	O 2	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	4	Total 4	O 4	0	0
61	H5	3	Total 3	O 3	0	0
61	L5	2	Total 2	O 2	0	0
61	M5	10	Total 10	O 10	0	0

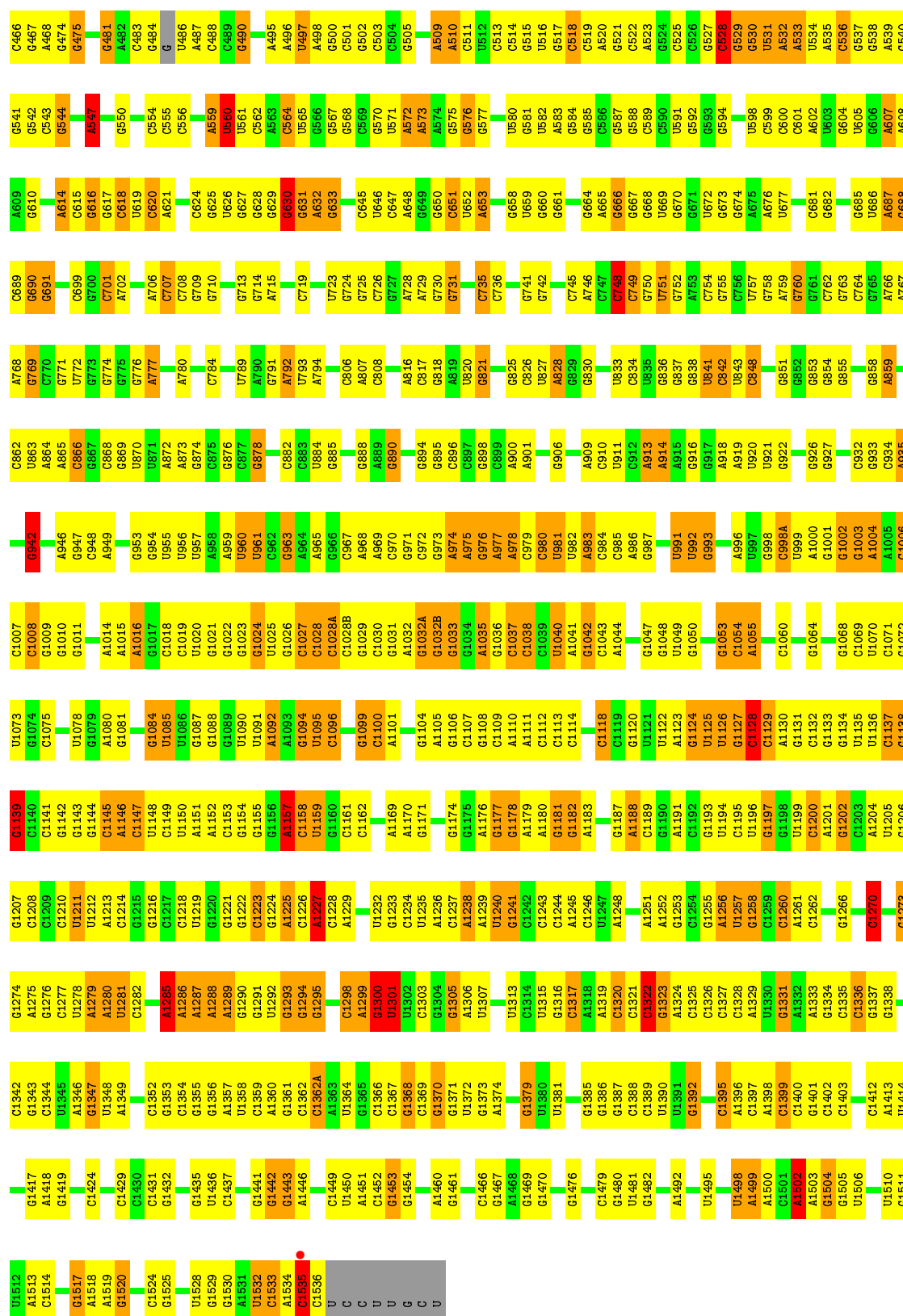
### 3 Residue-property plots

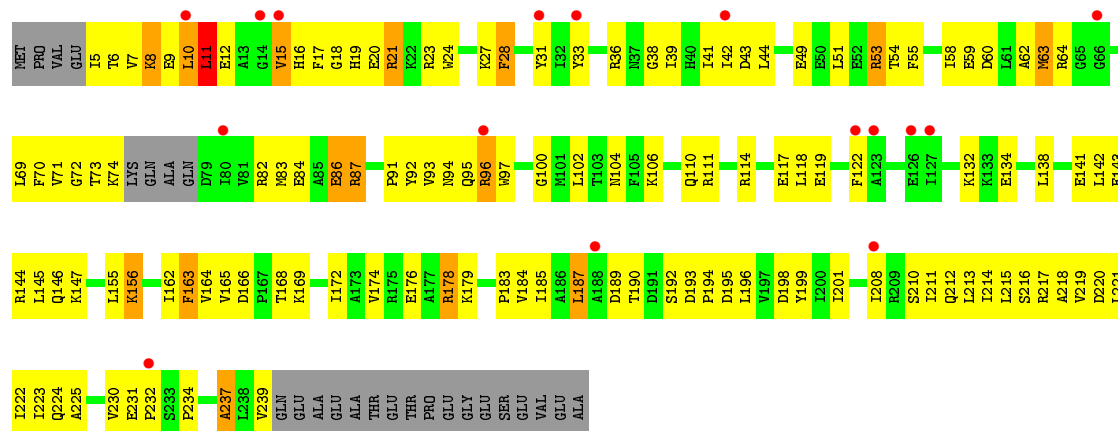
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

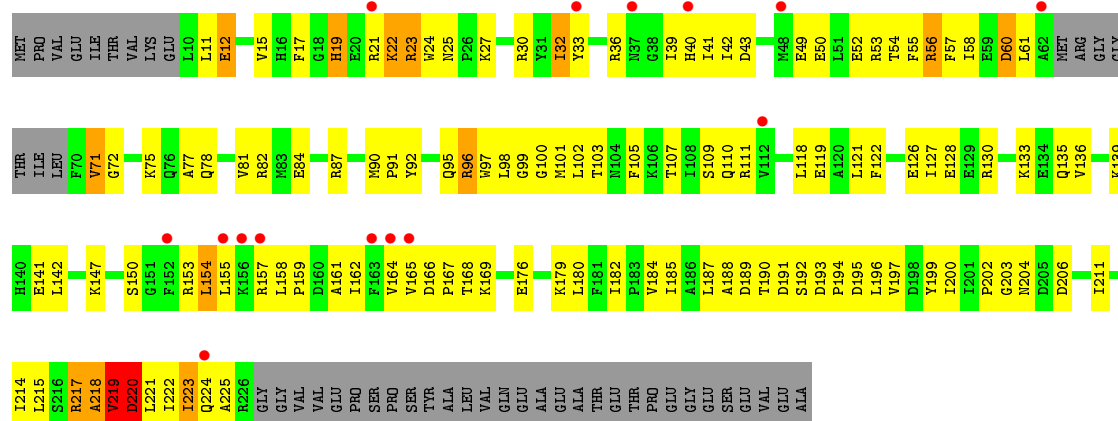




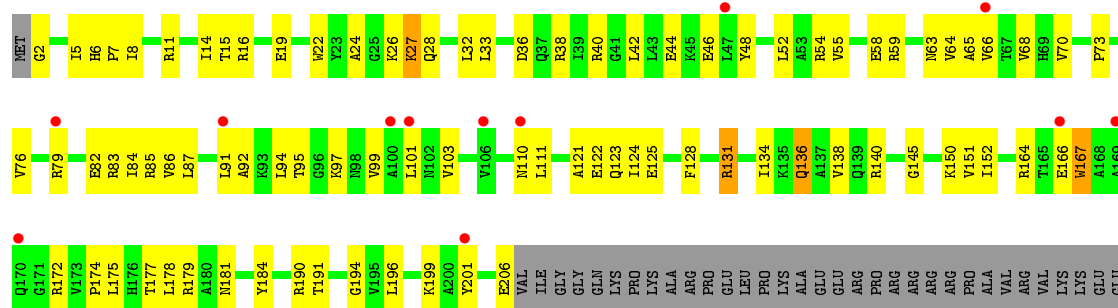




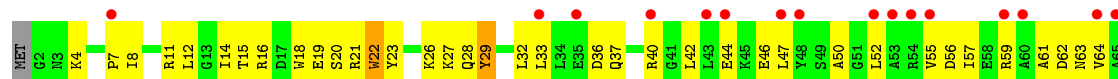
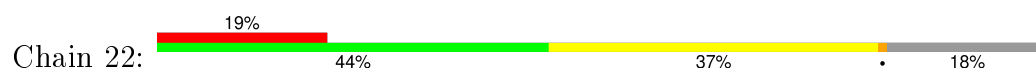
• Molecule 2: 30S ribosomal protein S2



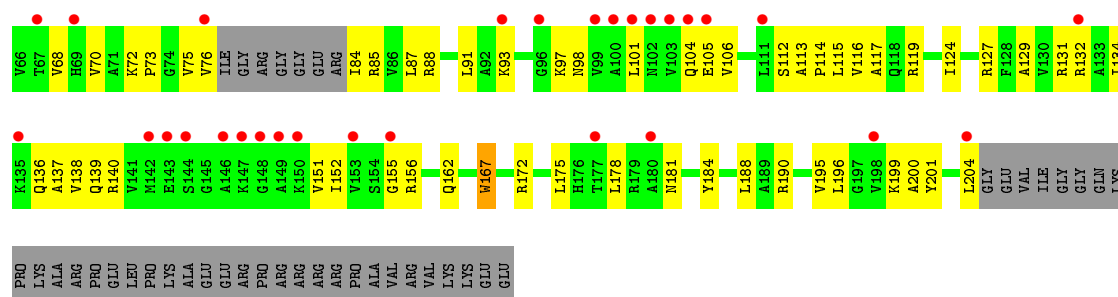
• Molecule 3: 30S ribosomal protein S3



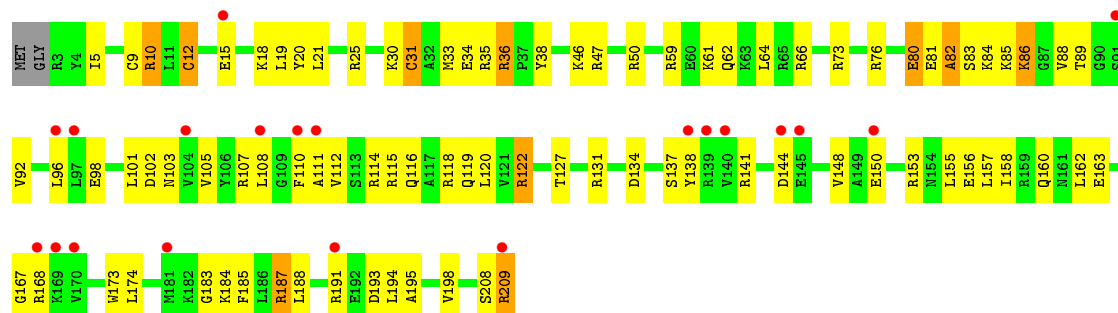
• Molecule 3: 30S ribosomal protein S3



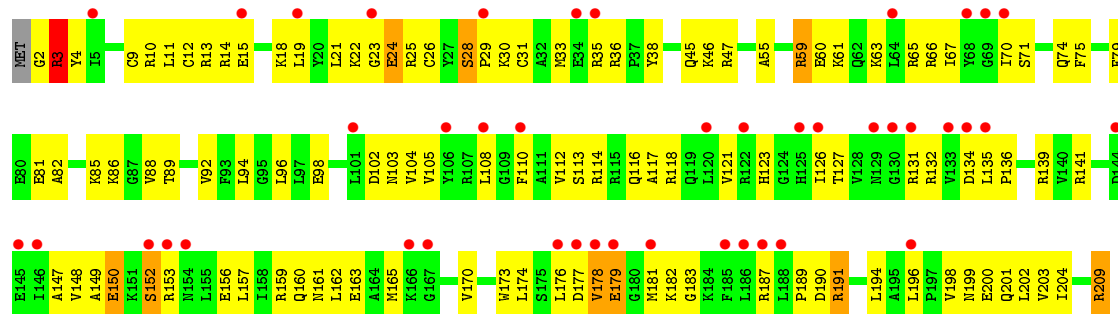




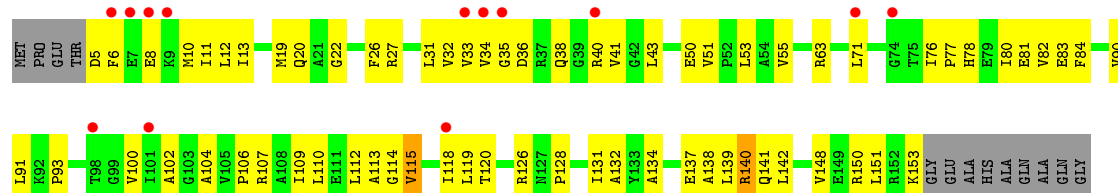
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

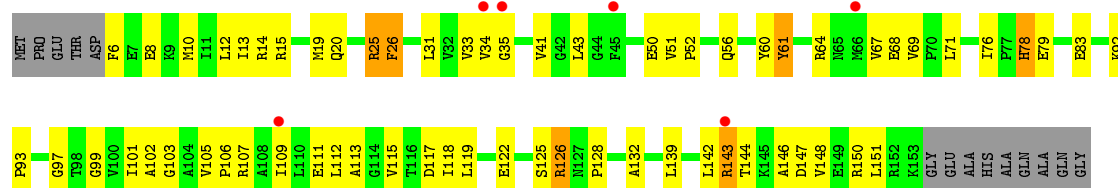


• Molecule 5: 30S ribosomal protein S5

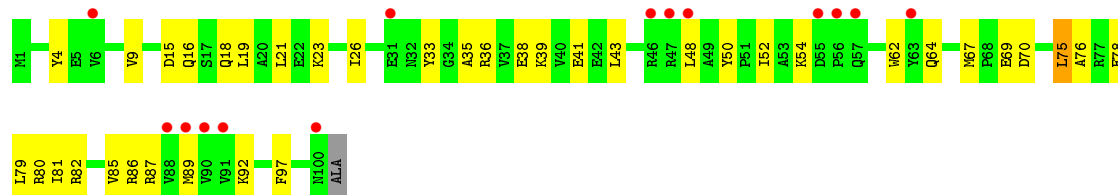


• Molecule 5: 30S ribosomal protein S5

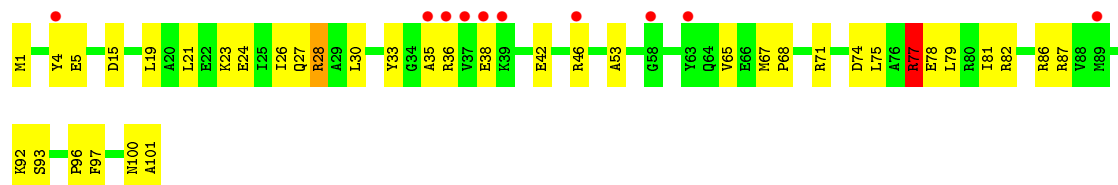




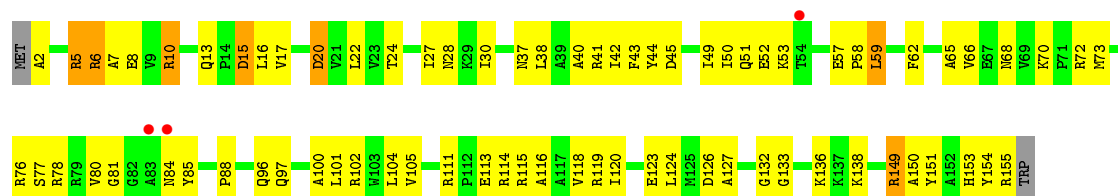
• Molecule 6: 30S ribosomal protein S6



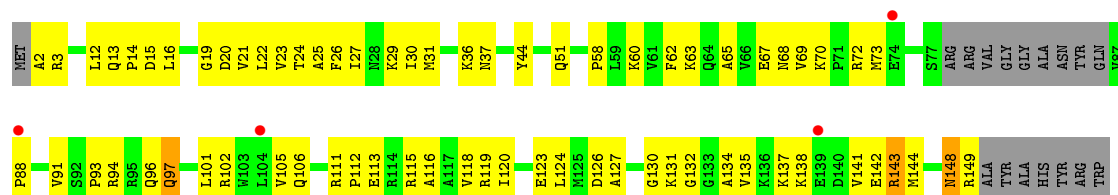
• Molecule 6: 30S ribosomal protein S6



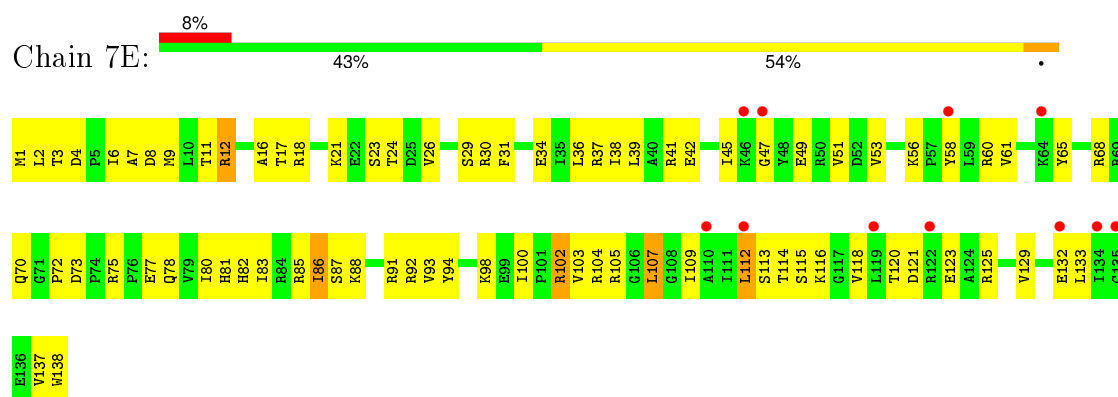
• Molecule 7: 30S ribosomal protein S7



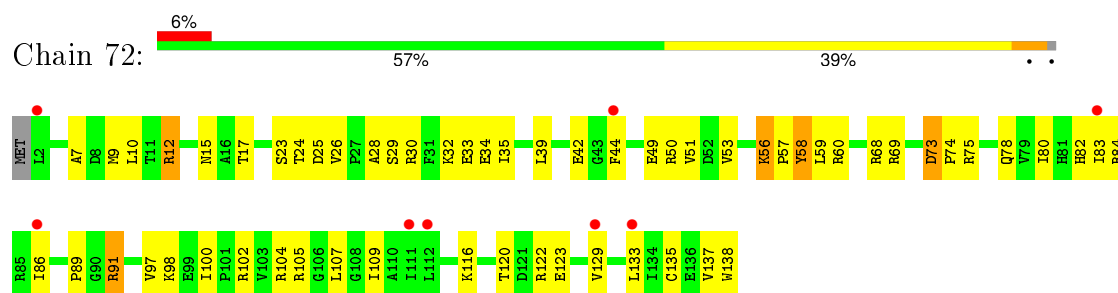
• Molecule 7: 30S ribosomal protein S7



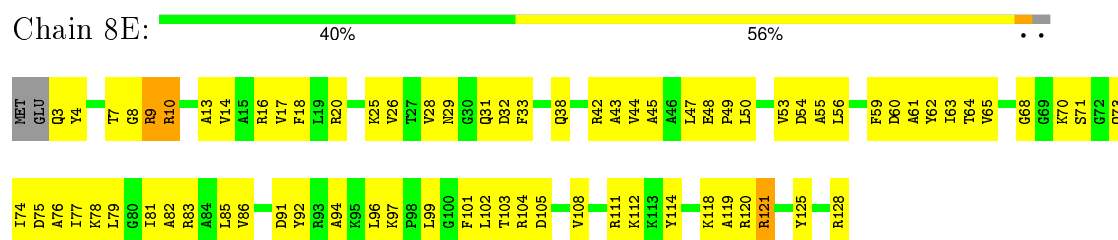
• Molecule 8: 30S ribosomal protein S8



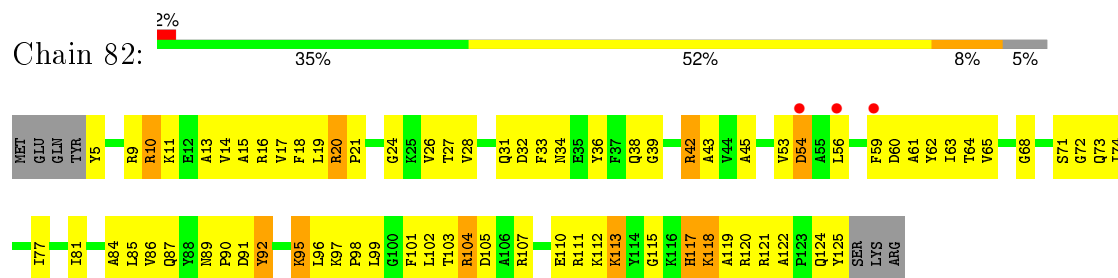
• Molecule 8: 30S ribosomal protein S8



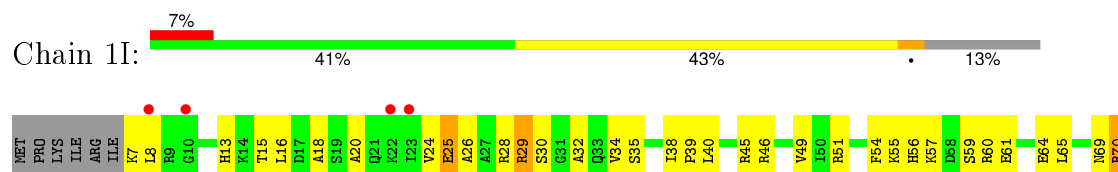
• Molecule 9: 30S ribosomal protein S9

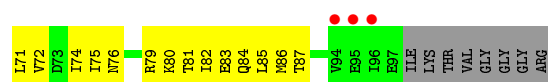


• Molecule 9: 30S ribosomal protein S9

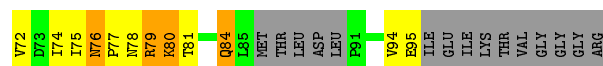
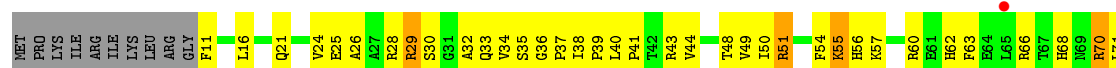


• Molecule 10: 30S ribosomal protein S10

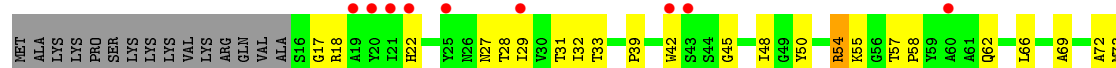




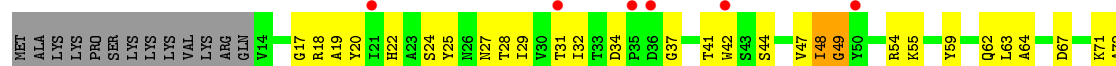
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

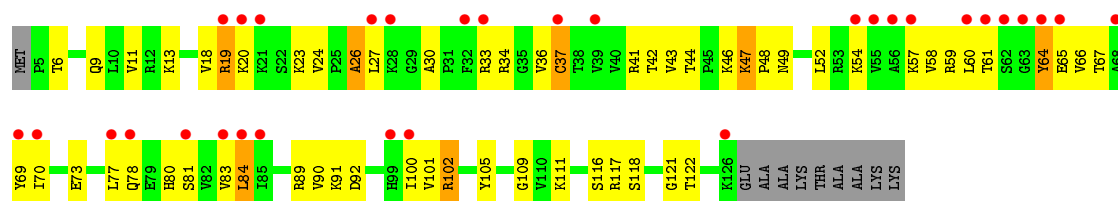


- Molecule 12: 30S ribosomal protein S12

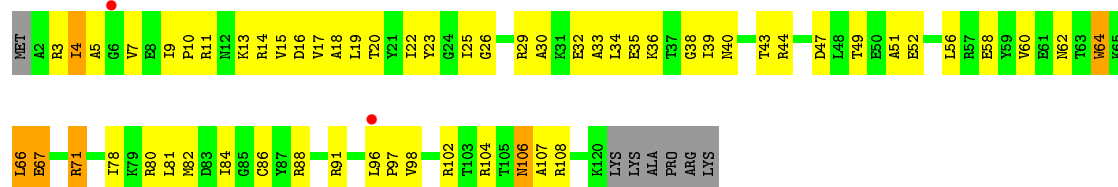


- Molecule 12: 30S ribosomal protein S12

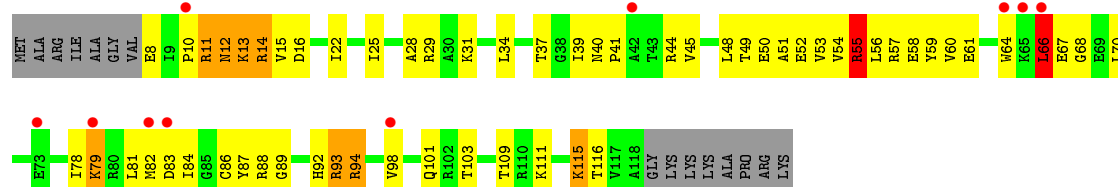
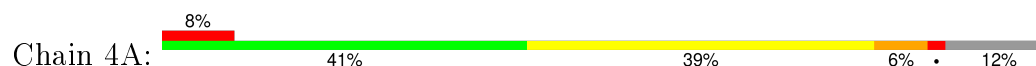




• Molecule 13: 30S ribosomal protein S13



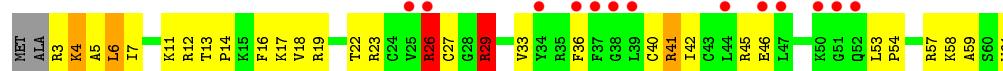
• Molecule 13: 30S ribosomal protein S13



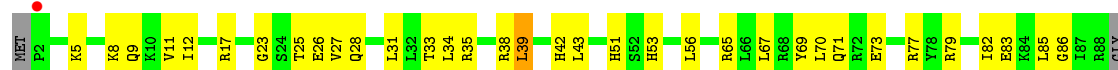
• Molecule 14: 30S ribosomal protein S14 type Z



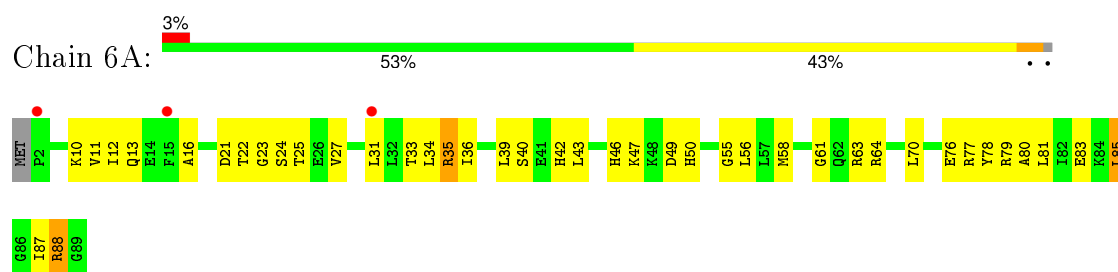
• Molecule 14: 30S ribosomal protein S14 type Z



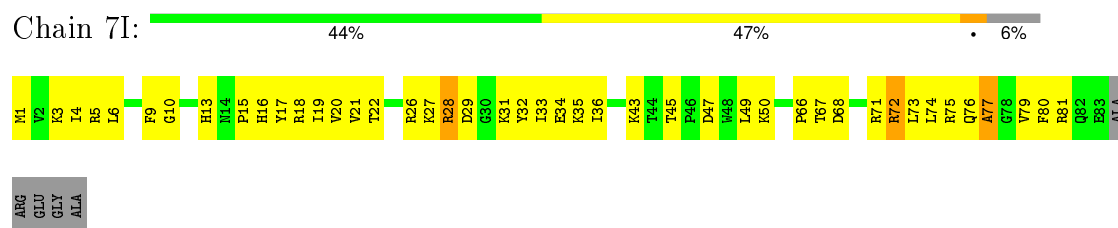
• Molecule 15: 30S ribosomal protein S15



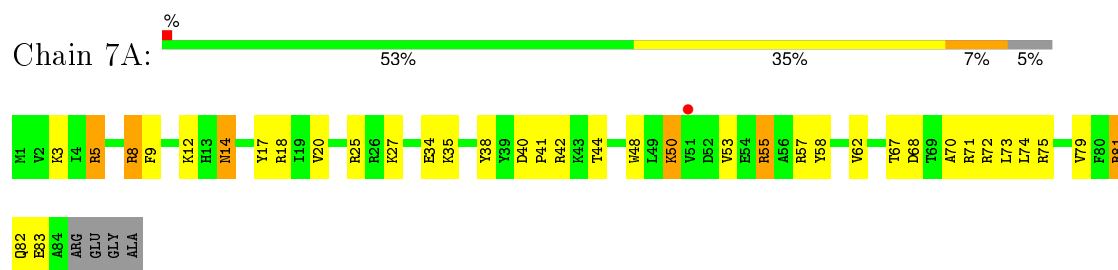
• Molecule 15: 30S ribosomal protein S15



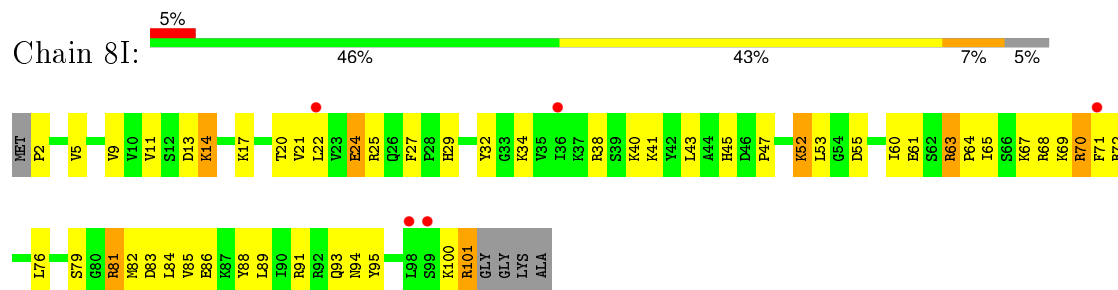
- Molecule 16: 30S ribosomal protein S16



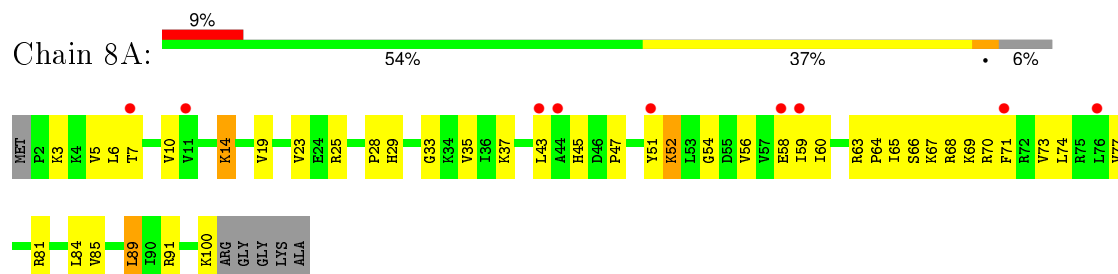
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

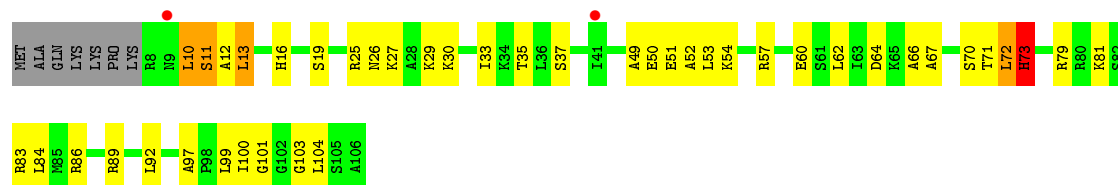


- Molecule 17: 30S ribosomal protein S17

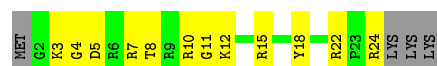


- Molecule 18: 30S ribosomal protein S18

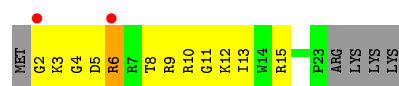




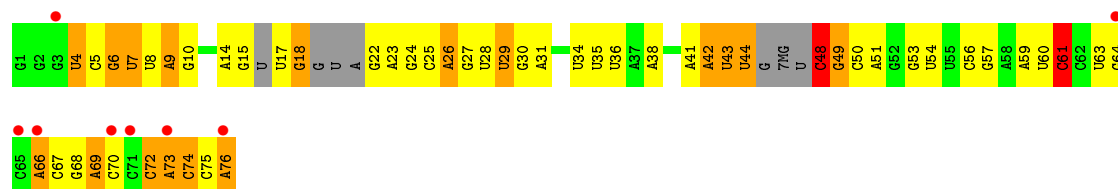
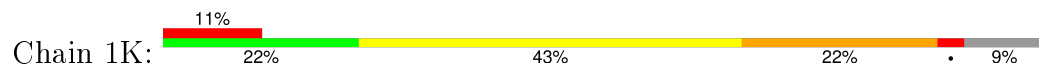
- Molecule 21: 30S ribosomal protein Thx



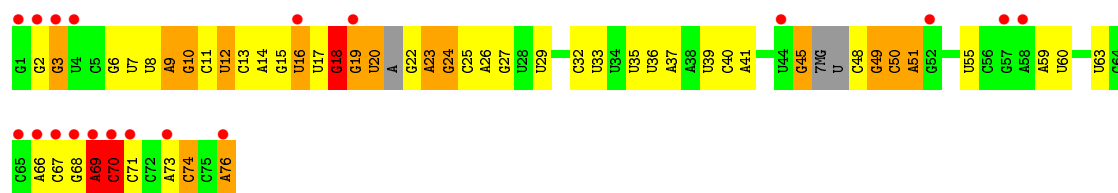
- Molecule 21: 30S ribosomal protein Thx



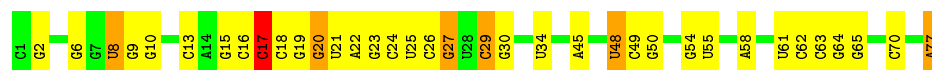
- Molecule 22: tRNA<sup>Lys</sup>



- Molecule 22: tRNA<sup>Lys</sup>

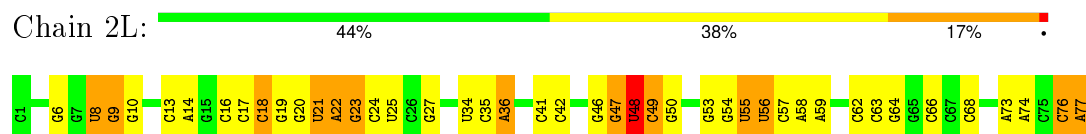


- Molecule 23: E. coli tRNA<sup>fMet</sup>

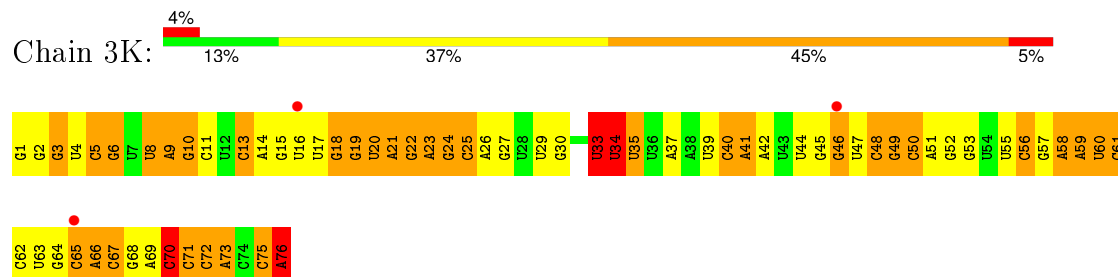


- Molecule 23: E. coli tRNA<sup>fMet</sup>

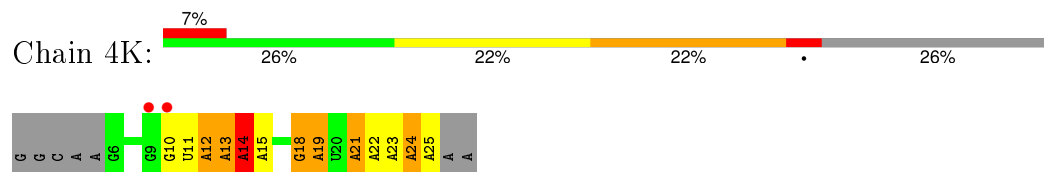




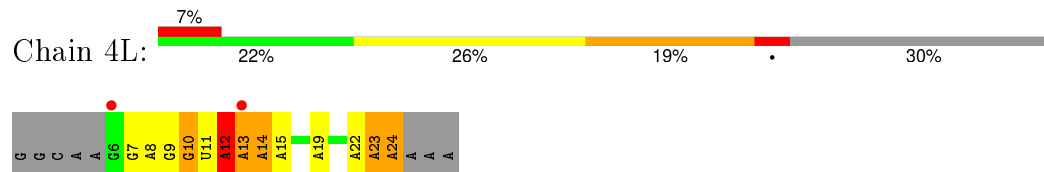
- Molecule 24: tRNA<sup>Lys</sup>



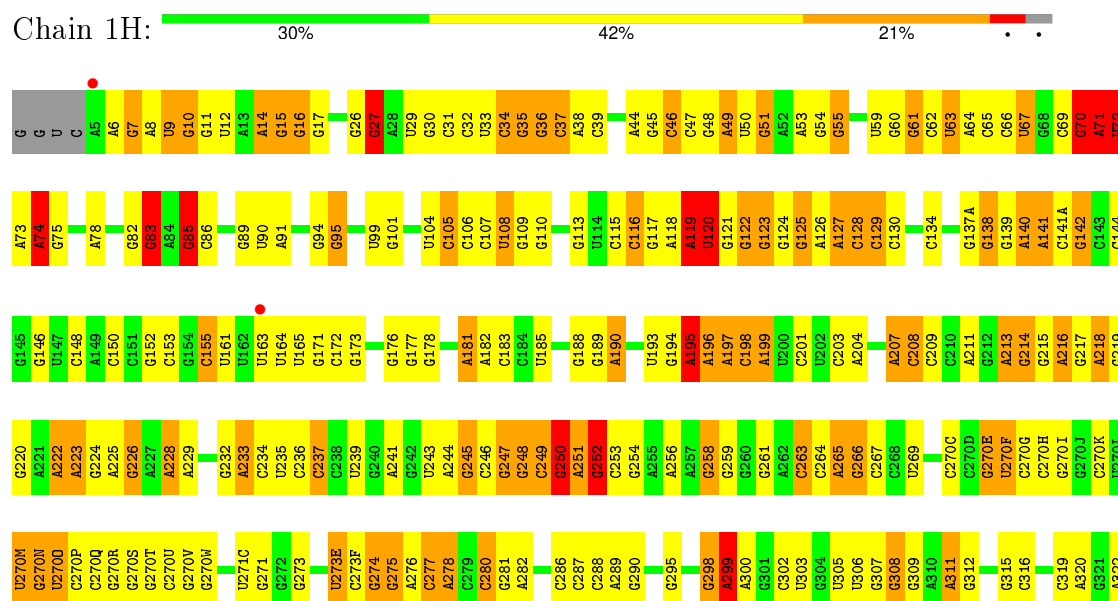
- Molecule 25: mRNA



- Molecule 25: mRNA

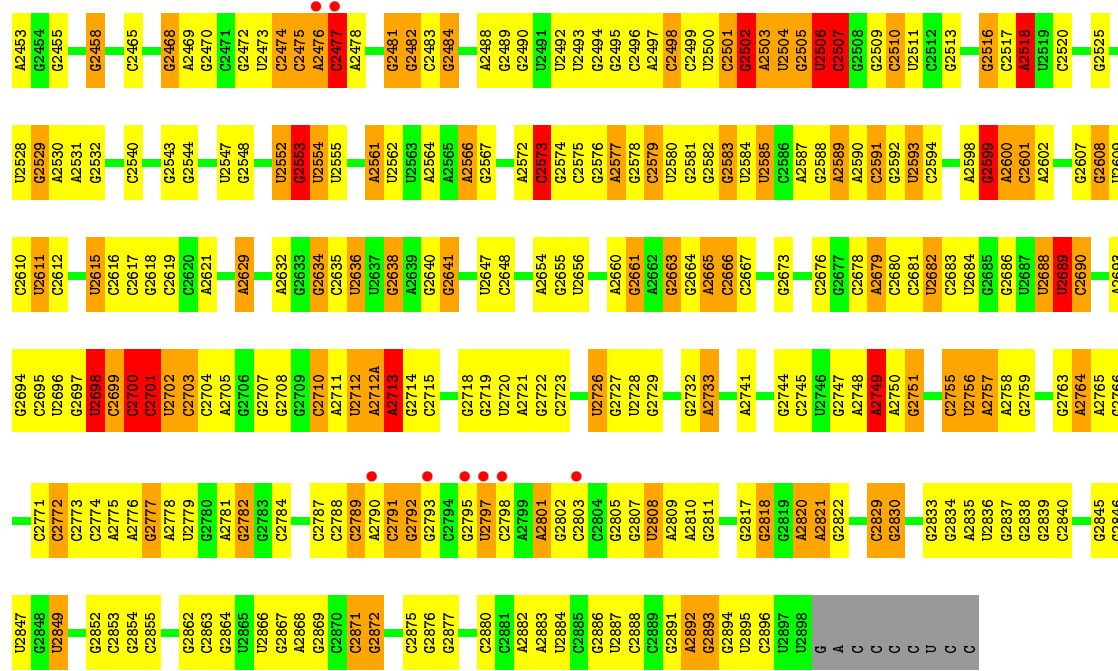


- Molecule 26: 23S rRNA

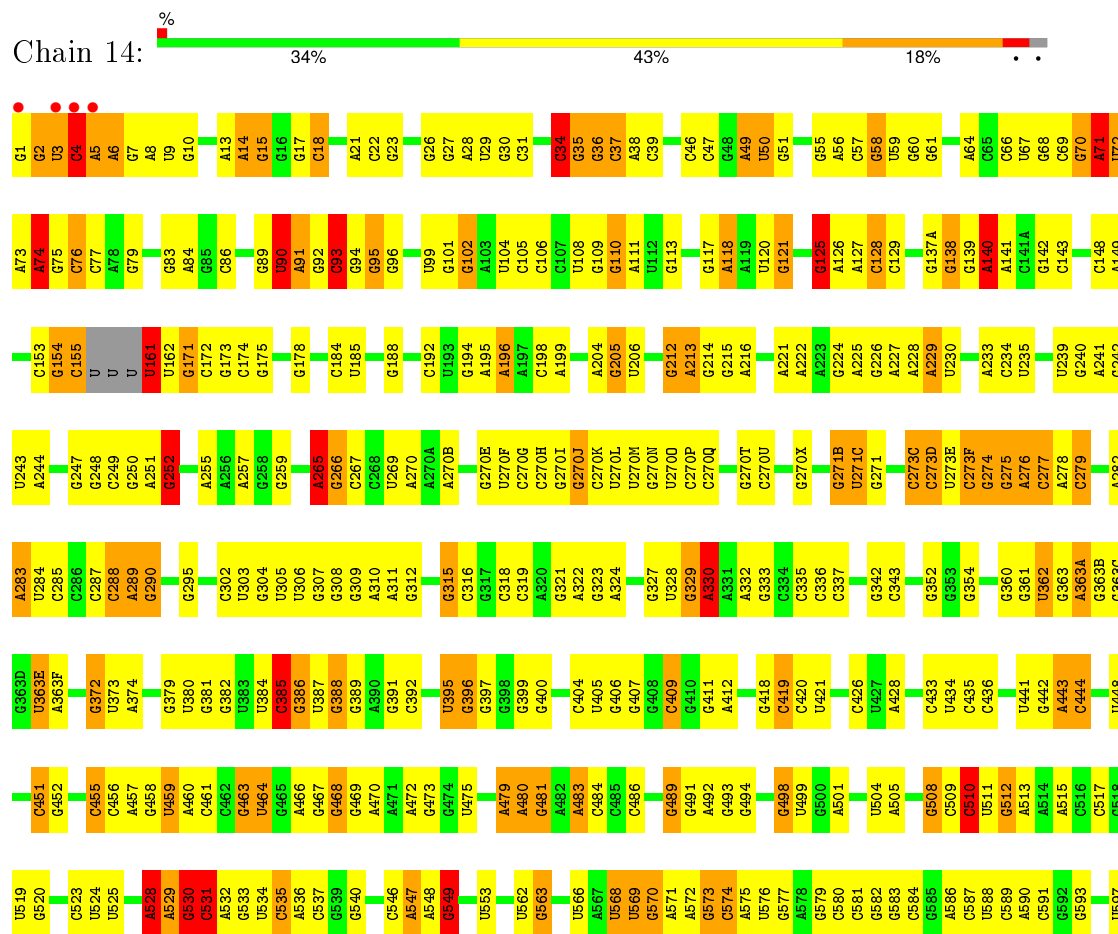


U1329	G1264	G1190	G1122	G989	G923	G850	A782	G717	C654Q	A608	C535	U464	C392	G323
C1330	A1265	G1191	C1123	A990	C923	U851	A783	A718	C654R	A609	A336	G465	A324	A324
A1331	G1192	C991	G1124	G852	A926	G853	A784	C719	G654S	G609A	C537	A466	C393	G325
C1332	G1193	G992	G1125	G853	G926	G854	G785	C720	A654T	G610	G539	G467	A394	G326
C1333	A1194	G993	A1126	G993	U930	C856	G786	C721		G612	C546	G468	U395	G327
A1336	G1195	C994	A1127	C995	U931	C857	U787	A722	U657	U613	C547	A470	G397	G329
G1337	U1198	C996	A1128	A996	G931	U858	A788	G723	C658	U614	A547	A471	A401	A331
G1338	U1199	G997	A1129	G997	G932	U859	C790	U724	C659	U615	A548	A472		
C1339	C1200	C998	U1130	C998	A933	G860	C791	G725	G660	G617	G549	G473	C404	C334
U1340	C1201	A1001	G1131	C999	G934	A861	G792	G726	G661	G618	G552	G474	C405	C335
A1341	G1202	G1002	G1135	U1001	C935	G862	A793	A727	G662	G618A	U553	U475	U405	C336
A1342	G1203	G1003	G1136	G1002	C936	G863	G794	G728	G663	G619	U554	U476	G406	
G1343	A1204	C1004	G1137	G1003	U937	G864	C795	G729	G664	G620	G556	A477	C337	
G1344	U1205	C1005	G1138	C1004	G938	C865	C796	C730	G665	G621	U557	A478	C409	G338
C1345	G1206	C1006	G1139	A941		A866	C797	C731	G666	A621	U558	A479	G410	U339
G1346	C1207	C1007	G1140	G942	G923	G873	C800	G734	U667	G622	G558	A480	A411	A340
G1347	C1208	C1008	U1141	U943	U943		A801	A735	C668	G623		A482	A412	
G1348	G1209	A1009	U1142	G944	G944	U877	A802	C736	A670	G625	C563	A483	G418	A346
A1349	A1210	A1010	A1143	A945	A945	A878	A803	G737	G672	U626	C564	A484	C419	A347
C1350	G1211	C1011	G1144	G946	G946	G879	A804	G738	G673	G627	C565	C484	C420	
C1351	G1212	U1012	C1144	G947	G947	G880	G805		G674	G628	U566	C485		
U1352	A1213	C1013	C1145	G948	G948	G881	C906	G741	A675	G630	U568	A491	U350	
A1353	G1214	U1014		G949	G949	G882	U807	G742	A676	A631	U569	A492	G351	G351
	G1215	G1016		G950	G950	G		G743	A677	A632	C426	A493	G352	G352
U1357	C1216	C951		C951	C951	C	C812				U427	G493	U427	G353
G1358	G1217	U1019	G1151	C952	C952	C	U813	U747	C678	A633	A428	G494	G354	G354
A1359	C1218	A1020	G1152	A953	A953	C	C814	G748	C679	C634	A429	G495	G355	G355
A1360	G1219	U1021	A1155	C954	C954	C	C915		C680	G635	G430	G496	G430	G356
	C1220	G1022	A1156	C955	C955	A	C916	A751	G681	G636	C574	G498	U431	A357
G1363	C1221	U1023	G1157	C956	C956	C	C817	G751	G682	A637	A575	U499	A432	U358
G1364	C1222	G1024	C1158	A957	A957	C	C818	A752	G683	G638	U576	G500	C433	
A1365	G1229A	G1025		U958	U958	A	G819	G753	C684	U639	G577	A501	C434	G361
A1366	C1230	U1026	C1161	C959	C959	G	A821	C754	A685	A502	A578	A502	C435	U362
G1367	G1231	A1027	G1162	C960	C960	C	U822	C755	G686	U504	G579	U504	G439	A363A
G1368	G1232	C961	G1163	C962	C962	C	U823	C756	C687	A505	C580	A505	G440	G363B
G1369	G1233	G1030	U1164	U962	U962	A	C825	U757	U688	G644	C581	G508	C452	G363C
C1370	G1236	C1031	U1165	U963	U963	A	U826		A689	C645	C582	C509	C453	C370
G1371	A1237	A1032	C1166	C964	C964	C	U827	G760	G690	G647	G583	C510	C454	A371
U1372	G1238	U1033	G1167	C965	C965	C	U828	A761	C691	G647	G584	U511	C445	G372
	A1241	G1034	G1168	G966	G966	C	U829	G762	C692	G651	G586	G512	C446	A363F
G1375	G1244	U1035	G1169	C970	C970	C	G831	A764	U694		A586	G513	C447	C364
C1376	G1245	G1036	G1170	C971	C971	C	G832	G765		A654	C589	A514	U447	G370
G1377	G1246	C1037	G1171	G972	G972	C	U833	C766	C698	A654A	A590	A515	U448	A371
A1378	A1247	G1038	G1172	C973	C973	C	U834	G767	A699	G654B	C591	C516	A449	G372
G1380	C1314	U1039	U1173	A973	A973	C	A835	G768	G700	G654C	G592	C517	G450	U373
G1381	G1250	G1040	G1174	G974	G974	C	G836	G769	G701	G654D	G593	C518	C451	A374
	C1251	C1041	G1175	C975	C975	C	C837	G770	G702	C	U594	G519	G452	G375
A1384	G1252	G1042	U1176	G976	G976	C	C838	G771	U703	C		U519	C453	C376
G1385	A1253	A1043	C1177	G977	G977	C	U839	C772	G704	C	G598	G520	A454	C377
C1386	G1254	A1044	G1178	G978	G978	C	C840	U773	A705	G	C599	A454	C455	
C1387	G1255	G1045	G1179	G979	G979	C	A841	U774	A706	C	C527	C527	C456	U380
G1388	C1256	A1046	C982	C982	C982	C	G842	G775		A	G601	A529	A457	U381
G1389	U1108	A1047	G983	C983	C983	C	G843	G776	U709	C	G602	G530	G458	U383
	G1183	A1048	U913	C984	C984	C	C844	G777	G710	C	A603	A531	U459	U384
G1392	G1184	C1049	A984	C985	C985	C	G845	G778		G	G604	C532	A460	C385
G1393	C1185	A1050	G985	C986	C986	C	G846	G779	U714	G654E	G605	A532	C461	G386
A1392	G1186	G1051	G986	G987	G987	C	G847	G780	G715	G654F	U606	G533	C462	
A1393	U1187	C1052	C987	A917	A917	C	A849	A781				U607	G463	G389
U1394	C1261	C1053	A	A988	A988	C								
A1395	U1263	A1053												

C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380																																																																																																																																																																																																																																																																																																																																																																																																																																										
G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315																																																																																																																																																																																																																																																																																																																																																																																																																																														
A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252																																																																																																																																																																																																																																																																																																																																																																																																																														
G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175																																																																																																																																																																																																																																																																																																																																																																																																																																											
G2037	G2038	G2039	G2040	G2041	G2042	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2060	G2061	G2062	G2063	G2064	G2065	G2066	G2067	G2068	G2069	G2070	G2071	G2072	G2073	G2074	G2075	G2076	G2077	G2078	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111																																																																																																																																																																																																																																																																																																																																																																																																																																
A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380
U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008					

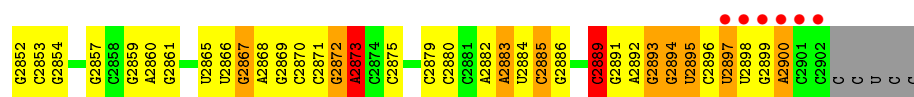


• Molecule 26: 23S rRNA

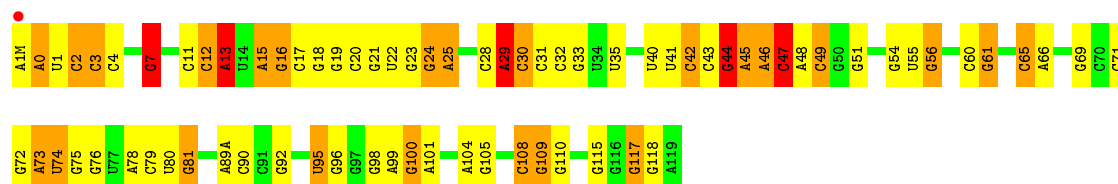




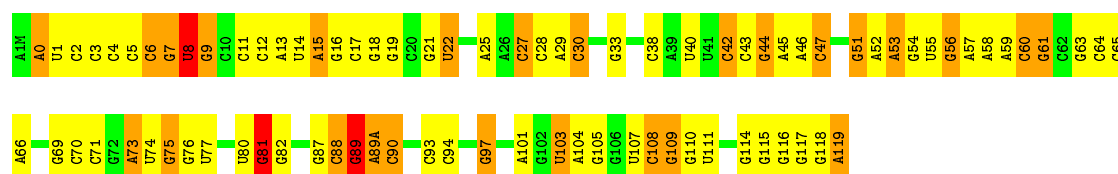
A2778	A2779	G2780	A2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	A2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	A2800	A2801	G2802	G2803	G2804	G2805	G2807	G2808	G2809	G2810	G2811	G2812	G2815	G2816	G2817	G2818	G2819	A2820	A2821	G2822	A2823	G2830	G2831	G2832	G2833	G2834	A2835	A2836	G2837	G2838	G2839	G2845	G2846	G2847	G2848	G2849	A2850	A2851																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C1683	C1684																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															</



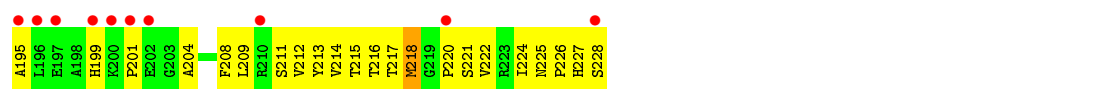
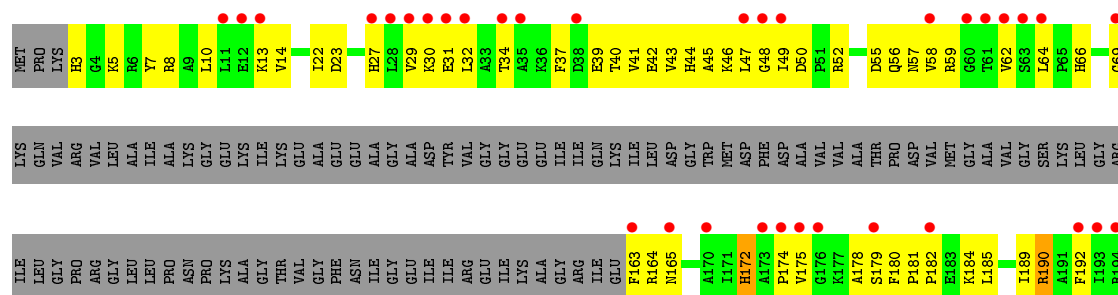
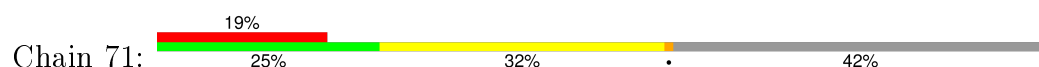
• Molecule 27: 5S rRNA



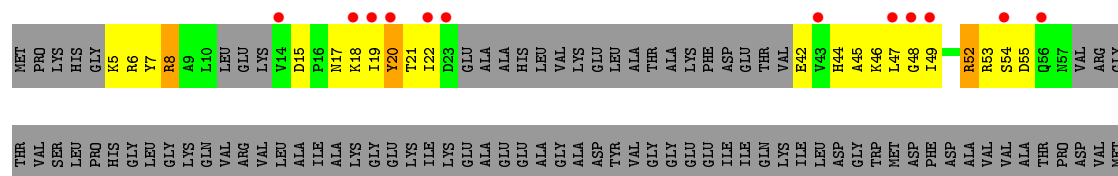
• Molecule 27: 5S rRNA

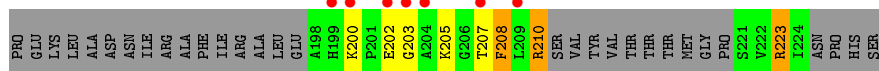
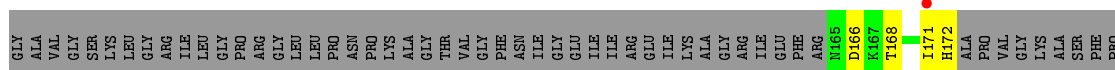


• Molecule 28: 50S ribosomal protein L1



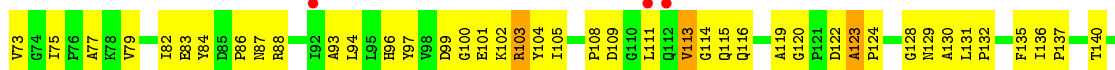
• Molecule 28: 50S ribosomal protein L1





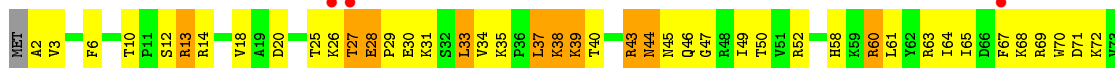
• Molecule 29: 50S ribosomal protein L2

Chain 11:



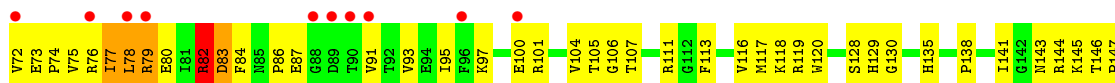
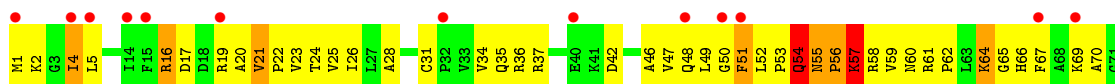
• Molecule 29: 50S ribosomal protein L2

Chain 19:

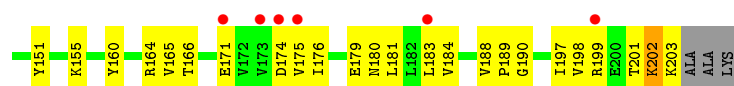


• Molecule 30: 50S ribosomal protein L3

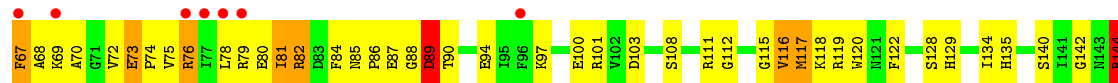
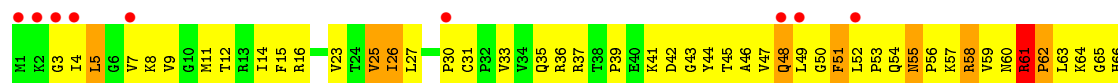
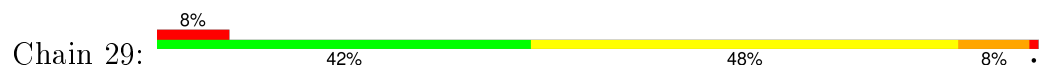
Chain 21:







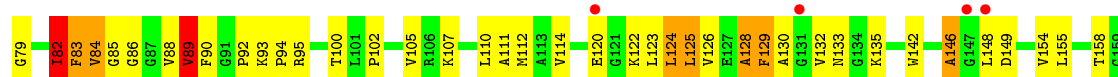
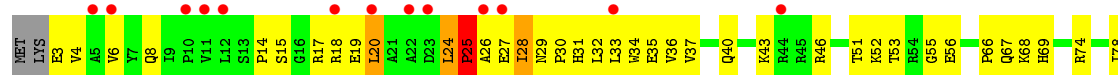
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4

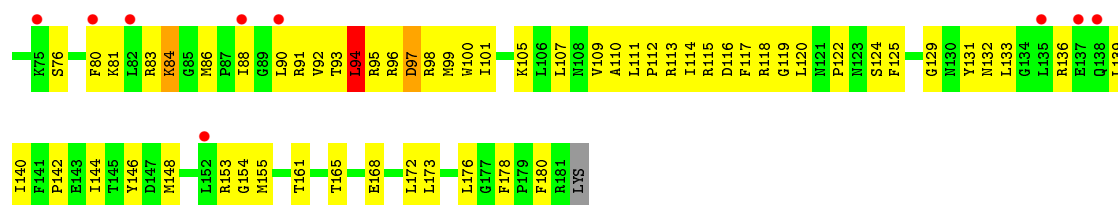


• Molecule 31: 50S ribosomal protein L4

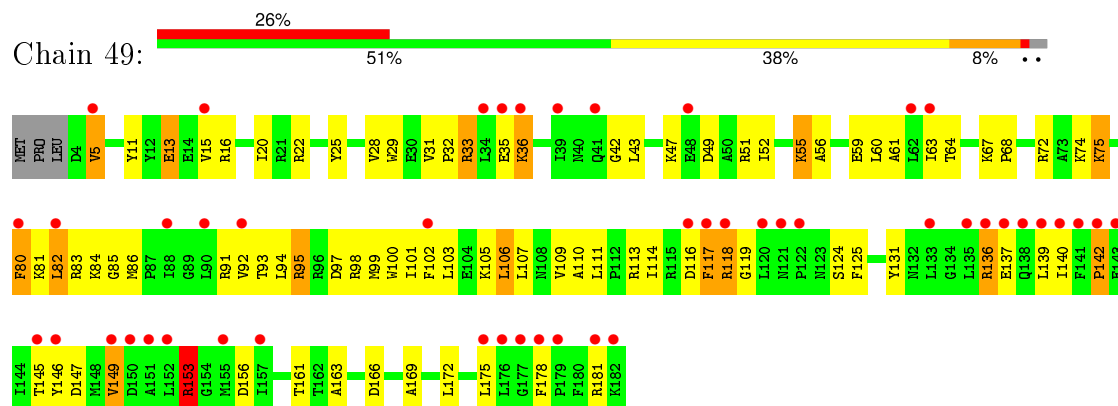


• Molecule 32: 50S ribosomal protein L5

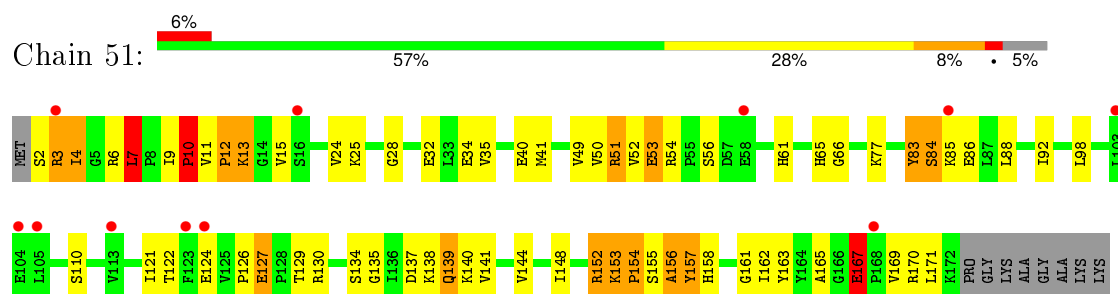




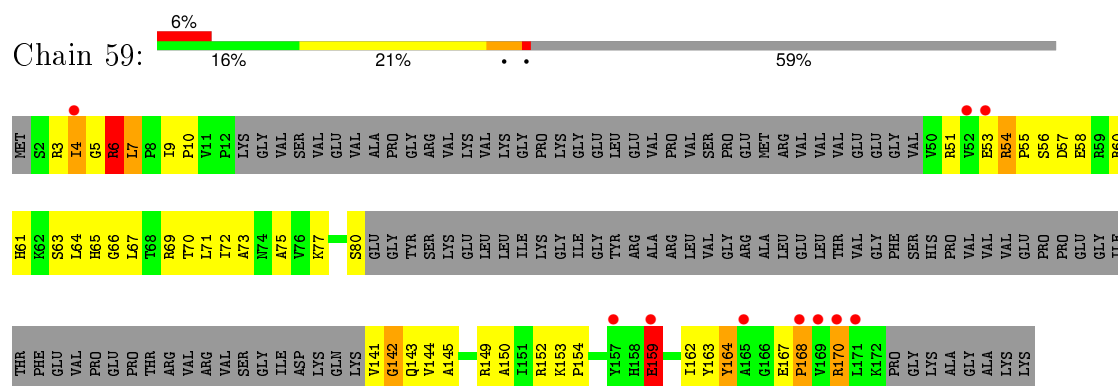
• Molecule 32: 50S ribosomal protein L5



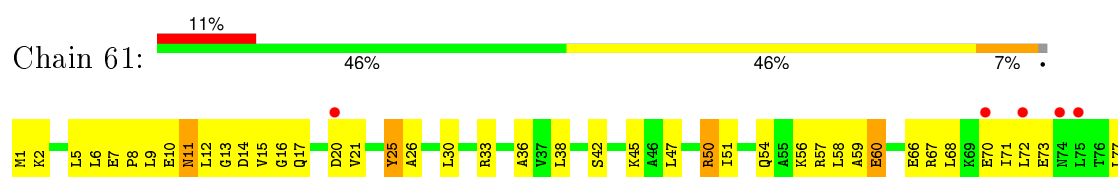
• Molecule 33: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L6

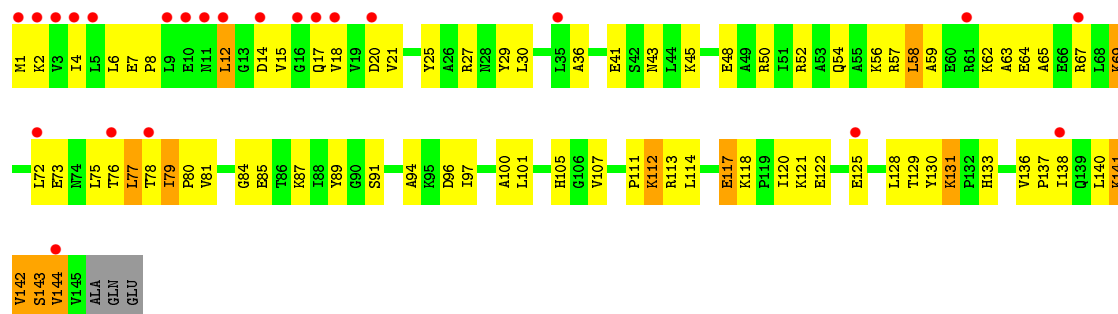


• Molecule 34: 50S ribosomal protein L9

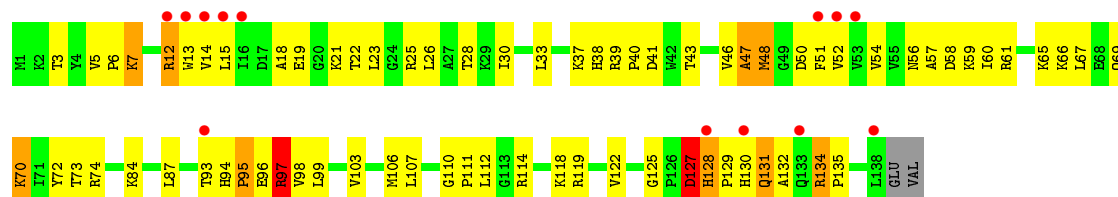




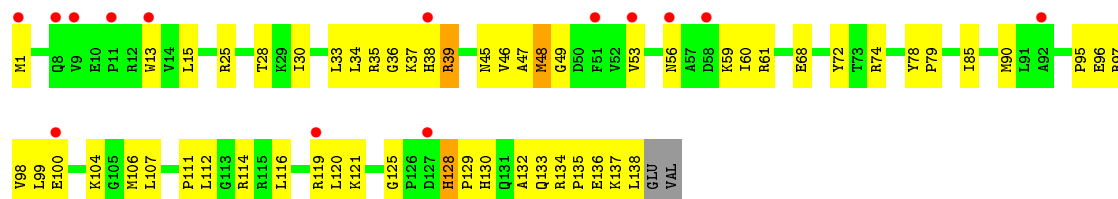
- Molecule 34: 50S ribosomal protein L9



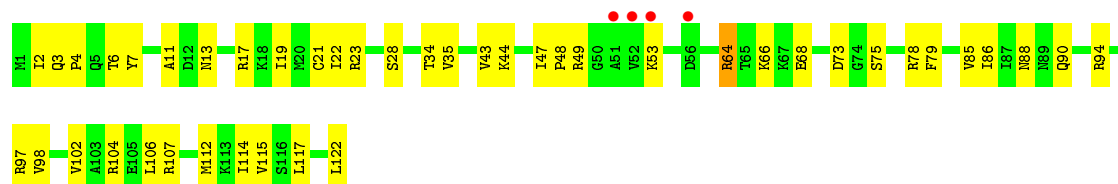
- Molecule 35: 50S ribosomal protein L13



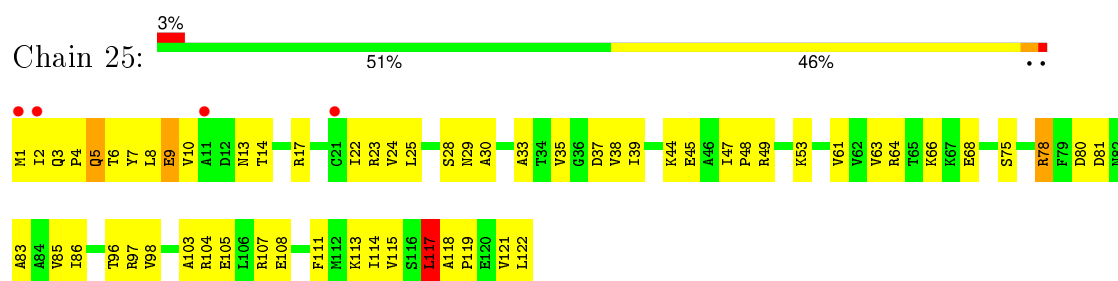
- Molecule 35: 50S ribosomal protein L13



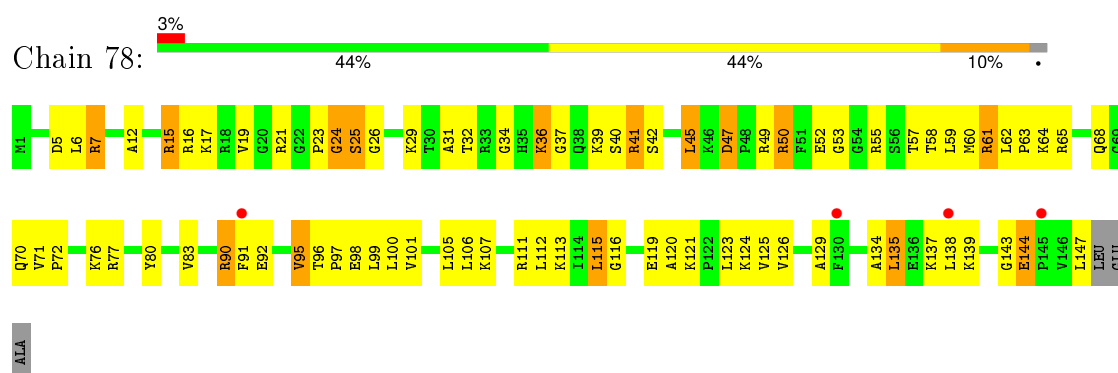
- Molecule 36: 50S ribosomal protein L14



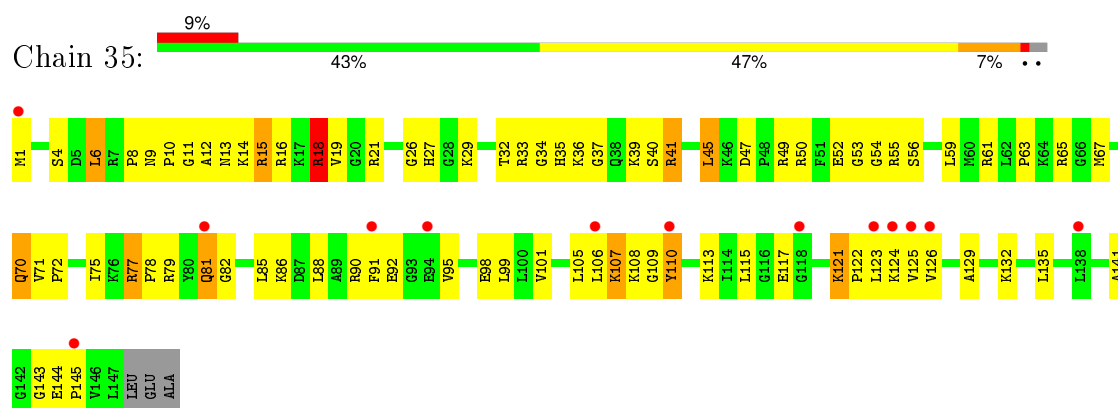
- Molecule 36: 50S ribosomal protein L14



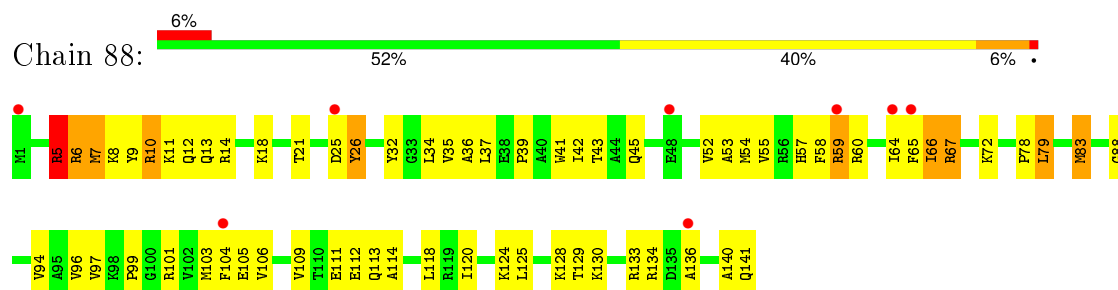
- Molecule 37: 50S ribosomal protein L15



- Molecule 37: 50S ribosomal protein L15

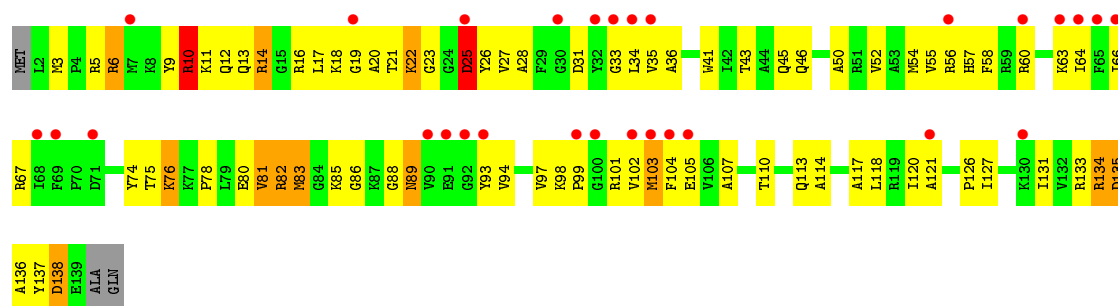


- Molecule 38: 50S ribosomal protein L16

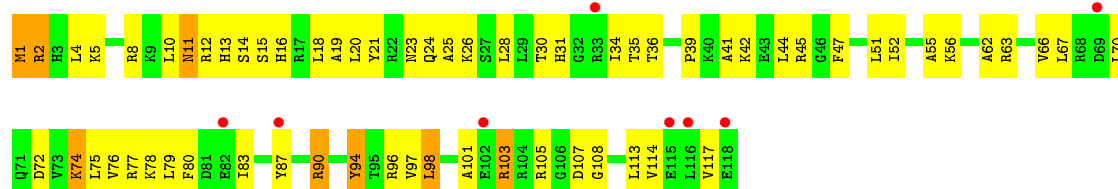


- Molecule 38: 50S ribosomal protein L16

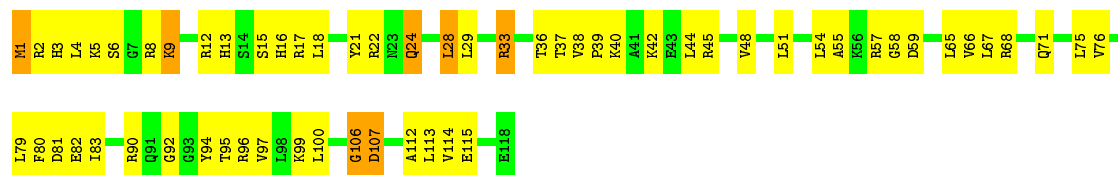




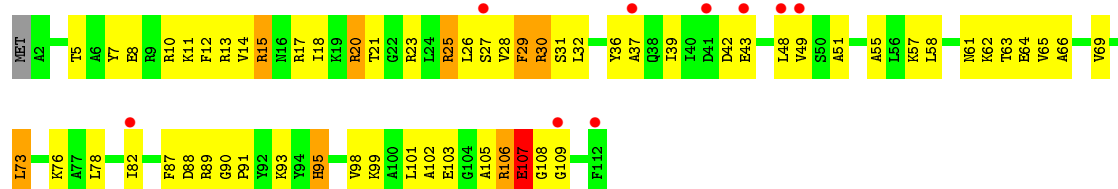
- Molecule 39: 50S ribosomal protein L17



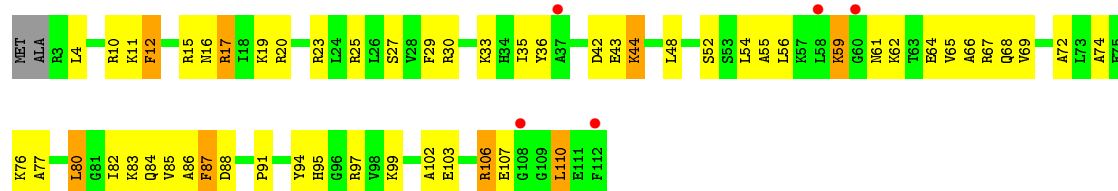
- Molecule 39: 50S ribosomal protein L17



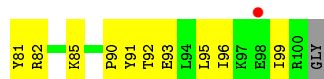
- Molecule 40: 50S ribosomal protein L18



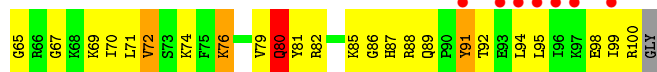
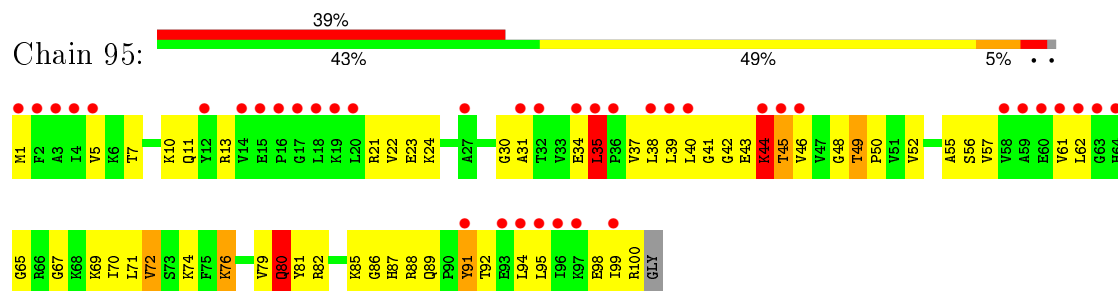
- Molecule 40: 50S ribosomal protein L18



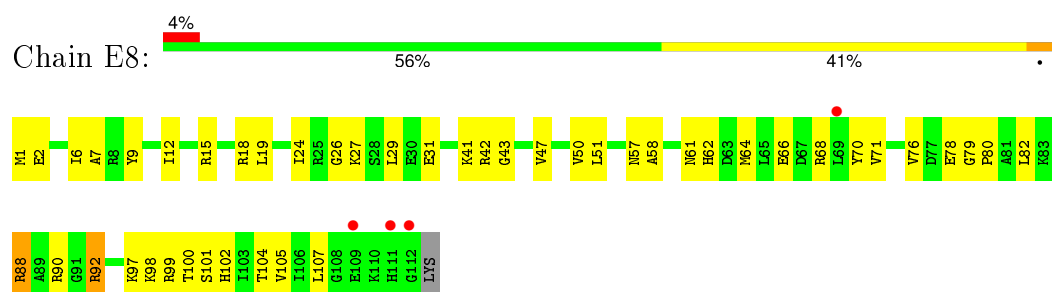




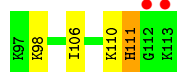
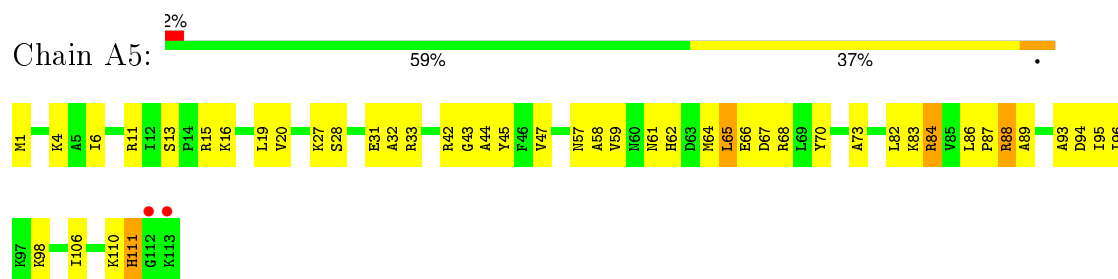
- Molecule 43: 50S ribosomal protein L21



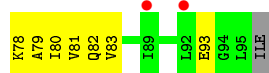
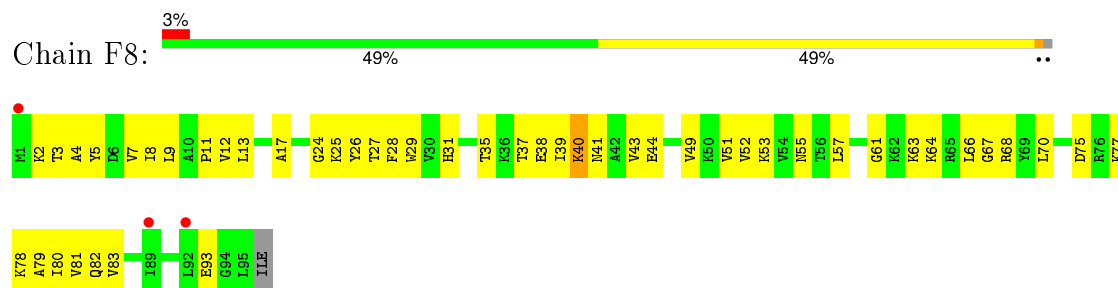
- Molecule 44: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L22

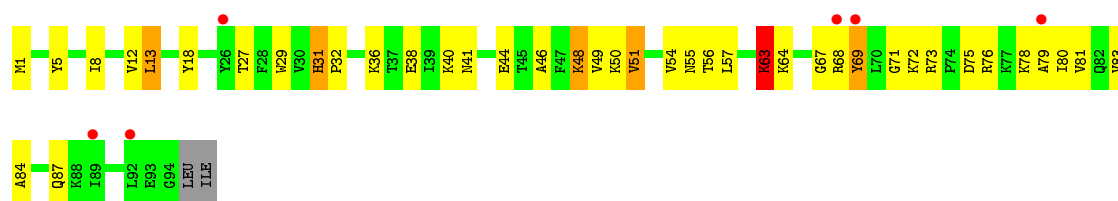


- Molecule 45: 50S ribosomal protein L23

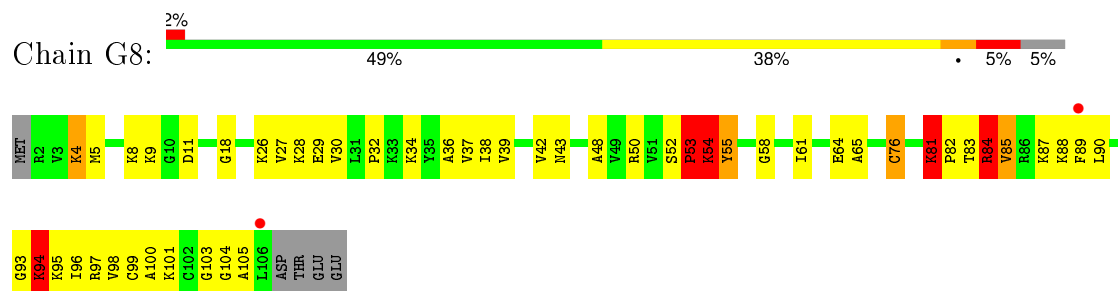


- Molecule 45: 50S ribosomal protein L23

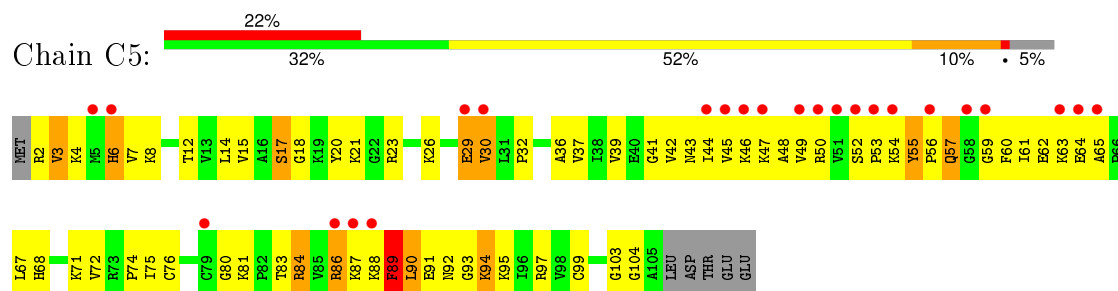




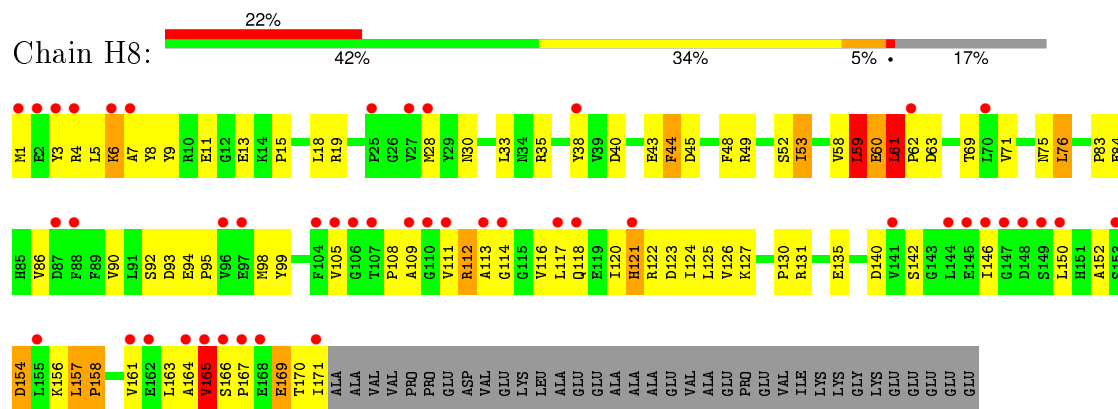
• Molecule 46: 50S ribosomal protein L24



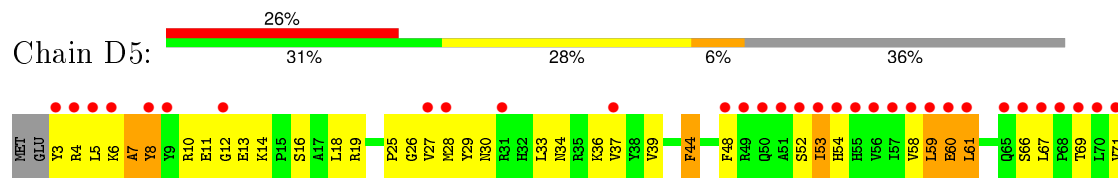
• Molecule 46: 50S ribosomal protein L24



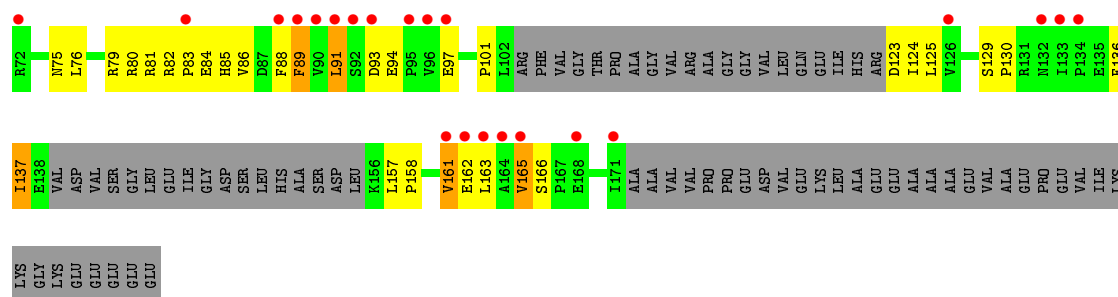
• Molecule 47: 50S ribosomal protein L25



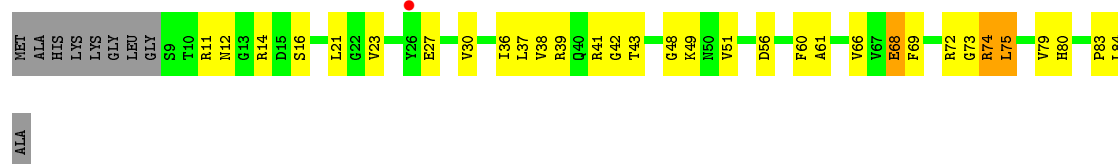
• Molecule 47: 50S ribosomal protein L25



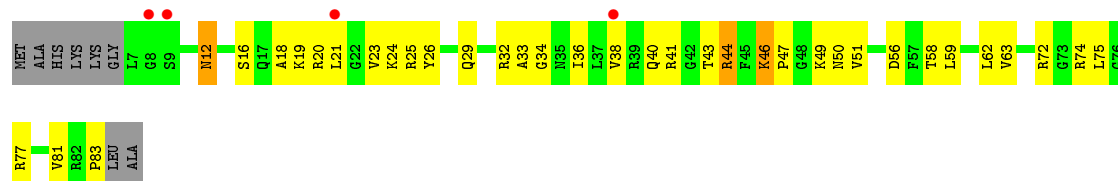




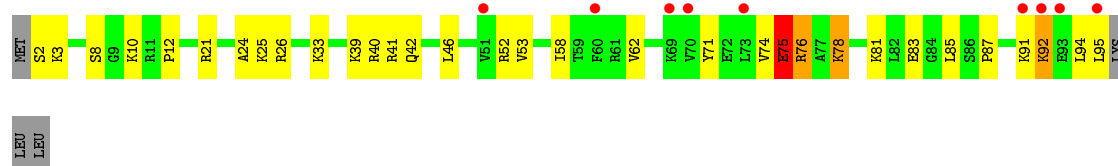
- Molecule 48: 50S ribosomal protein L27



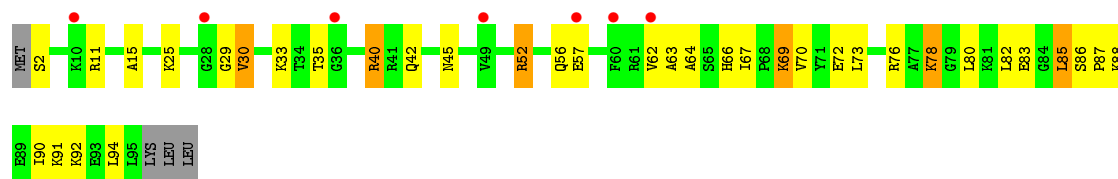
- Molecule 48: 50S ribosomal protein L27



- Molecule 49: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29

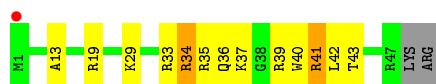




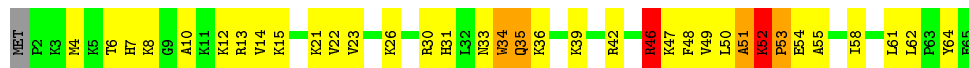
- Molecule 54: 50S ribosomal protein L34



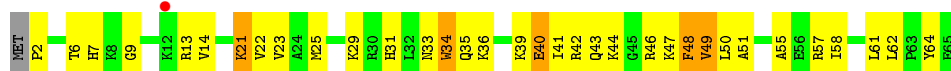
- Molecule 54: 50S ribosomal protein L34



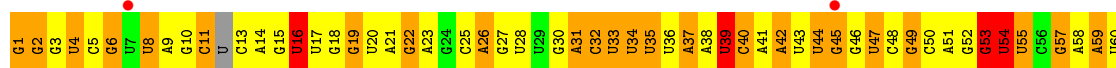
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA<sup>Lys</sup>



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.70 Å   449.50 Å   620.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	152.17 – 3.15 152.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.17-3.15) 91.9 (152.17-3.15)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.13 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.192   ,   0.247 0.202   ,   0.252	Depositor DCC
$R_{free}$ test set	2000 reflections (0.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 63.9	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 998591 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	296184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, PAR, U8U, 4SU, G7M, SF4, MG, ZN, 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	0.67	2/35994 (0.0%)	1.31	276/56171 (0.5%)
1	1G	0.58	0/36231	1.17	128/56544 (0.2%)
2	12	0.39	0/1752	0.71	0/2360
2	1E	0.46	1/1908 (0.1%)	0.69	3/2573 (0.1%)
3	22	0.39	0/1564	0.62	0/2109
3	2E	0.51	2/1629 (0.1%)	0.64	1/2195 (0.0%)
4	32	0.50	1/1732 (0.1%)	0.70	3/2318 (0.1%)
4	3E	0.54	2/1720 (0.1%)	0.69	0/2305
5	42	0.44	0/1150	0.66	1/1548 (0.1%)
5	4E	0.47	0/1158	0.68	1/1559 (0.1%)
6	52	0.52	0/855	0.66	1/1154 (0.1%)
6	5E	0.48	0/850	0.68	1/1147 (0.1%)
7	62	0.50	0/1127	0.67	0/1507
7	6E	0.39	0/1259	0.57	0/1686
8	72	0.36	0/1127	0.57	0/1517
8	7E	0.45	0/1135	0.72	2/1527 (0.1%)
9	82	0.37	0/971	0.71	0/1304
9	8E	0.42	0/1019	0.66	0/1367
10	1A	0.66	1/658 (0.2%)	0.63	0/885
10	1I	0.47	0/747	0.68	1/1006 (0.1%)
11	2A	0.38	0/850	0.58	0/1150
11	2I	0.40	0/838	0.62	0/1133
12	3A	0.44	0/972	0.70	0/1301
12	3I	0.55	0/972	0.78	1/1301 (0.1%)
13	4A	0.40	0/903	0.68	1/1211 (0.1%)
13	4I	0.49	0/952	0.67	0/1277
14	5A	0.40	0/495	0.71	1/657 (0.2%)
14	5I	0.45	0/500	0.73	1/664 (0.2%)
15	6A	0.42	0/744	0.58	0/992
15	6I	0.41	0/740	0.60	0/987
16	7A	0.48	1/721 (0.1%)	0.66	0/970
16	7I	0.44	0/716	0.69	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.41	0/836	0.59	0/1117
17	8I	0.48	2/847 (0.2%)	0.68	1/1131 (0.1%)
18	9A	0.44	0/549	0.63	0/732
18	9I	0.42	0/554	0.69	1/739 (0.1%)
19	AA	0.43	0/490	0.69	0/662
19	AI	0.49	0/668	0.73	0/899
20	BA	0.37	0/764	0.69	1/1007 (0.1%)
20	BI	0.40	0/748	0.76	1/986 (0.1%)
21	1B	0.44	0/192	0.63	0/252
21	1F	0.45	0/203	0.66	0/266
22	1K	0.58	0/1516	1.24	17/2350 (0.7%)
22	1L	0.48	0/1613	1.08	10/2504 (0.4%)
23	2K	0.74	0/1721	1.38	13/2682 (0.5%)
23	2L	0.63	0/1721	1.22	8/2682 (0.3%)
24	3K	0.49	0/1777	1.21	15/2767 (0.5%)
25	4K	0.77	0/495	1.38	6/771 (0.8%)
25	4L	0.69	0/470	1.27	2/732 (0.3%)
26	14	0.79	24/69023 (0.0%)	1.44	778/107740 (0.7%)
26	1H	0.88	50/68351 (0.1%)	1.58	1425/106700 (1.3%)
27	16	0.72	0/2928	1.46	42/4568 (0.9%)
27	1J	0.63	0/2928	1.30	18/4568 (0.4%)
28	71	0.34	0/1055	0.63	0/1425
28	79	0.31	0/459	0.57	0/608
29	11	0.75	6/2170 (0.3%)	0.93	4/2926 (0.1%)
29	19	0.58	0/2175	0.84	4/2933 (0.1%)
30	21	0.54	0/1591	0.86	2/2146 (0.1%)
30	29	0.68	5/1596 (0.3%)	1.00	7/2153 (0.3%)
31	31	0.55	0/1620	0.79	0/2194
31	39	0.48	0/1637	0.78	2/2218 (0.1%)
32	41	0.43	0/1481	0.74	1/1994 (0.1%)
32	49	0.53	3/1482 (0.2%)	0.72	1/1994 (0.1%)
33	51	0.56	1/1337 (0.1%)	0.85	4/1809 (0.2%)
33	59	0.50	1/582 (0.2%)	0.77	1/783 (0.1%)
34	61	0.42	0/1151	0.77	2/1558 (0.1%)
34	69	0.49	1/1146 (0.1%)	0.76	3/1551 (0.2%)
35	15	0.40	0/1131	0.65	1/1525 (0.1%)
35	58	0.49	1/1131 (0.1%)	0.73	1/1525 (0.1%)
36	25	0.56	2/942 (0.2%)	0.72	1/1269 (0.1%)
36	68	0.48	0/942	0.72	0/1269
37	35	0.61	1/1139 (0.1%)	0.90	1/1514 (0.1%)
37	78	0.54	0/1139	0.89	4/1514 (0.3%)
38	45	0.72	4/1120 (0.4%)	0.84	1/1498 (0.1%)
38	88	0.72	2/1134 (0.2%)	0.90	0/1519

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	55	0.50	0/981	0.80	1/1312 (0.1%)
39	98	0.45	0/981	0.80	1/1312 (0.1%)
40	65	0.49	0/886	0.83	2/1180 (0.2%)
40	A8	0.56	0/884	0.76	0/1178
41	75	0.61	3/1123 (0.3%)	0.72	0/1500
41	B8	0.62	2/1123 (0.2%)	0.76	1/1500 (0.1%)
42	85	0.49	0/977	0.70	0/1301
42	C8	0.55	1/968 (0.1%)	0.76	1/1289 (0.1%)
43	95	0.57	0/785	0.85	2/1052 (0.2%)
43	D8	0.52	0/785	0.81	2/1052 (0.2%)
44	A5	0.56	0/910	0.73	0/1220
44	E8	0.51	0/901	0.77	0/1209
45	B5	0.55	0/749	0.77	1/1007 (0.1%)
45	F8	0.60	0/757	0.81	2/1017 (0.2%)
46	C5	0.51	0/807	0.89	2/1076 (0.2%)
46	G8	0.68	2/809 (0.2%)	1.05	4/1080 (0.4%)
47	D5	0.49	0/1098	0.75	0/1487
47	H8	0.46	0/1403	0.75	2/1901 (0.1%)
48	E5	0.50	0/616	0.77	0/821
48	I8	0.75	2/614 (0.3%)	0.86	1/819 (0.1%)
49	F5	0.52	0/744	0.81	0/989
49	J8	0.59	0/744	0.83	1/989 (0.1%)
50	G5	0.52	0/560	0.75	0/741
50	K8	0.84	4/570 (0.7%)	0.86	0/755
51	H5	0.42	0/464	0.65	1/623 (0.2%)
51	L8	0.53	0/464	0.73	0/623
52	M8	0.41	0/375	0.86	2/507 (0.4%)
53	J5	0.49	0/448	0.70	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.54	0/409	0.84	1/540 (0.2%)
54	P8	0.62	0/409	0.88	0/540
55	M5	0.66	1/524 (0.2%)	0.81	1/691 (0.1%)
55	Q8	0.56	0/524	1.02	2/691 (0.3%)
56	3L	0.54	0/1729	1.28	17/2690 (0.6%)
All	All	0.70	128/317045 (0.0%)	1.28	2847/474982 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	3
4	3E	0	1
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	4
13	4A	0	3
13	4I	0	2
14	5A	0	3
14	5I	0	1
16	7I	0	2
18	9I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	3
20	BI	0	1
29	11	0	7
29	19	0	5
30	21	0	8
30	29	0	7
31	31	0	2
31	39	0	8
32	41	0	1
32	49	0	6
33	51	0	5
33	59	0	5
34	61	0	4
34	69	0	3
35	58	0	2
37	35	0	4
37	78	0	4
38	45	0	4
39	55	0	1
40	65	0	1
40	A8	0	1
41	75	0	1
42	85	0	4
42	C8	0	4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
43	95	0	3
43	D8	0	3
44	A5	0	1
45	F8	0	1
46	C5	0	3
46	G8	0	4
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	4
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	169

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	2572	A	N7-C5	24.38	1.53	1.39
26	14	2572	A	N9-C8	-21.02	1.21	1.37
26	14	2572	A	C5-C4	-18.45	1.25	1.38
26	14	2572	A	C5-C6	-15.84	1.26	1.41
26	1H	774	A	N9-C4	-12.29	1.30	1.37

The worst 5 of 2847 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2572	A	N9-C4-C5	28.35	117.14	105.80
26	14	2572	A	C4-C5-C6	24.01	129.00	117.00
26	14	2572	A	C4-C5-N7	-20.90	100.25	110.70
26	1H	1899	G	N3-C4-N9	-19.20	114.48	126.00
26	14	2572	A	N7-C8-N9	18.60	123.10	113.80

There are no chirality outliers.

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
4	3E	82	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	754	0
1	1G	32368	0	16343	752	1
2	12	1721	0	1758	119	0
2	1E	1874	0	1926	112	0
3	22	1541	0	1606	76	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1765	101	0
4	3E	1690	0	1738	92	0
5	42	1134	0	1200	69	0
5	4E	1142	0	1204	51	0
6	52	842	0	857	28	0
6	5E	837	0	852	29	0
7	62	1115	0	1165	57	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	54	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	72	0
9	8E	1000	0	1031	69	0
10	1A	646	0	662	48	0
10	1I	734	0	761	53	0
11	2A	835	0	847	47	0
11	2I	823	0	833	37	0
12	3A	956	0	1046	54	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	55	0
13	4I	942	0	997	48	0
14	5A	486	0	524	28	0
14	5I	491	0	530	36	0
15	6A	733	0	771	34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	26	0
16	7A	705	0	725	37	0
16	7I	700	0	720	51	0
17	8A	823	0	891	41	0
17	8I	834	0	904	59	0
18	9A	544	0	605	25	0
18	9I	549	0	607	22	0
19	AA	481	0	468	19	0
19	AI	654	0	675	52	0
20	BA	762	0	861	39	0
20	BI	746	0	843	50	0
21	1B	188	0	195	17	0
21	1F	199	0	208	15	0
22	1K	1477	0	758	30	0
22	1L	1563	0	799	31	0
23	2K	1646	0	844	19	0
23	2L	1646	0	844	33	0
24	3K	1611	0	817	74	0
25	4K	439	0	218	10	0
25	4L	417	0	207	11	0
26	14	61630	0	31072	1406	1
26	1H	61028	0	30762	1443	0
27	16	2617	0	1328	70	0
27	1J	2617	0	1328	79	0
28	7I	1033	0	1048	71	0
28	79	456	0	460	31	0
29	11	2120	0	2197	151	0
29	19	2125	0	2199	133	0
30	21	1558	0	1624	96	0
30	29	1563	0	1629	134	0
31	31	1585	0	1632	94	0
31	39	1602	0	1649	96	0
32	41	1457	0	1514	91	0
32	49	1458	0	1516	72	0
33	51	1312	0	1384	64	0
33	59	573	0	597	43	0
34	61	1136	0	1223	60	0
34	69	1131	0	1218	73	0
35	15	1104	0	1180	51	0
35	58	1104	0	1180	58	0
36	25	932	0	996	55	0
36	68	932	0	996	41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	35	1122	0	1206	93	0
37	78	1122	0	1206	109	0
38	45	1099	0	1154	94	0
38	88	1113	0	1157	56	0
39	55	967	0	1033	56	0
39	98	967	0	1033	64	0
40	65	876	0	938	57	0
40	A8	875	0	936	54	0
41	75	1109	0	1169	74	0
41	B8	1109	0	1170	60	0
42	85	959	0	1019	54	0
42	C8	950	0	1011	53	0
43	95	774	0	849	82	0
43	D8	774	0	849	58	0
44	A5	899	0	964	34	0
44	E8	890	0	951	33	0
45	B5	735	0	785	43	0
45	F8	743	0	794	39	0
46	C5	794	0	886	74	0
46	G8	796	0	886	53	0
47	D5	1074	0	1086	63	0
47	H8	1373	0	1402	81	0
48	E5	608	0	622	37	0
48	I8	606	0	625	31	0
49	F5	737	0	813	41	0
49	J8	737	0	813	28	0
50	G5	558	0	610	33	0
50	K8	568	0	614	31	0
51	H5	459	0	512	15	0
51	L8	459	0	512	18	0
52	M8	366	0	370	31	0
53	J5	434	0	454	24	0
53	N8	369	0	388	22	0
54	L5	401	0	436	13	0
54	P8	401	0	436	17	0
55	M5	516	0	582	34	0
55	Q8	516	0	582	49	0
56	3L	1601	0	814	69	0
57	11	3	0	0	0	0
57	13	150	0	0	0	0
57	14	454	0	0	0	0
57	16	12	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	93	0	0	0	0
57	1H	502	0	0	0	0
57	1I	1	0	0	0	0
57	1J	6	0	0	0	0
57	2I	3	0	0	0	0
57	29	4	0	0	0	0
57	2K	3	0	0	0	0
57	2L	4	0	0	0	0
57	3I	1	0	0	0	0
57	31	1	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	4I	2	0	0	0	0
57	45	3	0	0	0	0
57	55	1	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	88	1	0	0	0	0
57	BI	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	45	3	0
58	1G	42	0	45	2	0
59	32	8	0	0	2	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	12	0	0	1	0
61	13	319	0	0	23	0
61	14	1015	0	0	117	0
61	16	26	0	0	6	0
61	19	12	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1F	1	0	0	0	0
61	1G	226	0	0	16	0
61	1H	1158	0	0	132	0
61	1I	1	0	0	0	0
61	1J	18	0	0	2	0
61	1K	1	0	0	0	0
61	2I	6	0	0	1	0
61	29	6	0	0	0	0
61	2K	7	0	0	0	0
61	2L	1	0	0	0	0
61	3I	9	0	0	0	0
61	32	3	0	0	0	0
61	35	5	0	0	1	0
61	39	8	0	0	1	0
61	3A	1	0	0	0	0
61	3E	3	0	0	0	0
61	3I	3	0	0	1	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4E	3	0	0	1	0
61	4K	4	0	0	0	0
61	4L	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	1	0	0	1	0
61	6A	3	0	0	0	0
61	6I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	6	0	0	1	0
61	85	2	0	0	0	0
61	88	2	0	0	0	0
61	8A	1	0	0	0	0
61	8E	1	0	0	0	0
61	8I	2	0	0	0	0
61	A5	2	0	0	0	0
61	B5	1	0	0	0	0
61	BA	3	0	0	1	0
61	BI	5	0	0	0	0
61	C5	4	0	0	0	0
61	C8	2	0	0	0	0
61	E8	3	0	0	0	0
61	F8	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	G8	2	0	0	0	0
61	H5	3	0	0	0	0
61	I8	5	0	0	1	0
61	J8	3	0	0	0	0
61	K8	2	0	0	0	0
61	L5	2	0	0	0	0
61	L8	2	0	0	0	0
61	M5	10	0	0	0	0
61	P8	1	0	0	0	0
61	Q8	9	0	0	2	0
All	All	296184	0	196367	8846	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 19.

The worst 5 of 8846 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)
37:35:81:GLN:NE2	37:35:106:LEU:HA	1.45	1.29
15:6A:27:VAL:O	15:6A:31:LEU:HD13	1.26	1.27
26:14:2572:A:C5	30:29:144:ARG:NH1	2.04	1.25
37:35:81:GLN:CD	37:35:106:LEU:HA	1.58	1.24
29:19:69:ARG:NH2	29:19:130:ALA:H	1.33	1.21

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]	2.17	0.03

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	206/256 (80%)	175 (85%)	24 (12%)	7 (3%)	5	29
2	1E	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	21	65
3	22	192/239 (80%)	169 (88%)	23 (12%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	19	63
4	3E	205/209 (98%)	188 (92%)	16 (8%)	1 (0%)	34	76
5	42	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	26	71
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	135/156 (86%)	122 (90%)	12 (9%)	1 (1%)	26	71
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	13	53
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	26	71
9	82	119/128 (93%)	108 (91%)	9 (8%)	2 (2%)	11	50
9	8E	124/128 (97%)	105 (85%)	18 (14%)	1 (1%)	24	67
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	89/105 (85%)	82 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	98 (88%)	11 (10%)	2 (2%)	11	49
11	2I	109/129 (84%)	95 (87%)	12 (11%)	2 (2%)	11	49
12	3A	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	5	30
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	24	67
13	4A	109/126 (86%)	92 (84%)	15 (14%)	2 (2%)	11	49
13	4I	117/126 (93%)	98 (84%)	18 (15%)	1 (1%)	21	65
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	11	49
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	5	29
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	13	53
19	AA	56/93 (60%)	49 (88%)	4 (7%)	3 (5%)	2	17
19	AI	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	7	39
20	BA	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	9	44
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	244 (90%)	17 (6%)	10 (4%)	4	27
29	19	272/276 (99%)	245 (90%)	21 (8%)	6 (2%)	8	43
30	21	201/206 (98%)	156 (78%)	36 (18%)	9 (4%)	3	22
30	29	202/206 (98%)	154 (76%)	39 (19%)	9 (4%)	3	22
31	31	200/210 (95%)	179 (90%)	20 (10%)	1 (0%)	34	76
31	39	202/210 (96%)	161 (80%)	31 (15%)	10 (5%)	3	19
32	41	177/182 (97%)	153 (86%)	21 (12%)	3 (2%)	11	50
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	17	61
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	2	15
33	59	68/180 (38%)	49 (72%)	14 (21%)	5 (7%)	1	8
34	61	144/148 (97%)	116 (81%)	26 (18%)	2 (1%)	14	55
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	9	44
35	15	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	26	71
35	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	6	35
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	24	67
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	116 (80%)	25 (17%)	4 (3%)	6	36
37	78	145/150 (97%)	115 (79%)	26 (18%)	4 (3%)	6	36
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	6	35
38	88	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	4	28
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	102 (88%)	13 (11%)	1 (1%)	21	65
40	65	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	10	48
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	116 (88%)	15 (12%)	0	100	100
41	B8	131/146 (90%)	118 (90%)	12 (9%)	1 (1%)	24	67
42	85	114/118 (97%)	101 (89%)	12 (10%)	1 (1%)	21	65
42	C8	113/118 (96%)	100 (88%)	10 (9%)	3 (3%)	6	37
43	95	98/101 (97%)	75 (76%)	19 (19%)	4 (4%)	3	25
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	3	25
44	A5	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	21	65
44	E8	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
45	B5	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	8	43
45	F8	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	17	61
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	10
46	G8	103/110 (94%)	85 (82%)	13 (13%)	5 (5%)	3	20
47	D5	126/206 (61%)	99 (79%)	20 (16%)	7 (6%)	2	17
47	H8	169/206 (82%)	132 (78%)	31 (18%)	6 (4%)	4	28
48	E5	75/85 (88%)	64 (85%)	9 (12%)	2 (3%)	6	37
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	17	61
49	J8	92/98 (94%)	85 (92%)	4 (4%)	3 (3%)	5	30
50	G5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	12	52
50	K8	66/72 (92%)	58 (88%)	6 (9%)	2 (3%)	5	34
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
52	M8	45/71 (63%)	30 (67%)	14 (31%)	1 (2%)	8	43
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	5	31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	3	20
All	All	10975/12333 (89%)	9578 (87%)	1200 (11%)	197 (2%)	11	49

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU
29	11	273	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%)	172 (94%)	10 (6%)	27	66
2	1E	200/220 (91%)	183 (92%)	17 (8%)	13	46
3	22	154/188 (82%)	147 (96%)	7 (4%)	34	73
3	2E	159/188 (85%)	151 (95%)	8 (5%)	30	70
4	32	180/181 (99%)	167 (93%)	13 (7%)	18	55
4	3E	178/181 (98%)	166 (93%)	12 (7%)	20	58
5	42	114/123 (93%)	104 (91%)	10 (9%)	12	43
5	4E	115/123 (94%)	112 (97%)	3 (3%)	54	85
6	52	90/90 (100%)	86 (96%)	4 (4%)	35	73
6	5E	90/90 (100%)	85 (94%)	5 (6%)	26	66
7	62	114/127 (90%)	105 (92%)	9 (8%)	15	51
7	6E	125/127 (98%)	109 (87%)	16 (13%)	5	24
8	72	118/119 (99%)	107 (91%)	11 (9%)	11	40
8	7E	119/119 (100%)	111 (93%)	8 (7%)	20	58
9	82	92/99 (93%)	80 (87%)	12 (13%)	5	23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	91 (94%)	6 (6%)	23	62
10	1A	71/92 (77%)	63 (89%)	8 (11%)	7	30
10	1I	81/92 (88%)	79 (98%)	2 (2%)	55	85
11	2A	85/99 (86%)	82 (96%)	3 (4%)	43	79
11	2I	84/99 (85%)	82 (98%)	2 (2%)	57	86
12	3A	103/109 (94%)	92 (89%)	11 (11%)	8	32
12	3I	103/109 (94%)	97 (94%)	6 (6%)	25	64
13	4A	91/101 (90%)	81 (89%)	10 (11%)	8	31
13	4I	94/101 (93%)	85 (90%)	9 (10%)	10	38
14	5A	49/50 (98%)	43 (88%)	6 (12%)	6	26
14	5I	49/50 (98%)	47 (96%)	2 (4%)	37	75
15	6A	79/80 (99%)	74 (94%)	5 (6%)	22	61
15	6I	79/80 (99%)	75 (95%)	4 (5%)	29	69
16	7A	72/74 (97%)	66 (92%)	6 (8%)	14	48
16	7I	72/74 (97%)	69 (96%)	3 (4%)	36	74
17	8A	94/97 (97%)	89 (95%)	5 (5%)	28	67
17	8I	95/97 (98%)	87 (92%)	8 (8%)	14	47
18	9A	58/77 (75%)	56 (97%)	2 (3%)	44	80
18	9I	58/77 (75%)	55 (95%)	3 (5%)	29	68
19	AA	52/80 (65%)	49 (94%)	3 (6%)	25	64
19	AI	71/80 (89%)	64 (90%)	7 (10%)	10	36
20	BA	76/82 (93%)	72 (95%)	4 (5%)	28	67
20	BI	75/82 (92%)	72 (96%)	3 (4%)	38	76
21	1B	17/22 (77%)	16 (94%)	1 (6%)	24	63
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	71	109/181 (60%)	104 (95%)	5 (5%)	33	73
28	79	48/181 (26%)	41 (85%)	7 (15%)	4	18
29	11	214/218 (98%)	194 (91%)	20 (9%)	11	40
29	19	214/218 (98%)	198 (92%)	16 (8%)	17	53
30	21	165/166 (99%)	158 (96%)	7 (4%)	36	74
30	29	165/166 (99%)	155 (94%)	10 (6%)	23	62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	151 (94%)	10 (6%)	23	62
31	39	163/166 (98%)	159 (98%)	4 (2%)	55	85
32	41	153/156 (98%)	142 (93%)	11 (7%)	18	55
32	49	153/156 (98%)	141 (92%)	12 (8%)	16	51
33	51	142/148 (96%)	134 (94%)	8 (6%)	26	66
33	59	59/148 (40%)	54 (92%)	5 (8%)	13	46
34	61	122/124 (98%)	114 (93%)	8 (7%)	21	59
34	69	122/124 (98%)	115 (94%)	7 (6%)	25	65
35	15	117/119 (98%)	112 (96%)	5 (4%)	35	74
35	58	117/119 (98%)	107 (92%)	10 (8%)	13	46
36	25	100/100 (100%)	96 (96%)	4 (4%)	38	76
36	68	100/100 (100%)	98 (98%)	2 (2%)	63	88
37	35	114/116 (98%)	106 (93%)	8 (7%)	19	57
37	78	114/116 (98%)	109 (96%)	5 (4%)	35	73
38	45	109/111 (98%)	98 (90%)	11 (10%)	9	35
38	88	109/111 (98%)	99 (91%)	10 (9%)	11	40
39	55	101/101 (100%)	96 (95%)	5 (5%)	30	70
39	98	101/101 (100%)	93 (92%)	8 (8%)	15	51
40	65	87/88 (99%)	79 (91%)	8 (9%)	11	40
40	A8	86/88 (98%)	75 (87%)	11 (13%)	5	24
41	75	117/127 (92%)	104 (89%)	13 (11%)	8	31
41	B8	117/127 (92%)	105 (90%)	12 (10%)	9	34
42	85	93/94 (99%)	86 (92%)	7 (8%)	17	53
42	C8	92/94 (98%)	83 (90%)	9 (10%)	10	37
43	95	82/82 (100%)	75 (92%)	7 (8%)	13	46
43	D8	82/82 (100%)	79 (96%)	3 (4%)	41	78
44	A5	92/92 (100%)	84 (91%)	8 (9%)	13	44
44	E8	91/92 (99%)	81 (89%)	10 (11%)	8	31
45	B5	74/78 (95%)	69 (93%)	5 (7%)	20	57
45	F8	75/78 (96%)	72 (96%)	3 (4%)	38	76
46	C5	85/91 (93%)	77 (91%)	8 (9%)	11	39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	85/91 (93%)	77 (91%)	8 (9%)	11	39
47	D5	118/179 (66%)	111 (94%)	7 (6%)	24	63
47	H8	152/179 (85%)	143 (94%)	9 (6%)	24	63
48	E5	61/67 (91%)	59 (97%)	2 (3%)	45	80
48	I8	61/67 (91%)	60 (98%)	1 (2%)	70	90
49	F5	79/83 (95%)	74 (94%)	5 (6%)	22	61
49	J8	79/83 (95%)	76 (96%)	3 (4%)	40	77
50	G5	62/67 (92%)	57 (92%)	5 (8%)	15	49
50	K8	62/67 (92%)	58 (94%)	4 (6%)	21	60
51	H5	50/52 (96%)	45 (90%)	5 (10%)	9	36
51	L8	50/52 (96%)	47 (94%)	3 (6%)	24	63
52	M8	42/63 (67%)	38 (90%)	4 (10%)	11	38
53	J5	48/52 (92%)	46 (96%)	2 (4%)	36	74
53	N8	43/52 (83%)	40 (93%)	3 (7%)	19	57
54	L5	38/42 (90%)	35 (92%)	3 (8%)	15	51
54	P8	38/42 (90%)	34 (90%)	4 (10%)	8	33
55	M5	54/55 (98%)	52 (96%)	2 (4%)	41	78
55	Q8	54/55 (98%)	52 (96%)	2 (4%)	41	78
All	All	9274/10193 (91%)	8636 (93%)	638 (7%)	19	57

5 of 638 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	121	HIS
6	52	28	ARG
44	A5	67	ASP
50	K8	4	SER
2	12	191	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	40	HIS
5	42	127	ASN
47	D5	75	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	12	224	GLN
5	42	78	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	362 (24%)	32 (2%)
1	1G	1503/1522 (98%)	365 (24%)	35 (2%)
22	1K	65/76 (85%)	32 (49%)	3 (4%)
22	1L	69/76 (90%)	37 (53%)	3 (4%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	75/76 (98%)	49 (65%)	3 (4%)
25	4K	19/27 (70%)	10 (52%)	1 (5%)
25	4L	18/27 (66%)	10 (55%)	1 (5%)
26	14	2852/2917 (97%)	745 (26%)	45 (1%)
26	1H	2828/2917 (96%)	684 (24%)	52 (1%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
56	3L	73/76 (96%)	44 (60%)	5 (6%)
All	All	9389/9634 (97%)	2432 (25%)	189 (2%)

5 of 2432 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	28	G

5 of 189 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2225	A
1	1G	429	U
26	14	1992	G
26	1H	2476	A
27	16	108	C

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

23 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	2.46	4 (26%)	17,34,37	2.08	2 (11%)
22	T6A	1K	37	22	23,34,35	2.73	5 (21%)	26,49,52	3.63	6 (23%)
22	PSU	1K	39	22	15,21,22	0.98	1 (6%)	16,30,33	1.70	3 (18%)
22	5MU	1K	54	22	13,22,23	1.66	2 (15%)	16,32,35	1.36	1 (6%)
22	PSU	1K	55	22	15,21,22	1.01	1 (6%)	16,30,33	2.51	4 (25%)
22	U8U	1L	34	25,22	15,24,25	2.54	4 (26%)	17,34,37	1.87	2 (11%)
22	T6A	1L	37	22	23,34,35	2.55	5 (21%)	26,49,52	3.48	8 (30%)
22	PSU	1L	39	22	15,21,22	0.96	1 (6%)	16,30,33	1.87	4 (25%)
22	5MU	1L	54	22	13,22,23	1.68	2 (15%)	16,32,35	1.33	1 (6%)
22	PSU	1L	55	22	15,21,22	1.04	1 (6%)	16,30,33	2.19	4 (25%)
23	OMC	2K	33	23	15,22,23	2.23	4 (26%)	20,31,34	1.72	3 (15%)
23	G7M	2K	47	23	18,26,27	3.37	6 (33%)	21,39,42	1.77	3 (14%)
23	5MU	2K	55	23	13,22,23	1.67	2 (15%)	16,32,35	1.29	1 (6%)
23	PSU	2K	56	23	15,21,22	1.03	1 (6%)	16,30,33	1.83	3 (18%)
23	4SU	2K	8	23	12,21,22	3.28	2 (16%)	15,30,33	0.99	1 (6%)
23	OMC	2L	33	23	15,22,23	2.57	4 (26%)	20,31,34	1.49	3 (15%)
23	G7M	2L	47	23	18,26,27	3.34	5 (27%)	21,39,42	2.75	5 (23%)
23	5MU	2L	55	23	13,22,23	1.71	2 (15%)	16,32,35	1.26	1 (6%)
23	PSU	2L	56	23	15,21,22	1.09	1 (6%)	16,30,33	2.08	2 (12%)
23	4SU	2L	8	23	12,21,22	3.36	2 (16%)	15,30,33	0.66	0
24	PSU	3K	39	24	15,21,22	1.13	2 (13%)	16,30,33	2.18	3 (18%)
56	T6A	3L	37	56	23,34,35	2.58	4 (17%)	26,49,52	3.10	9 (34%)
56	PSU	3L	39	56	15,21,22	1.27	3 (20%)	16,30,33	4.68	5 (31%)

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
22	U8U	1L	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1L	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1L	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	G7M	2K	47	23	-	0/3/25/26	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	G7M	2L	47	23	-	0/3/25/26	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
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
56	T6A	3L	37	56	-	0/15/41/42	0/3/3/3
56	PSU	3L	39	56	-	0/7/25/26	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	34	U8U	C2-S2	-4.02	1.58	1.66
22	1K	34	U8U	C2-S2	-3.48	1.59	1.66
22	1L	54	5MU	C4-N3	-3.21	1.27	1.33
23	2L	55	5MU	C4-N3	-3.09	1.27	1.33
22	1K	54	5MU	C4-N3	-3.09	1.27	1.33

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	3L	39	PSU	C5-C1'-C2'	-16.75	86.99	115.44
22	1K	37	T6A	N3-C2-N1	-13.30	118.42	128.87
22	1L	37	T6A	N3-C2-N1	-12.71	118.89	128.87
56	3L	37	T6A	N3-C2-N1	-10.81	120.38	128.87
23	2L	47	G7M	C1'-N9-C4	-9.38	116.34	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	34	U8U	1	0
22	1K	54	5MU	1	0
22	1L	37	T6A	2	0
23	2K	55	5MU	2	0
23	2K	8	4SU	1	0
23	2L	47	G7M	4	0
23	2L	55	5MU	3	0
23	2L	56	PSU	3	0
23	2L	8	4SU	2	0
56	3L	37	T6A	2	0
56	3L	39	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1269 ligands modelled in this entry, 1265 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	PAR	13	1749	-	45,45,45	0.83	0	60,67,67	1.88	14 (23%)
58	PAR	1G	1691	-	45,45,45	0.69	0	60,67,67	1.68	14 (23%)
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
58	PAR	13	1749	-	-	0/18/94/94	0/4/4/4
58	PAR	1G	1691	-	-	0/18/94/94	0/4/4/4
59	SF4	32	301	-	-	0/0/48/48	0/6/5/5
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	C22-C12-C62	-4.80	102.69	110.14
58	13	1749	PAR	C14-O33-C33	-4.39	106.32	118.00
58	1G	1691	PAR	O11-C11-C21	-4.34	100.30	108.16
58	1G	1691	PAR	O11-C42-C32	-3.56	100.31	108.92
58	1G	1691	PAR	C13-O52-C52	-3.10	109.76	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	13	1749	PAR	3	0
58	1G	1691	PAR	2	0
59	32	301	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	69	1
4	3E	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3E	36:ARG	C	37:PRO	N	1.17
1	69	79:ILE	C	80:PRO	N	1.16
1	1A	76:ASN	C	77:PRO	N	1.12

## 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%)	-0.82	2 (0%) 95 95	58, 99, 162, 246	0
1	1G	1506/1522 (98%)	-0.86	1 (0%) 95 95	73, 114, 168, 253	0
2	12	210/256 (82%)	0.45	15 (7%) 19 10	127, 152, 169, 182	0
2	1E	231/256 (90%)	0.44	16 (6%) 20 10	105, 136, 157, 168	0
3	22	196/239 (82%)	1.11	45 (22%) 1 1	122, 138, 165, 170	0
3	2E	205/239 (85%)	0.46	12 (5%) 26 13	81, 103, 128, 138	0
4	32	208/209 (99%)	0.99	43 (20%) 1 1	98, 118, 136, 144	0
4	3E	207/209 (99%)	0.55	20 (9%) 10 5	80, 101, 121, 129	0
5	42	148/162 (91%)	0.40	6 (4%) 41 25	104, 121, 137, 147	0
5	4E	149/162 (91%)	0.55	13 (8%) 13 6	79, 96, 112, 121	0
6	52	101/101 (100%)	0.59	10 (9%) 9 4	83, 101, 118, 131	0
6	5E	100/101 (99%)	0.88	14 (14%) 4 2	83, 100, 115, 121	0
7	62	139/156 (89%)	0.17	4 (2%) 55 39	111, 124, 135, 141	0
7	6E	154/156 (98%)	-0.07	3 (1%) 70 54	101, 115, 132, 141	0
8	72	137/138 (99%)	0.41	8 (5%) 26 13	104, 124, 136, 142	0
8	7E	138/138 (100%)	0.57	11 (7%) 15 7	91, 106, 118, 127	0
9	82	121/128 (94%)	0.20	3 (2%) 61 45	110, 151, 165, 175	0
9	8E	126/128 (98%)	-0.19	0 100 100	89, 128, 147, 153	0
10	1A	80/105 (76%)	-0.01	1 (1%) 79 67	116, 145, 154, 156	0
10	1I	91/105 (86%)	0.24	7 (7%) 16 8	80, 121, 156, 161	0
11	2A	113/129 (87%)	0.82	16 (14%) 4 2	86, 110, 123, 130	0
11	2I	111/129 (86%)	0.91	16 (14%) 3 2	77, 102, 118, 125	0
12	3A	122/132 (92%)	1.17	31 (25%) 1 0	84, 102, 126, 145	0
12	3I	122/132 (92%)	0.40	5 (4%) 41 25	67, 77, 99, 122	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	111/126 (88%)	0.61	10 (9%) 12 5	109, 138, 154, 162	0
13	4I	119/126 (94%)	0.12	2 (1%) 73 59	84, 113, 128, 142	0
14	5A	59/61 (96%)	0.79	13 (22%) 1 1	122, 135, 145, 150	0
14	5I	60/61 (98%)	-0.33	0 100 100	82, 92, 108, 112	0
15	6A	88/89 (98%)	0.07	3 (3%) 49 32	89, 109, 128, 132	0
15	6I	87/89 (97%)	0.29	1 (1%) 82 71	83, 99, 116, 124	0
16	7A	84/88 (95%)	0.07	1 (1%) 81 69	92, 107, 125, 140	0
16	7I	83/88 (94%)	-0.26	0 100 100	97, 106, 136, 155	0
17	8A	99/105 (94%)	0.48	9 (9%) 11 5	95, 114, 127, 134	0
17	8I	100/105 (95%)	0.32	5 (5%) 32 17	88, 104, 115, 121	0
18	9A	67/88 (76%)	0.90	9 (13%) 4 2	93, 111, 130, 132	0
18	9I	68/88 (77%)	1.65	22 (32%) 1 0	87, 102, 124, 127	0
19	AA	62/93 (66%)	0.43	5 (8%) 15 7	123, 142, 153, 156	0
19	AI	81/93 (87%)	0.42	3 (3%) 45 28	91, 110, 132, 138	0
20	BA	99/106 (93%)	-0.06	2 (2%) 68 52	90, 110, 133, 142	0
20	BI	97/106 (91%)	-0.12	1 (1%) 84 74	104, 121, 147, 152	0
21	1B	22/27 (81%)	0.04	2 (9%) 11 5	119, 130, 141, 145	0
21	1F	23/27 (85%)	-0.35	0 100 100	89, 102, 110, 112	0
22	1K	64/76 (84%)	0.37	8 (12%) 5 3	84, 173, 191, 198	0
22	1L	68/76 (89%)	1.45	19 (27%) 1 0	115, 198, 216, 220	0
23	2K	72/77 (93%)	-0.54	0 100 100	74, 96, 123, 139	0
23	2L	72/77 (93%)	-0.48	0 100 100	81, 109, 138, 153	0
24	3K	75/76 (98%)	-0.33	3 (4%) 42 26	76, 207, 224, 234	0
25	4K	20/27 (74%)	0.14	2 (10%) 9 4	73, 133, 219, 222	0
25	4L	19/27 (70%)	0.30	2 (10%) 8 4	92, 146, 215, 217	0
26	14	2861/2917 (98%)	-0.59	18 (0%) 90 84	54, 86, 192, 250	0
26	1H	2833/2917 (97%)	-0.61	12 (0%) 93 90	44, 76, 171, 250	0
27	16	122/122 (100%)	-0.83	1 (0%) 87 79	69, 93, 114, 188	0
27	1J	122/122 (100%)	-0.87	0 100 100	87, 113, 134, 182	0
28	71	133/229 (58%)	1.48	44 (33%) 0 0	135, 198, 223, 231	0
28	79	57/229 (24%)	1.56	20 (35%) 0 0	141, 174, 199, 206	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	11	273/276 (98%)	0.32	7 (2%) 59 44	43, 68, 86, 96	0
29	19	274/276 (99%)	0.45	13 (4%) 35 20	52, 75, 91, 115	0
30	21	203/206 (98%)	0.66	29 (14%) 4 2	55, 93, 129, 137	0
30	29	204/206 (99%)	0.40	16 (7%) 16 8	63, 94, 125, 142	0
31	31	202/210 (96%)	0.11	6 (2%) 54 37	49, 80, 114, 128	0
31	39	204/210 (97%)	0.52	20 (9%) 10 5	60, 101, 144, 170	0
32	41	179/182 (98%)	0.46	15 (8%) 14 6	80, 101, 132, 143	0
32	49	179/182 (98%)	1.36	47 (26%) 1 0	107, 123, 144, 167	0
33	51	171/180 (95%)	0.34	11 (6%) 23 11	84, 103, 118, 126	0
33	59	74/180 (41%)	0.50	10 (13%) 4 2	127, 155, 176, 191	0
34	61	146/148 (98%)	0.68	17 (11%) 6 3	80, 125, 142, 155	0
34	69	145/148 (97%)	0.86	23 (15%) 3 1	86, 121, 142, 152	0
35	15	138/140 (98%)	0.74	14 (10%) 9 4	80, 104, 132, 141	0
35	58	138/140 (98%)	0.65	13 (9%) 11 5	67, 94, 126, 137	0
36	25	122/122 (100%)	0.38	4 (3%) 50 33	69, 87, 103, 112	0
36	68	122/122 (100%)	0.25	4 (3%) 50 33	61, 79, 95, 103	0
37	35	147/150 (98%)	0.52	13 (8%) 12 6	60, 102, 129, 139	0
37	78	147/150 (98%)	0.03	4 (2%) 58 42	50, 84, 111, 117	0
38	45	138/141 (97%)	1.28	29 (21%) 1 1	74, 100, 118, 130	0
38	88	141/141 (100%)	0.47	8 (5%) 27 14	61, 80, 100, 123	0
39	55	118/118 (100%)	-0.11	0 100 100	64, 80, 96, 107	0
39	98	118/118 (100%)	0.51	8 (6%) 20 10	66, 89, 106, 118	0
40	65	110/112 (98%)	0.55	5 (4%) 37 21	84, 106, 121, 127	0
40	A8	111/112 (99%)	0.58	9 (8%) 15 7	76, 88, 107, 116	0
41	75	133/146 (91%)	0.03	4 (3%) 54 37	76, 95, 122, 143	0
41	B8	133/146 (91%)	-0.17	1 (0%) 87 79	71, 94, 126, 141	0
42	85	116/118 (98%)	0.27	5 (4%) 39 23	67, 90, 121, 132	0
42	C8	115/118 (97%)	0.18	5 (4%) 39 23	60, 84, 111, 120	0
43	95	100/101 (99%)	1.72	39 (39%) 0 0	68, 117, 131, 142	0
43	D8	100/101 (99%)	0.82	11 (11%) 7 3	62, 103, 123, 129	0
44	A5	113/113 (100%)	0.18	2 (1%) 71 56	61, 75, 104, 155	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	E8	112/113 (99%)	0.44	4 (3%) 46 29	60, 76, 104, 136	0
45	B5	94/96 (97%)	0.35	6 (6%) 23 11	72, 83, 104, 119	0
45	F8	95/96 (98%)	0.21	3 (3%) 51 34	59, 74, 97, 107	0
46	C5	104/110 (94%)	1.12	24 (23%) 1 1	89, 114, 147, 154	0
46	G8	105/110 (95%)	0.11	2 (1%) 70 54	72, 94, 124, 135	0
47	D5	132/206 (64%)	1.66	54 (40%) 0 0	104, 132, 155, 163	0
47	H8	171/206 (83%)	1.27	46 (26%) 1 0	87, 118, 188, 193	0
48	E5	77/85 (90%)	0.65	4 (5%) 31 16	69, 87, 102, 123	0
48	I8	76/85 (89%)	-0.12	1 (1%) 79 67	59, 72, 85, 100	0
49	F5	94/98 (95%)	0.57	7 (7%) 17 9	66, 84, 115, 128	0
49	J8	94/98 (95%)	0.42	9 (9%) 10 5	54, 77, 114, 120	0
50	G5	66/72 (91%)	0.25	2 (3%) 54 37	81, 101, 121, 132	0
50	K8	68/72 (94%)	0.29	1 (1%) 76 62	67, 84, 98, 115	0
51	H5	58/60 (96%)	0.94	9 (15%) 3 1	77, 98, 128, 136	0
51	L8	58/60 (96%)	0.33	2 (3%) 49 32	65, 83, 107, 123	0
52	M8	47/71 (66%)	1.16	12 (25%) 1 0	102, 135, 150, 157	0
53	J5	56/60 (93%)	-0.10	0 100 100	59, 87, 127, 134	0
53	N8	48/60 (80%)	0.21	3 (6%) 23 12	55, 86, 128, 132	0
54	L5	47/49 (95%)	-0.19	1 (2%) 67 50	54, 62, 83, 88	0
54	P8	47/49 (95%)	-0.39	1 (2%) 67 50	49, 55, 72, 81	0
55	M5	64/65 (98%)	0.18	1 (1%) 74 61	68, 78, 93, 111	0
55	Q8	64/65 (98%)	-0.14	0 100 100	62, 70, 84, 97	0
56	3L	73/76 (96%)	0.11	3 (4%) 41 25	84, 205, 228, 235	0
All	All	20602/21967 (93%)	-0.02	1106 (5%) 29 15	43, 99, 165, 253	0

The worst 5 of 1106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	12.8
26	14	2901	C	9.8
32	49	138	GLN	8.4
44	A5	113	LYS	8.2
22	1L	71	C	8.2



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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	U8U	1K	34	23/24	0.95	0.14	-	81,89,100,107	0
22	T6A	1K	37	32/33	0.87	0.28	-	66,85,127,129	0
22	PSU	1K	55	20/21	0.92	0.14	-	107,132,143,147	0
22	T6A	1L	37	32/33	0.88	0.23	-	104,115,143,144	0
23	OMC	2K	33	21/22	0.96	0.14	-	73,80,83,87	0
23	4SU	2L	8	20/21	0.93	0.14	-	100,111,114,121	0
24	PSU	3K	39	20/21	0.95	0.09	-	109,116,128,137	0
23	PSU	2K	56	20/21	0.96	0.08	-	95,100,104,111	0
22	5MU	1K	54	21/22	0.91	0.18	-	118,126,140,143	0
23	OMC	2L	33	21/22	0.94	0.15	-	96,100,104,113	0
22	PSU	1L	55	20/21	0.88	0.21	-	126,149,158,158	0
56	PSU	3L	39	20/21	0.85	0.17	-	118,132,140,141	0
23	5MU	2K	55	21/22	0.95	0.09	-	90,103,110,112	0
22	PSU	1L	39	20/21	0.93	0.13	-	104,123,128,130	0
23	PSU	2L	56	20/21	0.93	0.10	-	106,110,116,120	0
22	5MU	1L	54	21/22	0.95	0.20	-	131,141,157,158	0
22	PSU	1K	39	20/21	0.96	0.11	-	79,97,103,106	0
56	T6A	3L	37	32/33	0.89	0.19	-	121,132,147,147	0
23	G7M	2L	47	24/25	0.96	0.12	-	114,121,128,132	0
23	G7M	2K	47	24/25	0.93	0.12	-	90,101,110,116	0
23	4SU	2K	8	20/21	0.95	0.13	-	87,92,97,98	0
23	5MU	2L	55	21/22	0.94	0.09	-	105,114,119,125	0
22	U8U	1L	34	23/24	0.91	0.17	-	115,123,131,134	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3029	1/1	0.99	0.35	64.89	49,49,49,49	0
57	MG	1H	3088	1/1	0.95	0.34	51.75	53,53,53,53	0
57	MG	13	1634	1/1	0.98	0.70	43.21	71,71,71,71	0
57	MG	14	3223	1/1	0.74	0.42	34.73	75,75,75,75	0
57	MG	14	3268	1/1	0.67	0.44	32.93	60,60,60,60	0
57	MG	1H	3090	1/1	0.91	0.48	32.85	57,57,57,57	0
57	MG	1H	3247	1/1	0.88	0.61	31.59	77,77,77,77	0
57	MG	1H	3230	1/1	0.91	0.36	30.12	78,78,78,78	0
57	MG	14	3243	1/1	0.69	0.41	28.58	86,86,86,86	0
57	MG	14	3080	1/1	0.98	0.38	27.09	46,46,46,46	0
57	MG	1H	3053	1/1	0.91	0.47	26.25	56,56,56,56	0
57	MG	14	3238	1/1	0.86	0.55	26.17	69,69,69,69	0
57	MG	14	3170	1/1	0.95	0.30	25.41	86,86,86,86	0
57	MG	14	3150	1/1	0.93	0.47	25.35	68,68,68,68	0
57	MG	1H	3057	1/1	0.90	0.40	24.72	53,53,53,53	0
57	MG	1H	3018	1/1	0.82	0.44	21.73	80,80,80,80	0
57	MG	13	1678	1/1	0.92	0.21	20.71	83,83,83,83	0
57	MG	1H	3180	1/1	0.67	0.38	20.47	76,76,76,76	0
57	MG	14	3061	1/1	0.98	0.34	20.32	61,61,61,61	0
57	MG	13	1654	1/1	0.96	0.32	20.21	75,75,75,75	0
57	MG	14	3212	1/1	0.83	0.43	20.17	80,80,80,80	0
57	MG	1H	3105	1/1	0.90	0.24	19.47	79,79,79,79	0
57	MG	13	1687	1/1	0.95	0.23	19.37	70,70,70,70	0
57	MG	1G	1647	1/1	0.94	0.25	19.24	115,115,115,115	0
57	MG	13	1602	1/1	0.99	0.41	18.64	88,88,88,88	0
57	MG	13	1620	1/1	0.88	0.35	18.36	58,58,58,58	0
57	MG	13	1627	1/1	0.96	0.29	18.12	64,64,64,64	0
57	MG	1H	3259	1/1	0.86	0.36	17.73	74,74,74,74	0
57	MG	14	3082	1/1	0.93	0.40	17.11	55,55,55,55	0
57	MG	14	3120	1/1	0.67	0.35	17.05	67,67,67,67	0
57	MG	14	3222	1/1	0.91	0.41	16.88	64,64,64,64	0
57	MG	13	1680	1/1	0.94	0.36	16.73	75,75,75,75	0
57	MG	14	3144	1/1	0.82	0.52	16.64	80,80,80,80	0
57	MG	1H	3061	1/1	0.95	0.28	16.47	68,68,68,68	0
57	MG	1H	3287	1/1	0.76	0.37	16.41	80,80,80,80	0
57	MG	1G	1613	1/1	0.82	0.52	16.37	73,73,73,73	0
57	MG	1G	1645	1/1	0.96	0.55	15.71	88,88,88,88	0
57	MG	14	3097	1/1	0.78	0.51	15.30	65,65,65,65	0
57	MG	14	3046	1/1	0.99	0.41	15.24	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3078	1/1	0.97	0.28	14.54	86,86,86,86	0
57	MG	1H	3045	1/1	0.95	0.29	14.50	54,54,54,54	0
57	MG	1G	1614	1/1	0.95	0.26	14.16	99,99,99,99	0
57	MG	14	3050	1/1	0.98	0.29	14.04	59,59,59,59	0
57	MG	14	3035	1/1	0.97	0.39	13.76	83,83,83,83	0
57	MG	1H	3014	1/1	0.87	0.50	13.41	75,75,75,75	0
57	MG	14	3137	1/1	0.98	0.22	13.34	72,72,72,72	0
57	MG	1G	1636	1/1	0.88	0.22	13.33	89,89,89,89	0
57	MG	14	3109	1/1	0.97	0.32	13.02	60,60,60,60	0
57	MG	13	1669	1/1	0.94	0.46	13.01	74,74,74,74	0
57	MG	1H	3128	1/1	0.77	0.22	12.83	64,64,64,64	0
57	MG	14	3136	1/1	0.94	0.37	12.75	59,59,59,59	0
57	MG	13	1650	1/1	0.70	0.37	12.61	100,100,100,100	0
57	MG	1H	3109	1/1	0.91	0.33	12.54	65,65,65,65	0
57	MG	14	3119	1/1	0.98	0.50	12.42	63,63,63,63	0
57	MG	14	3191	1/1	0.80	0.44	12.27	73,73,73,73	0
57	MG	14	3219	1/1	0.90	0.29	12.26	64,64,64,64	0
57	MG	14	3064	1/1	0.98	0.36	12.20	58,58,58,58	0
57	MG	1H	3232	1/1	0.95	0.31	12.19	65,65,65,65	0
57	MG	1H	3067	1/1	0.95	0.33	12.02	52,52,52,52	0
57	MG	1H	3004	1/1	0.95	0.23	12.00	54,54,54,54	0
57	MG	13	1611	1/1	0.97	0.24	11.97	79,79,79,79	0
57	MG	1H	3078	1/1	0.95	0.35	11.76	60,60,60,60	0
57	MG	1H	3249	1/1	0.78	0.22	11.62	61,61,61,61	0
57	MG	13	1645	1/1	0.82	0.23	11.50	93,93,93,93	0
57	MG	13	1671	1/1	0.93	0.32	11.35	71,71,71,71	0
57	MG	1H	3098	1/1	0.88	0.33	11.35	63,63,63,63	0
57	MG	13	1623	1/1	0.98	0.35	11.34	61,61,61,61	0
57	MG	14	3143	1/1	0.78	0.24	11.10	73,73,73,73	0
57	MG	1H	3036	1/1	0.82	0.20	11.03	78,78,78,78	0
57	MG	1G	1602	1/1	0.98	0.28	10.92	72,72,72,72	0
57	MG	1H	3124	1/1	0.95	0.24	10.76	74,74,74,74	0
57	MG	13	1642	1/1	0.88	0.26	10.54	107,107,107,107	0
57	MG	1H	3115	1/1	0.83	0.29	10.33	82,82,82,82	0
57	MG	1H	3221	1/1	0.90	0.21	10.31	60,60,60,60	0
57	MG	1H	3135	1/1	0.94	0.34	10.22	81,81,81,81	0
57	MG	1H	3043	1/1	0.99	0.28	9.98	70,70,70,70	0
57	MG	13	1668	1/1	0.86	0.23	9.92	95,95,95,95	0
57	MG	14	3074	1/1	0.93	0.27	9.86	62,62,62,62	0
57	MG	1H	3050	1/1	0.97	0.32	9.62	66,66,66,66	0
57	MG	1G	1611	1/1	0.95	0.39	9.55	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3229	1/1	0.84	0.29	9.54	74,74,74,74	0
57	MG	13	1616	1/1	0.94	0.31	9.50	48,48,48,48	0
57	MG	14	3019	1/1	0.99	0.33	9.31	58,58,58,58	0
57	MG	1H	3041	1/1	0.97	0.28	9.31	72,72,72,72	0
57	MG	14	3088	1/1	0.94	0.28	9.18	65,65,65,65	0
57	MG	16	205	1/1	0.72	0.20	9.17	81,81,81,81	0
57	MG	1H	3139	1/1	0.80	0.36	9.08	71,71,71,71	0
57	MG	1G	1640	1/1	0.94	0.18	8.75	100,100,100,100	0
57	MG	14	3018	1/1	0.97	0.26	8.63	49,49,49,49	0
57	MG	1H	3024	1/1	0.98	0.31	8.63	45,45,45,45	0
57	MG	14	3186	1/1	0.96	0.24	8.48	84,84,84,84	0
57	MG	1H	3120	1/1	0.83	0.16	8.48	63,63,63,63	0
57	MG	1H	3070	1/1	0.97	0.29	8.43	45,45,45,45	0
57	MG	1H	3035	1/1	0.92	0.24	8.40	57,57,57,57	0
57	MG	1H	3025	1/1	0.98	0.32	8.38	56,56,56,56	0
57	MG	13	1606	1/1	0.97	0.28	8.24	52,52,52,52	0
57	MG	1H	3056	1/1	0.97	0.28	7.96	52,52,52,52	0
57	MG	13	1608	1/1	0.97	0.23	7.82	75,75,75,75	0
57	MG	14	3024	1/1	0.91	0.26	7.78	58,58,58,58	0
57	MG	1H	3286	1/1	0.86	0.23	7.61	82,82,82,82	0
57	MG	14	3172	1/1	0.96	0.19	7.47	63,63,63,63	0
57	MG	14	3017	1/1	0.91	0.23	7.45	97,97,97,97	0
57	MG	1H	3116	1/1	0.89	0.30	7.12	63,63,63,63	0
57	MG	14	3175	1/1	0.91	0.24	7.04	90,90,90,90	0
57	MG	1G	1609	1/1	0.80	0.19	6.86	108,108,108,108	0
57	MG	14	3174	1/1	0.94	0.16	6.82	71,71,71,71	0
57	MG	14	3042	1/1	0.98	0.24	6.62	58,58,58,58	0
57	MG	1H	3240	1/1	0.96	0.24	6.59	72,72,72,72	0
57	MG	14	3030	1/1	0.94	0.22	6.52	68,68,68,68	0
57	MG	14	3105	1/1	0.92	0.26	6.51	55,55,55,55	0
57	MG	1H	3206	1/1	0.93	0.21	6.44	56,56,56,56	0
57	MG	14	3068	1/1	0.94	0.32	6.43	67,67,67,67	0
57	MG	14	3168	1/1	0.86	0.21	6.32	89,89,89,89	0
57	MG	1H	3268	1/1	0.98	0.25	6.28	81,81,81,81	0
57	MG	1G	1621	1/1	0.65	0.18	6.19	103,103,103,103	0
57	MG	13	1677	1/1	0.88	0.22	6.06	76,76,76,76	0
57	MG	1H	3091	1/1	0.90	0.26	6.05	57,57,57,57	0
57	MG	1G	1607	1/1	0.90	0.22	6.04	91,91,91,91	0
57	MG	1H	3079	1/1	0.98	0.30	6.03	47,47,47,47	0
57	MG	1G	1625	1/1	0.98	0.20	5.90	89,89,89,89	0
57	MG	1H	3146	1/1	0.96	0.25	5.88	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3139	1/1	0.90	0.22	5.87	58,58,58,58	0
57	MG	1H	3005	1/1	0.96	0.34	5.70	74,74,74,74	0
57	MG	2L	101	1/1	0.95	0.36	5.64	70,70,70,70	0
57	MG	1H	3082	1/1	0.95	0.23	5.58	49,49,49,49	0
57	MG	14	3254	1/1	0.94	0.21	5.56	81,81,81,81	0
57	MG	14	3047	1/1	0.97	0.33	5.55	42,42,42,42	0
57	MG	1G	1615	1/1	0.95	0.20	5.52	92,92,92,92	0
57	MG	1H	3038	1/1	0.95	0.23	5.50	53,53,53,53	0
57	MG	13	1651	1/1	0.94	0.21	5.41	68,68,68,68	0
57	MG	14	3037	1/1	0.77	0.21	5.38	63,63,63,63	0
57	MG	16	201	1/1	0.92	0.17	5.37	87,87,87,87	0
57	MG	2K	103	1/1	0.98	0.36	5.29	61,61,61,61	0
57	MG	13	1644	1/1	0.97	0.20	5.09	80,80,80,80	0
57	MG	1H	3179	1/1	0.95	0.25	5.07	49,49,49,49	0
57	MG	1H	3164	1/1	0.96	0.22	4.94	47,47,47,47	0
57	MG	1H	3465	1/1	0.97	0.26	4.87	53,53,53,53	0
57	MG	14	3049	1/1	0.93	0.27	4.84	63,63,63,63	0
57	MG	1H	3064	1/1	0.99	0.23	4.82	54,54,54,54	0
57	MG	1H	3054	1/1	0.79	0.34	4.77	59,59,59,59	0
57	MG	1H	3174	1/1	0.92	0.28	4.73	59,59,59,59	0
57	MG	1H	3153	1/1	0.97	0.18	4.58	59,59,59,59	0
57	MG	14	3259	1/1	0.85	0.19	4.48	97,97,97,97	0
57	MG	13	1684	1/1	0.75	0.22	4.46	85,85,85,85	0
57	MG	14	3083	1/1	0.97	0.21	4.20	61,61,61,61	0
57	MG	1H	3290	1/1	0.91	0.23	4.10	62,62,62,62	0
57	MG	14	3092	1/1	0.96	0.27	4.08	56,56,56,56	0
57	MG	14	3123	1/1	0.89	0.49	4.02	70,70,70,70	0
57	MG	1J	201	1/1	0.88	0.20	3.95	85,85,85,85	0
57	MG	14	3071	1/1	0.94	0.16	3.95	73,73,73,73	0
57	MG	1H	3101	1/1	0.92	0.18	3.86	58,58,58,58	0
57	MG	1H	3107	1/1	0.79	0.19	3.53	64,64,64,64	0
57	MG	1H	3173	1/1	0.95	0.15	3.52	63,63,63,63	0
57	MG	1H	3066	1/1	0.81	0.22	3.51	57,57,57,57	0
57	MG	1H	3008	1/1	0.91	0.26	3.50	57,57,57,57	0
57	MG	29	301	1/1	0.74	0.44	3.49	80,80,80,80	0
57	MG	14	3098	1/1	0.90	0.22	3.43	67,67,67,67	0
57	MG	1G	1604	1/1	0.86	0.17	3.37	87,87,87,87	0
57	MG	13	1610	1/1	0.98	0.15	3.31	79,79,79,79	0
57	MG	1H	3375	1/1	0.97	0.18	3.30	57,57,57,57	0
57	MG	13	1601	1/1	0.97	0.21	3.27	68,68,68,68	0
57	MG	14	3260	1/1	0.86	0.14	3.24	117,117,117,117	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3167	1/1	0.97	0.14	3.12	65,65,65,65	0
57	MG	14	3231	1/1	0.95	0.44	3.09	76,76,76,76	0
57	MG	14	3166	1/1	0.93	0.23	3.09	61,61,61,61	0
57	MG	1H	3074	1/1	0.96	0.21	3.00	48,48,48,48	0
57	MG	14	3028	1/1	0.99	0.21	2.97	60,60,60,60	0
57	MG	13	1683	1/1	0.99	0.21	2.94	67,67,67,67	0
57	MG	14	3073	1/1	0.97	0.23	2.89	57,57,57,57	0
57	MG	1H	3162	1/1	0.92	0.15	2.83	61,61,61,61	0
57	MG	14	3041	1/1	0.95	0.20	2.83	64,64,64,64	0
57	MG	1G	1644	1/1	0.94	0.35	2.78	67,67,67,67	0
57	MG	13	1646	1/1	0.45	0.17	2.73	109,109,109,109	0
57	MG	14	3111	1/1	0.91	0.15	2.65	79,79,79,79	0
57	MG	14	3007	1/1	0.93	0.28	2.59	50,50,50,50	0
57	MG	14	3205	1/1	0.96	0.18	2.59	77,77,77,77	0
57	MG	1H	3267	1/1	0.90	0.16	2.53	67,67,67,67	0
57	MG	1H	3154	1/1	0.94	0.18	2.47	75,75,75,75	0
57	MG	1H	3009	1/1	0.98	0.24	2.42	54,54,54,54	0
57	MG	1H	3123	1/1	0.93	0.21	2.30	71,71,71,71	0
57	MG	13	1607	1/1	0.98	0.27	2.16	74,74,74,74	0
57	MG	1G	1650	1/1	0.96	0.21	2.10	87,87,87,87	0
57	MG	13	1672	1/1	0.91	0.11	1.97	96,96,96,96	0
57	MG	1G	1630	1/1	0.96	0.22	1.97	113,113,113,113	0
57	MG	14	3052	1/1	0.94	0.32	1.97	62,62,62,62	0
57	MG	1G	1619	1/1	0.89	0.21	1.95	92,92,92,92	0
57	MG	1H	3250	1/1	0.97	0.19	1.90	67,67,67,67	0
57	MG	1H	3333	1/1	0.97	0.16	1.83	75,75,75,75	0
58	PAR	13	1749	42/42	0.96	0.20	1.82	64,70,78,81	0
57	MG	1H	3502	1/1	0.97	0.32	1.82	59,59,59,59	0
57	MG	14	3129	1/1	0.83	0.16	1.79	69,69,69,69	0
57	MG	14	3169	1/1	0.92	0.18	1.76	65,65,65,65	0
57	MG	1H	3499	1/1	0.99	0.26	1.72	67,67,67,67	0
57	MG	16	203	1/1	0.72	0.16	1.70	79,79,79,79	0
57	MG	55	201	1/1	0.59	0.33	1.70	83,83,83,83	0
57	MG	41	202	1/1	0.85	0.26	1.70	82,82,82,82	0
57	MG	1H	3172	1/1	0.99	0.14	1.66	73,73,73,73	0
57	MG	1H	3243	1/1	0.88	0.25	1.64	62,62,62,62	0
57	MG	1H	3349	1/1	0.99	0.17	1.63	53,53,53,53	0
57	MG	35	201	1/1	0.80	0.33	1.54	71,71,71,71	0
57	MG	21	303	1/1	0.82	0.22	1.50	69,69,69,69	0
57	MG	14	3187	1/1	0.97	0.15	1.38	80,80,80,80	0
57	MG	1H	3081	1/1	0.97	0.19	1.35	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3216	1/1	0.88	0.23	1.29	74,74,74,74	0
57	MG	1G	1657	1/1	0.79	0.13	1.28	105,105,105,105	0
57	MG	14	3033	1/1	0.92	0.14	1.27	74,74,74,74	0
57	MG	29	304	1/1	0.68	0.23	1.25	71,71,71,71	0
57	MG	14	3133	1/1	0.99	0.33	1.24	71,71,71,71	0
58	PAR	1G	1691	42/42	0.96	0.16	1.22	70,82,88,95	0
57	MG	14	3131	1/1	0.94	0.22	1.14	78,78,78,78	0
57	MG	13	1619	1/1	0.94	0.12	1.12	90,90,90,90	0
57	MG	1H	3037	1/1	0.95	0.17	1.11	55,55,55,55	0
57	MG	13	1626	1/1	0.86	0.14	1.08	87,87,87,87	0
57	MG	1H	3317	1/1	0.99	0.20	0.94	45,45,45,45	0
57	MG	1H	3223	1/1	0.98	0.18	0.92	64,64,64,64	0
57	MG	14	3273	1/1	0.98	0.19	0.90	58,58,58,58	0
57	MG	14	3032	1/1	0.97	0.18	0.77	47,47,47,47	0
57	MG	1H	3096	1/1	0.92	0.16	0.76	67,67,67,67	0
57	MG	14	3099	1/1	0.95	0.17	0.76	57,57,57,57	0
57	MG	13	1750	1/1	0.91	0.18	0.74	76,76,76,76	0
57	MG	85	201	1/1	0.99	0.20	0.66	72,72,72,72	0
57	MG	14	3025	1/1	0.97	0.19	0.62	58,58,58,58	0
57	MG	1H	3486	1/1	0.97	0.18	0.59	61,61,61,61	0
57	MG	14	3125	1/1	0.98	0.17	0.51	54,54,54,54	0
57	MG	1G	1624	1/1	0.88	0.19	0.32	87,87,87,87	0
57	MG	1H	3073	1/1	0.93	0.20	0.31	36,36,36,36	0
57	MG	1H	3167	1/1	0.99	0.15	0.30	63,63,63,63	0
57	MG	14	3132	1/1	0.94	0.17	0.25	58,58,58,58	0
57	MG	1H	3301	1/1	0.96	0.15	0.22	49,49,49,49	0
57	MG	1H	3148	1/1	0.89	0.23	0.15	65,65,65,65	0
60	ZN	5I	102	1/1	0.99	0.13	0.13	88,88,88,88	0
57	MG	1H	3389	1/1	0.99	0.16	0.08	59,59,59,59	0
57	MG	13	1633	1/1	0.96	0.13	0.00	85,85,85,85	0
57	MG	14	3347	1/1	0.98	0.13	-0.01	67,67,67,67	0
57	MG	13	1653	1/1	0.96	0.14	-0.02	66,66,66,66	0
57	MG	13	1710	1/1	0.94	0.12	-0.11	108,108,108,108	0
57	MG	1H	3313	1/1	0.96	0.11	-0.14	72,72,72,72	0
57	MG	1H	3001	1/1	0.97	0.16	-0.21	53,53,53,53	0
57	MG	14	3322	1/1	0.99	0.14	-0.25	74,74,74,74	0
57	MG	1G	1665	1/1	0.94	0.13	-0.28	97,97,97,97	0
59	SF4	3E	301	8/8	0.99	0.19	-0.28	71,78,87,91	0
57	MG	88	201	1/1	0.91	0.18	-0.28	82,82,82,82	0
57	MG	13	1751	1/1	0.96	0.14	-0.29	87,87,87,87	0
57	MG	13	1604	1/1	0.97	0.14	-0.31	112,112,112,112	0
57	MG	1H	3166	1/1	0.96	0.12	-0.33	70,70,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3287	1/1	0.99	0.17	-0.40	56,56,56,56	0
57	MG	1H	3373	1/1	0.97	0.14	-0.40	66,66,66,66	0
57	MG	29	303	1/1	0.82	0.16	-0.41	67,67,67,67	0
57	MG	13	1639	1/1	0.97	0.10	-0.43	84,84,84,84	0
57	MG	14	3159	1/1	0.94	0.18	-0.46	71,71,71,71	0
57	MG	14	3301	1/1	0.99	0.15	-0.47	56,56,56,56	0
57	MG	1H	3075	1/1	0.89	0.12	-0.48	60,60,60,60	0
57	MG	41	201	1/1	0.90	0.14	-0.51	75,75,75,75	0
57	MG	1H	3097	1/1	0.90	0.16	-0.55	51,51,51,51	0
57	MG	1G	1684	1/1	0.95	0.08	-0.56	121,121,121,121	0
57	MG	13	1697	1/1	0.99	0.09	-0.57	90,90,90,90	0
57	MG	1H	3316	1/1	0.96	0.14	-0.57	63,63,63,63	0
59	SF4	32	301	8/8	0.99	0.17	-0.58	100,111,117,118	0
57	MG	14	3090	1/1	0.94	0.13	-0.61	60,60,60,60	0
57	MG	1H	3368	1/1	0.97	0.15	-0.61	60,60,60,60	0
57	MG	1H	3431	1/1	0.93	0.16	-0.62	52,52,52,52	0
57	MG	14	3451	1/1	0.98	0.14	-0.63	77,77,77,77	0
57	MG	1H	3460	1/1	0.98	0.14	-0.72	62,62,62,62	0
57	MG	14	3318	1/1	0.90	0.15	-0.76	67,67,67,67	0
57	MG	14	3421	1/1	0.83	0.15	-0.81	75,75,75,75	0
57	MG	1G	1682	1/1	0.96	0.10	-0.81	127,127,127,127	0
57	MG	14	3305	1/1	0.99	0.17	-0.88	57,57,57,57	0
57	MG	14	3128	1/1	0.94	0.12	-0.89	60,60,60,60	0
57	MG	1H	3336	1/1	0.98	0.13	-0.93	61,61,61,61	0
57	MG	1H	3429	1/1	0.97	0.11	-0.94	75,75,75,75	0
57	MG	1H	3276	1/1	0.96	0.12	-0.96	98,98,98,98	0
57	MG	45	201	1/1	0.95	0.15	-0.96	72,72,72,72	0
57	MG	13	1726	1/1	0.98	0.08	-1.02	85,85,85,85	0
60	ZN	5A	101	1/1	0.98	0.09	-1.04	128,128,128,128	0
57	MG	13	1631	1/1	0.91	0.10	-1.05	73,73,73,73	0
57	MG	5I	101	1/1	0.75	0.08	-1.05	88,88,88,88	0
57	MG	1H	3319	1/1	0.99	0.13	-1.09	67,67,67,67	0
57	MG	13	1693	1/1	0.97	0.13	-1.14	72,72,72,72	0
57	MG	45	202	1/1	0.91	0.10	-1.23	102,102,102,102	0
57	MG	1H	3391	1/1	0.98	0.13	-1.26	49,49,49,49	0
57	MG	13	1695	1/1	0.99	0.11	-1.26	76,76,76,76	0
57	MG	14	3408	1/1	0.95	0.08	-1.30	78,78,78,78	0
57	MG	39	301	1/1	0.89	0.14	-1.31	95,95,95,95	0
57	MG	5E	201	1/1	0.97	0.20	-1.36	81,81,81,81	0
60	ZN	C5	202	1/1	0.96	0.15	-1.36	169,169,169,169	0
57	MG	14	3358	1/1	0.98	0.12	-1.39	54,54,54,54	0
57	MG	14	3307	1/1	0.99	0.12	-1.39	79,79,79,79	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3441	1/1	0.97	0.10	-1.41	94,94,94,94	0
57	MG	14	3038	1/1	0.90	0.08	-1.41	76,76,76,76	0
57	MG	Q8	101	1/1	0.96	0.15	-1.44	73,73,73,73	0
57	MG	14	3343	1/1	0.97	0.09	-1.49	63,63,63,63	0
60	ZN	G8	201	1/1	0.97	0.18	-1.51	146,146,146,146	0
57	MG	1H	3324	1/1	0.98	0.13	-1.51	47,47,47,47	0
57	MG	1H	3270	1/1	0.94	0.10	-1.52	71,71,71,71	0
57	MG	14	3450	1/1	0.98	0.10	-1.53	63,63,63,63	0
57	MG	13	1706	1/1	0.98	0.12	-1.65	71,71,71,71	0
57	MG	14	3281	1/1	0.99	0.16	-1.68	66,66,66,66	0
57	MG	14	3385	1/1	0.98	0.07	-1.70	70,70,70,70	0
57	MG	1G	1674	1/1	0.92	0.06	-1.75	107,107,107,107	0
57	MG	1H	3399	1/1	0.98	0.13	-1.78	61,61,61,61	0
57	MG	1H	3367	1/1	0.97	0.09	-1.78	54,54,54,54	0
57	MG	1H	3401	1/1	0.99	0.10	-1.81	52,52,52,52	0
57	MG	14	3317	1/1	0.96	0.10	-1.81	59,59,59,59	0
57	MG	1H	3335	1/1	0.96	0.09	-1.82	61,61,61,61	0
57	MG	14	3309	1/1	0.94	0.14	-1.86	73,73,73,73	0
57	MG	14	3178	1/1	0.91	0.09	-1.86	71,71,71,71	0
57	MG	13	1701	1/1	0.96	0.07	-1.87	70,70,70,70	0
57	MG	14	3413	1/1	0.97	0.10	-1.89	97,97,97,97	0
57	MG	1H	3468	1/1	0.98	0.11	-1.89	71,71,71,71	0
57	MG	14	3361	1/1	0.96	0.09	-1.91	69,69,69,69	0
57	MG	1G	1652	1/1	0.97	0.11	-1.92	82,82,82,82	0
57	MG	1G	1693	1/1	0.96	0.09	-1.94	92,92,92,92	0
57	MG	14	3153	1/1	0.98	0.09	-1.97	79,79,79,79	0
57	MG	11	302	1/1	0.98	0.11	-2.02	57,57,57,57	0
57	MG	14	3350	1/1	0.97	0.11	-2.05	56,56,56,56	0
57	MG	1H	3396	1/1	0.99	0.08	-2.07	60,60,60,60	0
57	MG	1G	1659	1/1	0.98	0.13	-2.16	79,79,79,79	0
57	MG	1H	3235	1/1	0.93	0.14	-2.18	65,65,65,65	0
57	MG	1H	3297	1/1	0.99	0.14	-2.21	49,49,49,49	0
57	MG	14	3288	1/1	0.99	0.14	-2.22	50,50,50,50	0
57	MG	13	1724	1/1	0.92	0.08	-2.27	114,114,114,114	0
57	MG	14	3158	1/1	0.92	0.12	-2.32	70,70,70,70	0
57	MG	1G	1672	1/1	0.97	0.03	-2.35	91,91,91,91	0
57	MG	1H	3315	1/1	0.95	0.10	-2.36	73,73,73,73	0
57	MG	1H	3359	1/1	0.95	0.12	-2.37	52,52,52,52	0
57	MG	13	1690	1/1	0.99	0.14	-2.43	68,68,68,68	0
57	MG	1G	1654	1/1	0.98	0.09	-2.44	93,93,93,93	0
57	MG	1H	3358	1/1	0.99	0.12	-2.44	67,67,67,67	0
57	MG	1H	3227	1/1	0.94	0.11	-2.47	70,70,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3333	1/1	0.98	0.14	-2.47	59,59,59,59	0
57	MG	14	3274	1/1	0.99	0.13	-2.48	62,62,62,62	0
57	MG	14	3341	1/1	0.99	0.07	-2.52	62,62,62,62	0
57	MG	14	3283	1/1	0.98	0.09	-2.53	74,74,74,74	0
57	MG	1H	3307	1/1	0.99	0.06	-2.53	57,57,57,57	0
57	MG	14	3344	1/1	0.96	0.09	-2.58	72,72,72,72	0
57	MG	13	1635	1/1	0.62	0.07	-2.58	85,85,85,85	0
57	MG	16	212	1/1	0.90	0.08	-2.66	88,88,88,88	0
57	MG	14	3393	1/1	0.97	0.09	-2.66	79,79,79,79	0
57	MG	14	3293	1/1	1.00	0.09	-2.74	51,51,51,51	0
57	MG	14	3294	1/1	1.00	0.11	-2.75	54,54,54,54	0
57	MG	1H	3321	1/1	0.97	0.09	-2.75	77,77,77,77	0
57	MG	14	3357	1/1	0.75	0.11	-2.95	84,84,84,84	0
57	MG	13	1624	1/1	0.95	0.12	-2.97	81,81,81,81	0
57	MG	14	3320	1/1	0.97	0.09	-2.98	83,83,83,83	0
57	MG	11	301	1/1	0.98	0.10	-3.02	46,46,46,46	0
57	MG	14	3276	1/1	0.96	0.11	-3.03	62,62,62,62	0
57	MG	1H	3310	1/1	0.98	0.10	-3.13	58,58,58,58	0
57	MG	1H	3340	1/1	0.97	0.11	-3.16	54,54,54,54	0
57	MG	1H	3501	1/1	0.87	0.05	-3.18	72,72,72,72	0
57	MG	1H	3414	1/1	0.97	0.13	-3.25	53,53,53,53	0
57	MG	13	1692	1/1	0.95	0.07	-3.25	81,81,81,81	0
57	MG	1H	3305	1/1	0.99	0.09	-3.28	53,53,53,53	0
57	MG	14	3327	1/1	0.99	0.06	-3.35	67,67,67,67	0
57	MG	14	3336	1/1	0.95	0.05	-3.43	83,83,83,83	0
57	MG	14	3289	1/1	0.98	0.12	-3.45	58,58,58,58	0
57	MG	1H	3304	1/1	0.99	0.11	-3.52	55,55,55,55	0
57	MG	14	3297	1/1	0.99	0.08	-3.70	74,74,74,74	0
57	MG	14	3295	1/1	0.99	0.11	-3.73	58,58,58,58	0
57	MG	1H	3454	1/1	0.95	0.08	-3.73	62,62,62,62	0
57	MG	14	3291	1/1	0.99	0.12	-3.75	66,66,66,66	0
57	MG	1H	3337	1/1	0.94	0.07	-3.84	73,73,73,73	0
57	MG	1H	3309	1/1	0.99	0.12	-3.87	48,48,48,48	0
57	MG	1G	1689	1/1	0.91	0.06	-3.89	126,126,126,126	0
57	MG	14	3335	1/1	0.98	0.07	-3.97	87,87,87,87	0
57	MG	13	1712	1/1	0.95	0.08	-4.12	75,75,75,75	0
57	MG	1H	3409	1/1	0.95	0.08	-4.20	69,69,69,69	0
57	MG	1H	3480	1/1	0.93	0.08	-4.34	78,78,78,78	0
57	MG	1H	3417	1/1	0.99	0.11	-4.39	56,56,56,56	0
57	MG	1H	3298	1/1	0.98	0.10	-4.45	61,61,61,61	0
57	MG	1H	3348	1/1	0.95	0.12	-4.46	65,65,65,65	0
57	MG	14	3286	1/1	0.98	0.05	-4.49	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3410	1/1	0.96	0.10	-4.53	56,56,56,56	0
57	MG	14	3334	1/1	0.98	0.11	-4.58	61,61,61,61	0
57	MG	1H	3327	1/1	0.99	0.05	-4.59	55,55,55,55	0
57	MG	1H	3500	1/1	0.93	0.06	-4.63	71,71,71,71	0
57	MG	14	3282	1/1	0.98	0.09	-4.71	58,58,58,58	0
57	MG	1H	3295	1/1	0.99	0.11	-4.78	52,52,52,52	0
57	MG	14	3306	1/1	0.99	0.10	-5.02	55,55,55,55	0
57	MG	1H	3390	1/1	1.00	0.08	-5.07	57,57,57,57	0
57	MG	1G	1651	1/1	0.98	0.08	-5.18	81,81,81,81	0
57	MG	14	3337	1/1	0.98	0.05	-5.21	76,76,76,76	0
57	MG	1H	3150	1/1	0.97	0.09	-5.27	50,50,50,50	0
57	MG	1H	3363	1/1	0.96	0.09	-5.37	61,61,61,61	0
57	MG	1H	3462	1/1	0.99	0.07	-5.59	54,54,54,54	0
57	MG	1H	3366	1/1	0.94	0.08	-5.79	65,65,65,65	0
57	MG	1H	3048	1/1	0.94	0.06	-5.85	80,80,80,80	0
57	MG	1H	3404	1/1	0.98	0.09	-5.93	76,76,76,76	0
57	MG	1H	3292	1/1	0.98	0.10	-5.95	50,50,50,50	0
57	MG	1H	3392	1/1	0.98	0.06	-6.02	69,69,69,69	0
57	MG	1H	3395	1/1	0.92	0.11	-6.03	59,59,59,59	0
57	MG	1H	3323	1/1	0.94	0.06	-6.12	61,61,61,61	0
57	MG	14	3304	1/1	0.97	0.07	-6.18	59,59,59,59	0
57	MG	14	3364	1/1	0.98	0.05	-6.21	73,73,73,73	0
57	MG	1H	3344	1/1	0.97	0.08	-6.25	49,49,49,49	0
57	MG	14	3277	1/1	0.98	0.08	-6.27	67,67,67,67	0
57	MG	13	1698	1/1	0.95	0.04	-6.45	93,93,93,93	0
57	MG	1H	3086	1/1	0.85	0.07	-6.46	71,71,71,71	0
57	MG	13	1717	1/1	0.99	0.10	-6.59	66,66,66,66	0
57	MG	14	3362	1/1	0.99	0.05	-6.82	62,62,62,62	0
57	MG	1H	3490	1/1	0.97	0.07	-6.97	83,83,83,83	0
57	MG	1H	3328	1/1	0.98	0.08	-6.97	52,52,52,52	0
57	MG	14	3415	1/1	0.97	0.06	-7.02	77,77,77,77	0
57	MG	1H	3332	1/1	0.98	0.07	-7.03	63,63,63,63	0
57	MG	1H	3408	1/1	0.99	0.11	-7.09	50,50,50,50	0
57	MG	1H	3342	1/1	0.98	0.06	-7.71	71,71,71,71	0
57	MG	14	3138	1/1	0.95	0.08	-7.77	68,68,68,68	0
57	MG	1H	3418	1/1	0.96	0.05	-7.77	69,69,69,69	0
57	MG	1H	3341	1/1	0.98	0.09	-7.88	57,57,57,57	0
57	MG	1H	3385	1/1	0.93	0.08	-8.12	57,57,57,57	0
57	MG	14	3278	1/1	0.98	0.05	-8.19	65,65,65,65	0
57	MG	1G	1660	1/1	0.99	0.03	-9.13	96,96,96,96	0
57	MG	14	3368	1/1	0.98	0.07	-9.48	72,72,72,72	0
57	MG	14	3311	1/1	0.95	0.07	-9.88	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3392	1/1	0.97	0.06	-10.38	87,87,87,87	0
57	MG	14	3302	1/1	0.98	0.10	-10.39	68,68,68,68	0
57	MG	1H	3293	1/1	0.98	0.06	-11.17	63,63,63,63	0
57	MG	1H	3374	1/1	0.95	0.08	-11.26	55,55,55,55	0
57	MG	1H	3312	1/1	1.00	0.05	-12.13	76,76,76,76	0
57	MG	13	1731	1/1	0.97	0.05	-13.44	86,86,86,86	0
57	MG	14	3353	1/1	0.95	0.10	-16.06	67,67,67,67	0
57	MG	1H	3042	1/1	0.95	0.17	-	79,79,79,79	0
57	MG	14	3232	1/1	0.80	0.25	-	130,130,130,130	0
57	MG	M5	101	1/1	0.91	0.17	-	77,77,77,77	0
57	MG	1G	1670	1/1	0.93	0.08	-	108,108,108,108	0
57	MG	1G	1605	1/1	0.95	0.29	-	92,92,92,92	0
57	MG	14	3342	1/1	0.97	0.09	-	58,58,58,58	0
57	MG	14	3192	1/1	0.82	0.36	-	100,100,100,100	0
57	MG	1H	3046	1/1	0.93	0.56	-	73,73,73,73	0
57	MG	14	3021	1/1	0.97	0.32	-	53,53,53,53	0
57	MG	14	3445	1/1	0.97	0.03	-	87,87,87,87	0
57	MG	14	3375	1/1	0.98	0.05	-	91,91,91,91	0
57	MG	I8	101	1/1	0.97	0.04	-	65,65,65,65	0
57	MG	1H	3010	1/1	0.91	0.47	-	59,59,59,59	0
57	MG	14	3154	1/1	0.82	0.69	-	74,74,74,74	0
57	MG	1H	3281	1/1	0.86	0.52	-	69,69,69,69	0
57	MG	1H	3034	1/1	0.96	0.19	-	54,54,54,54	0
57	MG	1H	3080	1/1	0.95	0.72	-	82,82,82,82	0
57	MG	13	1732	1/1	0.99	0.08	-	108,108,108,108	0
57	MG	1H	3451	1/1	0.93	0.04	-	95,95,95,95	0
57	MG	14	3303	1/1	0.89	0.13	-	63,63,63,63	0
57	MG	1H	3434	1/1	0.89	0.10	-	73,73,73,73	0
57	MG	13	1736	1/1	0.91	0.06	-	95,95,95,95	0
57	MG	1H	3467	1/1	0.92	0.08	-	77,77,77,77	0
57	MG	13	1744	1/1	0.94	0.16	-	94,94,94,94	0
57	MG	14	3444	1/1	0.87	0.12	-	87,87,87,87	0
57	MG	1H	3497	1/1	0.98	0.07	-	97,97,97,97	0
57	MG	14	3349	1/1	0.98	0.08	-	81,81,81,81	0
57	MG	14	3045	1/1	0.91	0.23	-	64,64,64,64	0
57	MG	1H	3329	1/1	0.98	0.13	-	55,55,55,55	0
57	MG	1H	3003	1/1	0.96	0.19	-	57,57,57,57	0
57	MG	13	1621	1/1	0.93	0.24	-	67,67,67,67	0
57	MG	14	3091	1/1	0.95	0.23	-	85,85,85,85	0
57	MG	14	3011	1/1	0.96	0.47	-	72,72,72,72	0
57	MG	14	3023	1/1	0.99	0.30	-	54,54,54,54	0
57	MG	14	3183	1/1	0.90	0.58	-	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1688	1/1	0.84	0.06	-	100,100,100,100	0
57	MG	14	3262	1/1	0.95	0.14	-	72,72,72,72	0
57	MG	1H	3199	1/1	0.79	0.38	-	75,75,75,75	0
57	MG	14	3181	1/1	0.92	0.20	-	63,63,63,63	0
57	MG	1G	1635	1/1	0.90	0.45	-	97,97,97,97	0
57	MG	14	3437	1/1	0.98	0.03	-	93,93,93,93	0
57	MG	1H	3141	1/1	0.95	0.21	-	67,67,67,67	0
57	MG	1H	3220	1/1	0.76	0.40	-	73,73,73,73	0
57	MG	1H	3218	1/1	0.93	0.74	-	70,70,70,70	0
57	MG	1H	3200	1/1	0.82	0.35	-	73,73,73,73	0
57	MG	1H	3013	1/1	0.96	0.34	-	60,60,60,60	0
57	MG	14	3252	1/1	0.99	0.19	-	67,67,67,67	0
57	MG	1H	3176	1/1	0.89	0.33	-	67,67,67,67	0
57	MG	14	3443	1/1	0.78	0.07	-	108,108,108,108	0
57	MG	1H	3006	1/1	0.89	0.14	-	86,86,86,86	0
57	MG	2K	102	1/1	0.94	0.06	-	92,92,92,92	0
57	MG	1H	3439	1/1	0.88	0.14	-	81,81,81,81	0
57	MG	1H	3411	1/1	0.86	0.07	-	81,81,81,81	0
57	MG	1H	3084	1/1	0.89	0.14	-	82,82,82,82	0
57	MG	1H	3355	1/1	0.99	0.10	-	68,68,68,68	0
57	MG	1H	3244	1/1	0.77	0.41	-	84,84,84,84	0
57	MG	13	1723	1/1	0.97	0.06	-	84,84,84,84	0
57	MG	14	3292	1/1	0.98	0.13	-	61,61,61,61	0
57	MG	1G	1655	1/1	0.85	0.07	-	120,120,120,120	0
57	MG	1H	3456	1/1	0.98	0.05	-	72,72,72,72	0
57	MG	1H	3498	1/1	0.90	0.12	-	85,85,85,85	0
57	MG	14	3127	1/1	0.99	0.34	-	48,48,48,48	0
57	MG	1H	3016	1/1	0.99	0.40	-	49,49,49,49	0
57	MG	13	1628	1/1	0.69	0.36	-	96,96,96,96	0
57	MG	1H	3258	1/1	0.92	0.21	-	79,79,79,79	0
57	MG	1H	3165	1/1	0.94	0.32	-	72,72,72,72	0
57	MG	16	211	1/1	0.85	0.08	-	84,84,84,84	0
57	MG	1G	1638	1/1	0.85	0.58	-	88,88,88,88	0
57	MG	1H	3076	1/1	0.93	0.25	-	76,76,76,76	0
57	MG	1H	3095	1/1	0.95	0.36	-	65,65,65,65	0
57	MG	14	3407	1/1	0.92	0.10	-	74,74,74,74	0
57	MG	14	3173	1/1	0.85	0.28	-	69,69,69,69	0
57	MG	14	3184	1/1	0.93	0.34	-	60,60,60,60	0
57	MG	1H	3253	1/1	0.97	0.69	-	76,76,76,76	0
57	MG	14	3397	1/1	0.98	0.14	-	64,64,64,64	0
57	MG	1H	3413	1/1	0.97	0.08	-	78,78,78,78	0
57	MG	1H	3027	1/1	0.99	0.40	-	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1700	1/1	0.98	0.07	-	93,93,93,93	0
57	MG	1H	3152	1/1	0.98	0.19	-	87,87,87,87	0
57	MG	2L	103	1/1	0.68	0.57	-	80,80,80,80	0
57	MG	14	3005	1/1	0.78	0.37	-	70,70,70,70	0
57	MG	14	3370	1/1	0.93	0.08	-	81,81,81,81	0
57	MG	1H	3322	1/1	0.96	0.04	-	82,82,82,82	0
57	MG	14	3269	1/1	0.89	0.30	-	102,102,102,102	0
57	MG	1H	3279	1/1	0.85	0.99	-	71,71,71,71	0
57	MG	1H	3127	1/1	0.96	0.34	-	56,56,56,56	0
57	MG	1G	1664	1/1	0.98	0.05	-	91,91,91,91	0
57	MG	14	3251	1/1	0.95	0.23	-	82,82,82,82	0
57	MG	14	3227	1/1	0.89	0.34	-	83,83,83,83	0
57	MG	1H	3278	1/1	0.74	0.21	-	82,82,82,82	0
57	MG	13	1685	1/1	0.96	0.12	-	101,101,101,101	0
57	MG	13	1618	1/1	0.82	0.33	-	64,64,64,64	0
57	MG	14	3077	1/1	0.97	0.41	-	80,80,80,80	0
57	MG	14	3151	1/1	0.93	0.23	-	72,72,72,72	0
57	MG	14	3329	1/1	0.97	0.06	-	90,90,90,90	0
57	MG	14	3194	1/1	0.90	0.21	-	68,68,68,68	0
57	MG	14	3237	1/1	0.67	0.50	-	72,72,72,72	0
57	MG	1H	3189	1/1	0.91	0.31	-	87,87,87,87	0
57	MG	21	302	1/1	0.94	0.32	-	50,50,50,50	0
57	MG	14	3233	1/1	0.90	0.26	-	79,79,79,79	0
57	MG	14	3419	1/1	0.98	0.05	-	70,70,70,70	0
57	MG	14	3001	1/1	0.90	0.05	-	103,103,103,103	0
57	MG	1G	1668	1/1	0.92	0.07	-	111,111,111,111	0
57	MG	14	3239	1/1	0.91	0.36	-	87,87,87,87	0
57	MG	16	206	1/1	0.69	0.41	-	81,81,81,81	0
57	MG	14	3152	1/1	0.86	0.32	-	67,67,67,67	0
57	MG	1H	3007	1/1	0.87	0.29	-	68,68,68,68	0
57	MG	1H	3331	1/1	0.99	0.07	-	66,66,66,66	0
57	MG	14	3354	1/1	0.96	0.15	-	78,78,78,78	0
57	MG	14	3244	1/1	0.84	0.68	-	77,77,77,77	0
57	MG	14	3044	1/1	0.85	0.81	-	76,76,76,76	0
57	MG	14	3438	1/1	0.95	0.07	-	93,93,93,93	0
57	MG	1G	1634	1/1	0.94	0.19	-	93,93,93,93	0
57	MG	14	3346	1/1	0.98	0.11	-	75,75,75,75	0
57	MG	1H	3193	1/1	0.88	0.61	-	84,84,84,84	0
57	MG	14	3060	1/1	0.98	0.30	-	74,74,74,74	0
57	MG	1H	3443	1/1	0.99	0.08	-	67,67,67,67	0
57	MG	14	3366	1/1	0.86	0.12	-	76,76,76,76	0
57	MG	13	1612	1/1	0.90	0.26	-	85,85,85,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3205	1/1	0.73	0.17	-	77,77,77,77	0
57	MG	13	1661	1/1	0.62	0.11	-	102,102,102,102	0
57	MG	13	1658	1/1	0.90	0.12	-	88,88,88,88	0
57	MG	1H	3194	1/1	0.85	0.45	-	66,66,66,66	0
57	MG	1H	3379	1/1	0.96	0.11	-	86,86,86,86	0
57	MG	14	3210	1/1	0.93	0.33	-	80,80,80,80	0
57	MG	1H	3318	1/1	0.99	0.15	-	54,54,54,54	0
57	MG	1G	1612	1/1	0.95	0.34	-	67,67,67,67	0
57	MG	1H	3444	1/1	0.96	0.07	-	77,77,77,77	0
57	MG	13	1663	1/1	0.83	0.35	-	71,71,71,71	0
57	MG	14	3386	1/1	0.98	0.07	-	56,56,56,56	0
57	MG	1H	3246	1/1	0.83	0.38	-	85,85,85,85	0
57	MG	13	1727	1/1	0.97	0.07	-	110,110,110,110	0
57	MG	1H	3487	1/1	0.86	0.08	-	91,91,91,91	0
57	MG	1G	1626	1/1	0.78	0.29	-	73,73,73,73	0
57	MG	1H	3238	1/1	0.85	0.34	-	78,78,78,78	0
57	MG	14	3096	1/1	0.88	0.34	-	65,65,65,65	0
57	MG	13	1682	1/1	0.84	0.68	-	90,90,90,90	0
57	MG	31	301	1/1	0.96	0.06	-	61,61,61,61	0
57	MG	14	3394	1/1	0.97	0.06	-	78,78,78,78	0
57	MG	14	3388	1/1	0.96	0.07	-	82,82,82,82	0
57	MG	14	3412	1/1	0.95	0.04	-	120,120,120,120	0
57	MG	1H	3168	1/1	0.93	0.27	-	80,80,80,80	0
57	MG	1H	3196	1/1	0.90	0.55	-	88,88,88,88	0
57	MG	1H	3302	1/1	0.99	0.07	-	47,47,47,47	0
57	MG	14	3201	1/1	0.97	0.47	-	58,58,58,58	0
57	MG	1H	3145	1/1	0.97	0.24	-	46,46,46,46	0
57	MG	1H	3474	1/1	0.96	0.09	-	89,89,89,89	0
57	MG	1H	3068	1/1	0.94	0.61	-	69,69,69,69	0
57	MG	1H	3406	1/1	0.96	0.05	-	87,87,87,87	0
57	MG	1H	3382	1/1	0.97	0.04	-	70,70,70,70	0
57	MG	1H	3142	1/1	0.94	0.52	-	85,85,85,85	0
57	MG	1H	3294	1/1	0.99	0.13	-	56,56,56,56	0
57	MG	1H	3447	1/1	0.96	0.12	-	97,97,97,97	0
57	MG	1H	3058	1/1	0.94	0.28	-	53,53,53,53	0
57	MG	14	3053	1/1	0.87	0.30	-	77,77,77,77	0
57	MG	14	3207	1/1	0.91	0.10	-	71,71,71,71	0
57	MG	14	3121	1/1	0.87	0.31	-	77,77,77,77	0
57	MG	1H	3383	1/1	0.99	0.05	-	78,78,78,78	0
57	MG	14	3016	1/1	0.67	0.56	-	73,73,73,73	0
57	MG	1G	1677	1/1	0.95	0.06	-	105,105,105,105	0
57	MG	13	1686	1/1	0.92	0.21	-	96,96,96,96	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3199	1/1	0.84	0.38	-	84,84,84,84	0
57	MG	13	1609	1/1	0.95	0.25	-	58,58,58,58	0
57	MG	13	1721	1/1	0.95	0.07	-	70,70,70,70	0
57	MG	16	208	1/1	0.99	0.05	-	67,67,67,67	0
57	MG	1H	3020	1/1	0.74	0.19	-	107,107,107,107	0
57	MG	1G	1663	1/1	0.95	0.07	-	87,87,87,87	0
57	MG	1G	1649	1/1	0.94	0.12	-	115,115,115,115	0
57	MG	14	3429	1/1	0.92	0.05	-	98,98,98,98	0
57	MG	14	3448	1/1	0.90	0.06	-	92,92,92,92	0
57	MG	14	3220	1/1	0.93	0.53	-	88,88,88,88	0
57	MG	1H	3022	1/1	0.90	0.18	-	81,81,81,81	0
57	MG	1G	1606	1/1	0.94	0.27	-	67,67,67,67	0
57	MG	14	3242	1/1	0.86	0.11	-	95,95,95,95	0
57	MG	14	3241	1/1	0.78	0.33	-	84,84,84,84	0
57	MG	1H	3254	1/1	0.90	0.62	-	82,82,82,82	0
57	MG	1H	3421	1/1	0.96	0.05	-	78,78,78,78	0
57	MG	14	3162	1/1	0.65	0.30	-	67,67,67,67	0
57	MG	14	3345	1/1	0.98	0.08	-	68,68,68,68	0
57	MG	14	3086	1/1	0.91	0.22	-	61,61,61,61	0
57	MG	14	3434	1/1	0.93	0.06	-	82,82,82,82	0
57	MG	1H	3265	1/1	0.91	0.12	-	89,89,89,89	0
57	MG	14	3206	1/1	0.64	0.55	-	95,95,95,95	0
57	MG	14	3157	1/1	0.68	0.32	-	99,99,99,99	0
57	MG	14	3218	1/1	0.97	0.28	-	54,54,54,54	0
57	MG	14	3246	1/1	0.98	0.23	-	76,76,76,76	0
57	MG	1G	1681	1/1	0.99	0.04	-	85,85,85,85	0
57	MG	11	303	1/1	0.75	0.51	-	65,65,65,65	0
57	MG	14	3234	1/1	0.91	0.16	-	64,64,64,64	0
57	MG	13	1730	1/1	0.96	0.15	-	82,82,82,82	0
57	MG	1H	3291	1/1	0.83	0.46	-	88,88,88,88	0
57	MG	1H	3284	1/1	0.74	0.62	-	75,75,75,75	0
57	MG	1H	3263	1/1	0.88	1.00	-	93,93,93,93	0
57	MG	14	3134	1/1	0.94	0.26	-	98,98,98,98	0
57	MG	1H	3326	1/1	0.94	0.07	-	49,49,49,49	0
57	MG	14	3258	1/1	0.82	0.76	-	83,83,83,83	0
57	MG	14	3114	1/1	0.95	0.39	-	63,63,63,63	0
57	MG	14	3113	1/1	0.86	0.41	-	73,73,73,73	0
57	MG	1H	3114	1/1	0.89	0.41	-	78,78,78,78	0
57	MG	1H	3111	1/1	0.94	0.31	-	80,80,80,80	0
57	MG	13	1746	1/1	0.98	0.08	-	83,83,83,83	0
57	MG	14	3225	1/1	0.89	0.36	-	80,80,80,80	0
57	MG	1G	1656	1/1	0.99	0.19	-	105,105,105,105	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3340	1/1	0.97	0.11	-	73,73,73,73	0
57	MG	14	3051	1/1	0.98	0.39	-	62,62,62,62	0
57	MG	1H	3212	1/1	0.86	0.35	-	77,77,77,77	0
57	MG	1H	3062	1/1	0.94	0.43	-	66,66,66,66	0
57	MG	14	3319	1/1	0.94	0.11	-	91,91,91,91	0
57	MG	13	1733	1/1	0.94	0.06	-	73,73,73,73	0
57	MG	1H	3489	1/1	0.88	0.08	-	125,125,125,125	0
57	MG	14	3230	1/1	0.93	0.23	-	70,70,70,70	0
57	MG	1H	3422	1/1	0.96	0.07	-	79,79,79,79	0
57	MG	13	1729	1/1	0.95	0.05	-	91,91,91,91	0
57	MG	1H	3117	1/1	0.98	0.51	-	72,72,72,72	0
57	MG	14	3185	1/1	0.84	0.28	-	89,89,89,89	0
57	MG	1H	3085	1/1	0.98	0.29	-	71,71,71,71	0
57	MG	1H	3234	1/1	0.96	0.19	-	72,72,72,72	0
57	MG	1G	1690	1/1	0.94	0.07	-	118,118,118,118	0
57	MG	14	3006	1/1	0.97	0.24	-	66,66,66,66	0
57	MG	16	202	1/1	0.93	0.28	-	73,73,73,73	0
57	MG	13	1694	1/1	0.99	0.17	-	79,79,79,79	0
57	MG	13	1708	1/1	0.94	0.07	-	76,76,76,76	0
57	MG	14	3374	1/1	0.74	0.07	-	96,96,96,96	0
57	MG	1H	3208	1/1	0.81	0.23	-	76,76,76,76	0
57	MG	14	3084	1/1	0.98	0.34	-	56,56,56,56	0
57	MG	14	3453	1/1	0.99	0.04	-	88,88,88,88	0
57	MG	1H	3248	1/1	0.93	0.14	-	79,79,79,79	0
57	MG	1H	3446	1/1	0.98	0.04	-	93,93,93,93	0
57	MG	1H	3412	1/1	0.98	0.13	-	66,66,66,66	0
57	MG	1H	3169	1/1	0.98	0.20	-	85,85,85,85	0
57	MG	1H	3177	1/1	0.83	0.25	-	81,81,81,81	0
57	MG	1H	3491	1/1	0.99	0.13	-	75,75,75,75	0
57	MG	1H	3012	1/1	0.96	0.41	-	42,42,42,42	0
57	MG	13	1720	1/1	0.96	0.07	-	86,86,86,86	0
57	MG	14	3149	1/1	0.90	0.29	-	96,96,96,96	0
57	MG	1H	3407	1/1	0.98	0.06	-	50,50,50,50	0
57	MG	1J	204	1/1	0.98	0.06	-	82,82,82,82	0
57	MG	13	1617	1/1	0.94	0.23	-	53,53,53,53	0
57	MG	1G	1637	1/1	0.89	0.20	-	77,77,77,77	0
57	MG	1H	3459	1/1	0.91	0.10	-	91,91,91,91	0
57	MG	1H	3040	1/1	0.96	0.15	-	60,60,60,60	0
57	MG	1G	1675	1/1	0.95	0.07	-	88,88,88,88	0
57	MG	14	3087	1/1	0.97	0.09	-	97,97,97,97	0
57	MG	1H	3472	1/1	0.94	0.07	-	93,93,93,93	0
57	MG	14	3140	1/1	0.98	0.31	-	81,81,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3181	1/1	0.92	0.53	-	77,77,77,77	0
57	MG	14	3315	1/1	0.92	0.05	-	81,81,81,81	0
57	MG	14	3213	1/1	0.83	0.45	-	87,87,87,87	0
57	MG	1H	3251	1/1	0.95	0.22	-	78,78,78,78	0
57	MG	14	3076	1/1	0.94	0.20	-	77,77,77,77	0
57	MG	14	3124	1/1	0.91	0.27	-	64,64,64,64	0
57	MG	1H	3361	1/1	0.99	0.08	-	53,53,53,53	0
57	MG	1H	3136	1/1	0.79	0.84	-	73,73,73,73	0
57	MG	1H	3182	1/1	0.92	0.44	-	72,72,72,72	0
57	MG	1H	3288	1/1	0.93	0.38	-	80,80,80,80	0
57	MG	1H	3241	1/1	0.83	0.55	-	71,71,71,71	0
57	MG	13	1715	1/1	0.98	0.09	-	110,110,110,110	0
57	MG	13	1745	1/1	0.97	0.05	-	117,117,117,117	0
57	MG	14	3211	1/1	0.85	0.38	-	78,78,78,78	0
57	MG	1H	3103	1/1	0.79	0.43	-	82,82,82,82	0
57	MG	1H	3211	1/1	0.90	0.34	-	80,80,80,80	0
57	MG	1H	3496	1/1	0.67	0.06	-	94,94,94,94	0
57	MG	14	3198	1/1	0.88	0.21	-	81,81,81,81	0
57	MG	14	3093	1/1	0.97	0.39	-	51,51,51,51	0
57	MG	14	3029	1/1	0.98	0.26	-	59,59,59,59	0
57	MG	1H	3130	1/1	0.93	0.23	-	67,67,67,67	0
57	MG	13	1689	1/1	0.59	0.40	-	99,99,99,99	0
57	MG	29	302	1/1	0.99	0.29	-	40,40,40,40	0
57	MG	13	1740	1/1	0.97	0.04	-	92,92,92,92	0
57	MG	1H	3449	1/1	0.98	0.12	-	69,69,69,69	0
57	MG	1H	3186	1/1	0.88	0.24	-	57,57,57,57	0
57	MG	13	1664	1/1	0.91	0.30	-	81,81,81,81	0
57	MG	1H	3051	1/1	0.99	0.16	-	93,93,93,93	0
57	MG	14	3399	1/1	0.97	0.09	-	78,78,78,78	0
57	MG	14	3008	1/1	0.97	0.11	-	72,72,72,72	0
57	MG	78	201	1/1	0.89	0.24	-	75,75,75,75	0
57	MG	1H	3060	1/1	0.99	0.37	-	55,55,55,55	0
57	MG	1H	3202	1/1	0.94	0.39	-	58,58,58,58	0
57	MG	1J	205	1/1	0.95	0.05	-	95,95,95,95	0
57	MG	2L	102	1/1	0.93	0.36	-	96,96,96,96	0
57	MG	14	3094	1/1	0.96	0.28	-	85,85,85,85	0
57	MG	13	1743	1/1	0.95	0.05	-	87,87,87,87	0
57	MG	1H	3163	1/1	0.93	0.28	-	59,59,59,59	0
57	MG	1H	3225	1/1	0.95	0.40	-	67,67,67,67	0
57	MG	1H	3147	1/1	0.96	0.15	-	51,51,51,51	0
57	MG	1H	3432	1/1	0.97	0.09	-	75,75,75,75	0
57	MG	1G	1666	1/1	0.90	0.05	-	106,106,106,106	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3070	1/1	0.97	0.38	-	52,52,52,52	0
57	MG	1H	3372	1/1	0.94	0.07	-	89,89,89,89	0
57	MG	13	1666	1/1	0.88	0.42	-	77,77,77,77	0
57	MG	14	3203	1/1	0.96	0.18	-	89,89,89,89	0
57	MG	1H	3143	1/1	0.90	0.45	-	89,89,89,89	0
57	MG	14	3432	1/1	0.99	0.10	-	83,83,83,83	0
57	MG	1H	3440	1/1	0.96	0.04	-	87,87,87,87	0
57	MG	1H	3275	1/1	0.84	0.21	-	95,95,95,95	0
57	MG	1H	3094	1/1	0.97	0.12	-	52,52,52,52	0
57	MG	1H	3393	1/1	0.94	0.10	-	56,56,56,56	0
57	MG	1H	3453	1/1	0.97	0.04	-	83,83,83,83	0
57	MG	1H	3482	1/1	0.91	0.06	-	72,72,72,72	0
57	MG	1G	1610	1/1	0.91	0.13	-	114,114,114,114	0
57	MG	14	3300	1/1	0.98	0.14	-	57,57,57,57	0
57	MG	13	1699	1/1	0.95	0.06	-	73,73,73,73	0
57	MG	13	1622	1/1	0.88	0.21	-	81,81,81,81	0
57	MG	1H	3019	1/1	0.74	0.27	-	78,78,78,78	0
57	MG	1H	3093	1/1	0.83	0.63	-	71,71,71,71	0
57	MG	1H	3352	1/1	0.98	0.15	-	72,72,72,72	0
57	MG	13	1725	1/1	0.98	0.06	-	71,71,71,71	0
57	MG	14	3299	1/1	0.99	0.06	-	60,60,60,60	0
57	MG	14	3022	1/1	0.97	0.41	-	60,60,60,60	0
57	MG	13	1660	1/1	0.88	0.55	-	83,83,83,83	0
57	MG	14	3418	1/1	0.99	0.05	-	75,75,75,75	0
57	MG	1G	1623	1/1	0.82	0.31	-	77,77,77,77	0
57	MG	14	3062	1/1	0.97	0.25	-	85,85,85,85	0
57	MG	14	3398	1/1	0.97	0.13	-	83,83,83,83	0
57	MG	14	3257	1/1	0.75	0.58	-	87,87,87,87	0
57	MG	1H	3021	1/1	0.89	0.16	-	90,90,90,90	0
57	MG	14	3104	1/1	0.93	0.36	-	81,81,81,81	0
57	MG	14	3122	1/1	0.97	0.07	-	104,104,104,104	0
57	MG	14	3267	1/1	0.66	0.15	-	83,83,83,83	0
57	MG	1H	3122	1/1	0.88	0.52	-	73,73,73,73	0
57	MG	14	3048	1/1	0.94	0.75	-	75,75,75,75	0
57	MG	1G	1694	1/1	0.95	0.48	-	98,98,98,98	0
57	MG	1H	3485	1/1	0.96	0.05	-	76,76,76,76	0
57	MG	1H	3184	1/1	0.96	0.41	-	67,67,67,67	0
57	MG	14	3190	1/1	0.75	0.87	-	82,82,82,82	0
57	MG	1H	3436	1/1	0.94	0.10	-	65,65,65,65	0
57	MG	14	3389	1/1	0.98	0.07	-	81,81,81,81	0
57	MG	1H	3195	1/1	0.86	0.28	-	73,73,73,73	0
57	MG	1H	3347	1/1	0.97	0.10	-	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3290	1/1	0.98	0.09	-	64,64,64,64	0
57	MG	1G	1631	1/1	0.82	0.29	-	107,107,107,107	0
57	MG	1G	1620	1/1	0.64	0.76	-	79,79,79,79	0
57	MG	14	3439	1/1	0.93	0.05	-	96,96,96,96	0
57	MG	1H	3140	1/1	0.93	0.22	-	62,62,62,62	0
57	MG	14	3331	1/1	0.99	0.09	-	66,66,66,66	0
57	MG	1H	3351	1/1	0.99	0.08	-	69,69,69,69	0
57	MG	1H	3257	1/1	0.98	0.25	-	84,84,84,84	0
57	MG	14	3177	1/1	0.95	0.35	-	79,79,79,79	0
57	MG	16	207	1/1	0.77	0.26	-	77,77,77,77	0
57	MG	1H	3217	1/1	0.97	0.16	-	59,59,59,59	0
57	MG	1H	3384	1/1	0.98	0.11	-	73,73,73,73	0
57	MG	1H	3118	1/1	0.97	0.12	-	60,60,60,60	0
57	MG	1H	3264	1/1	0.96	0.18	-	74,74,74,74	0
57	MG	14	3188	1/1	0.86	0.40	-	66,66,66,66	0
57	MG	1H	3138	1/1	0.86	0.41	-	55,55,55,55	0
57	MG	1H	3160	1/1	0.98	0.46	-	67,67,67,67	0
57	MG	13	1614	1/1	0.97	0.59	-	64,64,64,64	0
57	MG	1G	1601	1/1	0.94	0.46	-	86,86,86,86	0
57	MG	1H	3357	1/1	0.97	0.09	-	68,68,68,68	0
57	MG	1H	3493	1/1	0.72	0.19	-	94,94,94,94	0
57	MG	1G	1628	1/1	0.87	0.24	-	124,124,124,124	0
57	MG	14	3270	1/1	0.93	0.28	-	83,83,83,83	0
57	MG	1H	3228	1/1	0.91	0.49	-	69,69,69,69	0
57	MG	1H	3197	1/1	0.95	0.34	-	67,67,67,67	0
57	MG	1H	3011	1/1	0.87	0.67	-	72,72,72,72	0
57	MG	1H	3469	1/1	0.97	0.04	-	100,100,100,100	0
57	MG	14	3112	1/1	0.93	0.37	-	88,88,88,88	0
57	MG	1H	3119	1/1	0.86	0.19	-	71,71,71,71	0
57	MG	1G	1676	1/1	0.98	0.04	-	86,86,86,86	0
57	MG	14	3228	1/1	0.92	0.15	-	81,81,81,81	0
57	MG	14	3355	1/1	0.99	0.12	-	59,59,59,59	0
57	MG	13	1704	1/1	0.92	0.13	-	105,105,105,105	0
57	MG	13	1688	1/1	0.94	0.25	-	90,90,90,90	0
57	MG	1H	3398	1/1	0.98	0.12	-	50,50,50,50	0
57	MG	1G	1603	1/1	0.98	0.20	-	81,81,81,81	0
57	MG	14	3200	1/1	0.91	0.21	-	69,69,69,69	0
57	MG	39	302	1/1	0.90	0.10	-	63,63,63,63	0
57	MG	14	3209	1/1	0.95	0.79	-	64,64,64,64	0
57	MG	1H	3112	1/1	0.91	0.39	-	66,66,66,66	0
57	MG	1J	206	1/1	0.95	0.05	-	94,94,94,94	0
57	MG	1H	3233	1/1	0.77	0.34	-	70,70,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3298	1/1	0.99	0.03	-	79,79,79,79	0
57	MG	1H	3464	1/1	0.97	0.08	-	62,62,62,62	0
57	MG	13	1625	1/1	0.73	0.27	-	96,96,96,96	0
57	MG	14	3414	1/1	0.97	0.06	-	85,85,85,85	0
57	MG	14	3039	1/1	0.95	0.19	-	73,73,73,73	0
57	MG	1H	3033	1/1	0.95	0.26	-	62,62,62,62	0
57	MG	1H	3343	1/1	0.99	0.07	-	74,74,74,74	0
57	MG	14	3147	1/1	0.88	0.29	-	72,72,72,72	0
57	MG	14	3285	1/1	0.98	0.05	-	59,59,59,59	0
57	MG	1H	3455	1/1	0.85	0.06	-	103,103,103,103	0
57	MG	1H	3424	1/1	0.98	0.05	-	68,68,68,68	0
57	MG	1H	3325	1/1	0.93	0.11	-	69,69,69,69	0
57	MG	13	1652	1/1	0.91	0.48	-	89,89,89,89	0
57	MG	14	3436	1/1	0.91	0.07	-	108,108,108,108	0
57	MG	14	3435	1/1	0.84	0.08	-	103,103,103,103	0
57	MG	1H	3484	1/1	0.90	0.07	-	90,90,90,90	0
57	MG	1H	3216	1/1	0.97	0.21	-	57,57,57,57	0
57	MG	13	1636	1/1	0.88	0.21	-	75,75,75,75	0
57	MG	1H	3188	1/1	0.83	0.38	-	74,74,74,74	0
57	MG	1H	3063	1/1	0.98	0.27	-	52,52,52,52	0
57	MG	14	3193	1/1	0.91	0.15	-	70,70,70,70	0
57	MG	14	3059	1/1	0.99	0.41	-	69,69,69,69	0
57	MG	1H	3069	1/1	0.75	0.46	-	65,65,65,65	0
57	MG	14	3072	1/1	0.97	0.25	-	69,69,69,69	0
57	MG	1H	3365	1/1	0.99	0.09	-	70,70,70,70	0
57	MG	1H	3438	1/1	0.93	0.05	-	75,75,75,75	0
57	MG	1H	3129	1/1	0.69	0.31	-	76,76,76,76	0
57	MG	14	3403	1/1	0.95	0.08	-	76,76,76,76	0
57	MG	1H	3478	1/1	0.94	0.06	-	85,85,85,85	0
57	MG	1H	3314	1/1	0.98	0.13	-	75,75,75,75	0
57	MG	14	3380	1/1	0.89	0.12	-	93,93,93,93	0
57	MG	1G	1687	1/1	0.94	0.06	-	95,95,95,95	0
57	MG	1H	3334	1/1	0.92	0.10	-	82,82,82,82	0
57	MG	1H	3350	1/1	0.97	0.12	-	69,69,69,69	0
57	MG	13	1667	1/1	0.68	0.43	-	97,97,97,97	0
57	MG	1H	3495	1/1	0.88	0.07	-	98,98,98,98	0
57	MG	1H	3131	1/1	0.86	0.52	-	67,67,67,67	0
57	MG	1H	3430	1/1	0.97	0.06	-	85,85,85,85	0
57	MG	14	3249	1/1	0.99	0.28	-	60,60,60,60	0
57	MG	14	3405	1/1	0.94	0.04	-	83,83,83,83	0
57	MG	1H	3231	1/1	0.90	0.42	-	65,65,65,65	0
57	MG	14	3043	1/1	0.94	0.27	-	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1618	1/1	0.81	0.19	-	86,86,86,86	0
57	MG	1H	3126	1/1	0.91	0.45	-	70,70,70,70	0
57	MG	14	3095	1/1	0.94	0.21	-	85,85,85,85	0
57	MG	13	1719	1/1	0.94	0.15	-	72,72,72,72	0
57	MG	14	3176	1/1	0.90	0.08	-	88,88,88,88	0
57	MG	1H	3207	1/1	0.70	0.15	-	56,56,56,56	0
57	MG	1G	1692	1/1	0.81	0.36	-	105,105,105,105	0
57	MG	14	3146	1/1	0.88	0.44	-	76,76,76,76	0
57	MG	14	3332	1/1	0.98	0.07	-	63,63,63,63	0
57	MG	1H	3137	1/1	0.96	0.09	-	72,72,72,72	0
57	MG	13	1747	1/1	0.97	0.13	-	72,72,72,72	0
57	MG	1H	3065	1/1	0.93	0.17	-	56,56,56,56	0
57	MG	13	1647	1/1	0.97	0.22	-	104,104,104,104	0
57	MG	14	3118	1/1	0.95	0.30	-	66,66,66,66	0
57	MG	14	3446	1/1	0.94	0.04	-	109,109,109,109	0
57	MG	1H	3483	1/1	0.94	0.05	-	106,106,106,106	0
57	MG	1H	3039	1/1	0.99	0.12	-	90,90,90,90	0
57	MG	14	3360	1/1	0.98	0.06	-	83,83,83,83	0
57	MG	1H	3171	1/1	0.89	0.43	-	68,68,68,68	0
57	MG	1H	3209	1/1	0.85	0.23	-	78,78,78,78	0
57	MG	14	3377	1/1	0.97	0.16	-	67,67,67,67	0
57	MG	1H	3044	1/1	0.96	0.28	-	62,62,62,62	0
57	MG	14	3015	1/1	0.92	0.27	-	77,77,77,77	0
57	MG	14	3280	1/1	0.93	0.12	-	54,54,54,54	0
57	MG	1H	3354	1/1	0.97	0.10	-	62,62,62,62	0
57	MG	14	3135	1/1	0.84	0.37	-	71,71,71,71	0
57	MG	14	3165	1/1	0.89	0.11	-	78,78,78,78	0
57	MG	1H	3159	1/1	0.90	0.37	-	56,56,56,56	0
57	MG	14	3363	1/1	0.97	0.11	-	68,68,68,68	0
57	MG	14	3425	1/1	0.91	0.06	-	122,122,122,122	0
57	MG	14	3352	1/1	0.98	0.06	-	65,65,65,65	0
57	MG	1H	3271	1/1	0.88	0.20	-	74,74,74,74	0
57	MG	14	3423	1/1	0.79	0.06	-	144,144,144,144	0
57	MG	14	3040	1/1	0.98	0.33	-	64,64,64,64	0
57	MG	13	1735	1/1	0.89	0.07	-	118,118,118,118	0
57	MG	14	3411	1/1	0.96	0.05	-	74,74,74,74	0
57	MG	14	3142	1/1	0.91	0.31	-	82,82,82,82	0
57	MG	1H	3380	1/1	0.93	0.14	-	55,55,55,55	0
57	MG	16	210	1/1	0.95	0.09	-	88,88,88,88	0
57	MG	1H	3428	1/1	0.86	0.08	-	87,87,87,87	0
57	MG	16	209	1/1	0.96	0.10	-	73,73,73,73	0
57	MG	1J	202	1/1	0.96	0.22	-	94,94,94,94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3377	1/1	0.96	0.11	-	76,76,76,76	0
57	MG	14	3379	1/1	0.98	0.10	-	94,94,94,94	0
57	MG	14	3089	1/1	0.91	0.22	-	56,56,56,56	0
57	MG	13	1674	1/1	0.88	0.36	-	78,78,78,78	0
57	MG	1G	1616	1/1	0.82	0.23	-	86,86,86,86	0
57	MG	14	3248	1/1	0.70	0.35	-	75,75,75,75	0
57	MG	14	3328	1/1	0.95	0.07	-	93,93,93,93	0
57	MG	14	3428	1/1	0.91	0.09	-	104,104,104,104	0
57	MG	14	3155	1/1	0.68	0.26	-	66,66,66,66	0
57	MG	1H	3320	1/1	0.98	0.05	-	67,67,67,67	0
57	MG	1G	1653	1/1	0.92	0.08	-	110,110,110,110	0
57	MG	13	1676	1/1	0.93	0.26	-	101,101,101,101	0
57	MG	14	3261	1/1	0.90	0.21	-	102,102,102,102	0
57	MG	13	1722	1/1	0.90	0.05	-	92,92,92,92	0
57	MG	1H	3476	1/1	0.90	0.07	-	93,93,93,93	0
57	MG	1H	3364	1/1	0.97	0.03	-	106,106,106,106	0
57	MG	14	3326	1/1	0.90	0.09	-	74,74,74,74	0
57	MG	14	3416	1/1	0.89	0.07	-	66,66,66,66	0
57	MG	14	3055	1/1	0.89	0.35	-	57,57,57,57	0
57	MG	14	3026	1/1	0.96	0.32	-	72,72,72,72	0
57	MG	14	3369	1/1	0.98	0.19	-	56,56,56,56	0
57	MG	14	3058	1/1	0.89	0.25	-	66,66,66,66	0
57	MG	1H	3161	1/1	0.96	0.29	-	72,72,72,72	0
57	MG	1G	1658	1/1	0.98	0.05	-	94,94,94,94	0
57	MG	14	3196	1/1	0.97	0.17	-	90,90,90,90	0
57	MG	1H	3356	1/1	0.98	0.10	-	58,58,58,58	0
57	MG	1H	3353	1/1	0.99	0.09	-	57,57,57,57	0
57	MG	14	3221	1/1	0.90	0.51	-	73,73,73,73	0
57	MG	1H	3433	1/1	0.95	0.10	-	86,86,86,86	0
57	MG	14	3250	1/1	0.97	0.18	-	65,65,65,65	0
57	MG	14	3057	1/1	0.90	0.36	-	41,41,41,41	0
57	MG	13	1696	1/1	0.96	0.03	-	86,86,86,86	0
57	MG	13	1613	1/1	0.96	0.28	-	65,65,65,65	0
57	MG	14	3383	1/1	0.92	0.07	-	101,101,101,101	0
57	MG	1G	1622	1/1	0.93	0.35	-	76,76,76,76	0
57	MG	1H	3475	1/1	0.97	0.13	-	88,88,88,88	0
57	MG	1H	3023	1/1	0.83	0.39	-	81,81,81,81	0
57	MG	1H	3283	1/1	0.91	0.47	-	82,82,82,82	0
57	MG	13	1649	1/1	0.85	0.37	-	78,78,78,78	0
57	MG	45	203	1/1	0.96	0.48	-	71,71,71,71	0
57	MG	1H	3047	1/1	0.88	0.28	-	61,61,61,61	0
57	MG	14	3130	1/1	0.96	0.32	-	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3463	1/1	0.95	0.07	-	82,82,82,82	0
57	MG	1H	3198	1/1	0.75	0.26	-	76,76,76,76	0
57	MG	14	3400	1/1	0.92	0.06	-	86,86,86,86	0
57	MG	13	1605	1/1	0.96	0.31	-	68,68,68,68	0
57	MG	1G	1643	1/1	0.90	0.39	-	67,67,67,67	0
57	MG	14	3296	1/1	0.92	0.09	-	59,59,59,59	0
57	MG	14	3420	1/1	0.99	0.12	-	65,65,65,65	0
57	MG	1H	3394	1/1	0.98	0.14	-	70,70,70,70	0
57	MG	1H	3092	1/1	0.85	0.34	-	57,57,57,57	0
57	MG	1H	3420	1/1	0.98	0.07	-	64,64,64,64	0
57	MG	1H	3425	1/1	0.96	0.07	-	83,83,83,83	0
57	MG	1H	3269	1/1	0.83	0.22	-	73,73,73,73	0
57	MG	14	3356	1/1	0.98	0.13	-	61,61,61,61	0
57	MG	1H	3303	1/1	0.97	0.11	-	63,63,63,63	0
57	MG	1H	3445	1/1	0.98	0.03	-	97,97,97,97	0
57	MG	14	3145	1/1	0.96	0.44	-	74,74,74,74	0
57	MG	1H	3261	1/1	0.98	0.22	-	67,67,67,67	0
57	MG	1H	3285	1/1	0.87	0.55	-	87,87,87,87	0
57	MG	1H	3427	1/1	0.95	0.04	-	88,88,88,88	0
57	MG	14	3009	1/1	0.90	0.20	-	68,68,68,68	0
57	MG	14	3348	1/1	0.96	0.05	-	88,88,88,88	0
57	MG	1H	3224	1/1	0.94	0.28	-	63,63,63,63	0
57	MG	1H	3017	1/1	0.94	0.18	-	55,55,55,55	0
57	MG	1H	3387	1/1	0.97	0.10	-	64,64,64,64	0
57	MG	1H	3175	1/1	0.96	0.31	-	65,65,65,65	0
57	MG	1H	3002	1/1	0.98	0.31	-	39,39,39,39	0
57	MG	1H	3252	1/1	0.94	0.32	-	80,80,80,80	0
57	MG	1G	1680	1/1	0.97	0.04	-	103,103,103,103	0
57	MG	1H	3370	1/1	0.98	0.11	-	70,70,70,70	0
57	MG	14	3202	1/1	0.72	0.23	-	90,90,90,90	0
57	MG	14	3215	1/1	0.89	0.30	-	64,64,64,64	0
57	MG	1G	1661	1/1	0.98	0.05	-	111,111,111,111	0
57	MG	1H	3113	1/1	0.96	0.36	-	82,82,82,82	0
57	MG	2L	104	1/1	0.94	0.41	-	72,72,72,72	0
57	MG	13	1691	1/1	0.96	0.12	-	79,79,79,79	0
57	MG	P8	101	1/1	0.80	0.44	-	66,66,66,66	0
57	MG	1H	3442	1/1	0.95	0.11	-	86,86,86,86	0
57	MG	13	1603	1/1	0.81	0.36	-	76,76,76,76	0
57	MG	1H	3388	1/1	0.99	0.14	-	57,57,57,57	0
57	MG	14	3417	1/1	0.99	0.07	-	87,87,87,87	0
57	MG	1H	3266	1/1	0.93	0.15	-	75,75,75,75	0
57	MG	14	3020	1/1	0.98	0.38	-	51,51,51,51	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1629	1/1	0.98	0.67	-	83,83,83,83	0
57	MG	1H	3400	1/1	0.95	0.21	-	67,67,67,67	0
57	MG	1H	3457	1/1	0.95	0.10	-	82,82,82,82	0
57	MG	14	3441	1/1	0.88	0.08	-	72,72,72,72	0
57	MG	1H	3071	1/1	0.98	0.43	-	54,54,54,54	0
57	MG	13	1716	1/1	0.98	0.08	-	66,66,66,66	0
57	MG	14	3312	1/1	0.95	0.06	-	77,77,77,77	0
57	MG	1H	3296	1/1	0.99	0.18	-	49,49,49,49	0
57	MG	1H	3450	1/1	0.94	0.04	-	87,87,87,87	0
57	MG	13	1742	1/1	0.94	0.08	-	100,100,100,100	0
57	MG	1H	3104	1/1	0.94	0.20	-	62,62,62,62	0
57	MG	1G	1673	1/1	0.98	0.09	-	84,84,84,84	0
57	MG	1H	3214	1/1	0.96	0.43	-	92,92,92,92	0
57	MG	14	3338	1/1	0.95	0.06	-	72,72,72,72	0
57	MG	1G	1671	1/1	0.94	0.06	-	117,117,117,117	0
57	MG	14	3365	1/1	0.95	0.09	-	88,88,88,88	0
57	MG	14	3067	1/1	0.93	0.34	-	68,68,68,68	0
57	MG	1H	3083	1/1	0.84	0.21	-	74,74,74,74	0
57	MG	1H	3210	1/1	0.65	0.32	-	74,74,74,74	0
57	MG	13	1637	1/1	0.91	0.26	-	86,86,86,86	0
57	MG	13	1670	1/1	0.85	0.33	-	78,78,78,78	0
57	MG	14	3431	1/1	0.95	0.06	-	90,90,90,90	0
57	MG	1H	3402	1/1	0.98	0.09	-	73,73,73,73	0
57	MG	14	3010	1/1	0.88	0.31	-	69,69,69,69	0
57	MG	2K	101	1/1	0.78	0.30	-	95,95,95,95	0
57	MG	1H	3133	1/1	0.85	0.42	-	80,80,80,80	0
57	MG	13	1711	1/1	0.96	0.05	-	99,99,99,99	0
57	MG	1H	3416	1/1	0.97	0.16	-	48,48,48,48	0
57	MG	14	3406	1/1	0.94	0.15	-	76,76,76,76	0
57	MG	13	1734	1/1	0.94	0.06	-	86,86,86,86	0
57	MG	14	3160	1/1	0.98	0.30	-	51,51,51,51	0
57	MG	1H	3437	1/1	0.97	0.04	-	57,57,57,57	0
57	MG	13	1615	1/1	0.97	0.24	-	91,91,91,91	0
57	MG	1H	3477	1/1	0.97	0.10	-	65,65,65,65	0
57	MG	14	3272	1/1	0.66	0.30	-	77,77,77,77	0
57	MG	1H	3185	1/1	0.93	0.36	-	90,90,90,90	0
57	MG	1G	1648	1/1	0.93	0.23	-	86,86,86,86	0
57	MG	1H	3190	1/1	0.73	0.47	-	74,74,74,74	0
57	MG	1H	3338	1/1	0.99	0.18	-	53,53,53,53	0
57	MG	14	3271	1/1	0.90	0.45	-	80,80,80,80	0
57	MG	14	3156	1/1	0.95	0.41	-	75,75,75,75	0
57	MG	1H	3203	1/1	0.93	0.28	-	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3072	1/1	0.95	0.69	-	73,73,73,73	0
57	MG	14	3171	1/1	0.73	0.22	-	73,73,73,73	0
57	MG	3I	201	1/1	0.97	0.16	-	57,57,57,57	0
57	MG	1H	3308	1/1	1.00	0.07	-	61,61,61,61	0
57	MG	14	3240	1/1	0.93	0.30	-	85,85,85,85	0
57	MG	1G	1646	1/1	0.86	0.67	-	84,84,84,84	0
57	MG	14	3161	1/1	0.97	0.30	-	73,73,73,73	0
57	MG	1H	3494	1/1	0.97	0.03	-	126,126,126,126	0
57	MG	1H	3245	1/1	0.93	0.57	-	69,69,69,69	0
57	MG	1H	3369	1/1	0.94	0.16	-	74,74,74,74	0
57	MG	14	3034	1/1	0.94	0.36	-	57,57,57,57	0
57	MG	14	3402	1/1	0.96	0.08	-	88,88,88,88	0
57	MG	14	3373	1/1	0.98	0.06	-	93,93,93,93	0
57	MG	13	1713	1/1	0.88	0.08	-	89,89,89,89	0
57	MG	1H	3099	1/1	0.93	0.13	-	60,60,60,60	0
57	MG	1H	3492	1/1	0.98	0.06	-	105,105,105,105	0
57	MG	13	1641	1/1	0.96	0.43	-	69,69,69,69	0
57	MG	14	3108	1/1	0.82	0.11	-	90,90,90,90	0
57	MG	1H	3170	1/1	0.92	0.72	-	72,72,72,72	0
57	MG	1H	3256	1/1	0.98	0.34	-	71,71,71,71	0
57	MG	14	3430	1/1	0.96	0.04	-	90,90,90,90	0
57	MG	14	3395	1/1	0.98	0.04	-	78,78,78,78	0
57	MG	1G	1608	1/1	0.95	0.23	-	91,91,91,91	0
57	MG	1H	3052	1/1	0.92	0.32	-	57,57,57,57	0
57	MG	14	3275	1/1	0.99	0.09	-	61,61,61,61	0
57	MG	1G	1679	1/1	0.92	0.05	-	91,91,91,91	0
57	MG	1H	3144	1/1	0.80	0.48	-	75,75,75,75	0
57	MG	1H	3110	1/1	0.91	0.15	-	84,84,84,84	0
57	MG	14	3224	1/1	0.69	0.38	-	80,80,80,80	0
57	MG	1G	1685	1/1	0.97	0.06	-	109,109,109,109	0
57	MG	14	3313	1/1	0.95	0.07	-	72,72,72,72	0
57	MG	14	3101	1/1	0.96	0.47	-	64,64,64,64	0
57	MG	1H	3026	1/1	0.98	0.44	-	40,40,40,40	0
57	MG	1H	3028	1/1	0.97	0.26	-	51,51,51,51	0
57	MG	1H	3087	1/1	0.85	0.16	-	68,68,68,68	0
57	MG	14	3325	1/1	0.94	0.05	-	78,78,78,78	0
57	MG	13	1662	1/1	0.91	0.21	-	119,119,119,119	0
57	MG	13	1629	1/1	0.96	0.29	-	98,98,98,98	0
57	MG	1H	3236	1/1	0.92	0.32	-	75,75,75,75	0
57	MG	13	1648	1/1	0.82	0.30	-	90,90,90,90	0
57	MG	14	3056	1/1	0.94	0.66	-	82,82,82,82	0
57	MG	14	3208	1/1	0.91	0.31	-	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3219	1/1	0.98	0.14	-	62,62,62,62	0
57	MG	1H	3237	1/1	0.98	0.18	-	61,61,61,61	0
57	MG	14	3427	1/1	0.82	0.08	-	102,102,102,102	0
57	MG	1H	3330	1/1	0.97	0.12	-	57,57,57,57	0
57	MG	14	3195	1/1	0.92	0.23	-	105,105,105,105	0
57	MG	1H	3149	1/1	0.90	0.15	-	61,61,61,61	0
57	MG	BI	201	1/1	0.91	0.03	-	103,103,103,103	0
57	MG	13	1714	1/1	0.93	0.10	-	93,93,93,93	0
57	MG	13	1673	1/1	0.95	0.14	-	90,90,90,90	0
57	MG	1G	1641	1/1	0.76	0.34	-	78,78,78,78	0
57	MG	1H	3049	1/1	0.94	0.28	-	68,68,68,68	0
57	MG	1H	3397	1/1	0.94	0.07	-	85,85,85,85	0
57	MG	1H	3134	1/1	0.88	0.31	-	76,76,76,76	0
57	MG	14	3163	1/1	0.86	0.64	-	72,72,72,72	0
57	MG	14	3321	1/1	0.94	0.06	-	89,89,89,89	0
57	MG	1H	3435	1/1	0.93	0.05	-	94,94,94,94	0
57	MG	1H	3345	1/1	0.96	0.15	-	56,56,56,56	0
57	MG	14	3235	1/1	0.93	0.50	-	69,69,69,69	0
57	MG	13	1738	1/1	0.90	0.09	-	97,97,97,97	0
57	MG	E5	101	1/1	0.91	0.43	-	72,72,72,72	0
57	MG	14	3409	1/1	0.99	0.14	-	80,80,80,80	0
57	MG	1H	3419	1/1	0.99	0.06	-	63,63,63,63	0
57	MG	1H	3262	1/1	0.90	0.17	-	68,68,68,68	0
57	MG	14	3256	1/1	0.95	0.12	-	91,91,91,91	0
57	MG	14	3382	1/1	0.98	0.09	-	91,91,91,91	0
57	MG	1H	3059	1/1	0.86	0.21	-	66,66,66,66	0
57	MG	14	3447	1/1	0.96	0.06	-	101,101,101,101	0
57	MG	14	3164	1/1	0.86	0.33	-	65,65,65,65	0
57	MG	1G	1617	1/1	0.90	0.23	-	61,61,61,61	0
57	MG	1H	3360	1/1	0.94	0.09	-	60,60,60,60	0
57	MG	14	3266	1/1	0.52	0.24	-	84,84,84,84	0
57	MG	1H	3378	1/1	0.96	0.06	-	84,84,84,84	0
57	MG	1I	201	1/1	0.79	0.12	-	100,100,100,100	0
57	MG	14	3182	1/1	0.90	0.57	-	67,67,67,67	0
57	MG	14	3396	1/1	0.97	0.09	-	62,62,62,62	0
57	MG	14	3351	1/1	0.93	0.06	-	72,72,72,72	0
57	MG	1G	1678	1/1	0.93	0.03	-	115,115,115,115	0
57	MG	14	3081	1/1	0.95	0.74	-	74,74,74,74	0
57	MG	14	3440	1/1	0.97	0.04	-	94,94,94,94	0
57	MG	1H	3346	1/1	0.99	0.11	-	58,58,58,58	0
57	MG	14	3107	1/1	0.86	0.42	-	81,81,81,81	0
57	MG	14	3454	1/1	0.82	0.20	-	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3310	1/1	0.89	0.09	-	68,68,68,68	0
57	MG	1H	3300	1/1	0.99	0.11	-	54,54,54,54	0
57	MG	1H	3158	1/1	0.96	0.59	-	68,68,68,68	0
57	MG	13	1657	1/1	0.95	0.43	-	73,73,73,73	0
57	MG	14	3264	1/1	0.84	0.32	-	90,90,90,90	0
57	MG	13	1681	1/1	0.94	0.40	-	86,86,86,86	0
57	MG	14	3110	1/1	0.93	0.18	-	86,86,86,86	0
57	MG	1G	1642	1/1	0.90	0.30	-	82,82,82,82	0
57	MG	14	3452	1/1	0.91	0.09	-	113,113,113,113	0
57	MG	14	3308	1/1	0.89	0.08	-	96,96,96,96	0
57	MG	14	3148	1/1	0.96	0.37	-	69,69,69,69	0
57	MG	1J	203	1/1	0.75	0.30	-	93,93,93,93	0
57	MG	14	3217	1/1	0.94	0.30	-	76,76,76,76	0
57	MG	13	1665	1/1	0.70	0.46	-	82,82,82,82	0
57	MG	14	3012	1/1	0.96	0.20	-	68,68,68,68	0
57	MG	14	3381	1/1	0.98	0.05	-	52,52,52,52	0
57	MG	14	3442	1/1	0.91	0.07	-	95,95,95,95	0
57	MG	14	3316	1/1	0.95	0.07	-	102,102,102,102	0
57	MG	1H	3277	1/1	0.60	0.18	-	77,77,77,77	0
57	MG	1H	3339	1/1	0.99	0.09	-	50,50,50,50	0
57	MG	1G	1632	1/1	0.95	0.16	-	132,132,132,132	0
57	MG	14	3359	1/1	0.98	0.11	-	67,67,67,67	0
57	MG	14	3378	1/1	0.95	0.04	-	93,93,93,93	0
57	MG	14	3384	1/1	0.97	0.06	-	95,95,95,95	0
57	MG	1H	3488	1/1	0.90	0.05	-	113,113,113,113	0
57	MG	14	3376	1/1	0.97	0.11	-	52,52,52,52	0
57	MG	1H	3280	1/1	0.79	0.42	-	80,80,80,80	0
57	MG	14	3371	1/1	0.95	0.05	-	83,83,83,83	0
57	MG	1H	3426	1/1	0.98	0.08	-	57,57,57,57	0
57	MG	14	3449	1/1	0.94	0.09	-	95,95,95,95	0
57	MG	14	3106	1/1	0.94	0.49	-	82,82,82,82	0
57	MG	14	3410	1/1	0.97	0.05	-	85,85,85,85	0
57	MG	1H	3458	1/1	0.96	0.12	-	87,87,87,87	0
57	MG	14	3422	1/1	0.92	0.09	-	84,84,84,84	0
57	MG	1H	3448	1/1	0.95	0.09	-	62,62,62,62	0
57	MG	14	3126	1/1	0.98	0.43	-	64,64,64,64	0
57	MG	1H	3204	1/1	0.97	0.22	-	86,86,86,86	0
57	MG	14	3255	1/1	0.92	0.14	-	87,87,87,87	0
57	MG	1H	3032	1/1	0.98	0.14	-	61,61,61,61	0
57	MG	1H	3213	1/1	0.89	0.14	-	92,92,92,92	0
57	MG	14	3323	1/1	0.97	0.08	-	72,72,72,72	0
57	MG	1H	3125	1/1	0.78	0.34	-	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3089	1/1	0.99	0.44	-	51,51,51,51	0
57	MG	14	3204	1/1	0.83	0.19	-	90,90,90,90	0
57	MG	14	3330	1/1	0.90	0.06	-	113,113,113,113	0
57	MG	1H	3423	1/1	1.00	0.10	-	55,55,55,55	0
57	MG	1H	3306	1/1	0.99	0.09	-	60,60,60,60	0
57	MG	14	3103	1/1	0.98	0.52	-	68,68,68,68	0
57	MG	1H	3289	1/1	0.74	0.40	-	82,82,82,82	0
57	MG	14	3391	1/1	0.96	0.09	-	86,86,86,86	0
57	MG	14	3433	1/1	0.97	0.05	-	71,71,71,71	0
57	MG	1H	3077	1/1	0.86	0.55	-	74,74,74,74	0
57	MG	14	3247	1/1	0.97	0.25	-	67,67,67,67	0
57	MG	1H	3121	1/1	0.75	0.42	-	79,79,79,79	0
57	MG	1H	3362	1/1	0.97	0.07	-	60,60,60,60	0
57	MG	1H	3100	1/1	0.97	0.19	-	44,44,44,44	0
57	MG	14	3027	1/1	0.90	0.31	-	83,83,83,83	0
57	MG	14	3002	1/1	0.99	0.12	-	49,49,49,49	0
57	MG	1H	3299	1/1	0.98	0.06	-	50,50,50,50	0
57	MG	14	3279	1/1	0.97	0.09	-	62,62,62,62	0
57	MG	1H	3201	1/1	0.95	0.37	-	65,65,65,65	0
57	MG	1H	3260	1/1	0.95	0.25	-	65,65,65,65	0
57	MG	14	3063	1/1	0.71	0.31	-	76,76,76,76	0
57	MG	14	3284	1/1	0.99	0.07	-	57,57,57,57	0
57	MG	13	1675	1/1	0.97	0.41	-	79,79,79,79	0
57	MG	14	3013	1/1	0.70	0.24	-	74,74,74,74	0
57	MG	1G	1639	1/1	0.83	0.18	-	97,97,97,97	0
57	MG	1H	3156	1/1	0.95	0.33	-	61,61,61,61	0
57	MG	1H	3242	1/1	0.81	0.27	-	80,80,80,80	0
57	MG	1H	3255	1/1	0.86	0.14	-	88,88,88,88	0
57	MG	14	3115	1/1	0.95	0.39	-	71,71,71,71	0
57	MG	1H	3466	1/1	0.88	0.05	-	83,83,83,83	0
57	MG	1H	3132	1/1	0.96	0.23	-	75,75,75,75	0
57	MG	14	3079	1/1	0.98	0.30	-	64,64,64,64	0
57	MG	13	1659	1/1	0.78	0.42	-	75,75,75,75	0
57	MG	13	1707	1/1	0.97	0.04	-	90,90,90,90	0
57	MG	14	3263	1/1	0.92	0.45	-	80,80,80,80	0
57	MG	1H	3405	1/1	0.98	0.11	-	69,69,69,69	0
57	MG	35	202	1/1	0.62	0.22	-	75,75,75,75	0
57	MG	13	1718	1/1	0.98	0.09	-	78,78,78,78	0
57	MG	1G	1686	1/1	0.90	0.07	-	92,92,92,92	0
57	MG	13	1640	1/1	0.94	0.24	-	71,71,71,71	0
57	MG	14	3426	1/1	0.96	0.04	-	80,80,80,80	0
57	MG	21	301	1/1	0.94	0.36	-	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3014	1/1	0.96	0.17	-	72,72,72,72	0
57	MG	L8	101	1/1	0.88	0.39	-	72,72,72,72	0
57	MG	14	3085	1/1	0.98	0.31	-	65,65,65,65	0
57	MG	14	3179	1/1	0.68	0.35	-	74,74,74,74	0
57	MG	1H	3403	1/1	0.94	0.18	-	89,89,89,89	0
57	MG	13	1737	1/1	0.94	0.10	-	147,147,147,147	0
57	MG	1H	3311	1/1	0.99	0.10	-	53,53,53,53	0
57	MG	1H	3215	1/1	0.93	0.27	-	65,65,65,65	0
57	MG	13	1679	1/1	0.87	0.23	-	86,86,86,86	0
57	MG	14	3003	1/1	0.96	0.19	-	65,65,65,65	0
57	MG	7A	101	1/1	0.75	0.23	-	89,89,89,89	0
57	MG	1H	3371	1/1	0.91	0.05	-	85,85,85,85	0
57	MG	1G	1633	1/1	0.88	0.41	-	100,100,100,100	0
57	MG	14	3075	1/1	0.75	0.46	-	70,70,70,70	0
57	MG	14	3180	1/1	0.81	0.31	-	69,69,69,69	0
57	MG	14	3401	1/1	0.99	0.10	-	66,66,66,66	0
57	MG	1H	3381	1/1	0.98	0.11	-	95,95,95,95	0
57	MG	14	3116	1/1	0.63	0.39	-	87,87,87,87	0
57	MG	13	1703	1/1	0.98	0.07	-	95,95,95,95	0
57	MG	1H	3229	1/1	0.86	0.34	-	73,73,73,73	0
57	MG	1H	3452	1/1	0.87	0.09	-	89,89,89,89	0
57	MG	1H	3376	1/1	0.90	0.06	-	88,88,88,88	0
57	MG	1G	1669	1/1	0.96	0.09	-	114,114,114,114	0
57	MG	1H	3031	1/1	0.98	0.38	-	53,53,53,53	0
57	MG	14	3424	1/1	0.90	0.05	-	107,107,107,107	0
57	MG	1H	3191	1/1	0.94	0.13	-	95,95,95,95	0
57	MG	1H	3272	1/1	0.87	0.73	-	95,95,95,95	0
57	MG	1H	3106	1/1	0.95	0.43	-	74,74,74,74	0
57	MG	13	1728	1/1	0.98	0.08	-	91,91,91,91	0
57	MG	1H	3222	1/1	0.92	0.11	-	68,68,68,68	0
57	MG	14	3189	1/1	0.97	0.48	-	69,69,69,69	0
57	MG	1G	1667	1/1	0.94	0.06	-	100,100,100,100	0
57	MG	1H	3015	1/1	0.88	0.24	-	72,72,72,72	0
57	MG	14	3387	1/1	0.93	0.05	-	97,97,97,97	0
57	MG	14	3324	1/1	0.88	0.09	-	107,107,107,107	0
57	MG	14	3054	1/1	0.88	0.40	-	67,67,67,67	0
57	MG	14	3069	1/1	0.88	0.42	-	67,67,67,67	0
57	MG	1H	3481	1/1	0.93	0.06	-	92,92,92,92	0
57	MG	1H	3273	1/1	0.88	0.26	-	57,57,57,57	0
57	MG	1H	3386	1/1	0.94	0.06	-	84,84,84,84	0
57	MG	14	3066	1/1	0.97	0.18	-	53,53,53,53	0
57	MG	13	1741	1/1	0.86	0.14	-	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1662	1/1	0.97	0.11	-	76,76,76,76	0
57	MG	1H	3470	1/1	0.90	0.08	-	100,100,100,100	0
57	MG	13	1630	1/1	0.92	0.27	-	92,92,92,92	0
57	MG	1H	3274	1/1	0.93	0.29	-	70,70,70,70	0
57	MG	14	3214	1/1	0.98	0.15	-	73,73,73,73	0
57	MG	13	1632	1/1	0.95	0.13	-	77,77,77,77	0
57	MG	14	3253	1/1	0.94	0.18	-	63,63,63,63	0
57	MG	1H	3471	1/1	0.83	0.12	-	82,82,82,82	0
57	MG	1H	3030	1/1	0.99	0.23	-	45,45,45,45	0
57	MG	1H	3102	1/1	0.95	0.46	-	70,70,70,70	0
57	MG	1H	3473	1/1	0.97	0.07	-	85,85,85,85	0
57	MG	1H	3183	1/1	0.46	0.35	-	92,92,92,92	0
57	MG	14	3372	1/1	0.94	0.09	-	73,73,73,73	0
57	MG	13	1643	1/1	0.57	0.21	-	89,89,89,89	0
57	MG	1H	3178	1/1	0.89	0.12	-	93,93,93,93	0
57	MG	1H	3108	1/1	0.79	0.41	-	82,82,82,82	0
57	MG	1H	3192	1/1	0.82	0.32	-	82,82,82,82	0
57	MG	14	3141	1/1	0.97	0.36	-	50,50,50,50	0
57	MG	1G	1627	1/1	0.85	0.25	-	86,86,86,86	0
57	MG	13	1656	1/1	0.78	0.50	-	62,62,62,62	0
57	MG	14	3102	1/1	0.90	0.20	-	86,86,86,86	0
57	MG	1H	3479	1/1	0.96	0.04	-	89,89,89,89	0
57	MG	14	3236	1/1	0.76	0.22	-	88,88,88,88	0
57	MG	14	3036	1/1	0.81	0.24	-	76,76,76,76	0
57	MG	1H	3155	1/1	0.98	0.18	-	75,75,75,75	0
57	MG	13	1655	1/1	0.72	0.46	-	71,71,71,71	0
57	MG	13	1748	1/1	0.87	0.09	-	115,115,115,115	0
57	MG	16	204	1/1	0.83	0.27	-	90,90,90,90	0
57	MG	14	3314	1/1	0.97	0.06	-	75,75,75,75	0
57	MG	1H	3157	1/1	0.90	0.28	-	64,64,64,64	0
57	MG	C5	201	1/1	0.92	0.04	-	110,110,110,110	0
57	MG	14	3265	1/1	0.69	0.51	-	79,79,79,79	0
57	MG	14	3390	1/1	0.94	0.06	-	82,82,82,82	0
57	MG	13	1705	1/1	0.98	0.07	-	76,76,76,76	0
57	MG	14	3031	1/1	0.32	0.26	-	105,105,105,105	0
57	MG	14	3197	1/1	0.97	0.14	-	56,56,56,56	0
57	MG	1H	3055	1/1	0.94	0.34	-	72,72,72,72	0
57	MG	14	3404	1/1	0.97	0.09	-	94,94,94,94	0
57	MG	1H	3151	1/1	0.97	0.18	-	91,91,91,91	0
57	MG	14	3367	1/1	0.99	0.05	-	60,60,60,60	0
57	MG	1H	3187	1/1	0.93	0.08	-	88,88,88,88	0
57	MG	13	1709	1/1	0.98	0.09	-	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1702	1/1	0.98	0.12	-	76,76,76,76	0
57	MG	14	3226	1/1	0.79	0.27	-	78,78,78,78	0
57	MG	14	3065	1/1	0.98	0.28	-	54,54,54,54	0
57	MG	1G	1683	1/1	0.89	0.09	-	96,96,96,96	0
57	MG	14	3100	1/1	0.96	0.32	-	43,43,43,43	0
57	MG	1H	3226	1/1	0.86	0.15	-	64,64,64,64	0
57	MG	14	3339	1/1	1.00	0.07	-	86,86,86,86	0
57	MG	14	3117	1/1	0.96	0.36	-	66,66,66,66	0
57	MG	1H	3239	1/1	0.99	0.09	-	67,67,67,67	0
57	MG	13	1638	1/1	0.97	0.46	-	58,58,58,58	0
57	MG	13	1739	1/1	0.88	0.06	-	104,104,104,104	0
57	MG	1H	3282	1/1	0.45	0.25	-	96,96,96,96	0
57	MG	14	3004	1/1	0.93	0.88	-	77,77,77,77	0
57	MG	14	3245	1/1	0.94	0.36	-	79,79,79,79	0
57	MG	1H	3461	1/1	0.97	0.05	-	85,85,85,85	0
57	MG	1H	3415	1/1	0.99	0.10	-	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.