



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2016 – 06:19 PM EDT

PDB ID : 5IB8
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and near-cognate tRNA^{Lys} with U-G mismatch in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 3.13 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

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-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

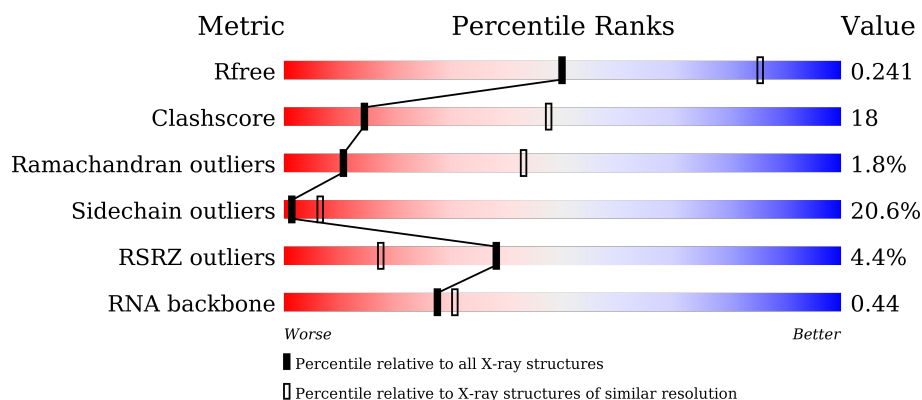
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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.



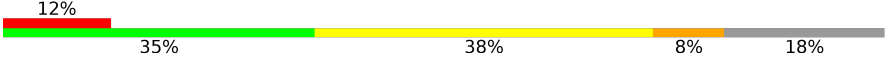


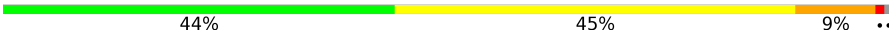

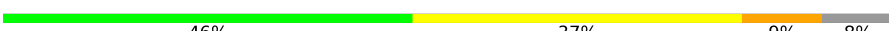





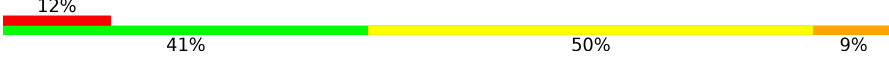

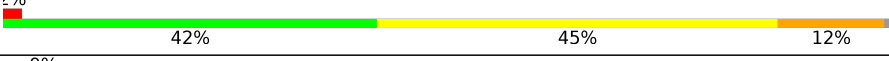
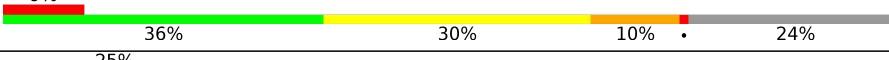
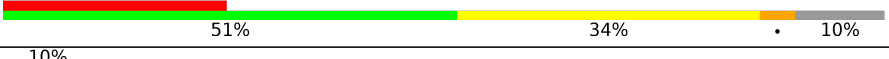
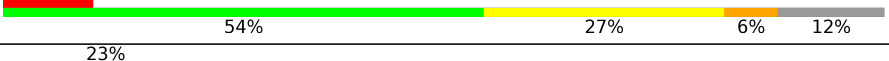
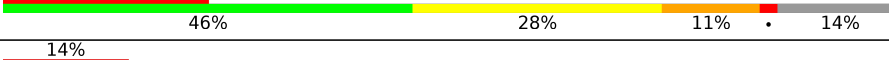


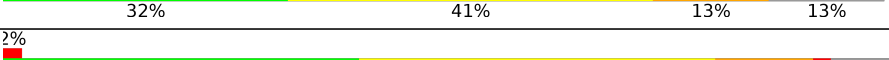




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)
RNA backbone	2183	1016 (3.58-2.70)

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 ≥ 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	

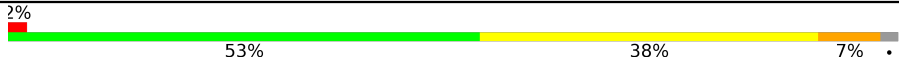

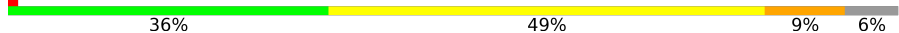



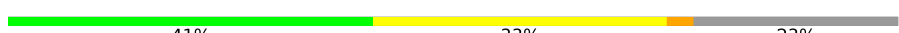
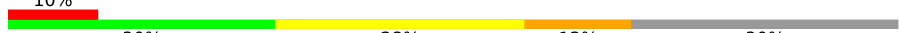







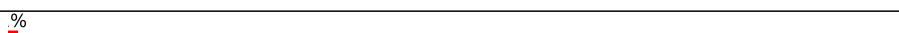
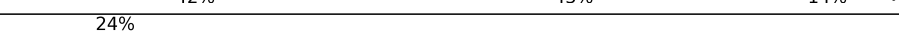


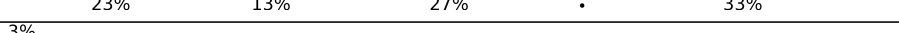
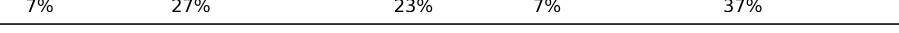

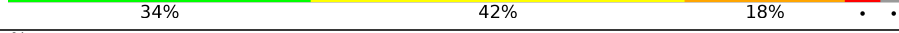


Continued on next page...

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	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
41	75	146	




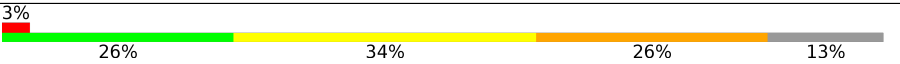
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
54	L5	49	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1601	-	-	-	X
57	MG	13	1607	-	-	-	X
57	MG	13	1609	-	-	-	X
57	MG	13	1614	-	-	-	X
57	MG	13	1615	-	-	-	X
57	MG	13	1624	-	-	-	X
57	MG	13	1625	-	-	-	X
57	MG	13	1628	-	-	-	X
57	MG	13	1629	-	-	-	X
57	MG	13	1630	-	-	-	X
57	MG	13	1634	-	-	-	X
57	MG	13	1635	-	-	-	X
57	MG	13	1638	-	-	-	X
57	MG	13	1643	-	-	-	X
57	MG	13	1649	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1696	-	-	-	X
57	MG	14	3005	-	-	-	X
57	MG	14	3009	-	-	-	X
57	MG	14	3016	-	-	-	X
57	MG	14	3032	-	-	-	X
57	MG	14	3034	-	-	-	X
57	MG	14	3038	-	-	-	X
57	MG	14	3042	-	-	-	X
57	MG	14	3045	-	-	-	X
57	MG	14	3046	-	-	-	X
57	MG	14	3050	-	-	-	X
57	MG	14	3052	-	-	-	X
57	MG	14	3054	-	-	-	X
57	MG	14	3058	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3066	-	-	-	X
57	MG	14	3068	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3075	-	-	-	X
57	MG	14	3078	-	-	-	X
57	MG	14	3080	-	-	-	X
57	MG	14	3082	-	-	-	X
57	MG	14	3086	-	-	-	X
57	MG	14	3091	-	-	-	X
57	MG	14	3094	-	-	-	X
57	MG	14	3095	-	-	-	X
57	MG	14	3096	-	-	-	X
57	MG	14	3102	-	-	-	X
57	MG	14	3105	-	-	-	X
57	MG	14	3106	-	-	-	X
57	MG	14	3113	-	-	-	X
57	MG	14	3119	-	-	-	X
57	MG	14	3123	-	-	-	X
57	MG	14	3124	-	-	-	X
57	MG	14	3130	-	-	-	X
57	MG	14	3132	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3142	-	-	-	X
57	MG	14	3145	-	-	-	X
57	MG	14	3147	-	-	-	X
57	MG	14	3149	-	-	-	X
57	MG	14	3159	-	-	-	X
57	MG	14	3160	-	-	-	X
57	MG	14	3165	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	14	3182	-	-	-	X
57	MG	14	3194	-	-	-	X
57	MG	14	3228	-	-	-	X
57	MG	14	3240	-	-	-	X
57	MG	14	3302	-	-	-	X
57	MG	16	202	-	-	-	X
57	MG	16	204	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1606	-	-	-	X
57	MG	1G	1607	-	-	-	X
57	MG	1G	1614	-	-	-	X
57	MG	1G	1626	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1G	1632	-	-	-	X
57	MG	1G	1647	-	-	-	X
57	MG	1G	1648	-	-	-	X
57	MG	1G	1651	-	-	-	X
57	MG	1G	1670	-	-	-	X
57	MG	1G	1679	-	-	-	X
57	MG	1H	3007	-	-	-	X
57	MG	1H	3015	-	-	-	X
57	MG	1H	3017	-	-	-	X
57	MG	1H	3019	-	-	-	X
57	MG	1H	3021	-	-	-	X
57	MG	1H	3036	-	-	-	X
57	MG	1H	3041	-	-	-	X
57	MG	1H	3052	-	-	-	X
57	MG	1H	3055	-	-	-	X
57	MG	1H	3063	-	-	-	X
57	MG	1H	3074	-	-	-	X
57	MG	1H	3075	-	-	-	X
57	MG	1H	3082	-	-	-	X
57	MG	1H	3084	-	-	-	X
57	MG	1H	3086	-	-	-	X
57	MG	1H	3090	-	-	-	X
57	MG	1H	3093	-	-	-	X
57	MG	1H	3107	-	-	-	X
57	MG	1H	3112	-	-	-	X
57	MG	1H	3116	-	-	-	X
57	MG	1H	3119	-	-	-	X
57	MG	1H	3126	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3154	-	-	-	X
57	MG	1H	3160	-	-	-	X
57	MG	1H	3169	-	-	-	X
57	MG	1H	3179	-	-	-	X
57	MG	1H	3191	-	-	-	X
57	MG	1H	3198	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3207	-	-	-	X
57	MG	1H	3215	-	-	-	X
57	MG	1H	3218	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3237	-	-	-	X
57	MG	1H	3240	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3394	-	-	-	X
57	MG	1H	3413	-	-	-	X
57	MG	1H	3427	-	-	-	X
57	MG	1H	3432	-	-	-	X
57	MG	1H	3497	-	-	-	X
57	MG	1H	3532	-	-	-	X
57	MG	1H	3541	-	-	-	X
57	MG	1H	3548	-	-	-	X
57	MG	2L	101	-	-	-	X
58	SF4	32	302	-	-	X	-
60	SPE	14	3458	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	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	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	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	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	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			

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			

- Molecule 23 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	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^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- 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
			442	198	94	130	20			
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2831	Total	C	N	O	P	0	0	0
			60991	27142	11416	19602	2831			
26	14	2825	Total	C	N	O	P	0	0	0
			60857	27083	11390	19559	2825			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1546	978	295	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	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
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	B5	94	Total	C	N	O	0	0	0
			735	477	133	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	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^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	66	Total	C	N	O	P	0	0	0
			1402	627	244	465	66			

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

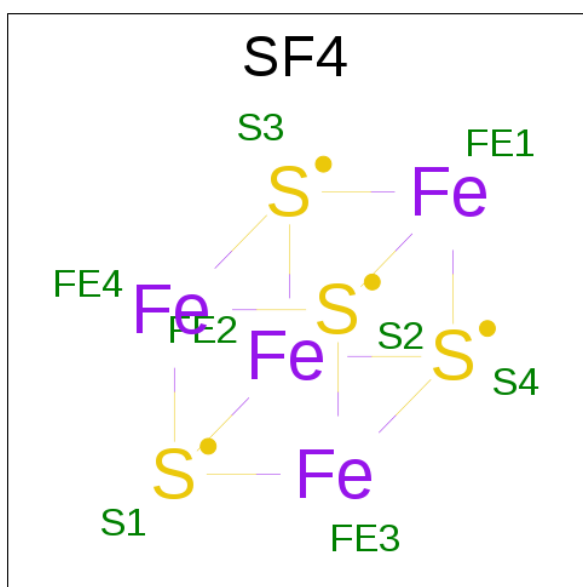
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	1	Total 1	Mg 1	0	0
57	19	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	32	1	Total 1	Mg 1	0	0
57	2I	1	Total 1	Mg 1	0	0
57	13	141	Total 141	Mg 141	0	0
57	1J	10	Total 10	Mg 10	0	0
57	35	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0
57	16	12	Total 12	Mg 12	0	0
57	42	2	Total 2	Mg 2	0	0
57	B5	1	Total 1	Mg 1	0	0
57	25	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0
57	21	3	Total 3	Mg 3	0	0
57	31	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	I8	2	Total 2	Mg 2	0	0
57	52	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0

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	1	Total 1	Mg 1	0	0
57	1G	125	Total 125	Mg 125	0	0
57	1H	552	Total 552	Mg 552	0	0
57	E5	2	Total 2	Mg 2	0	0
57	88	3	Total 3	Mg 3	0	0
57	14	460	Total 460	Mg 460	0	0
57	F8	1	Total 1	Mg 1	0	0
57	41	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

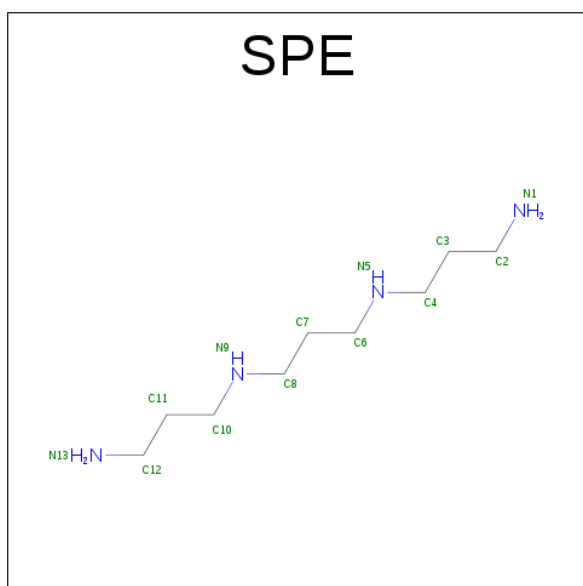


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C5	1	Total	Zn	0	0
			1	1		
59	5A	1	Total	Zn	0	0
			1	1		
59	G8	1	Total	Zn	0	0
			1	1		
59	5I	1	Total	Zn	0	0
			1	1		

- Molecule 60 is THERMINE (three-letter code: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1G	1	Total	C	N	0	0
			13	9	4		
60	14	1	Total	C	N	0	0
			13	9	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	354	Total 354	O 354	0	0
61	3E	2	Total 2	O 2	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	7I	2	Total 2	O 2	0	0
61	BI	3	Total 3	O 3	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	5	Total 5	O 5	0	0
61	1H	1720	Total 1720	O 1720	0	0
61	16	12	Total 12	O 12	0	0
61	11	10	Total 10	O 10	0	0
61	21	6	Total 6	O 6	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	68	2	Total 2	O 2	0	0
61	78	13	Total 13	O 13	0	0
61	98	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B8	1	Total 1	O 1	0	0
61	C8	4	Total 4	O 4	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	3	Total 3	O 3	0	0
61	G8	3	Total 3	O 3	0	0
61	I8	6	Total 6	O 6	0	0
61	J8	5	Total 5	O 5	0	0
61	L8	4	Total 4	O 4	0	0
61	N8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	364	Total 364	O 364	0	0
61	32	4	Total 4	O 4	0	0
61	42	1	Total 1	O 1	0	0
61	52	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	4A	2	Total 2	O 2	0	0
61	6A	3	Total 3	O 3	0	0
61	7A	4	Total 4	O 4	0	0
61	9A	2	Total 2	O 2	0	0
61	BA	3	Total 3	O 3	0	0

Continued on next page...

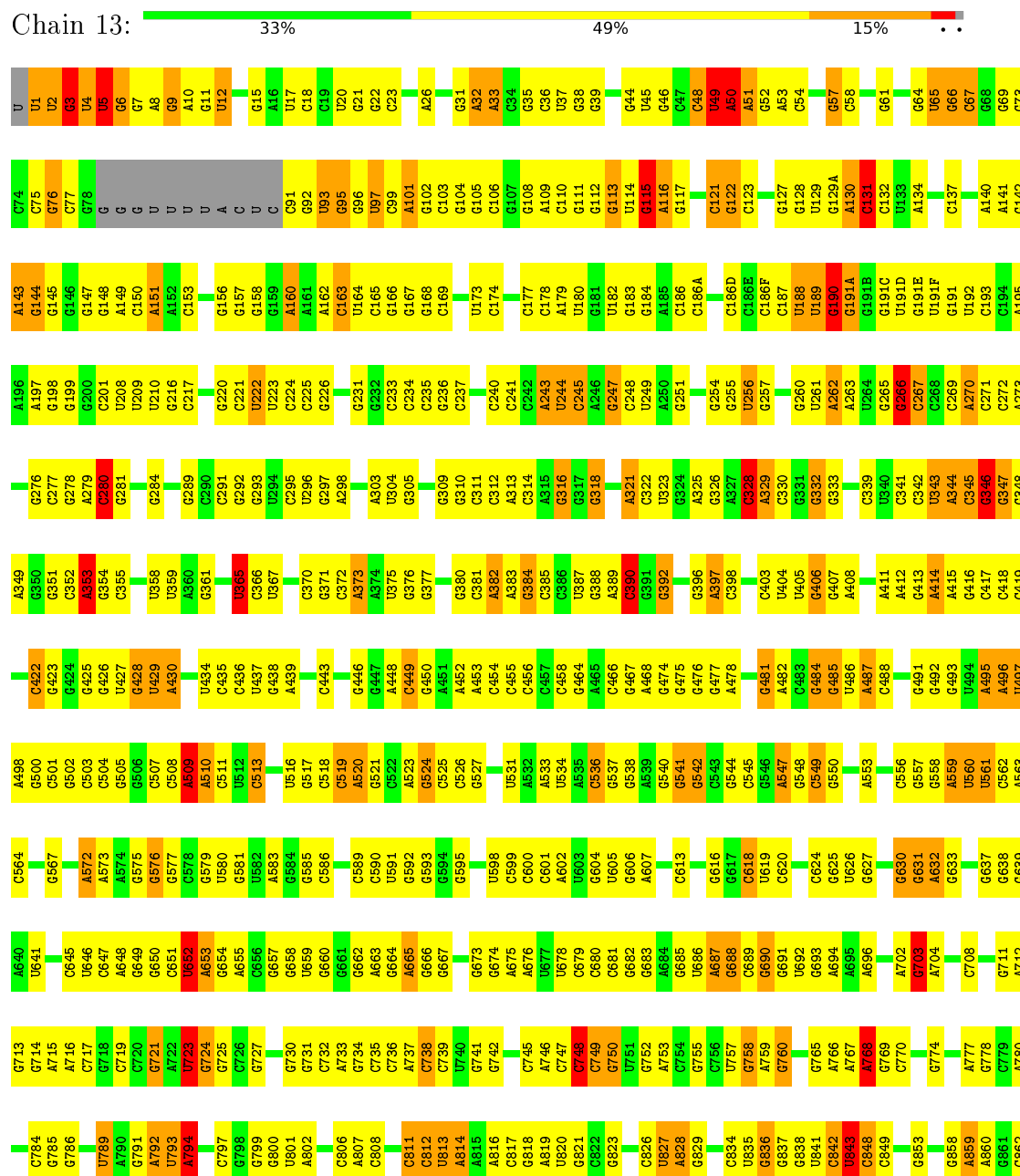
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2L	8	Total 8	O 8	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1303	Total 1303	O 1303	0	0
61	1J	27	Total 27	O 27	0	0
61	19	14	Total 14	O 14	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	15	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	35	8	Total 8	O 8	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	F5	1	Total 1	O 1	0	0
61	H5	1	Total 1	O 1	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	8	Total 8	O 8	0	0

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

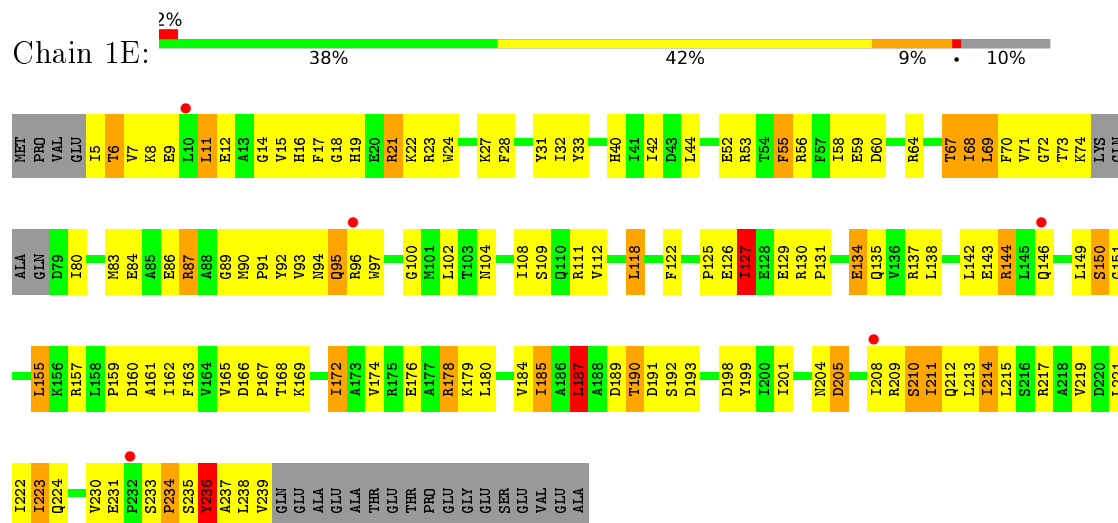


[illegible]

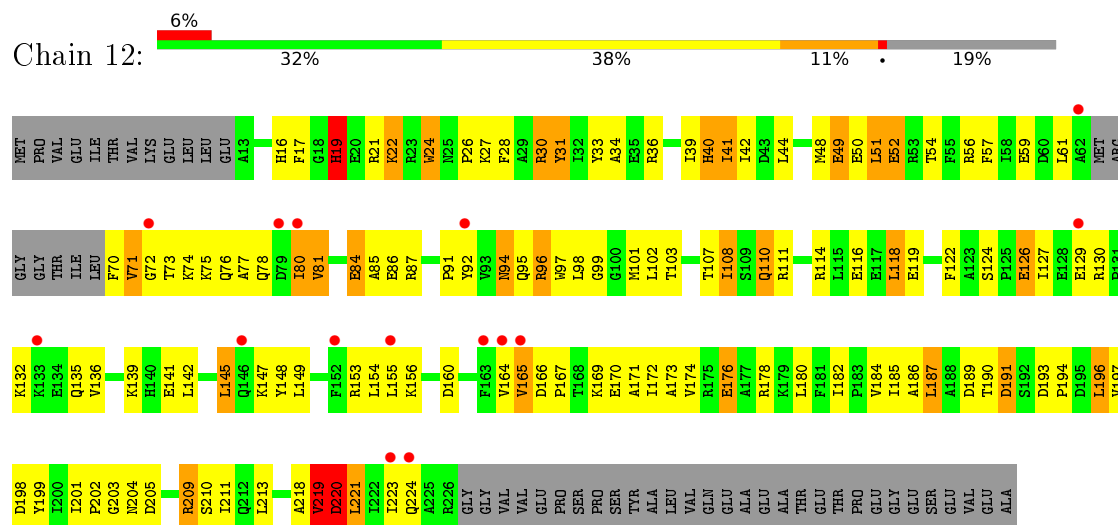
C1466	U1380	G1255	A1191	A1130	A1055	C995	C931	G858	A768	G688	G610	A547	G477	G392
G1467	U1381	A1256	C1195	G1131	U1056	A996	C932	A659	G769	C689	A611	A548	G481	A393
A1468	C1382	U1257	C1196	G1132	G1057	U997	C933	G861	C770	G690	A614	U551	G482	A397
G1469	G1258	G1288	G1196	G1133	G1058	G998	C934	G862	G771	G691	G616	U552	C483	C398
G1470	A1324	C1259	G1197	G1134	C1059	A935A	C935	U663	G776	U692	G617	U553	G484	
G1471	G1387	C1260	G1198	U1135	U1062	U999	C936	U664	A777	A694	G618	C554	G485	G406
		A1261	U1199	U1136	U1063	A1000	C937	A865	G778		G619	C555	U486	G407
G1474	U1391	C1262	C1200	C1137	G1064	G1001	A938		C779	U697	U619	C556		A408
	G1392	C1263	G1201	G1138	U1065	G1002	C939	C868	A780	G698	U620	C557	G490	A409
C1478	C1395	G1264	G1202	G1139	U1085	G1003	C940	C869			A621	U558	G491	G410
C1479	U1330	G1265	C1203	C1140	G1068	A1004	G941	C870	A781		G622	A559	G492	A411
	A1396	G1266	A1204	G1141	G1088	A1005	U943	U871	G784	A702	C623	U560		A412
G1487	C1397	C1267	U1205	G1142	C1071	C1006	U944	A872	A787	A706	C624	U561	A495	G443
	A1398	A1268	G1206	G1143	G1072	C1007		A873			G625	C562	A496	A414
C1490	C1399	A1269	C1207	G1144	G1072	C1008		A874	G791	G709	G626	C563	U497	
G1491	C1400	G1334	C1208	C1145	G1073	C1009	G947	G875	G792	G710	G627	C564	G498	C419
A1492	G1401	C1336	C1209	A1146	U1078	G1010	C948	C876	U793	G710	G628	U565	A498	U420
A1493	C1402	G1337	G1210	G1147	G1079	G1011		G877	A794	G713	G629	C566	C501	U421
	C1403	U1211	U1211	U1148	A1080	G1012	G951	C878		G714	G630	C567	C502	G422
		U1212	U1212	U1149	G1081	A1014	U952	C879	U801		G631	C568	C503	G423
	C1409	G1213	A1213	U1150	G1082	A1015	C953	C879	A802		G632	U571	C504	G424
	G1410	C1214	C1214	A1151	U1083	A1016	U957	C883	G803		G633	A572	G505	G425
	C1411	G1215	A1152	G1084	U1085	G1017	A958	U884	U804		G634	A573	C506	G426
	C1412	G1216	C1153	U1085		C1018	A959	G885	C805		G635	A574	C507	U427
	A1413	C1217	G1154	C1019		C1019	U960						A509	G428
G1505	U1414	C1218	G1155	U1020	G1088	U1020	U961	A889	C811	U723	A640	G575	A510	U429
	G1415	U1219	A1157	G1220	G1094	G1022	C962	G890		G724	U641	C576	C511	A430
	U1507	C1282	G1220	A1157	G1094	G1022	C963		A816	G725	A642	C577	C513	
C1508	G1419	C1283	G1221	U1095	C1158	G1023	A964	G894	C817	G726	U646	C578	U516	C433
		A1285	G1221	U1159	C1086	G1024	C965	G895	G818	G727	C647	U580	C517	U434
U1510	G1422	C1286	G1222	G1160	C1087	U1025	A965		A819	G728	C647	U581	C518	C435
G1511	G1423	A1287	G1223	C1161	C1088	G1026	G966	G898	U820	A729	C651	U582	C519	C436
	C1424	C1288	G1224	C1162	C1089	G1027	C967	C999	G821	G730	U652	U583	A520	U437
			C1226	C1163	A1101	C1028A	A968	A900	C822	G731	A653	G584	A521	G438
C1513	C1429	G1291	A1227	G1164	A1102	G1028B	C970	C904	G825	C735	G660	G585	A523	A439
C1514	C1354	C1228	C1165	C1165	C1103	G1029	C971	U905	C826	C736	G661	C586	G524	A440
C1515	C1355	U1292	C1166	G1104	G1104	C1030	C972	G906	U827	C737	G662	C587	C525	C442
G1516	G1431	G1293	C1167	A1105	A1105	G1031	C973		A828	A737	A663	C588	C526	C443
	G1432	C1230	U1231	A1170	G1106	A1032	A974	A909	G829	C738	G664	U591	G527	C444
C1517	A1518	U1232	U1232	G1171	C1107	G1032A	C975	C910	U833	U740	A665	C592	C528	C445
A1519	C1433	C1295	C1295	G1175	G1108	G1032B	G976	C912	C834	G741	A666	C593	C529	C446
C1520	G1435	C1297	U1233	A1176	A1111	G1034	C978	C913	U835	U743	G667	C594	G529	C447
G1521	U1436	C1298	U1234	C1172	C1112	C1037	C980	A914	G837	C744	G668	C595	U531	C448
U1522	G1437	A1299	U1235	G1173	C1109	G1033	A977	U911	G838	C745		C596	A532	C449
	C1438	G1300	C1237	A1179	G1118	U1040	U981	A915	U841	C746	U672	C597	A533	A451
	C1439	U1301	A1238	A1176	C1119	G1042	U982	G916	G838	C749	G673	U598	U534	A452
G1526	G1440	C1302	U1239	G1175	G1121	G1043	C984	A918	C842	G750	G674	C599	A535	C456
C1527	C1441	C1366	U1240	G1177	U1121	C1044	C985	A919	U843	C751	A675	C600	C536	C457
U1528	G1442	C1367	G1304	G1178	G1182	A1045	U986	U920	C848	C754	U676	C601	C537	C458
G1529	G1443	G1368	G1305	A1179	A1183	C1046	C987	U921	U841	C755	U677	A602	A538	C459
C1530	A1446	C1369	C1244	A1180	U1122	A1047	G988	G922	G851	G756	U678	U603	A539	G464
		U1307	A1245	G1181	G1120	G1048	G989	C924	G852	C679	C679	G604	G540	A465
U1532	C1449	G1371	C1246	A1181	U1121	G1048	C990	C924	G853	A759	G683	U605	G541	C466
C1533	A1534	U1372	A1247	A1183	A1123	G1048	U991	G925	G854		A684	G606	G542	C467
C1535	A1451	G1373	C1248	G1184	A1123	G1048	U992	G926	G855	G765	A694	A607	C543	A468
C	U	C1452	A1249	G1185	U1125	G1048	U993	G927	C856	A766		A608	C544	G474
U	C	G1453	A1250	G1186	U1126	G1048	U994	G928	C857	A767		A609	G546	G475
U	C	G1454	A1251	G1187	U1126	G1048	U995	G929	C858					G476
U	C	G1455	A1252	A1188	C1128	C1054	U996	G930	C859					
U	C	G1456	G1253	C1128	C1128	C1054	U997	G931	C860					
U	U	G1457	G1254	C1129	C1129	C1054	A994							

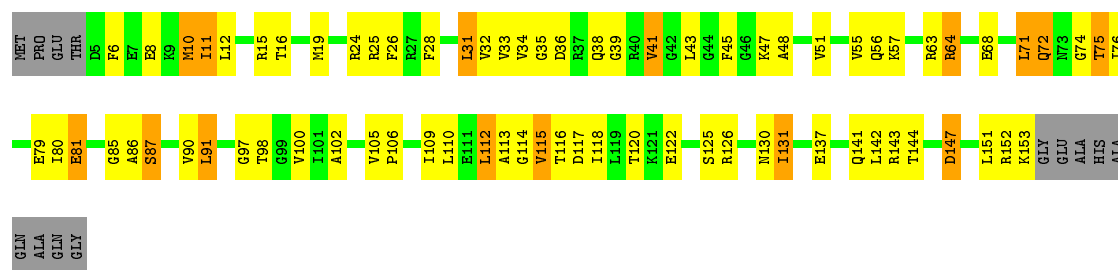
C D

- Molecule 2: 30S ribosomal protein S2



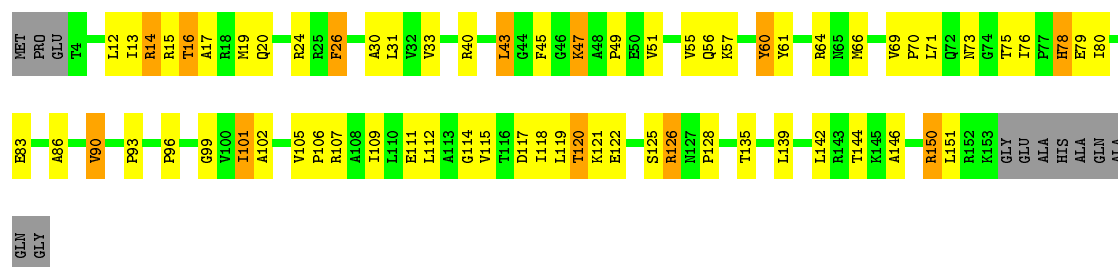
- Molecule 2: 30S ribosomal protein S2





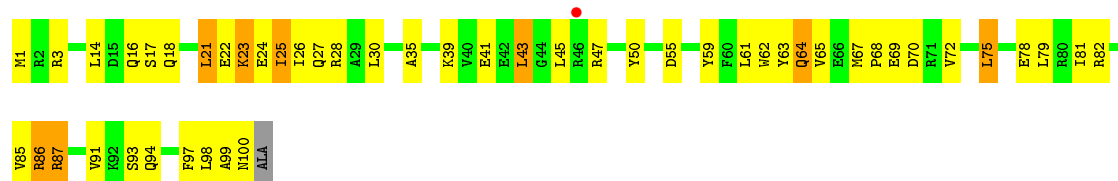
• Molecule 5: 30S ribosomal protein S5

Chain 42: 51% 34% 7% 7%



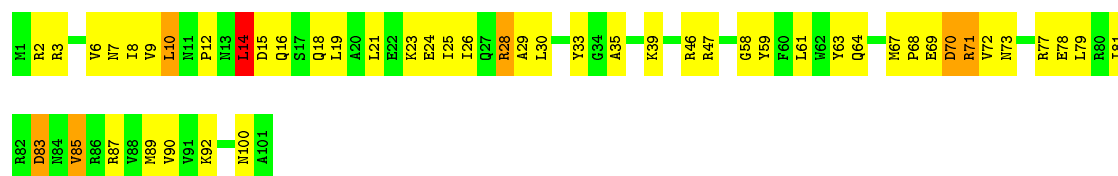
• Molecule 6: 30S ribosomal protein S6

Chain 5E: 50% 41% 8%



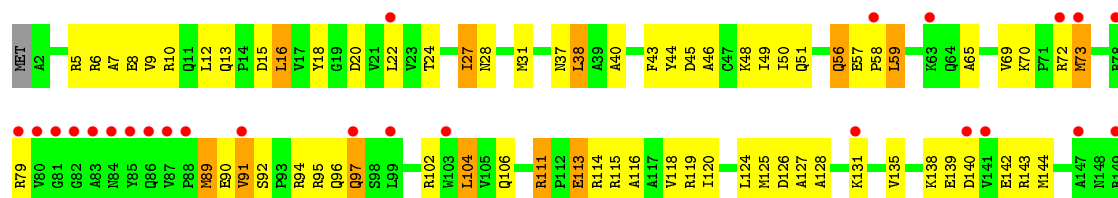
• Molecule 6: 30S ribosomal protein S6

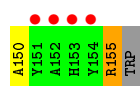
Chain 52: 51% 42% 6%



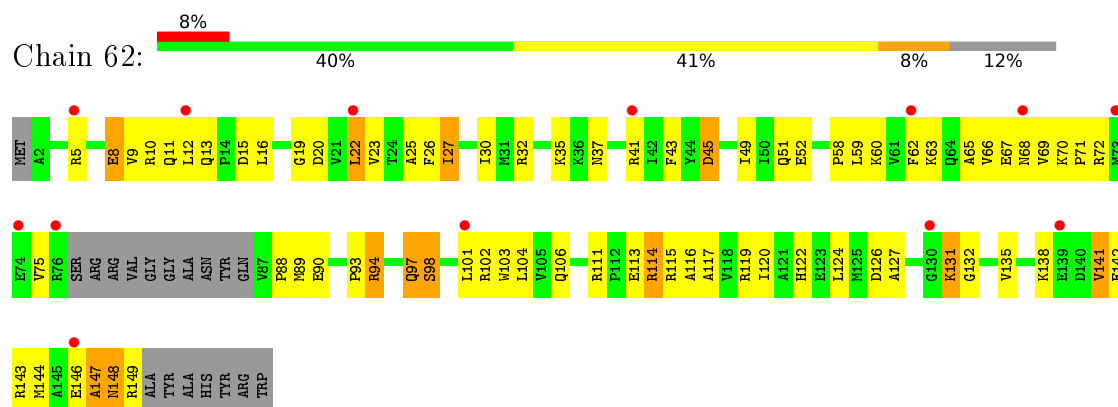
• Molecule 7: 30S ribosomal protein S7

Chain 6E: 19% 53% 38% 8%

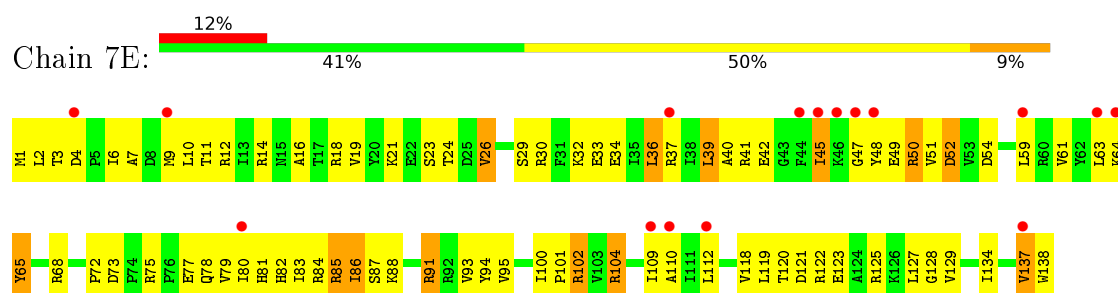




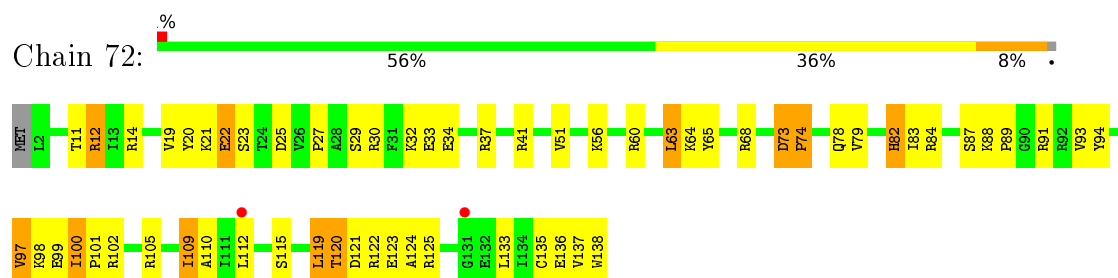
• Molecule 7: 30S ribosomal protein S7



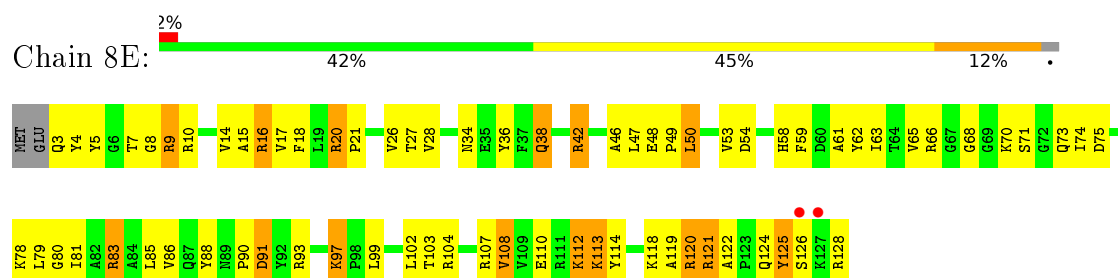
• Molecule 8: 30S ribosomal protein S8



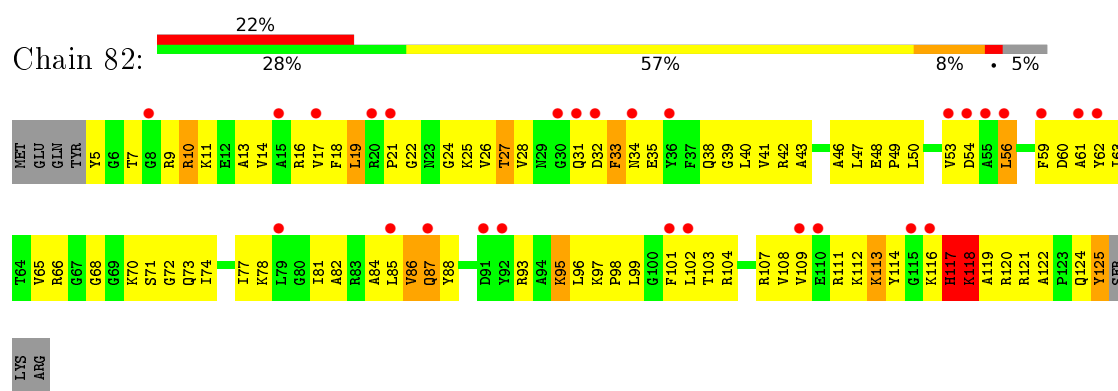
• Molecule 8: 30S ribosomal protein S8



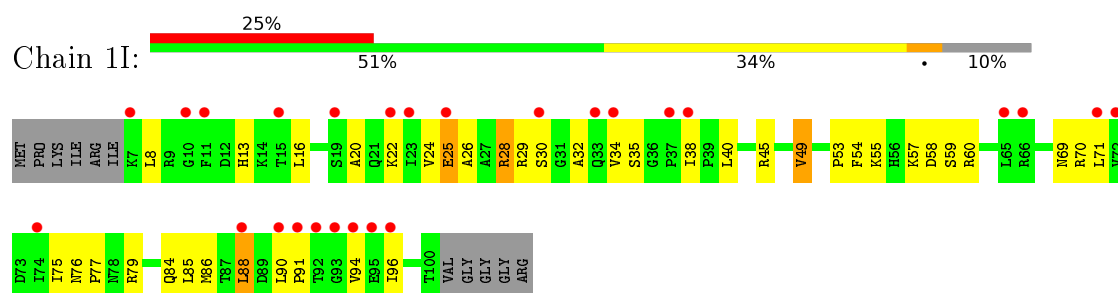
• Molecule 9: 30S ribosomal protein S9



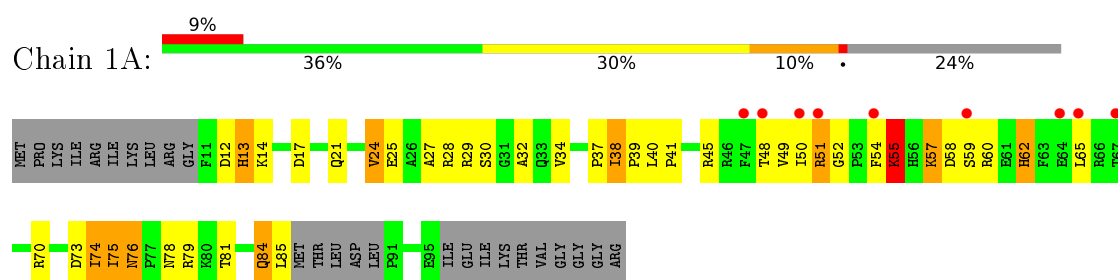
• Molecule 9: 30S ribosomal protein S9



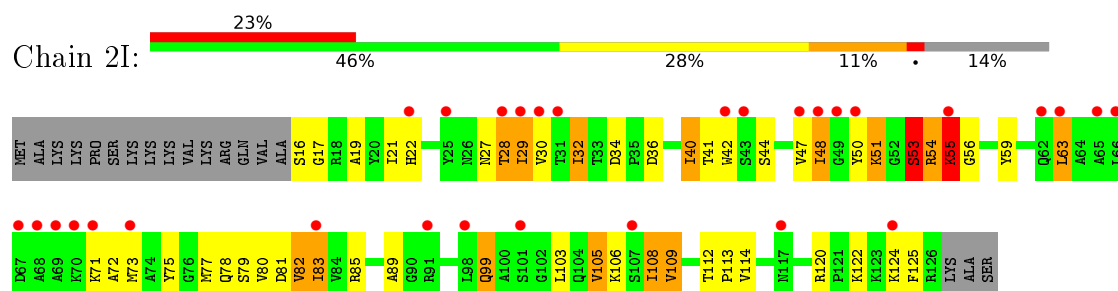
• Molecule 10: 30S ribosomal protein S10



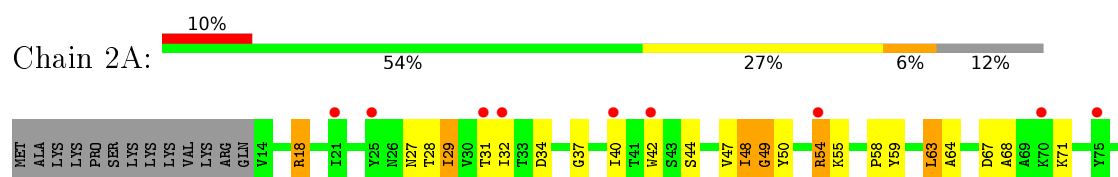
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

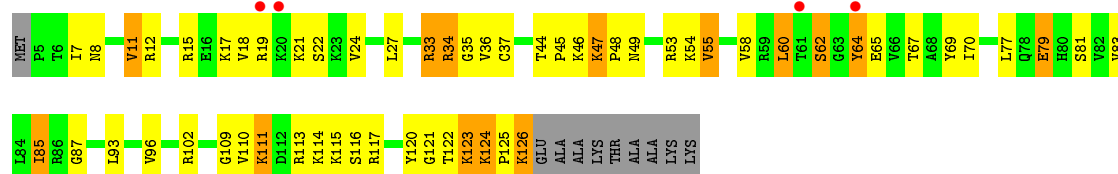


• Molecule 11: 30S ribosomal protein S11

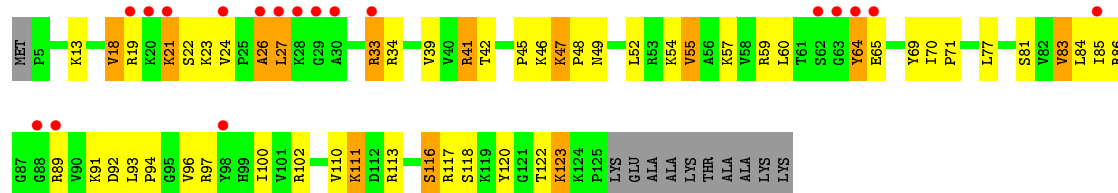




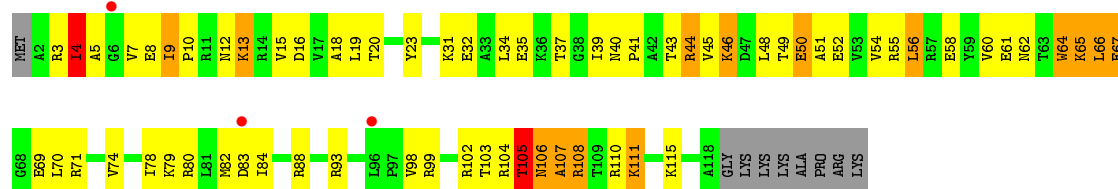
- Molecule 12: 30S ribosomal protein S12



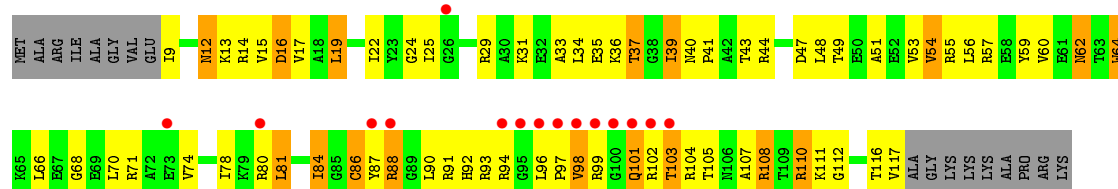
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

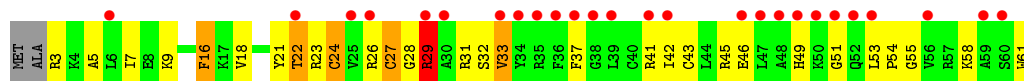
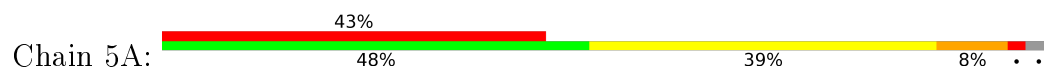


- Molecule 14: 30S ribosomal protein S14 type Z

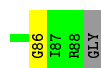
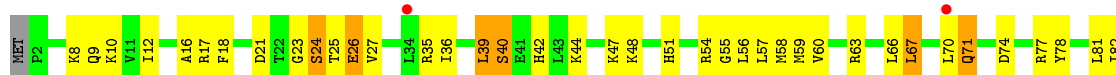




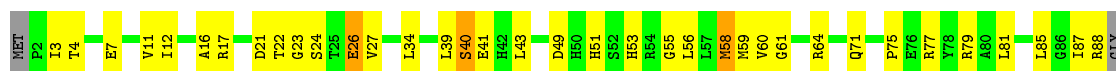
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

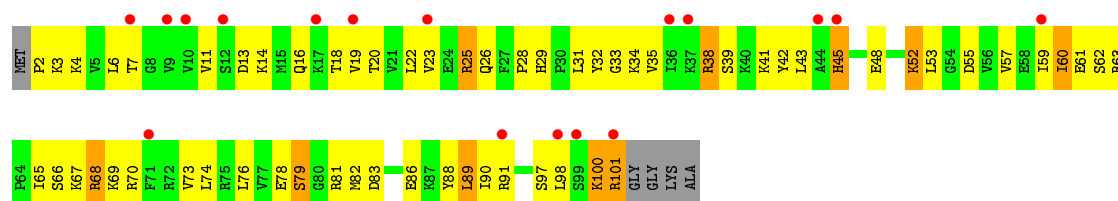


- Molecule 16: 30S ribosomal protein S16

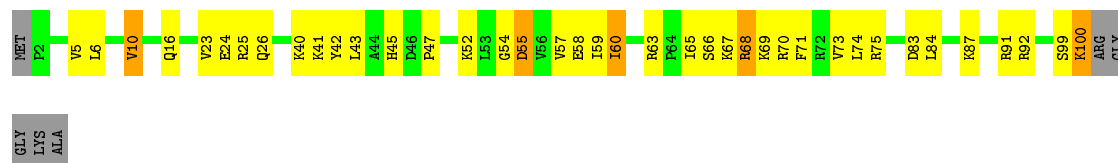


- Molecule 17: 30S ribosomal protein S17

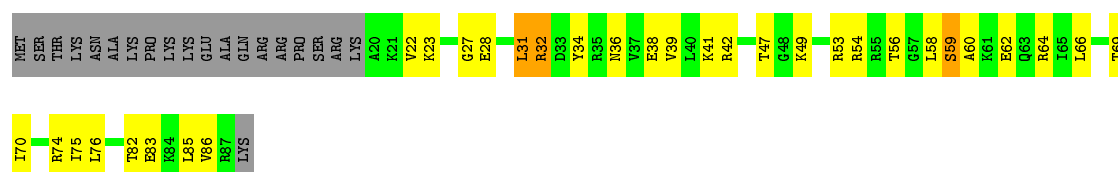




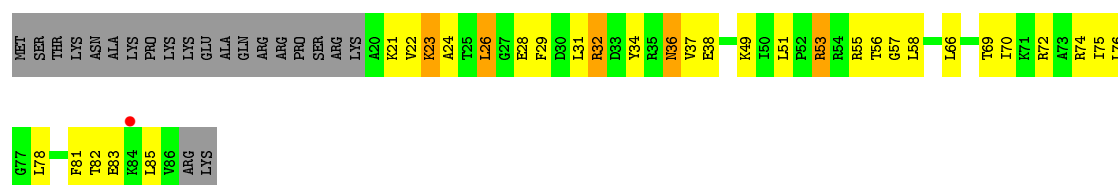
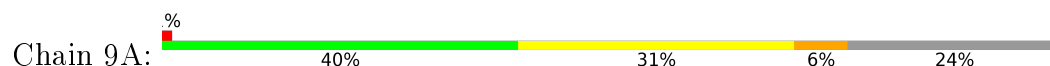
• Molecule 17: 30S ribosomal protein S17



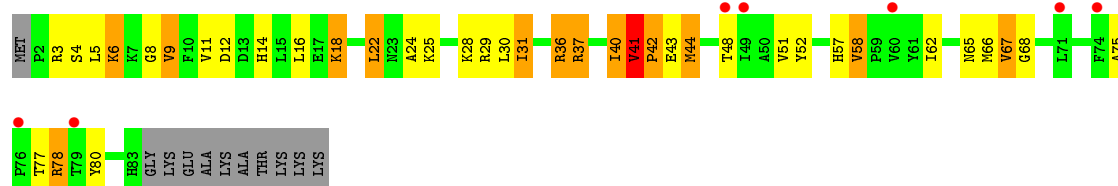
• Molecule 18: 30S ribosomal protein S18



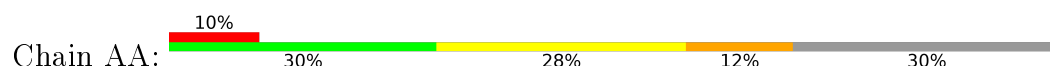
• Molecule 18: 30S ribosomal protein S18

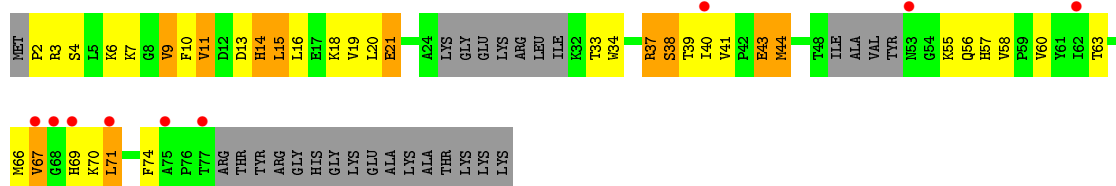


• Molecule 19: 30S ribosomal protein S19

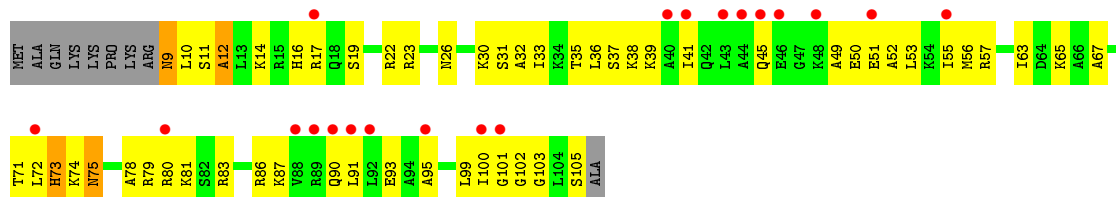


• Molecule 19: 30S ribosomal protein S19

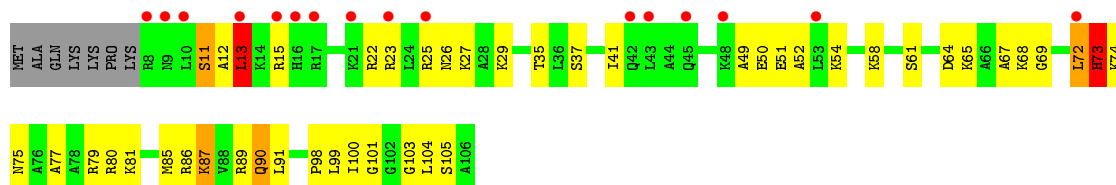




• Molecule 20: 30S ribosomal protein S20



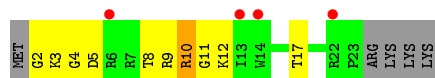
• Molecule 20: 30S ribosomal protein S20



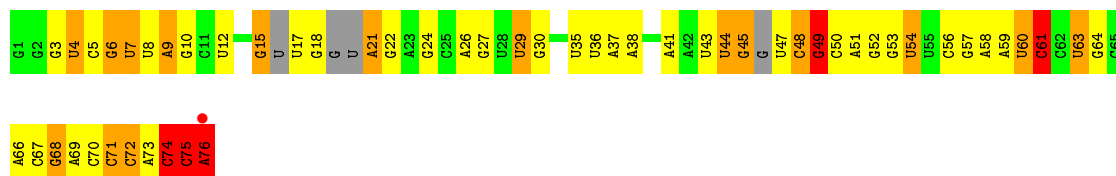
• Molecule 21: 30S ribosomal protein Thx



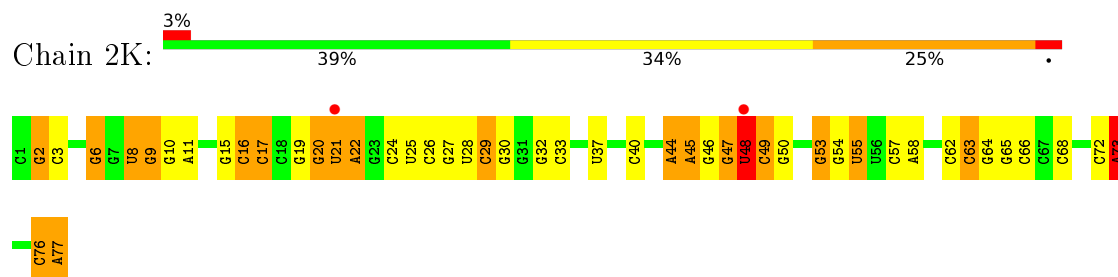
• Molecule 21: 30S ribosomal protein Thx



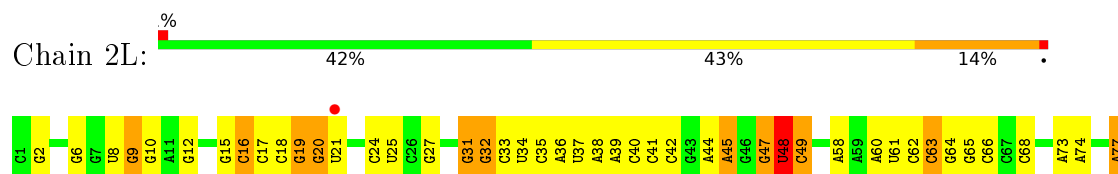
• Molecule 22: tRNA^{Lys}



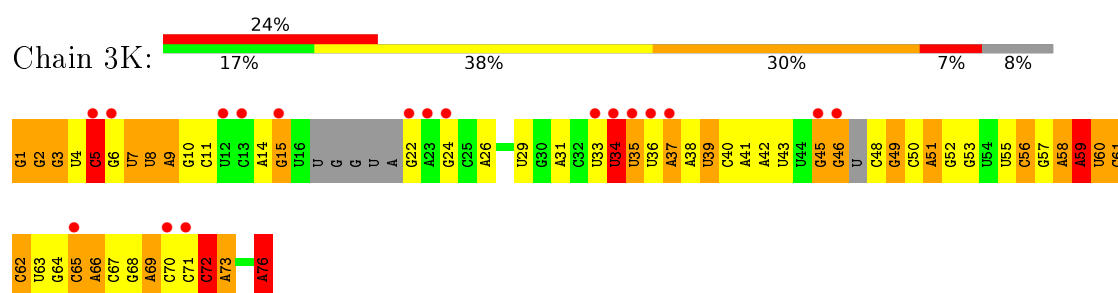
- Molecule 23: tRNA^{fMet}



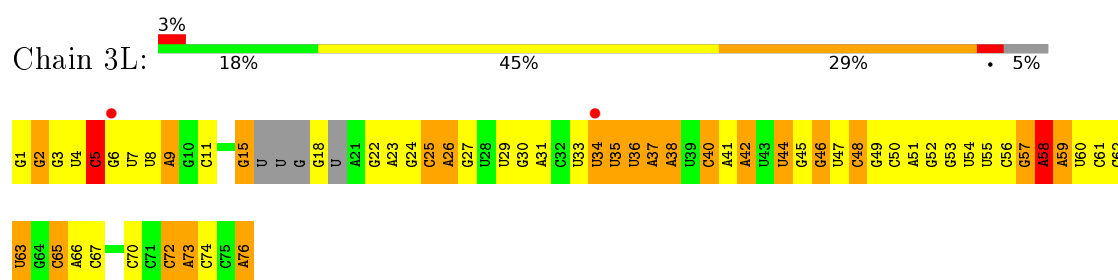
- Molecule 23: tRNA^{fMet}



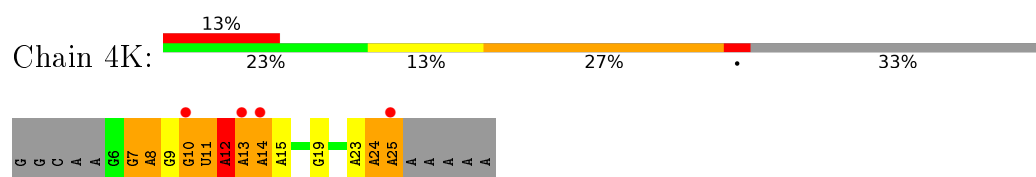
- Molecule 24: tRNA^{Lys}



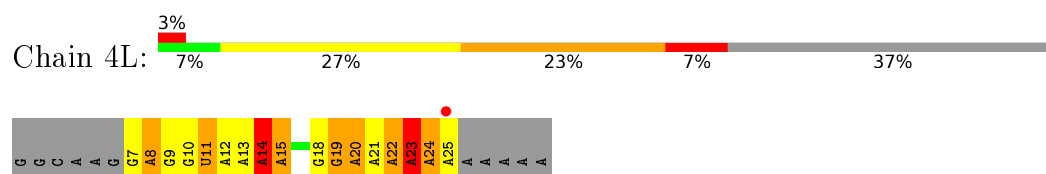
- Molecule 24: tRNA^{Lys}

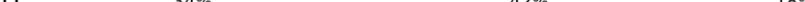


- Molecule 25: mRNA



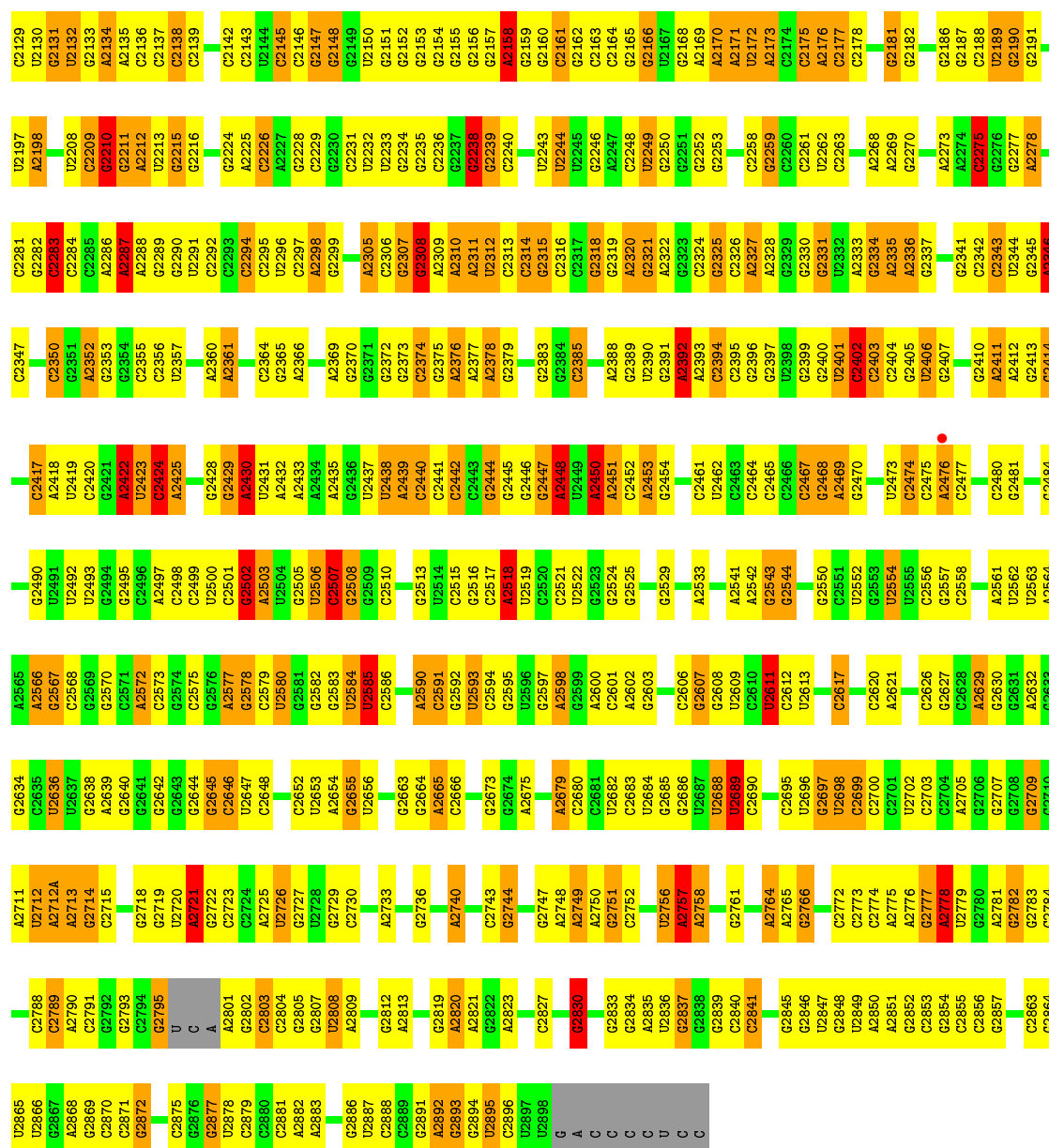
- Molecule 25: mRNA



Chain 1H: 

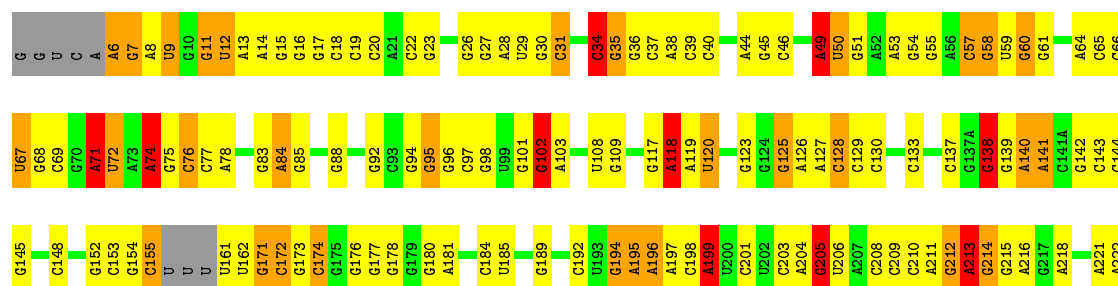


C2061	U1991	G1915	G1826	G1759	G1660	C1531	G1455	C1387	G1313	G1244	A1177	G1106	A1046
A2062	G1992	A1916	C1827	A1760	G1661	C1532	C1458	G1388	C1314	G1245	C1178	G1107	G1047
C2063	G1993		G1828	C1761	C1662	C1533	G1459	G1389		A1246	C1179	U1108	A1048
C2064	A1919	A1919	A1762	A1762		G1534	G1459	U1390	C1318	A1247	C1180	C1109	C1049
C2065	G1995	C1920	G1763	G1763	G1665	U1535	G1460	U1391	C1319	U1248	C1181	G1110	A1050
C2066	G1996		G1764	G1764	G1666	A1536	G1461	A1392	C1320	U1249	A1182	A1111	G1051
G2067	U1926	U1926	C1832	G1765	G1667	C1537	C1464	A1393	A1321	G1250	G1183	G1112	C1052
U2068			U1833	U1766	A1668	G1538		U1394	A1322			U1113	A1053
G2069	G1929	G1929	U1834	C1767	A1669	G1539	C1467	U1395	U1323	A1253	G1186	G1114	A1054
G2070	A2001	G1930	G1835	U1768	C1670	G1540	U1396	U1397	G1324	U1254	G1187	C1121	G
A2071	U1931	U1931	G1836	G1769	U1671	U1541	A1468	G1398		U1255	U1188	C1122	A
	A1932	A1932	C1837	G1770	U1672	G1542	A1470		C1327	G1256	A1189	G1123	U
G2074	G1933	G1933	C1838	G1771	G1674	A1543	A1471	C1403	U1329	C1257	G1190	C1124	G
U2075			G1839	G1772	C1675	C1544		C1404	G1330	G1259	G1192	G1125	U
			A1843	A1773	A1676	A1545	G1475	U1399	A1331	C1261	A1194	G1126	U
C2081	G2009	A1937	C1843	U1775	G1678	C1547		C1398	G1332	A1262	G1195	A1128	G
A2082	U1938	U1938	A1847	U1776	G1681	C1548	G1478	C1407	U1337	U1263	C1196	U1129	C
G2083	G2012	U1939	G1776	U1777	G1682	C1549	G1479	A1408	G1338	G1264	G1197	U1130	U
C2084	A2013	U1940	U1778	U1778	G1683	C1550		G1409	G1339	A1265	U1199	G1131	U
C2085	A2014	C1941	G1779	U1779	C1684	C1551	G1483	G1410	U1341	U1267	U1200	C1135	A
U2086	A2015	G1942	A1780	A1780	C1685		G1484			G1268	C1201	G1136	A
G2087	U2016	G1945	C1781	G1781	G1686	A1554	G1485	U1415			C1202	G1137	A
	U2017	U1946	C1782	C1782	C1687	G1555	A1486	G1416	G1344	G1271	G1203	G1138	G
U2092	A2020		G1858	A1783	U1621	C1556	G1487	C1417	C1345	U1272	A1204	G1139	C
G2093	G2021	G1949	A1859	A1784	G1622	C1557	G1488	A1418	G1346	U1273	C1205	C1140	A
A2094	U2022	G1950	G1860	A1785	G1623	C1558	U1489	A1419	G1347	U1274	G1206	U1141	G
C2095	G2023	U1951	C1861	A1786	G1624	A1559	U1490	U1420	A1348		C1207	U1142	C
G2096	A1952	A1952	G1862	A1787	C1625	G1560	G1491	G1421	A1349		C1208	A1142A	C
U2097	C2025	G1953	C1863	C1788	U1693	C1561	G1492	G1422		A1278	G1209	A1143	A
G2098	G1954	U1954	U1864	A1789	G1695	C1562	C1493	G1423	U1357	A1284	C1210	G1144	U
U2099	U2026		U1865	G1790	G1696	C1563	A1494	G1424	G1358	G1285	U1211		C
C2100	G2027	U1955	G1869	A1791	G1697	A1566	A1495	G1425	A1359	U1287	G1212	C1147	U
G2101	U2028	U1956	C1870	A1792	G1698	A1567	A1496	G1426	A1360				A
U2102	G2029		A1871	G1792	G1699	C1568	U1497	A1427					U
C2103	A2030	G1959	C1872	C1793	A1700	G1569	C1506	C1428			A1213		U
G2104	G2031		G1878	U1794		A1569	A1507	G1429	C1363	U1288		G1151	U
C2105	G2032	U1963	C1883	C1795	G1703	A1570	A1508	C1430	G1364	C1289	C1217	G1152	U
G2106	A2033	G1964		U1796	G1704	A1571	A1509	U1431	A1365	C1290	C1218	C1153	A
C2107		C1965	C1886	C1797	G1705	A1572	C1509	C1432	A1366	C1291	G1219	G1154	A
C2108	G2036	A1966	G1887	U1798	U1706	C1573	A1510	U1433	A1367	U1292	A1220	A1155	A
U2109	G2037	C1967	G1888	G1799	U1707	C1574	A1511	A1434	G1368	C1293	C1221	A1156	G
G2110	G2038	G1968	C1889	C1800	U1709	C1575	G1512	A1435	G1369	U1294	C1222	G1157	A
C2111	C2039	A1969	A1890	G1801	C1710	U1576	C1513	G1436	C1370	C1295	C1223		C
G2112	C2040	A1970	G1891	A1802		C1577	U1514	C1437	G1371	G1296	G1224	G1160	U
U2113		A1971	G1892	U1803	G1726	C1578	U1515	U1438	U1372		C1225	C1161	G
A2114	C2043	A1972	C1895	C1806	U1727	A1579	U1516	A1439	A1373			G1162	C
G2115		G1973		G1807	G1728	G1647	C1517	A1440	G1374	U1300	G1229A	G1163	G
A2117	G2048	C1974	U1898	A1729	G1729	G1648	C1518	G1441	C1375	C1301	C1230	G1164	U
U2118	C2050	G1975	G1899	U1730	U1730	G1649	G1519	G1442	G1376	A1302	G1231	U1165	A
A2119	A2051		A1900	G1811			U1520	G1443	G1377	G1303		C1166	A
G2120	G2052	A1981	C1902	G1814	G1731	C1585	G1521	A1444	A1378	C1304	G1235	U1167	U
C2121	C1982	C1982	A1815	G1815	U1732	A1586	G1522		A1379	C1305	G1236	G1168	A
A2054	G1983	C1983	G1816	G1816	G1750	A1587	G1523		G1380	G1306	A1237	G1169	G
G2055	G1904	G1904	C1816	G1816	C1751		G1524	G1448	G1381	A1307	G1238	G1170	C
G2124	G2056	G1985	A1819	A1819	C1752	U1590	G1525	A1449	G1382	A1308	G1239	G1171	U
G2125	A2057	A1986	U1820	U1820	C1756	G1591	G1526	G1449A	C1383	G1309	U1240	G1173	C
A2126	G2058		A1821	A1821	G1757	C1592	G1527		A1384	G1310	A1241	A1174	A
G2127	U2059	G1989	U1757	U1757	C1657	G1593	A1528		G1385	G1311	A1242	U1175	C
C2128	A2060	C1990	G1758	G1758	U1659	G1595	G1530	U1454	C1386	U1312	G1243	G1176	U



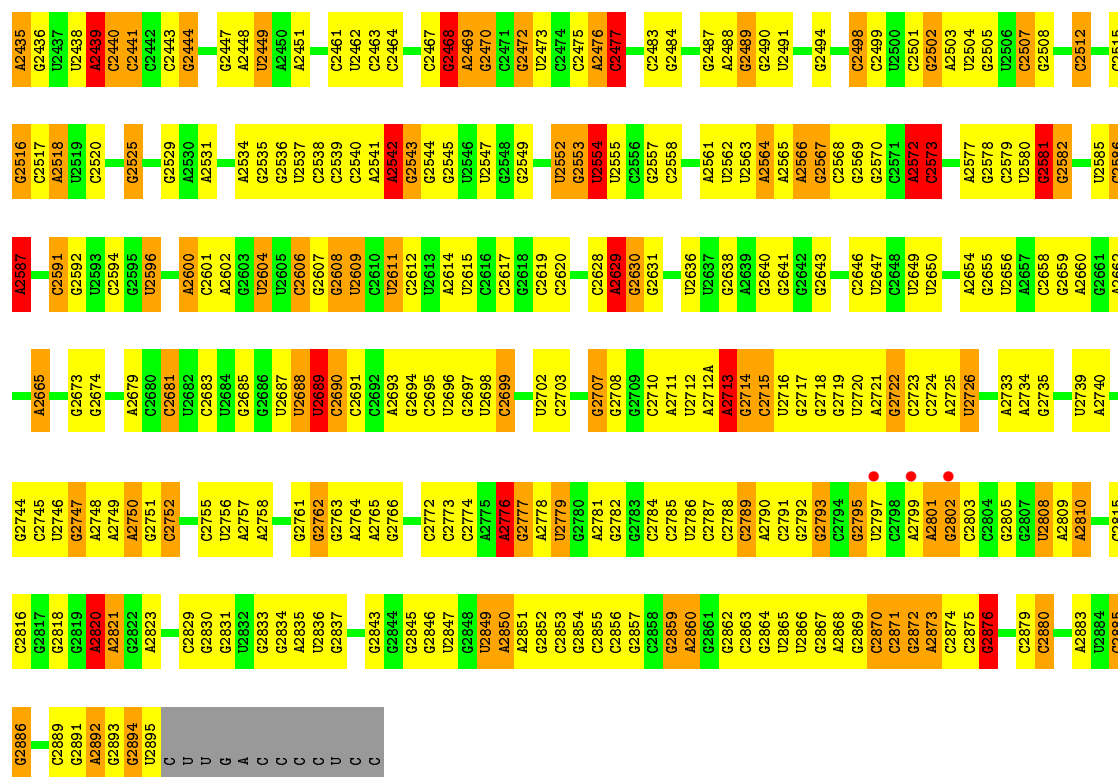
• Molecule 26: 23S ribosomal RNA

Chain 14: 35% 41% 17%

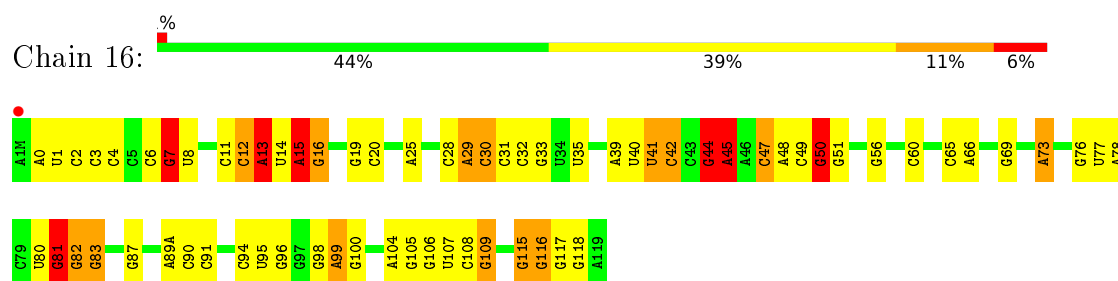




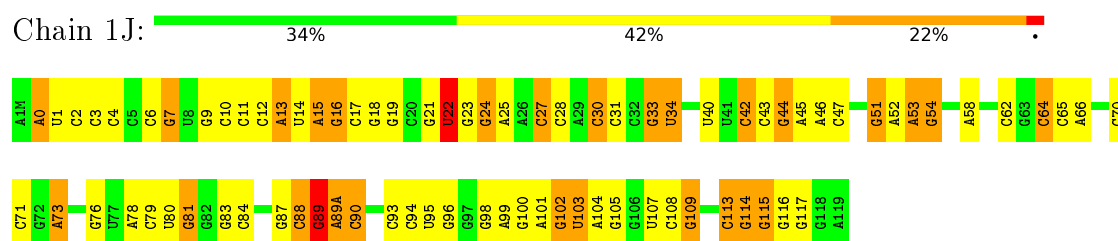
G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G3212	G3213	G3214	G3215	G3216	G3217	G3218	G3219	G3220	G3221	G3222	G3223	G3224	G3225	G3226	G3227	G3228	G3229	G3230	G3231	G3232	G3233	G3234	G3235	G3236	G3237	G3238	G3239	G3240	G3241	G3242	G3243	G3244	G3245	G3246	G3247	G3248	G3249	G3250	G3251	G3252	G3253	G3254	G3255	G3256	G3257	G3258	G3259	G3260	G3261	G3262	G3263	G3264	G3265	G3266	G3267	G3268	G3269	G3270	G3271	G3272	G3273	G3274	G3275	G3276	G3277	G3278	G3279	G3280	G3281	G3282	G3283	G3284	G3285	G3286	G3287	G3288	G3289	G3290	G3291	G3292	G3293	G3294	G3295	G3296	G3297	G3298	G3299	G3300	G3301	G3302	G3303	G3304	G3305	G3306	G3307	G3308	G3309	G3310	G3311	G3312	G3313	G3314	G3315	G3316	G3317	G3318	G3319	G3320	G3321	G3322	G3323	G3324	G3325	G3326	G3327	G3328	G3329	G3330	G3331	G3332	G3333	G3334	G3335	G3336	G3337	G3338	G3339	G3340	G3341	G3342	G3343	G3344	G3345	G3346	G3347	G3348	G3349	G3350	G3351	G3352	G3353	G3354	G3355	G3356	G3357	G3358	G3359	G3360	G3361	G3362	G3363	G3364	G3365	G3366	G3367	G3368	G3369	G3370	G3371	G3372	G3373	G3374	G3375	G3376	G3377	G3378	G3379	G3380	G3381	G3382	G3383	G3384	G3385	G3386	G3387	G3388	G3389	G3390	G3391	G3392	G3393	G3394	G3395	G3396	G3397	G3398	G3399	G3400	G3401	G3402	G3403	G3404	G3405	G3406	G3407	G3408	G3409	G3410	G3411	G3412	G3413	G3414	G3415	G3416	G3417	G3418	G3419	G3420	G3421	G3422	G3423	G3424	G3425	G3426	G3427	G3428	G3429	G3430	G3431	G3432	G3433	G3434	G3435	G3436	G3437	G3438	G3439	G3440	G3441	G3442	G3443	G3444	G3445	G3446	G3447	G3448	G3449	G3450	G3451	G3452	G3453	G3454	G3455	G3456	G3457	G3458	G3459	G3460	G3461	G3462	G3463	G3464	G3465	G3466	G3467	G3468	G3469	G3470	G3471	G3472	G3473	G3474	G3475	G3476	G3477	G3478	G3479	G3480	G3481	G3482	G3483	G3484	G3485	G3486	G3487	G3488	G3489	G3490	G3491	G3492	G3493	G3494	G3495	G3496	G3497	G3498	G3499	G3500	G3501	G3502	G3503	G3504	G3505	G3506	G3507	G3508	G3509	G3510	G3511	G3512	G3513	G3514	G3515	G3516	G3517	G3518	G3519	G3520	G3521	G3522	G3523	G3524	G3525	G3526	G3527	G3528	G3529	G3530	G3531	G3532	G3533	G3534	G3535	G3536	G3537	G3538	G3539	G3540	G3541	G3542	G3543	G3544	G3545	G3546	G3547	G3548	G3549	G3550	G3551	G3552	G3553	G3554	G3555	G3556	G3557	G3558	G3559	G3560	G3561	G3562	G3563	G3564	G3565	G3566	G3567	G3568	G3569	G3570	G3571	G3572	G3573	G3574	G3575	G3576	G3577	G3578	G3579	G3580	G3581	G3582	G3583	G3584	G3585	G3586	G3587	G3588	G3589	G3590	G3591	G3592	G3593	G3594	G3595	G3596	G3597	G3598	G3599	G3600	G3601	G3602	G3603	G3604	G3605	G3606	G3607	G3608	G3609	G3610	G3611	G3612	G3613	G3614	G3615	G3616	G3617	G3618	G3619	G3620	G3621	G3622	G3623	G3624	G3625	G3626	G3627	G3628	G3629	G3630	G3631	G3632	G3633	G3634	G3635	G3636	G3637	G3638	G3639	G3640	G3641	G3642	G3643	G3644	G3645	G3646	G3647	G3648	G3649	G3650	G3651	G3652	G3653	G3654	G3655	G3656	G3657	G3658	G3659	G3660	G3661	G3662	G3663	G3664	G3665	G3666	G3667	G3668	G3669	G3670	G3671	G3672	G3673	G3674	G3675	G3676	G3677	G3678	G3679	G3680	G3681	G3682	G3683	G3684	G3685	G3686	G3687	G3688	G3689	G3690	G3691	G3692	G3693	G3694	G3695	G3696	G3697	G3698	G3699	G3700	G3701	G3702	G3703	G3704	G3705	G3706	G3707	G3708	G3709	G3710	G3711	G3712	G3713	G3714	G3715	G3716	G3717	G3718	G3719	G3720	G3721	G3722	G3723	G3724	G3725	G3726	G3727	G3728	G3729	G3730	G3731	G3732	G3733	G3734	G3735	G3736	G3737	G3738	G3739	G3740	G3741	G3742	G3743	G3744	G374
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------



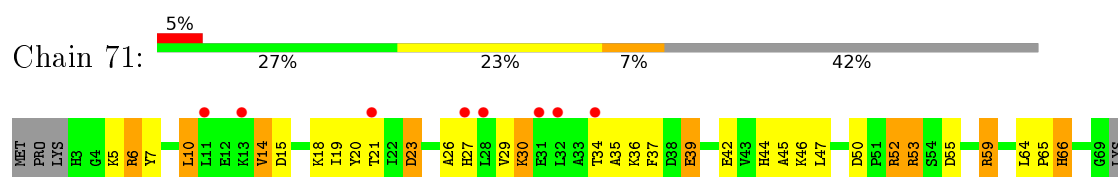
• Molecule 27: 5S ribosomal RNA

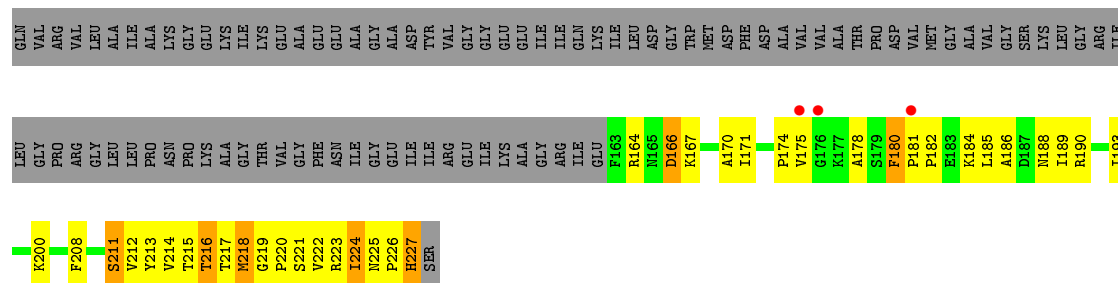


• Molecule 27: 5S ribosomal RNA



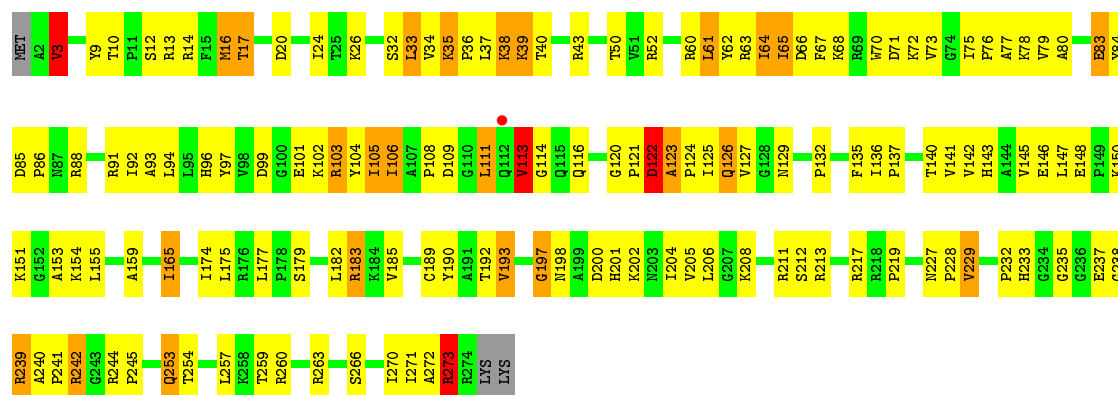
• Molecule 28: 50S ribosomal protein L1





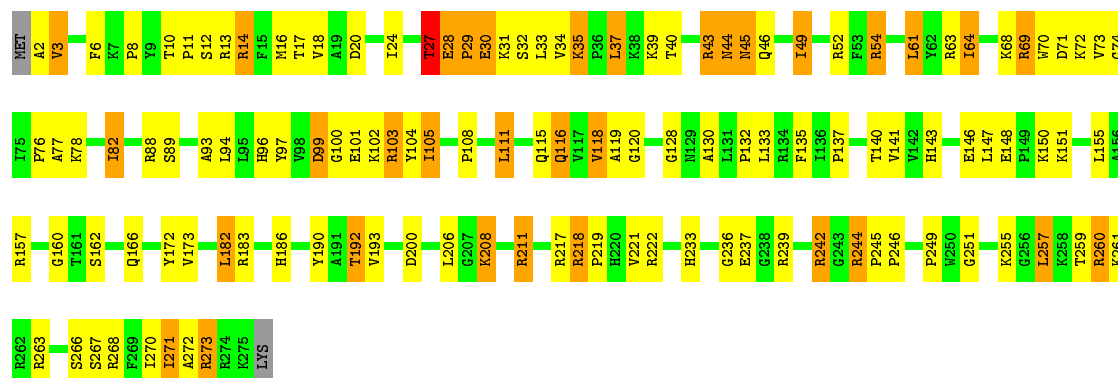
• Molecule 29: 50S ribosomal protein L2

Chain 11: 47% 42% 9% ..



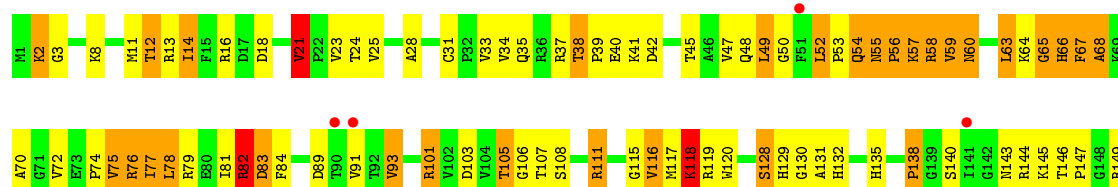
• Molecule 29: 50S ribosomal protein L2

Chain 19: 54% 33% 12% ..



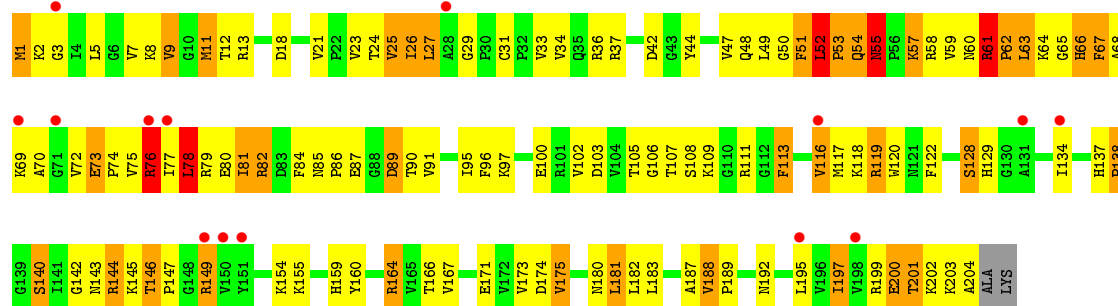
• Molecule 30: 50S ribosomal protein L3

Chain 21: 2% 44% 35% 17% ..

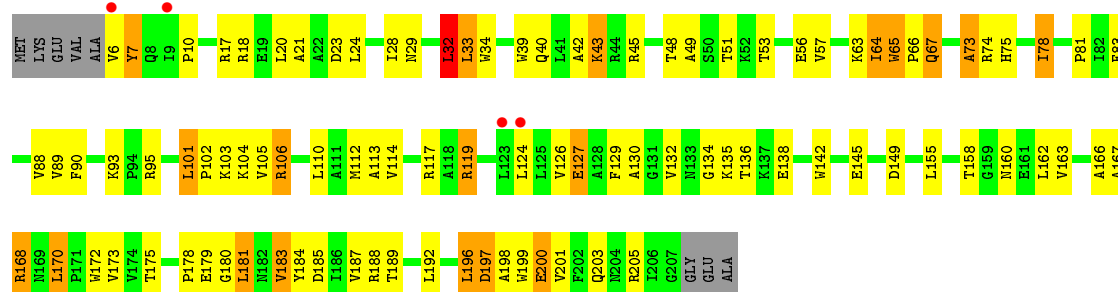




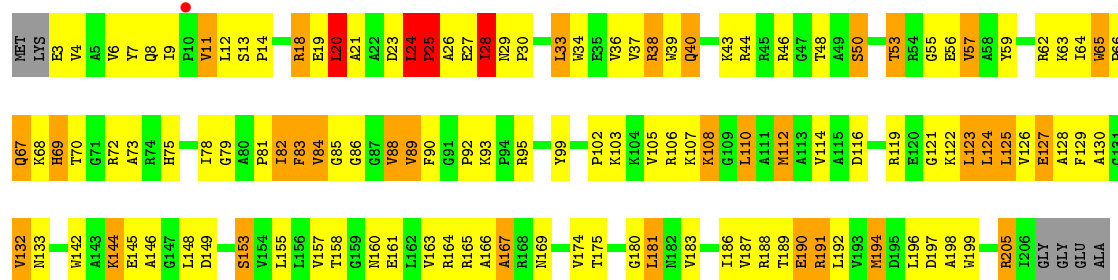
• Molecule 30: 50S ribosomal protein L3



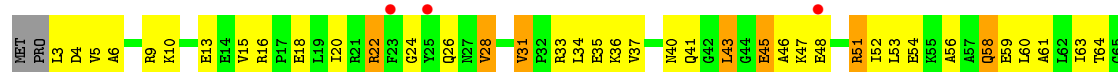
• Molecule 31: 50S ribosomal protein L4

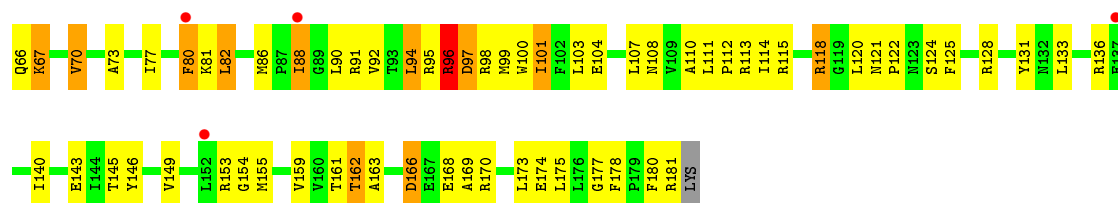


• Molecule 31: 50S ribosomal protein L4

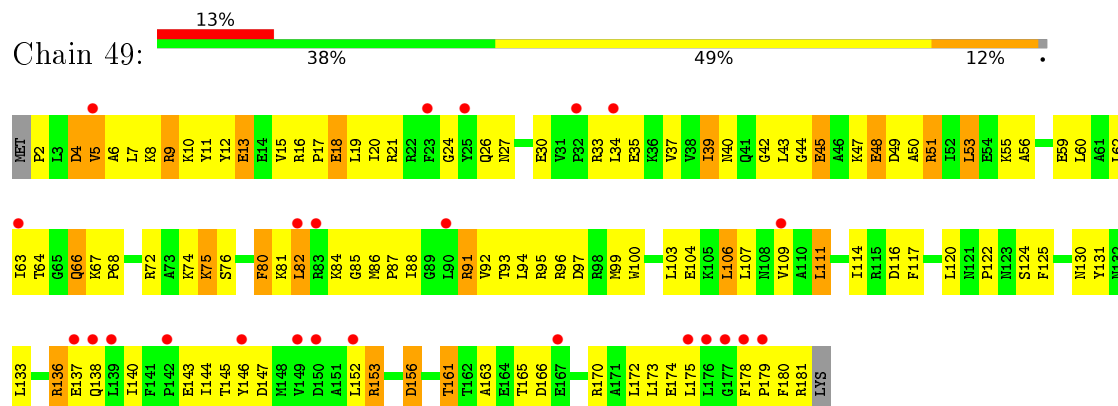


• Molecule 32: 50S ribosomal protein L5

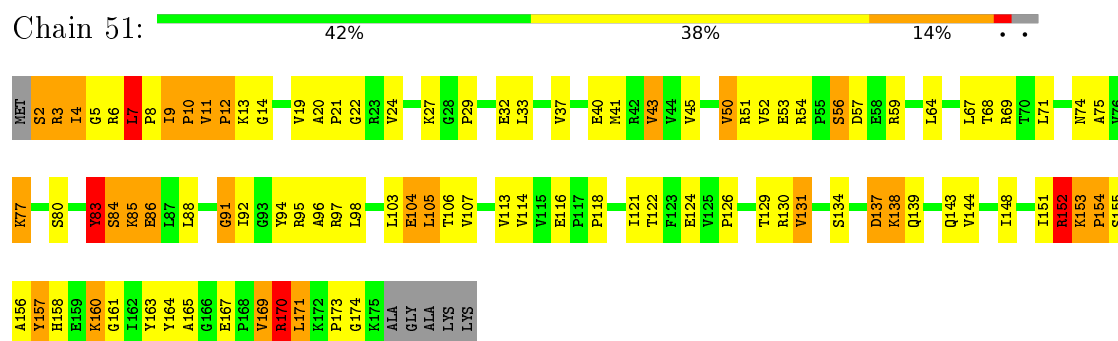




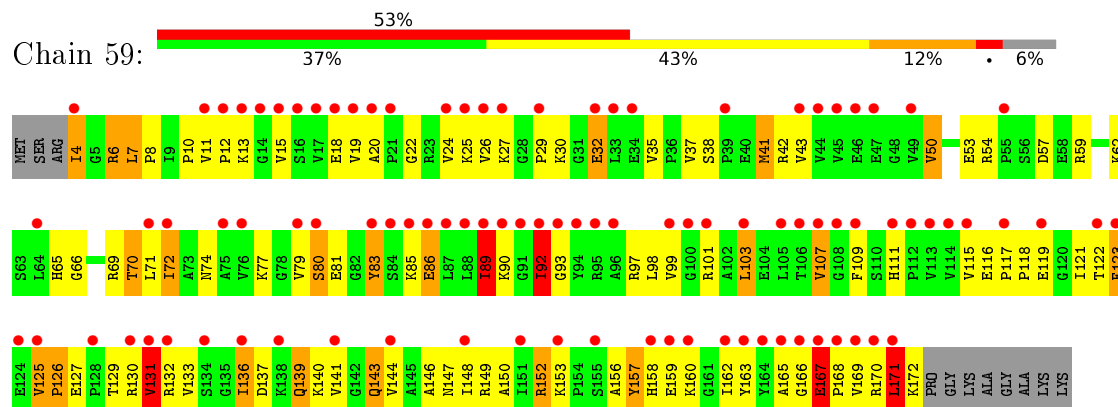
• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6

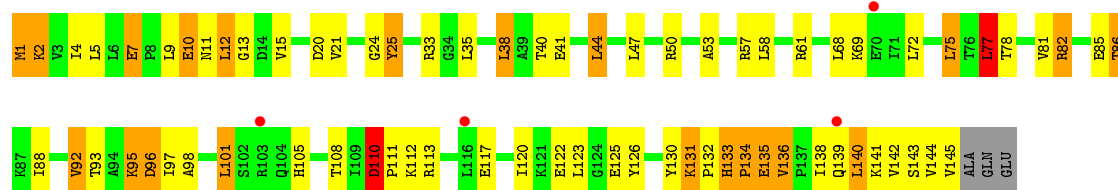


• Molecule 33: 50S ribosomal protein L6

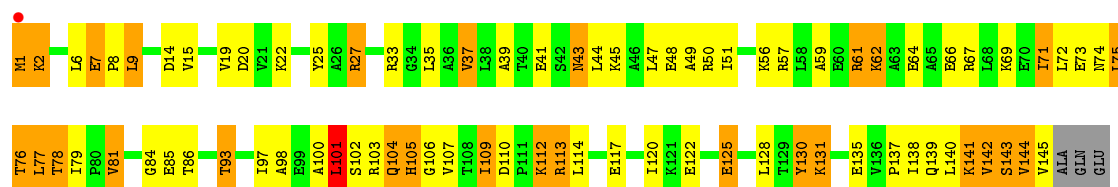
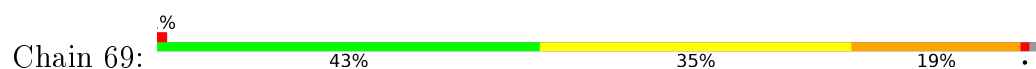


• Molecule 34: 50S ribosomal protein L9

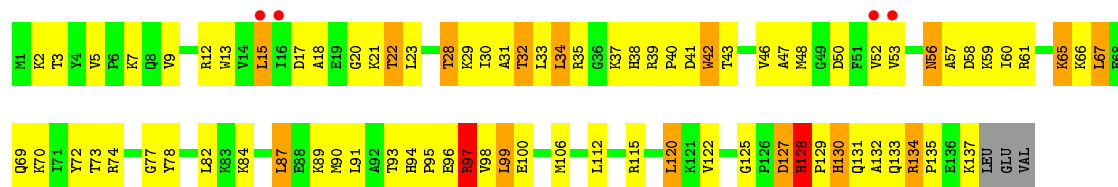




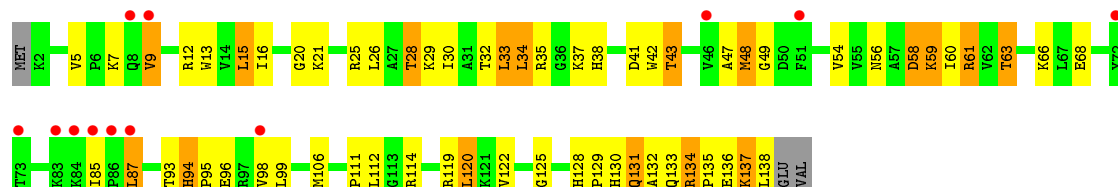
• Molecule 34: 50S ribosomal protein L9



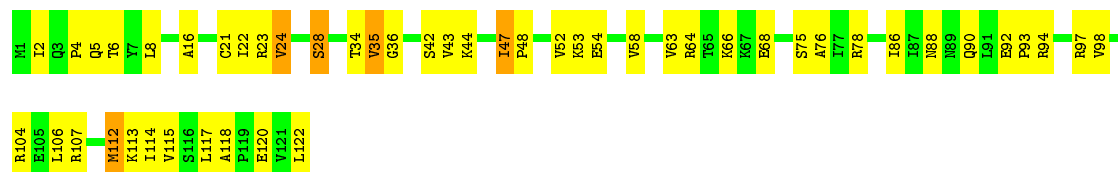
• Molecule 35: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L13

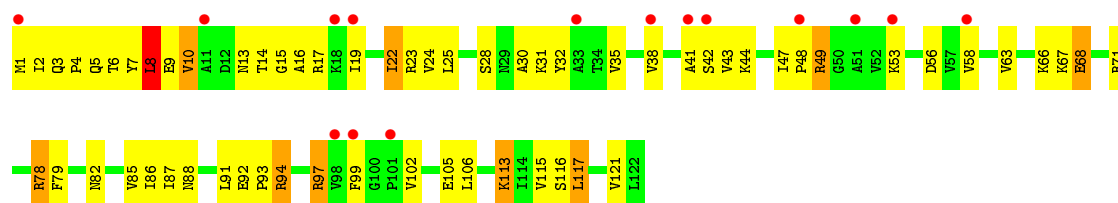


• Molecule 36: 50S ribosomal protein L14



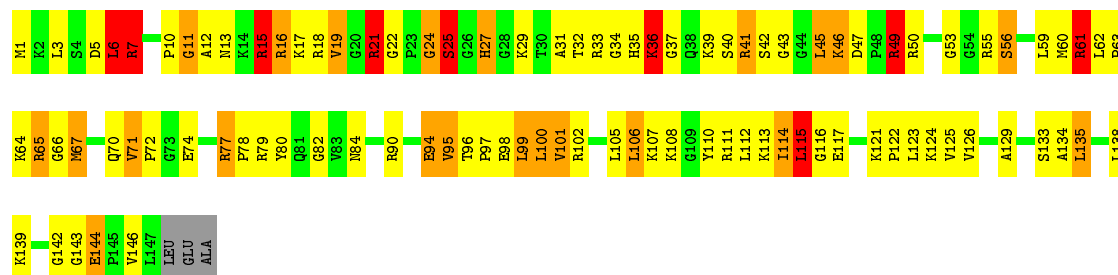
• Molecule 36: 50S ribosomal protein L14





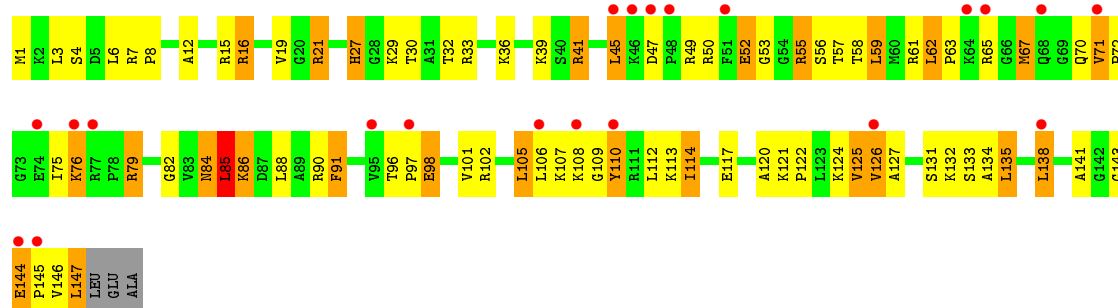
• Molecule 37: 50S ribosomal protein L15

Chain 78: 33% 44% 15% 6%



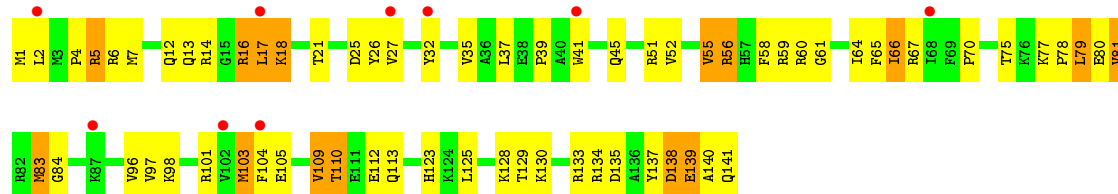
• Molecule 37: 50S ribosomal protein L15

Chain 35: 14% 43% 37% 17%



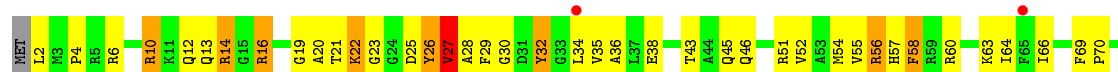
• Molecule 38: 50S ribosomal protein L16

Chain 88: 6% 52% 37% 11%



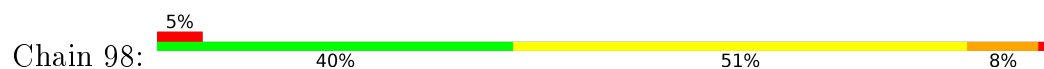
• Molecule 38: 50S ribosomal protein L16

Chain 45: 2% 41% 43% 13%

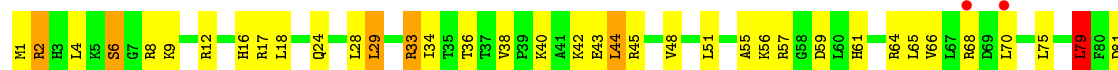




• Molecule 39: 50S ribosomal protein L17



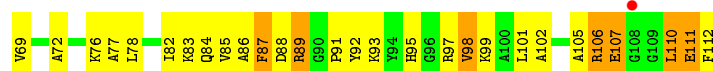
• Molecule 39: 50S ribosomal protein L17



• Molecule 40: 50S ribosomal protein L18

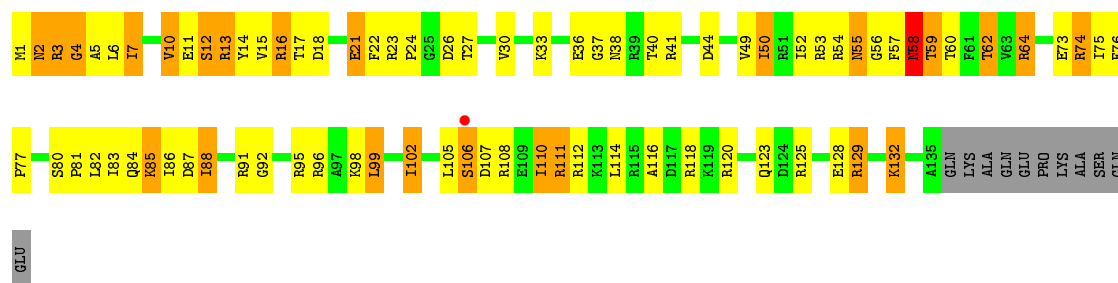


• Molecule 40: 50S ribosomal protein L18

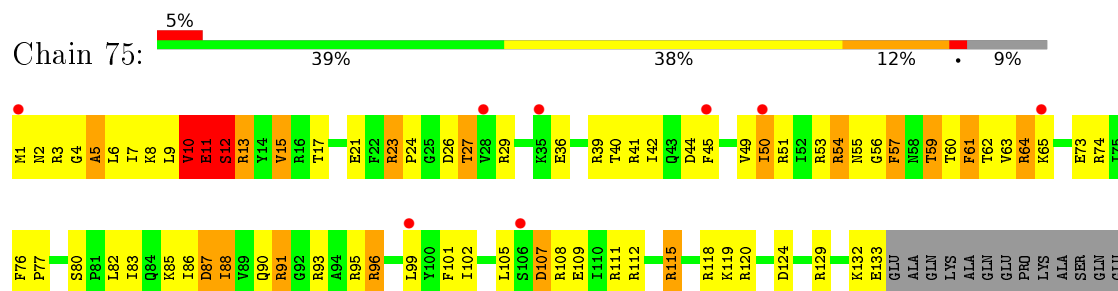


• Molecule 41: 50S ribosomal protein L19

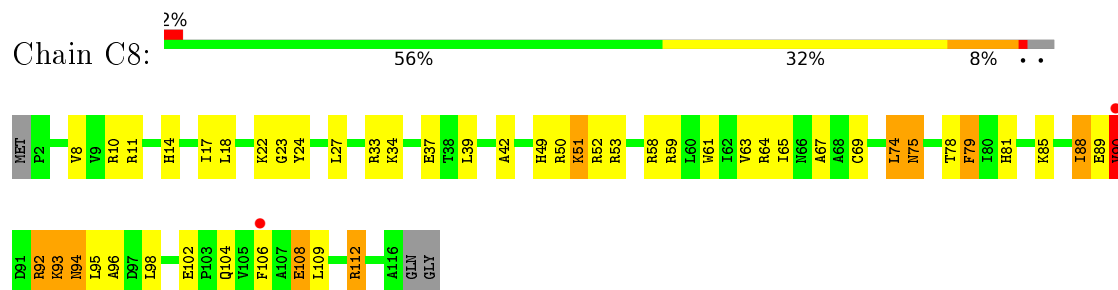




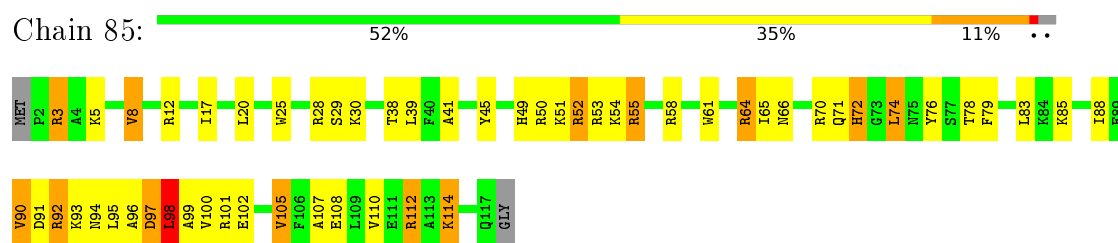
- Molecule 41: 50S ribosomal protein L19



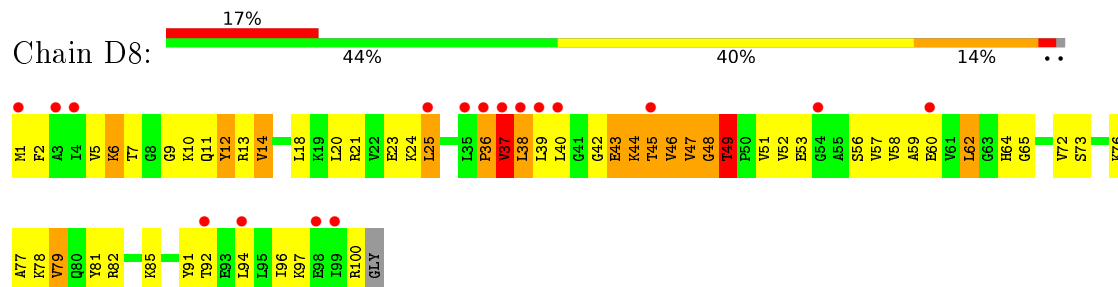
- Molecule 42: 50S ribosomal protein L20



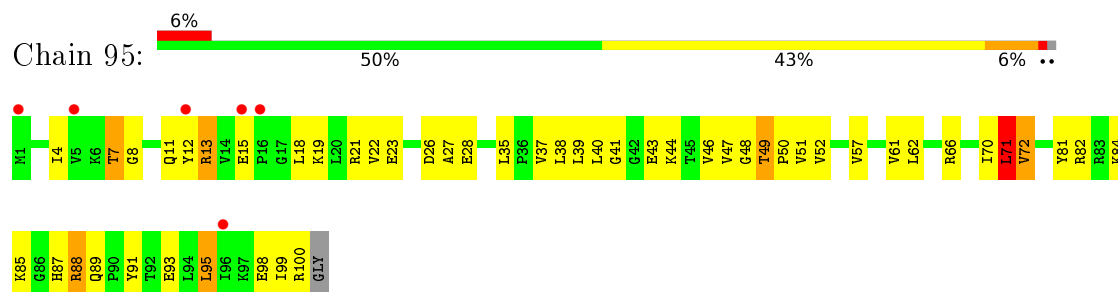
- Molecule 42: 50S ribosomal protein L20



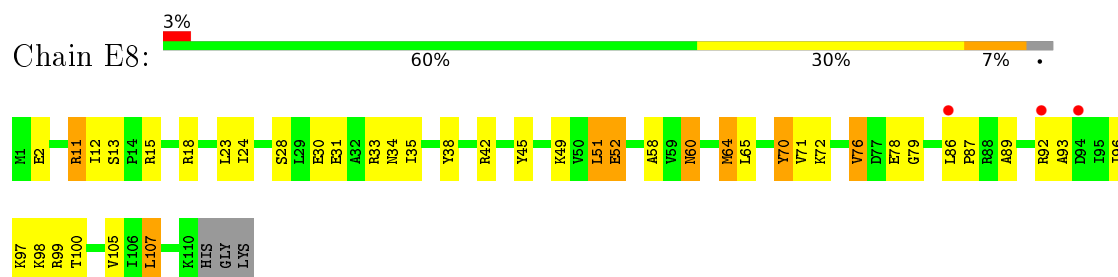
- Molecule 43: 50S ribosomal protein L21



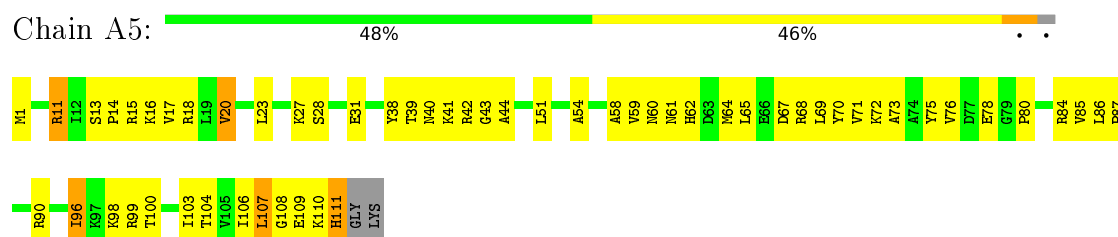
- Molecule 43: 50S ribosomal protein L21



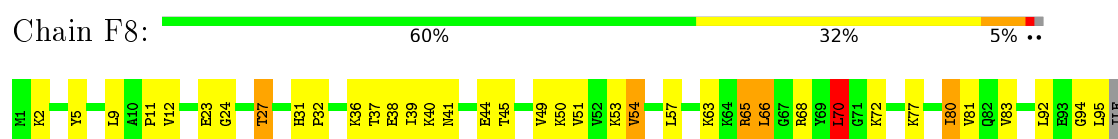
- Molecule 44: 50S ribosomal protein L22



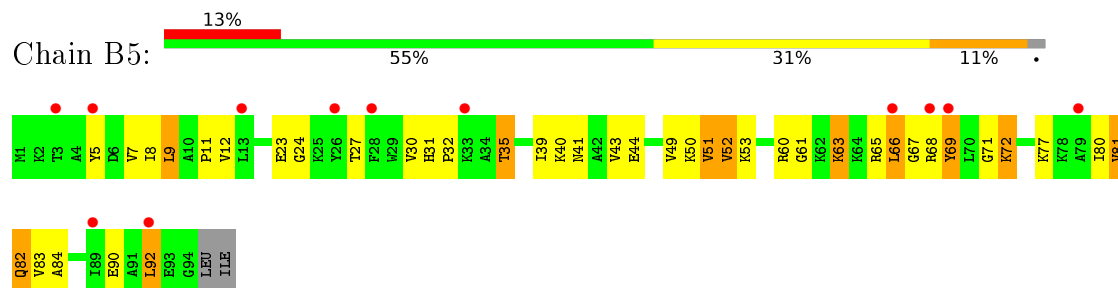
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23

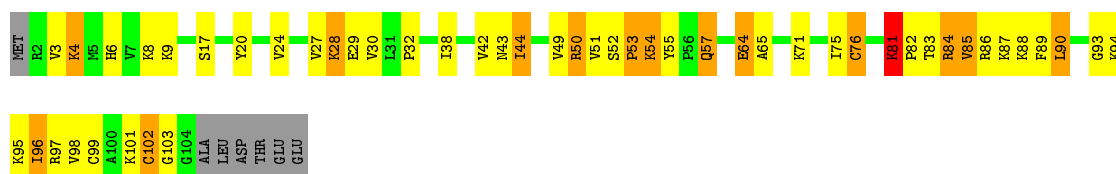


- Molecule 45: 50S ribosomal protein L23

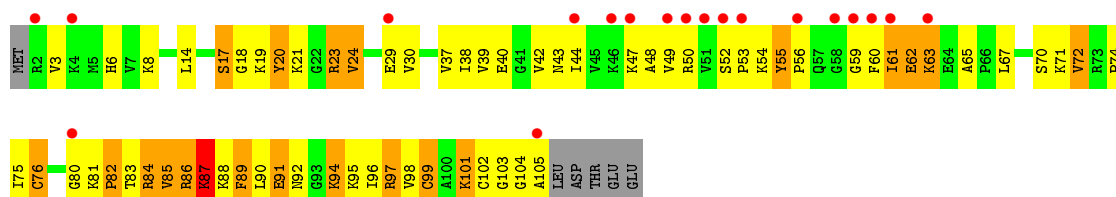


- Molecule 46: 50S ribosomal protein L24

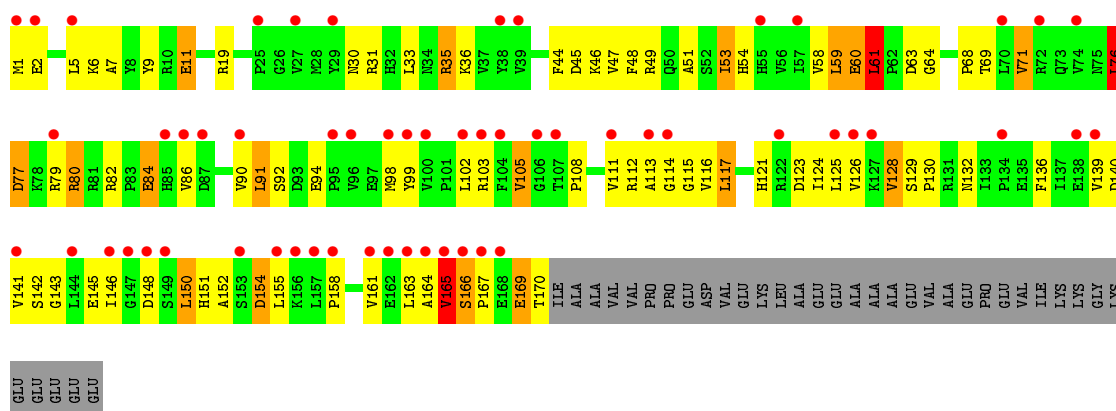




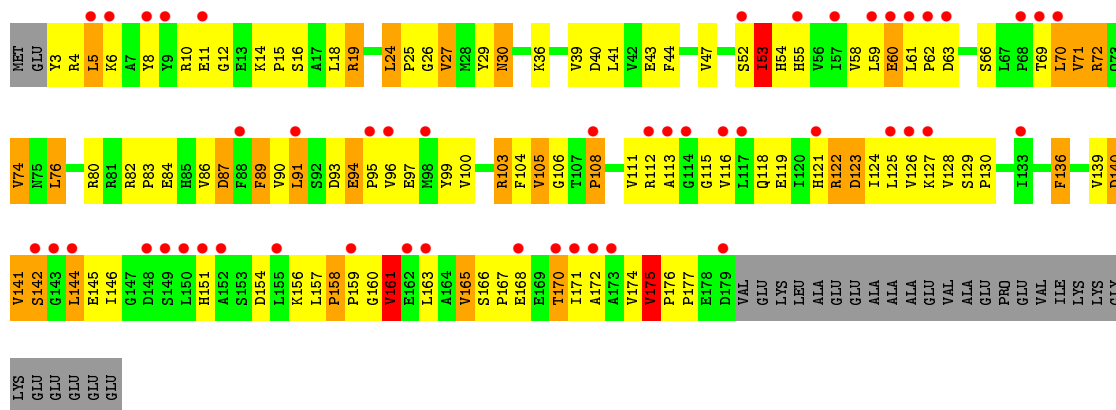
• Molecule 46: 50S ribosomal protein L24



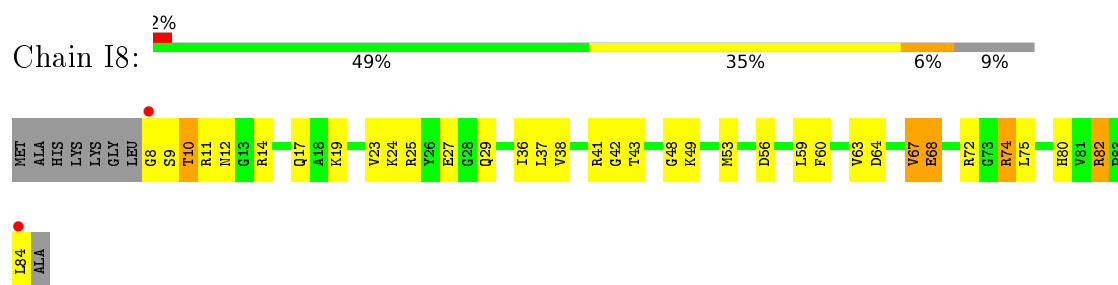
• Molecule 47: 50S ribosomal protein L25



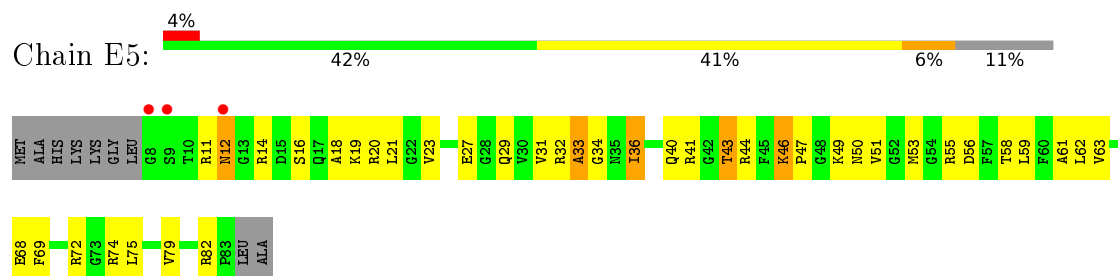
• Molecule 47: 50S ribosomal protein L25



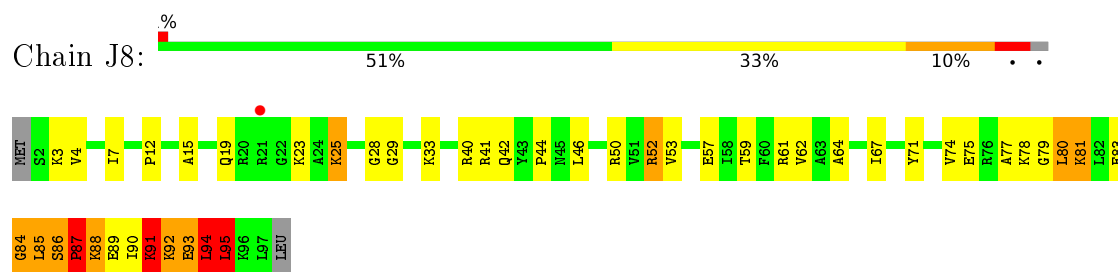
• Molecule 48: 50S ribosomal protein L27



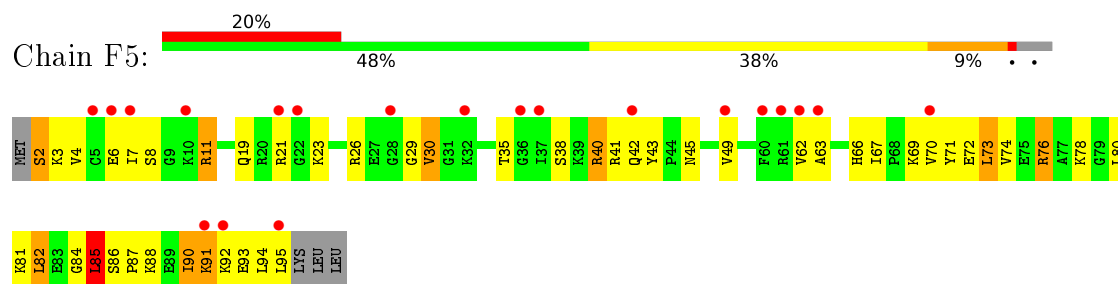
- Molecule 48: 50S ribosomal protein L27



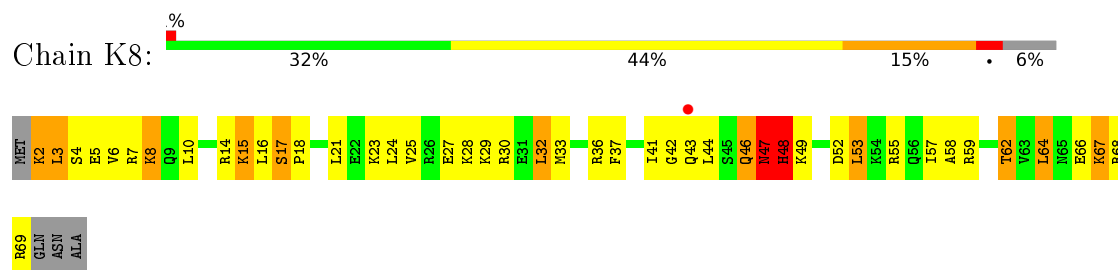
- Molecule 49: 50S ribosomal protein L28



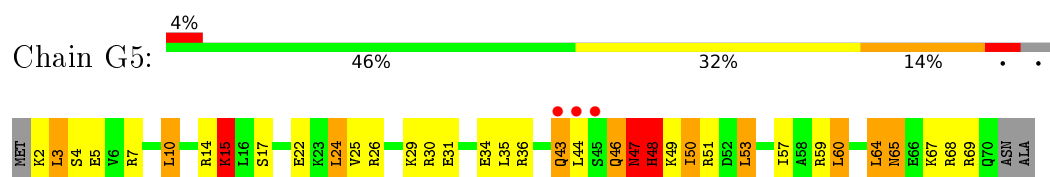
- Molecule 49: 50S ribosomal protein L28



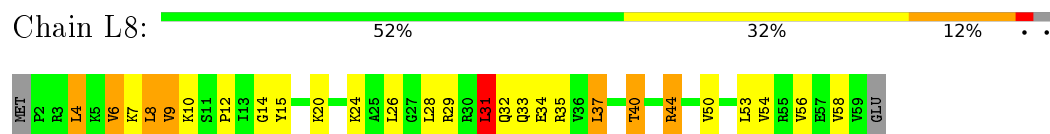
- Molecule 50: 50S ribosomal protein L29



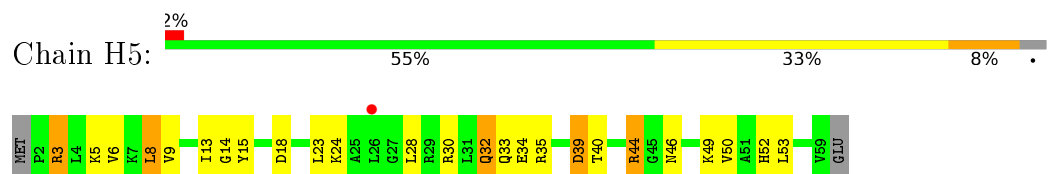
- Molecule 50: 50S ribosomal protein L29



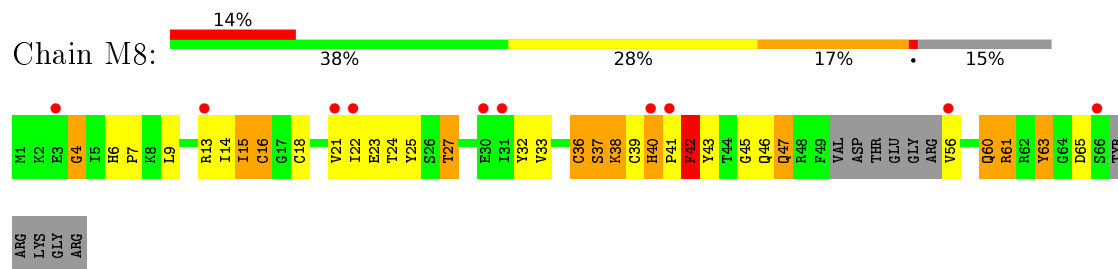
- Molecule 51: 50S ribosomal protein L30



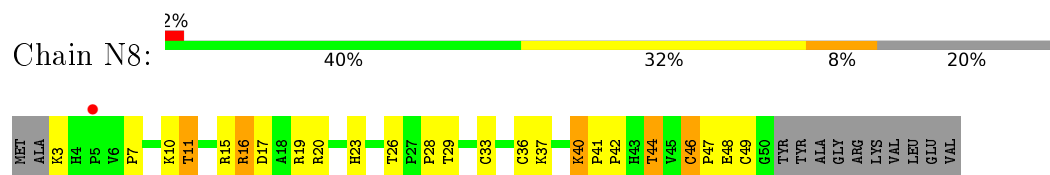
- Molecule 51: 50S ribosomal protein L30



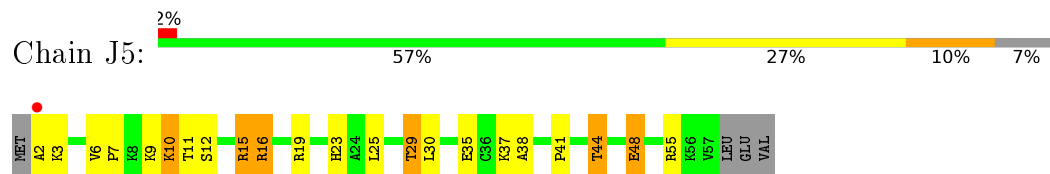
- Molecule 52: 50S ribosomal protein L31



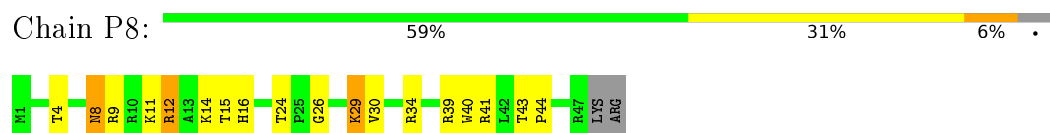
- Molecule 53: 50S ribosomal protein L32



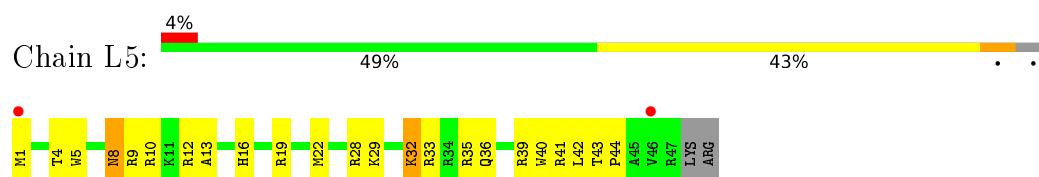
- Molecule 53: 50S ribosomal protein L32



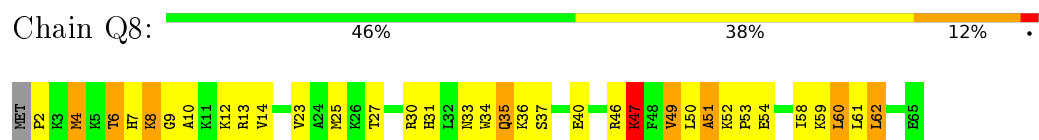
- Molecule 54: 50S ribosomal protein L34



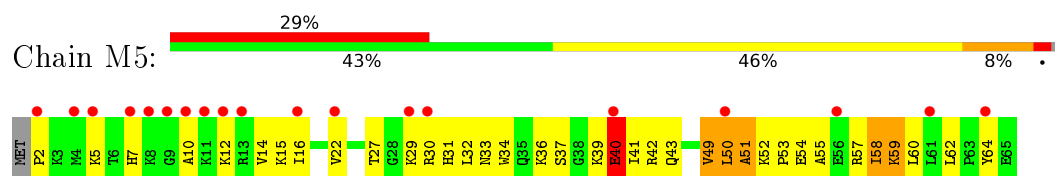
- Molecule 54: 50S ribosomal protein L34



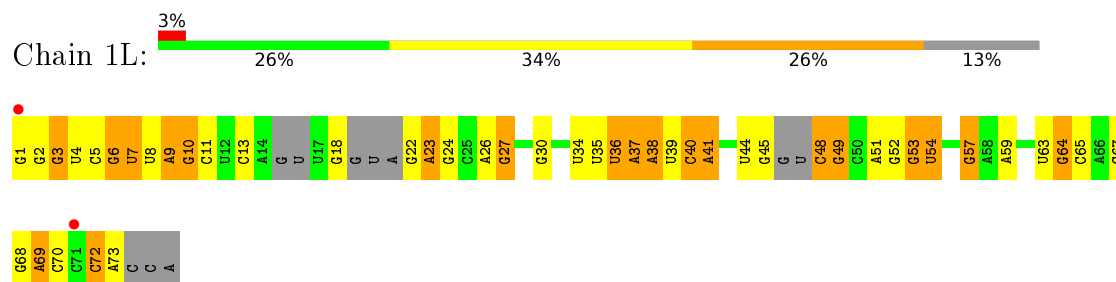
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA^{Lys}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.15Å 448.16Å 617.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.45 – 3.13 161.54 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.45-3.13) 90.9 (161.54-3.13)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.244 0.190 , 0.241	Depositor DCC
R_{free} test set	1833 reflections (0.20%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296999	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, U8U, H2U, 7MG, SF4, MG, 4SU, T6A, SPE, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.67	3/36095 (0.0%)	1.26	206/56332 (0.4%)
1	1G	0.60	2/36309 (0.0%)	1.18	153/56668 (0.3%)
2	12	0.38	0/1727	0.64	2/2326 (0.1%)
2	1E	0.40	0/1908	0.62	2/2573 (0.1%)
3	22	0.47	1/1560 (0.1%)	0.58	0/2104
3	2E	0.44	1/1629 (0.1%)	0.60	1/2195 (0.0%)
4	32	0.41	0/1732	0.60	0/2318
4	3E	0.49	1/1728 (0.1%)	0.64	3/2313 (0.1%)
5	42	0.40	0/1156	0.62	0/1557
5	4E	0.40	0/1158	0.61	0/1559
6	52	0.45	0/855	0.61	1/1154 (0.1%)
6	5E	0.47	0/850	0.61	0/1147
7	62	0.39	0/1122	0.56	0/1500
7	6E	0.40	0/1259	0.51	0/1686
8	72	0.38	0/1127	0.59	0/1517
8	7E	0.40	0/1135	0.61	0/1527
9	82	0.36	0/971	0.62	0/1304
9	8E	0.38	0/1019	0.61	0/1367
10	1A	0.93	2/658 (0.3%)	0.57	0/885
10	1I	0.37	0/762	0.61	0/1027
11	2A	0.40	0/850	0.60	0/1150
11	2I	0.43	0/838	0.62	0/1133
12	3A	0.48	0/963	0.69	1/1290 (0.1%)
12	3I	0.57	0/972	0.76	0/1301
13	4A	0.34	0/889	0.58	0/1192
13	4I	0.46	0/943	0.65	0/1265
14	5A	0.40	0/495	0.66	0/657
14	5I	0.49	0/495	0.74	1/657 (0.2%)
15	6A	0.39	0/740	0.56	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.41	0/721	0.63	0/970
16	7I	0.40	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.48	0/847	0.66	0/1131
18	9A	0.44	0/549	0.64	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.71	0/700
19	AI	0.40	0/676	0.72	1/910 (0.1%)
20	BA	0.37	0/764	0.66	1/1007 (0.1%)
20	BI	0.36	0/748	0.60	1/986 (0.1%)
21	1B	0.37	0/192	0.58	0/252
21	1F	0.43	0/203	0.62	0/266
22	1K	0.57	0/1568	1.21	10/2434 (0.4%)
23	2K	0.73	0/1721	1.30	11/2682 (0.4%)
23	2L	0.67	1/1721 (0.1%)	1.17	4/2682 (0.1%)
24	3K	0.49	0/1654	1.14	11/2570 (0.4%)
24	3L	0.53	0/1705	1.15	12/2650 (0.5%)
25	4K	0.79	0/499	1.32	5/778 (0.6%)
25	4L	0.67	0/473	1.32	3/737 (0.4%)
26	14	0.84	35/68159 (0.1%)	1.43	876/106398 (0.8%)
26	1H	0.99	95/68309 (0.1%)	1.56	1280/106631 (1.2%)
27	16	0.74	0/2928	1.41	33/4568 (0.7%)
27	1J	0.65	0/2928	1.31	16/4568 (0.4%)
28	71	0.30	0/1049	0.54	0/1417
29	11	0.64	1/2170 (0.0%)	0.85	2/2926 (0.1%)
29	19	0.62	1/2175 (0.0%)	0.79	2/2933 (0.1%)
30	21	0.57	0/1579	0.90	5/2131 (0.2%)
30	29	0.56	0/1596	0.82	2/2153 (0.1%)
31	31	0.62	0/1620	0.84	1/2194 (0.0%)
31	39	0.53	1/1637 (0.1%)	0.80	1/2218 (0.0%)
32	41	0.43	0/1481	0.67	0/1994
32	49	0.45	1/1483 (0.1%)	0.62	1/1997 (0.1%)
33	51	0.52	0/1354	0.85	2/1833 (0.1%)
33	59	0.38	0/1320	0.68	2/1787 (0.1%)
34	61	0.43	0/1146	0.71	2/1551 (0.1%)
34	69	0.48	1/1146 (0.1%)	0.68	1/1551 (0.1%)
35	15	0.42	0/1123	0.64	0/1515
35	58	0.51	0/1123	0.76	1/1514 (0.1%)
36	25	0.52	0/942	0.72	1/1269 (0.1%)
36	68	0.57	0/942	0.73	0/1269
37	35	0.52	0/1139	0.78	1/1514 (0.1%)
37	78	0.62	1/1139 (0.1%)	0.96	4/1514 (0.3%)
38	45	0.55	0/1120	0.82	0/1498
38	88	0.61	0/1138	0.90	1/1523 (0.1%)
39	55	0.50	0/981	0.77	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	98	0.48	0/981	0.79	1/1312 (0.1%)
40	65	0.46	0/886	0.75	1/1180 (0.1%)
40	A8	0.53	0/891	0.78	1/1187 (0.1%)
41	75	0.51	0/1123	0.76	1/1500 (0.1%)
41	B8	0.55	0/1133	0.76	1/1514 (0.1%)
42	85	0.46	0/977	0.67	1/1301 (0.1%)
42	C8	0.59	0/968	0.76	1/1289 (0.1%)
43	95	0.46	0/781	0.79	1/1048 (0.1%)
43	D8	0.58	0/785	0.75	1/1052 (0.1%)
44	A5	0.53	0/897	0.69	0/1204
44	E8	0.56	0/886	0.75	0/1189
45	B5	0.56	0/749	0.73	0/1007
45	F8	0.62	0/764	0.80	1/1025 (0.1%)
46	C5	0.64	0/807	0.86	1/1076 (0.1%)
46	G8	0.65	0/796	0.94	2/1062 (0.2%)
47	D5	0.72	1/1443 (0.1%)	0.65	0/1960
47	H8	0.43	0/1395	0.73	2/1890 (0.1%)
48	E5	0.49	0/611	0.73	0/814
48	I8	0.62	0/619	0.81	0/825
49	F5	0.52	0/744	0.84	1/989 (0.1%)
49	J8	0.66	0/754	0.95	3/1003 (0.3%)
50	G5	0.51	0/578	0.70	0/766
50	K8	0.61	0/577	0.93	1/763 (0.1%)
51	H5	0.48	0/464	0.64	0/623
51	L8	0.48	0/464	0.77	1/623 (0.2%)
52	M8	0.45	0/485	0.78	0/652
53	J5	0.49	0/448	0.74	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.52	0/409	0.76	0/540
54	P8	0.67	0/409	0.88	1/540 (0.2%)
55	M5	0.65	0/524	0.85	0/691
55	Q8	0.60	0/524	0.90	1/691 (0.1%)
56	1L	0.47	1/1516 (0.1%)	0.95	1/2350 (0.0%)
All	All	0.74	149/316848 (0.0%)	1.26	2688/474550 (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	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	5
4	3E	0	1
8	72	0	1
9	82	0	2
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	3
13	4I	0	3
14	5A	0	1
16	7I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	3
20	BI	0	1
29	11	0	4
29	19	0	2
30	21	0	7
30	29	0	5
31	39	0	8
32	49	0	2
33	51	0	6
33	59	0	4
34	61	0	3
34	69	0	4
35	15	0	1
35	58	0	1
37	35	0	1
37	78	0	6
38	45	0	2
38	88	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	3
43	D8	0	3
44	A5	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
45	B5	0	2
46	C5	0	3
46	G8	0	3
47	D5	0	4
47	H8	0	5
49	F5	0	1
49	J8	0	3
50	G5	0	3
50	K8	0	3
52	M8	0	4
55	M5	0	4
55	Q8	0	2
All	All	0	151

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	D5	94	GLU	C-N	23.32	1.78	1.34
10	1A	38	ILE	C-N	19.43	1.71	1.34
26	1H	2430	A	N9-C4	-14.21	1.29	1.37
26	1H	774	A	N9-C4	-13.66	1.29	1.37
3	22	173	VAL	C-N	12.84	1.58	1.34

The worst 5 of 2688 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-18.59	114.85	126.00
26	1H	1332	G	C5-N7-C8	-17.78	95.41	104.30
26	1H	1332	G	C2-N3-C4	-17.15	103.32	111.90
26	1H	676	A	C2-N3-C4	-16.45	102.38	110.60
26	1H	783	A	C2-N3-C4	-16.44	102.38	110.60

There are no chirality outliers.

5 of 151 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide
2	1E	9	GLU	Peptide
4	3E	29	PRO	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	32246	0	16276	858	0
1	1G	32437	0	16372	887	2
2	12	1696	0	1730	94	0
2	1E	1874	0	1926	99	0
3	22	1537	0	1603	87	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1765	98	0
4	3E	1698	0	1761	84	0
5	42	1141	0	1198	41	0
5	4E	1142	0	1204	54	0
6	52	842	0	857	34	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	66	0
7	6E	1242	0	1286	54	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	75	0
9	8E	1000	0	1031	61	0
10	1A	646	0	662	41	0
10	1I	749	0	767	45	0
11	2A	835	0	847	27	0
11	2I	823	0	832	41	0
12	3A	947	0	1033	37	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	67	0
13	4I	933	0	992	51	0
14	5A	486	0	525	34	0
14	5I	486	0	524	28	0
15	6A	729	0	768	27	0
15	6I	729	0	768	31	0
16	7A	705	0	725	29	0
16	7I	700	0	720	49	0
17	8A	823	0	891	32	0
17	8I	834	0	904	62	0
18	9A	544	0	605	23	0
18	9I	549	0	607	23	0
19	AA	510	0	507	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	38	0
20	BA	762	0	861	40	0
20	BI	746	0	843	45	0
21	1B	188	0	195	11	0
21	1F	199	0	208	12	0
22	1K	1542	0	790	43	0
23	2K	1646	0	843	36	0
23	2L	1646	0	845	32	0
24	3K	1483	0	756	67	0
24	3L	1528	0	778	48	0
25	4K	442	0	219	9	0
25	4L	419	0	208	23	0
26	14	60857	0	30679	1311	1
26	1H	60991	0	30744	1358	1
27	16	2617	0	1328	56	0
27	1J	2617	0	1328	84	0
28	71	1027	0	1043	66	0
29	11	2120	0	2197	121	0
29	19	2125	0	2199	108	0
30	21	1546	0	1602	94	0
30	29	1563	0	1629	110	0
31	31	1585	0	1632	87	0
31	39	1602	0	1649	97	0
32	41	1457	0	1514	76	0
32	49	1459	0	1507	73	0
33	51	1328	0	1396	77	0
33	59	1295	0	1366	74	0
34	61	1131	0	1218	44	0
34	69	1131	0	1218	58	0
35	15	1096	0	1168	56	0
35	58	1096	0	1169	67	0
36	25	932	0	996	48	0
36	68	932	0	996	38	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	99	0
38	45	1099	0	1154	74	0
38	88	1117	0	1168	55	0
39	55	967	0	1033	47	0
39	98	967	0	1033	51	0
40	65	876	0	938	55	0
40	A8	881	0	943	55	0
41	75	1109	0	1170	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	B8	1119	0	1177	71	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	55	0
43	95	770	0	838	41	0
43	D8	774	0	849	42	0
44	A5	886	0	948	35	0
44	E8	876	0	941	27	0
45	B5	735	0	785	32	0
45	F8	750	0	814	33	0
46	C5	794	0	885	61	0
46	G8	783	0	869	48	0
47	D5	1411	0	1436	83	0
47	H8	1365	0	1391	60	0
48	E5	603	0	620	40	0
48	I8	611	0	631	32	0
49	F5	737	0	813	43	0
49	J8	747	0	817	35	0
50	G5	576	0	625	33	0
50	K8	575	0	634	45	0
51	H5	459	0	512	15	0
51	L8	459	0	512	22	0
52	M8	475	0	465	34	0
53	J5	434	0	454	23	0
53	N8	369	0	388	21	0
54	L5	401	0	436	21	0
54	P8	401	0	436	13	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1402	0	715	32	0
57	13	141	0	0	0	0
57	14	460	0	0	0	0
57	16	12	0	0	0	0
57	19	1	0	0	0	0
57	1G	125	0	0	0	0
57	1H	552	0	0	0	0
57	1J	10	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2I	1	0	0	0	0
57	2K	3	0	0	0	0
57	2L	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	31	1	0	0	0	0
57	32	1	0	0	0	0
57	35	2	0	0	0	0
57	39	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	2	0	0	0	0
57	45	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	B5	1	0	0	0	0
57	E5	2	0	0	0	0
57	F8	1	0	0	0	0
57	I8	2	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	32	8	0	0	2	0
58	3E	8	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	14	13	0	24	0	0
60	1G	13	0	22	3	0
61	11	10	0	0	6	0
61	13	354	0	0	20	0
61	14	1303	0	0	91	0
61	15	3	0	0	0	0
61	16	12	0	0	1	0
61	19	14	0	0	1	0
61	1A	2	0	0	0	0
61	1G	364	0	0	24	0
61	1H	1720	0	0	128	0
61	1I	2	0	0	0	0
61	1J	27	0	0	1	0
61	1K	1	0	0	0	0
61	21	6	0	0	1	0
61	25	8	0	0	0	0
61	29	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2A	1	0	0	0	0
61	2K	8	0	0	0	0
61	2L	8	0	0	0	0
61	31	6	0	0	0	0
61	32	4	0	0	1	0
61	35	8	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4A	2	0	0	0	0
61	4E	3	0	0	2	0
61	4K	5	0	0	0	0
61	4L	3	0	0	0	0
61	52	4	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5I	1	0	0	0	0
61	68	2	0	0	0	0
61	6A	3	0	0	0	0
61	75	1	0	0	0	0
61	78	13	0	0	4	0
61	7A	4	0	0	0	0
61	7I	2	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	98	1	0	0	2	0
61	9A	2	0	0	0	0
61	B5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	3	0	0	0	0
61	BI	3	0	0	1	0
61	C5	3	0	0	0	0
61	C8	4	0	0	0	0
61	E8	1	0	0	0	0
61	F5	1	0	0	0	0
61	F8	3	0	0	1	0
61	G8	3	0	0	0	0
61	H5	1	0	0	2	0
61	I8	6	0	0	0	0
61	J8	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	L5	1	0	0	0	0
61	L8	4	0	0	0	0
61	M5	8	0	0	2	0
61	N8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296999	0	196564	8532	2

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

The worst 5 of 8532 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)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.39
47:D5:94:GLU:C	47:D5:95:PRO:N	1.78	1.36
38:45:27:VAL:HB	38:45:28:ALA:HA	1.16	1.08
26:1H:1604:C:OP2	61:1H:3655:HOH:O	1.75	1.04
8:72:12:ARG:HH21	8:72:27:PRO:HD3	1.22	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	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	203/256 (79%)	173 (85%)	23 (11%)	7 (3%)	5 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	186 (82%)	39 (17%)	2 (1%)	21	62
3	22	191/239 (80%)	172 (90%)	19 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	34	74
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	34	74
4	3E	205/209 (98%)	193 (94%)	11 (5%)	1 (0%)	34	74
5	42	148/162 (91%)	142 (96%)	5 (3%)	1 (1%)	26	67
5	4E	147/162 (91%)	136 (92%)	10 (7%)	1 (1%)	26	67
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	134/156 (86%)	125 (93%)	8 (6%)	1 (1%)	26	67
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	13	48
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	26	67
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	24	64
9	8E	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	83 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	99 (89%)	10 (9%)	2 (2%)	11	43
11	2I	109/129 (84%)	93 (85%)	11 (10%)	5 (5%)	3	18
12	3A	119/132 (90%)	101 (85%)	14 (12%)	4 (3%)	5	25
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	24	64
13	4A	107/126 (85%)	89 (83%)	17 (16%)	1 (1%)	21	62
13	4I	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	21	62
14	5A	57/61 (93%)	49 (86%)	7 (12%)	1 (2%)	11	43
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	4	25
15	6A	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
15	6I	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	4 (4%)	1 (1%)	19	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	64 (98%)	1 (2%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	13	48
19	AA	59/93 (63%)	49 (83%)	7 (12%)	3 (5%)	2	16
19	AI	80/93 (86%)	69 (86%)	7 (9%)	4 (5%)	3	16
20	BA	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	9	38
20	BI	95/106 (90%)	83 (87%)	12 (13%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	7I	128/229 (56%)	121 (94%)	7 (6%)	0	100	100
29	11	271/276 (98%)	255 (94%)	10 (4%)	6 (2%)	8	37
29	19	272/276 (99%)	248 (91%)	21 (8%)	3 (1%)	17	56
30	21	201/206 (98%)	160 (80%)	28 (14%)	13 (6%)	1	10
30	29	202/206 (98%)	150 (74%)	40 (20%)	12 (6%)	2	12
31	31	200/210 (95%)	177 (88%)	22 (11%)	1 (0%)	34	74
31	39	202/210 (96%)	159 (79%)	36 (18%)	7 (4%)	4	25
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	11	44
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	30	70
33	51	172/180 (96%)	139 (81%)	23 (13%)	10 (6%)	2	12
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	4	24
34	61	143/148 (97%)	123 (86%)	18 (13%)	2 (1%)	14	50
34	69	143/148 (97%)	112 (78%)	28 (20%)	3 (2%)	9	38
35	15	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
35	58	135/140 (96%)	114 (84%)	16 (12%)	5 (4%)	4	24
36	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	120 (83%)	25 (17%)	0	100	100
37	78	145/150 (97%)	113 (78%)	21 (14%)	11 (8%)	1	7
38	45	136/141 (96%)	110 (81%)	23 (17%)	3 (2%)	8	37
38	88	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	3	19
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	21	62
39	98	116/118 (98%)	101 (87%)	15 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	65	108/112 (96%)	87 (81%)	19 (18%)	2 (2%)	10	41
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	62
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	13	48
41	B8	133/146 (91%)	118 (89%)	14 (10%)	1 (1%)	24	64
42	85	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
42	C8	113/118 (96%)	107 (95%)	2 (2%)	4 (4%)	4	25
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	5	28
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	28
44	A5	109/113 (96%)	101 (93%)	8 (7%)	0	100	100
44	E8	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
45	B5	92/96 (96%)	82 (89%)	8 (9%)	2 (2%)	8	37
45	F8	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	22 (22%)	6 (6%)	2	12
46	G8	101/110 (92%)	83 (82%)	14 (14%)	4 (4%)	4	21
47	D5	175/206 (85%)	133 (76%)	32 (18%)	10 (6%)	2	13
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	20
48	E5	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	14	50
48	I8	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
49	F5	92/98 (94%)	81 (88%)	10 (11%)	1 (1%)	17	56
49	J8	94/98 (96%)	80 (85%)	9 (10%)	5 (5%)	2	15
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	5	29
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	3	18
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	39 (70%)	17 (30%)	0	100	100
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	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%)	51 (82%)	11 (18%)	0	100	100
55	Q8	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11086/12104 (92%)	9718 (88%)	1167 (10%)	201 (2%)	11	43

5 of 201 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
29	11	239	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	179/220 (81%)	144 (80%)	35 (20%)	1	7
2	1E	200/220 (91%)	158 (79%)	42 (21%)	1	6
3	22	154/188 (82%)	123 (80%)	31 (20%)	1	7
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	7
4	32	180/181 (99%)	152 (84%)	28 (16%)	3	14
4	3E	180/181 (99%)	146 (81%)	34 (19%)	2	8
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	4
5	4E	115/123 (94%)	90 (78%)	25 (22%)	1	6
6	52	90/90 (100%)	78 (87%)	12 (13%)	5	20
6	5E	90/90 (100%)	73 (81%)	17 (19%)	2	8
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	7
7	6E	125/127 (98%)	105 (84%)	20 (16%)	3	13
8	72	118/119 (99%)	101 (86%)	17 (14%)	4	17
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	92/99 (93%)	73 (79%)	19 (21%)	1	6
9	8E	97/99 (98%)	70 (72%)	27 (28%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	54 (76%)	17 (24%)	1	3
10	1I	81/92 (88%)	75 (93%)	6 (7%)	17	51
11	2A	85/99 (86%)	71 (84%)	14 (16%)	3	12
11	2I	84/99 (85%)	66 (79%)	18 (21%)	1	6
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	7
12	3I	103/109 (94%)	76 (74%)	27 (26%)	0	2
13	4A	90/101 (89%)	68 (76%)	22 (24%)	1	3
13	4I	94/101 (93%)	67 (71%)	27 (29%)	0	1
14	5A	49/50 (98%)	40 (82%)	9 (18%)	2	9
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9	33
15	6I	79/80 (99%)	68 (86%)	11 (14%)	4	19
16	7A	72/74 (97%)	64 (89%)	8 (11%)	8	30
16	7I	72/74 (97%)	58 (81%)	14 (19%)	2	8
17	8A	94/97 (97%)	80 (85%)	14 (15%)	4	16
17	8I	95/97 (98%)	80 (84%)	15 (16%)	3	13
18	9A	58/77 (75%)	49 (84%)	9 (16%)	3	14
18	9I	58/77 (75%)	50 (86%)	8 (14%)	4	19
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	4
19	AI	72/80 (90%)	57 (79%)	15 (21%)	1	6
20	BA	76/82 (93%)	68 (90%)	8 (10%)	8	32
20	BI	75/82 (92%)	67 (89%)	8 (11%)	8	31
21	1B	17/22 (77%)	16 (94%)	1 (6%)	24	60
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	5
28	7I	108/181 (60%)	87 (81%)	21 (19%)	2	8
29	11	214/218 (98%)	172 (80%)	42 (20%)	1	7
29	19	214/218 (98%)	167 (78%)	47 (22%)	1	5
30	21	162/166 (98%)	124 (76%)	38 (24%)	1	4
30	29	165/166 (99%)	125 (76%)	40 (24%)	1	3
31	31	161/166 (97%)	130 (81%)	31 (19%)	2	8
31	39	163/166 (98%)	123 (76%)	40 (24%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	120 (78%)	33 (22%)	1	6
32	49	152/156 (97%)	117 (77%)	35 (23%)	1	4
33	51	143/148 (97%)	109 (76%)	34 (24%)	1	3
33	59	140/148 (95%)	101 (72%)	39 (28%)	0	1
34	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	116/119 (98%)	91 (78%)	25 (22%)	1	6
35	58	116/119 (98%)	92 (79%)	24 (21%)	1	6
36	25	100/100 (100%)	82 (82%)	18 (18%)	2	9
36	68	100/100 (100%)	89 (89%)	11 (11%)	8	30
37	35	114/116 (98%)	76 (67%)	38 (33%)	0	0
37	78	114/116 (98%)	77 (68%)	37 (32%)	0	1
38	45	109/111 (98%)	82 (75%)	27 (25%)	1	3
38	88	110/111 (99%)	91 (83%)	19 (17%)	2	11
39	55	101/101 (100%)	86 (85%)	15 (15%)	4	16
39	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
40	65	87/88 (99%)	67 (77%)	20 (23%)	1	4
40	A8	87/88 (99%)	61 (70%)	26 (30%)	0	1
41	75	117/127 (92%)	85 (73%)	32 (27%)	0	1
41	B8	117/127 (92%)	84 (72%)	33 (28%)	0	1
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	11
42	C8	92/94 (98%)	80 (87%)	12 (13%)	5	21
43	95	81/82 (99%)	66 (82%)	15 (18%)	2	9
43	D8	82/82 (100%)	54 (66%)	28 (34%)	0	0
44	A5	91/92 (99%)	72 (79%)	19 (21%)	1	6
44	E8	90/92 (98%)	76 (84%)	14 (16%)	3	14
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	6
45	F8	77/78 (99%)	67 (87%)	10 (13%)	5	21
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
46	G8	84/91 (92%)	67 (80%)	17 (20%)	1	7
47	D5	156/179 (87%)	118 (76%)	38 (24%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	128 (85%)	23 (15%)	3	15
48	E5	61/67 (91%)	55 (90%)	6 (10%)	10	36
48	I8	62/67 (92%)	56 (90%)	6 (10%)	10	36
49	F5	79/83 (95%)	64 (81%)	15 (19%)	2	8
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	15
50	G5	63/67 (94%)	47 (75%)	16 (25%)	1	2
50	K8	64/67 (96%)	47 (73%)	17 (27%)	0	2
51	H5	50/52 (96%)	37 (74%)	13 (26%)	0	2
51	L8	50/52 (96%)	41 (82%)	9 (18%)	2	9
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	1
53	J5	48/52 (92%)	38 (79%)	10 (21%)	1	6
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	6
54	L5	38/42 (90%)	31 (82%)	7 (18%)	2	9
54	P8	38/42 (90%)	31 (82%)	7 (18%)	2	9
55	M5	54/55 (98%)	44 (82%)	10 (18%)	2	9
55	Q8	54/55 (98%)	43 (80%)	11 (20%)	1	6
All	All	9354/10012 (93%)	7424 (79%)	1930 (21%)	1	6

5 of 1930 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	1	MET
5	42	31	LEU
45	B5	66	LEU
48	I8	67	VAL
55	Q8	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
44	E8	40	ASN
55	Q8	31	HIS
30	29	54	GLN
41	B8	58	ASN
29	19	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1500/1522 (98%)	349 (23%)	39 (2%)
1	1G	1508/1522 (99%)	354 (23%)	40 (2%)
22	1K	69/76 (90%)	29 (42%)	5 (7%)
23	2K	76/77 (98%)	24 (31%)	2 (2%)
23	2L	76/77 (98%)	20 (26%)	1 (1%)
24	3K	67/76 (88%)	39 (58%)	2 (2%)
24	3L	69/76 (90%)	32 (46%)	2 (2%)
25	4K	19/30 (63%)	11 (57%)	2 (10%)
25	4L	18/30 (60%)	13 (72%)	1 (5%)
26	14	2820/2917 (96%)	664 (23%)	45 (1%)
26	1H	2824/2917 (96%)	601 (21%)	36 (1%)
27	16	121/122 (99%)	22 (18%)	3 (2%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
56	1L	62/76 (81%)	27 (43%)	4 (6%)
All	All	9350/9640 (96%)	2218 (23%)	184 (1%)

5 of 2218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2210	G
1	1G	466	C
26	14	2275	C
26	1H	2756	U
1	1G	87	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	H2U	1K	17	22	17,21,22	2.18	4 (23%)	23,30,33	2.71	5 (21%)
22	U8U	1K	34	25,22	15,24,25	2.53	4 (26%)	17,34,37	1.95	2 (11%)
22	T6A	1K	37	22	23,34,35	2.55	4 (17%)	26,49,52	3.57	8 (30%)
22	PSU	1K	39	22	15,21,22	0.95	1 (6%)	16,30,33	1.93	4 (25%)
22	5MU	1K	54	22	13,22,23	1.73	2 (15%)	16,32,35	1.79	1 (6%)
22	PSU	1K	55	22	15,21,22	1.08	1 (6%)	16,30,33	2.16	4 (25%)
56	5MU	1L	54	56	13,22,23	1.70	2 (15%)	16,32,35	1.40	1 (6%)
56	PSU	1L	55	56	15,21,22	1.07	1 (6%)	16,30,33	2.16	3 (18%)
23	OMC	2K	33	23	15,22,23	2.11	4 (26%)	20,31,34	1.68	3 (15%)
23	7MG	2K	47	23	20,26,27	3.50	7 (35%)	23,39,42	2.71	8 (34%)
23	5MU	2K	55	23	13,22,23	1.67	2 (15%)	16,32,35	1.43	1 (6%)
23	PSU	2K	56	23	15,21,22	1.05	2 (13%)	16,30,33	1.87	3 (18%)
23	4SU	2K	8	23	12,21,22	2.92	2 (16%)	15,30,33	0.87	1 (6%)
23	OMC	2L	33	23	15,22,23	2.25	4 (26%)	20,31,34	1.72	2 (10%)
23	7MG	2L	47	23	20,26,27	3.39	6 (30%)	23,39,42	2.36	7 (30%)
23	5MU	2L	55	23	13,22,23	1.72	2 (15%)	16,32,35	1.45	1 (6%)
23	PSU	2L	56	23	15,21,22	1.27	2 (13%)	16,30,33	2.15	4 (25%)
23	4SU	2L	8	23	12,21,22	3.35	2 (16%)	15,30,33	0.89	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/3/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2K	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C5-C4	-5.72	1.24	1.39
23	2L	47	7MG	C5-C4	-5.51	1.24	1.39
22	1K	17	H2U	C6-N1	-3.84	1.42	1.47
23	2K	55	5MU	C4-N3	-3.19	1.27	1.33
23	2L	55	5MU	C4-N3	-3.16	1.27	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	T6A	N3-C2-N1	-12.10	119.37	128.87
23	2L	47	7MG	C5-C4-N3	-7.93	118.67	126.74
23	2K	47	7MG	C5-C4-N3	-6.38	120.24	126.74
22	1K	34	U8U	C5-C4-N3	-6.21	119.62	125.19
22	1K	17	H2U	C4-N3-C2	-6.12	120.22	125.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	T6A	1	0
22	1K	54	5MU	3	0
56	1L	54	5MU	2	0
23	2K	33	OMC	1	0
23	2K	47	7MG	6	0
23	2K	55	5MU	5	0
23	2K	8	4SU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	33	OMC	3	0
23	2L	47	7MG	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1345 ligands modelled in this entry, 1341 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	$\# Z > 2$
60	SPE	14	3458	-	12,12,12	0.46	0	11,11,11	0.77	0
60	SPE	1G	1725	1	12,12,12	0.43	0	11,11,11	0.75	0
58	SF4	32	302	-	0,12,12	0.00	-	0,24,24	0.00	-
58	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
60	SPE	14	3458	-	-	0/10/10/10	0/0/0/0
60	SPE	1G	1725	1	-	0/10/10/10	0/0/0/0
58	SF4	32	302	-	-	0/0/48/48	0/6/5/5
58	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1G	1725	SPE	3	0
58	32	302	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
47	D5	1
10	1A	1
56	1L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1L	72:C	O3'	73:A	P	3.48
1	D5	94:GLU	C	95:PRO	N	1.78
1	1A	38:ILE	C	39:PRO	N	1.71
1	69	79:ILE	C	80:PRO	N	1.17
1	3E	36:ARG	C	37:PRO	N	1.15

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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 ²)	Q<0.9
1	13	1500/1522 (98%)	-0.52	0 100 100	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.47	3 (0%) 95 91	76, 123, 193, 253	0
2	12	207/256 (80%)	0.29	15 (7%) 18 7	139, 165, 185, 196	0
2	1E	231/256 (90%)	-0.07	5 (2%) 65 44	118, 145, 172, 180	0
3	22	195/239 (81%)	0.76	28 (14%) 3 1	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.34	11 (5%) 29 12	97, 117, 144, 155	0
4	32	208/209 (99%)	-0.32	0 100 100	104, 123, 142, 149	0
4	3E	207/209 (99%)	-0.20	1 (0%) 91 84	93, 118, 137, 144	0
5	42	150/162 (92%)	-0.23	0 100 100	106, 123, 139, 146	0
5	4E	149/162 (91%)	-0.06	0 100 100	87, 109, 128, 133	0
6	52	101/101 (100%)	-0.42	0 100 100	93, 110, 124, 135	0
6	5E	100/101 (99%)	-0.01	1 (1%) 84 70	92, 111, 127, 135	0
7	62	138/156 (88%)	0.84	13 (9%) 11 4	122, 135, 145, 151	0
7	6E	154/156 (98%)	1.00	29 (18%) 2 1	111, 127, 155, 174	0
8	72	137/138 (99%)	-0.07	2 (1%) 76 59	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.80	16 (11%) 6 2	102, 117, 129, 139	0
9	82	121/128 (94%)	1.36	28 (23%) 1 0	118, 161, 171, 178	0
9	8E	126/128 (98%)	-0.11	2 (1%) 74 56	96, 141, 159, 165	0
10	1A	80/105 (76%)	0.35	9 (11%) 7 2	122, 152, 167, 170	0
10	1I	94/105 (89%)	1.43	26 (27%) 1 0	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.78	13 (11%) 6 2	91, 116, 131, 138	0
11	2I	111/129 (86%)	1.39	30 (27%) 1 0	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.68	18 (14%) 3 1	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.12	4 (3%) 50 27	81, 89, 110, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.22	15 (13%) 4 2	125, 152, 170, 187	0
13	4I	117/126 (92%)	-0.05	3 (2%) 59 38	97, 125, 138, 145	0
14	5A	59/61 (96%)	2.06	26 (44%) 0 0	131, 146, 164, 167	0
14	5I	59/61 (96%)	0.51	3 (5%) 32 13	92, 106, 121, 129	0
15	6A	87/89 (97%)	-0.54	0 100 100	93, 117, 133, 137	0
15	6I	87/89 (97%)	0.12	2 (2%) 64 42	89, 107, 126, 130	0
16	7A	84/88 (95%)	-0.36	0 100 100	100, 116, 137, 159	0
16	7I	83/88 (94%)	-0.03	1 (1%) 81 65	107, 119, 145, 163	0
17	8A	99/105 (94%)	0.02	0 100 100	100, 112, 125, 131	0
17	8I	100/105 (95%)	1.10	17 (17%) 2 1	95, 114, 124, 128	0
18	9A	67/88 (76%)	-0.21	1 (1%) 76 59	101, 117, 135, 140	0
18	9I	68/88 (77%)	0.03	0 100 100	97, 113, 133, 138	0
19	AA	65/93 (69%)	0.62	9 (13%) 4 2	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.45	7 (8%) 13 4	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.87	16 (16%) 3 1	94, 119, 140, 153	0
20	BI	97/106 (91%)	0.90	20 (20%) 1 0	113, 127, 150, 157	0
21	1B	22/27 (81%)	1.10	4 (18%) 2 1	122, 139, 143, 150	0
21	1F	23/27 (85%)	-0.45	0 100 100	103, 110, 116, 123	0
22	1K	66/76 (86%)	0.03	1 (1%) 76 59	104, 183, 206, 213	0
23	2K	72/77 (93%)	-0.01	2 (2%) 56 34	75, 100, 133, 145	0
23	2L	72/77 (93%)	-0.23	1 (1%) 78 61	85, 120, 153, 162	0
24	3K	70/76 (92%)	1.14	18 (25%) 1 0	82, 225, 245, 249	0
24	3L	72/76 (94%)	-0.02	2 (2%) 56 34	87, 206, 223, 228	0
25	4K	20/30 (66%)	0.70	4 (20%) 1 0	81, 145, 215, 216	0
25	4L	19/30 (63%)	0.13	1 (5%) 30 12	101, 162, 218, 218	0
26	14	2825/2917 (96%)	-0.29	11 (0%) 93 86	62, 91, 198, 251	0
26	1H	2831/2917 (97%)	-0.32	3 (0%) 95 92	51, 79, 176, 251	0
27	16	122/122 (100%)	-0.57	1 (0%) 87 76	76, 98, 118, 204	0
27	1J	122/122 (100%)	-0.76	0 100 100	94, 133, 152, 210	0
28	7I	132/229 (57%)	0.36	11 (8%) 14 5	143, 206, 228, 235	0
29	11	273/276 (98%)	0.12	1 (0%) 93 86	48, 71, 88, 95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.12	0 100 100	56, 80, 94, 111	0
30	21	203/206 (98%)	0.18	4 (1%) 68 48	57, 90, 121, 133	0
30	29	204/206 (99%)	0.41	14 (6%) 20 7	66, 97, 133, 147	0
31	31	202/210 (96%)	0.20	4 (1%) 68 48	51, 82, 114, 134	0
31	39	204/210 (97%)	-0.12	1 (0%) 91 84	64, 105, 148, 175	0
32	41	179/182 (98%)	0.27	7 (3%) 43 21	90, 109, 139, 154	0
32	49	180/182 (98%)	0.59	24 (13%) 4 2	125, 147, 166, 179	0
33	51	174/180 (96%)	-0.31	0 100 100	82, 105, 123, 133	0
33	59	169/180 (93%)	2.49	95 (56%) 0 0	157, 203, 223, 233	0
34	61	145/148 (97%)	0.14	4 (2%) 56 34	82, 128, 147, 153	0
34	69	145/148 (97%)	-0.15	1 (0%) 89 79	91, 129, 149, 154	0
35	15	137/140 (97%)	0.59	12 (8%) 12 4	82, 110, 140, 150	0
35	58	137/140 (97%)	0.30	4 (2%) 55 32	71, 90, 122, 138	0
36	25	122/122 (100%)	1.04	15 (12%) 5 2	74, 90, 108, 120	0
36	68	122/122 (100%)	-0.22	0 100 100	67, 82, 98, 106	0
37	35	147/150 (98%)	0.65	21 (14%) 4 1	64, 106, 141, 158	0
37	78	147/150 (98%)	0.22	0 100 100	58, 84, 106, 114	0
38	45	138/141 (97%)	0.17	3 (2%) 65 44	79, 106, 127, 138	0
38	88	141/141 (100%)	0.63	9 (6%) 23 8	62, 83, 105, 133	0
39	55	118/118 (100%)	0.20	2 (1%) 73 53	68, 85, 100, 113	0
39	98	118/118 (100%)	0.55	6 (5%) 32 13	67, 86, 103, 117	0
40	65	110/112 (98%)	-0.09	3 (2%) 58 36	99, 124, 141, 145	0
40	A8	111/112 (99%)	0.14	4 (3%) 46 23	82, 95, 114, 127	0
41	75	133/146 (91%)	0.74	8 (6%) 25 10	82, 97, 127, 145	0
41	B8	135/146 (92%)	-0.28	1 (0%) 89 79	79, 96, 135, 151	0
42	85	116/118 (98%)	0.03	0 100 100	72, 101, 129, 136	0
42	C8	115/118 (97%)	0.19	2 (1%) 73 53	60, 82, 108, 115	0
43	95	100/101 (99%)	0.55	6 (6%) 25 10	72, 120, 140, 147	0
43	D8	100/101 (99%)	1.16	17 (17%) 2 1	62, 100, 120, 130	0
44	A5	111/113 (98%)	0.15	0 100 100	71, 81, 107, 139	0
44	E8	110/113 (97%)	0.26	3 (2%) 58 36	64, 77, 100, 113	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	0.85	12 (12%) 5 2	78, 90, 111, 121	0
45	F8	95/96 (98%)	-0.12	0 100 100	59, 74, 98, 108	0
46	C5	104/110 (94%)	1.02	19 (18%) 2 1	92, 119, 152, 158	0
46	G8	103/110 (93%)	-0.38	0 100 100	76, 97, 124, 134	0
47	D5	177/206 (85%)	1.44	50 (28%) 1 0	117, 159, 218, 223	0
47	H8	170/206 (82%)	1.59	57 (33%) 0 0	88, 121, 189, 196	0
48	E5	76/85 (89%)	0.32	3 (3%) 43 21	78, 97, 111, 120	0
48	I8	77/85 (90%)	0.22	2 (2%) 59 38	64, 79, 96, 108	0
49	F5	94/98 (95%)	1.19	20 (21%) 1 0	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.38	1 (1%) 84 70	61, 80, 117, 123	0
50	G5	69/72 (95%)	0.34	3 (4%) 39 18	90, 109, 132, 144	0
50	K8	68/72 (94%)	-0.15	1 (1%) 76 59	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.68	1 (1%) 73 53	81, 101, 126, 136	0
51	L8	58/60 (96%)	0.36	0 100 100	70, 84, 110, 122	0
52	M8	60/71 (84%)	1.13	10 (16%) 2 1	114, 150, 177, 181	0
53	J5	56/60 (93%)	0.13	1 (1%) 71 51	67, 90, 133, 143	0
53	N8	48/60 (80%)	0.27	1 (2%) 67 46	56, 85, 128, 135	0
54	L5	47/49 (95%)	0.47	2 (4%) 39 18	61, 69, 91, 100	0
54	P8	47/49 (95%)	-0.12	0 100 100	54, 59, 77, 89	0
55	M5	64/65 (98%)	1.22	19 (29%) 1 0	76, 86, 101, 117	0
55	Q8	64/65 (98%)	0.23	0 100 100	61, 75, 88, 101	0
56	1L	64/76 (84%)	0.13	2 (3%) 52 29	140, 201, 221, 227	0
All	All	20656/21744 (94%)	0.05	908 (4%) 38 17	48, 105, 181, 253	0

The worst 5 of 908 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	D8	37	VAL	14.5
47	H8	113	ALA	10.9
33	59	17	VAL	10.2
33	59	96	ALA	8.2
47	H8	146	ILE	8.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
22	U8U	1K	34	23/24	0.97	0.15	-	98,105,115,118	0
23	OMC	2K	33	21/22	0.96	0.25	-	85,89,90,91	0
23	OMC	2L	33	21/22	0.96	0.18	-	100,107,110,117	0
22	T6A	1K	37	32/33	0.93	0.20	-	91,108,133,134	0
23	5MU	2K	55	21/22	0.94	0.14	-	105,112,118,128	0
23	PSU	2K	56	20/21	0.94	0.12	-	102,108,119,120	0
23	4SU	2K	8	20/21	0.93	0.16	-	91,99,105,106	0
22	PSU	1K	55	20/21	0.88	0.15	-	115,126,136,137	0
22	H2U	1K	17	20/21	0.86	0.14	-	130,139,153,158	0
56	PSU	1L	55	20/21	0.85	0.10	-	121,135,144,145	0
23	PSU	2L	56	20/21	0.90	0.11	-	112,122,130,133	0
22	PSU	1K	39	20/21	0.94	0.11	-	100,119,123,124	0
56	5MU	1L	54	21/22	0.92	0.11	-	125,136,146,154	0
23	5MU	2L	55	21/22	0.96	0.14	-	115,126,133,135	0
22	5MU	1K	54	21/22	0.89	0.17	-	116,121,138,149	0
23	4SU	2L	8	20/21	0.94	0.15	-	108,116,123,125	0
23	7MG	2K	47	24/25	0.88	0.19	-	99,108,119,120	0
23	7MG	2L	47	24/25	0.94	0.13	-	124,131,143,146	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
57	MG	14	3068	1/1	0.82	0.47	72.24	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1628	1/1	0.94	0.59	68.00	90,90,90,90	0
57	MG	14	3133	1/1	0.71	0.92	51.84	89,89,89,89	0
57	MG	14	3147	1/1	0.97	0.74	40.26	86,86,86,86	0
57	MG	13	1659	1/1	0.93	0.39	29.23	109,109,109,109	0
57	MG	1G	1614	1/1	0.95	0.58	26.02	91,91,91,91	0
57	MG	1H	3548	1/1	0.80	0.42	25.00	98,98,98,98	0
57	MG	1H	3237	1/1	0.74	0.56	24.22	85,85,85,85	0
57	MG	14	3095	1/1	0.83	0.31	21.95	72,72,72,72	0
57	MG	1H	3112	1/1	0.96	0.25	20.91	79,79,79,79	0
57	MG	14	3142	1/1	0.91	0.37	20.18	98,98,98,98	0
57	MG	1H	3055	1/1	0.67	0.27	19.65	62,62,62,62	0
57	MG	1H	3215	1/1	0.76	0.46	19.38	94,94,94,94	0
57	MG	13	1614	1/1	0.90	0.32	18.83	102,102,102,102	0
57	MG	14	3165	1/1	0.54	0.66	18.47	97,97,97,97	0
57	MG	14	3132	1/1	0.90	0.26	18.41	90,90,90,90	0
57	MG	1H	3532	1/1	0.83	0.47	18.04	79,79,79,79	0
57	MG	14	3050	1/1	0.96	0.44	17.16	87,87,87,87	0
57	MG	13	1615	1/1	0.94	0.40	16.96	75,75,75,75	0
57	MG	1H	3086	1/1	0.77	0.29	16.59	67,67,67,67	0
57	MG	13	1634	1/1	0.97	0.33	16.28	91,91,91,91	0
57	MG	1H	3130	1/1	0.92	0.40	16.11	97,97,97,97	0
57	MG	1H	3207	1/1	0.95	0.40	16.11	77,77,77,77	0
57	MG	14	3194	1/1	0.58	0.50	14.47	84,84,84,84	0
57	MG	14	3130	1/1	0.77	0.28	13.50	92,92,92,92	0
57	MG	1G	1648	1/1	0.87	0.27	12.87	121,121,121,121	0
57	MG	1H	3154	1/1	0.85	0.43	12.85	67,67,67,67	0
57	MG	16	202	1/1	0.92	0.28	12.69	103,103,103,103	0
57	MG	1H	3191	1/1	0.92	0.30	12.65	79,79,79,79	0
57	MG	13	1630	1/1	0.97	0.25	12.63	86,86,86,86	0
57	MG	1H	3015	1/1	0.94	0.47	12.63	77,77,77,77	0
57	MG	14	3078	1/1	0.86	0.23	12.48	88,88,88,88	0
57	MG	14	3094	1/1	0.86	0.44	12.09	100,100,100,100	0
57	MG	1H	3225	1/1	0.92	0.35	11.39	74,74,74,74	0
57	MG	1H	3084	1/1	0.95	0.29	10.99	77,77,77,77	0
57	MG	14	3149	1/1	0.94	0.31	10.93	94,94,94,94	0
57	MG	14	3096	1/1	0.96	0.28	10.75	84,84,84,84	0
57	MG	13	1601	1/1	0.90	0.32	10.73	97,97,97,97	0
57	MG	14	3123	1/1	0.88	0.32	10.70	75,75,75,75	0
57	MG	14	3160	1/1	0.80	0.45	10.51	85,85,85,85	0
57	MG	1H	3082	1/1	0.91	0.32	10.49	69,69,69,69	0
57	MG	1G	1626	1/1	0.97	0.28	10.28	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3106	1/1	0.94	0.33	10.10	79,79,79,79	0
57	MG	1H	3093	1/1	0.87	0.31	9.95	73,73,73,73	0
57	MG	1H	3206	1/1	0.98	0.34	9.72	55,55,55,55	0
57	MG	1H	3119	1/1	0.85	0.23	9.62	79,79,79,79	0
57	MG	1H	3041	1/1	0.99	0.28	9.61	57,57,57,57	0
57	MG	14	3124	1/1	0.79	0.35	9.59	64,64,64,64	0
57	MG	14	3034	1/1	0.94	0.28	9.12	75,75,75,75	0
57	MG	13	1629	1/1	0.78	0.32	9.11	100,100,100,100	0
57	MG	13	1635	1/1	0.99	0.44	8.87	83,83,83,83	0
57	MG	1H	3413	1/1	0.83	0.34	8.73	93,93,93,93	0
57	MG	1H	3036	1/1	0.93	0.28	8.32	73,73,73,73	0
57	MG	1H	3240	1/1	0.91	0.20	7.94	86,86,86,86	0
57	MG	1G	1647	1/1	0.54	0.23	7.78	99,99,99,99	0
57	MG	1H	3169	1/1	0.73	0.27	7.66	91,91,91,91	0
57	MG	1H	3179	1/1	0.97	0.24	7.55	74,74,74,74	0
57	MG	14	3240	1/1	0.94	0.25	7.07	63,63,63,63	0
57	MG	1H	3074	1/1	0.88	0.25	6.99	75,75,75,75	0
57	MG	13	1624	1/1	0.96	0.30	6.89	83,83,83,83	0
57	MG	1G	1651	1/1	0.87	0.29	6.89	97,97,97,97	0
57	MG	1H	3107	1/1	0.82	0.35	6.76	62,62,62,62	0
57	MG	14	3119	1/1	0.91	0.32	6.74	69,69,69,69	0
57	MG	14	3052	1/1	0.91	0.32	6.68	59,59,59,59	0
57	MG	14	3102	1/1	0.89	0.28	6.58	94,94,94,94	0
57	MG	14	3005	1/1	0.91	0.33	6.47	83,83,83,83	0
57	MG	1H	3116	1/1	0.93	0.21	6.25	82,82,82,82	0
57	MG	2L	101	1/1	0.97	0.43	6.23	83,83,83,83	0
57	MG	1H	3007	1/1	0.82	0.24	5.83	57,57,57,57	0
57	MG	14	3145	1/1	0.78	0.39	5.70	71,71,71,71	0
57	MG	14	3046	1/1	0.91	0.20	5.56	77,77,77,77	0
57	MG	1H	3021	1/1	0.98	0.28	5.56	60,60,60,60	0
57	MG	19	301	1/1	0.95	0.30	5.34	61,61,61,61	0
57	MG	14	3086	1/1	0.88	0.27	5.16	73,73,73,73	0
57	MG	13	1696	1/1	0.94	0.18	5.01	114,114,114,114	0
57	MG	1H	3427	1/1	0.86	0.23	4.70	102,102,102,102	0
57	MG	14	3302	1/1	0.94	0.26	4.69	94,94,94,94	0
57	MG	14	3054	1/1	0.92	0.28	4.60	67,67,67,67	0
57	MG	1H	3198	1/1	0.96	0.26	4.58	75,75,75,75	0
57	MG	14	3075	1/1	0.96	0.28	4.54	65,65,65,65	0
57	MG	14	3105	1/1	0.96	0.17	4.49	92,92,92,92	0
57	MG	14	3113	1/1	0.89	0.34	4.44	74,74,74,74	0
57	MG	14	3009	1/1	0.82	0.28	4.42	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1643	1/1	0.93	0.22	4.20	95,95,95,95	0
57	MG	1H	3160	1/1	0.81	0.24	4.19	79,79,79,79	0
57	MG	1G	1670	1/1	0.88	0.16	4.18	109,109,109,109	0
57	MG	1H	3052	1/1	0.97	0.28	4.11	58,58,58,58	0
57	MG	14	3091	1/1	0.96	0.31	3.97	92,92,92,92	0
57	MG	1H	3218	1/1	0.90	0.32	3.95	70,70,70,70	0
57	MG	14	3058	1/1	0.96	0.24	3.90	83,83,83,83	0
57	MG	13	1638	1/1	0.55	0.56	3.86	103,103,103,103	0
57	MG	14	3042	1/1	0.94	0.28	3.72	54,54,54,54	0
57	MG	14	3016	1/1	0.96	0.27	3.69	69,69,69,69	0
57	MG	16	204	1/1	0.81	0.19	3.68	89,89,89,89	0
57	MG	14	3069	1/1	0.85	0.22	3.60	56,56,56,56	0
57	MG	14	3159	1/1	0.77	0.27	3.58	80,80,80,80	0
57	MG	1H	3063	1/1	0.94	0.24	3.57	59,59,59,59	0
57	MG	14	3066	1/1	0.96	0.25	3.47	63,63,63,63	0
57	MG	13	1609	1/1	0.97	0.19	3.46	88,88,88,88	0
57	MG	13	1607	1/1	0.97	0.23	3.41	83,83,83,83	0
57	MG	1H	3017	1/1	0.97	0.27	3.38	56,56,56,56	0
57	MG	1H	3090	1/1	0.74	0.27	3.24	82,82,82,82	0
57	MG	14	3045	1/1	0.85	0.23	3.23	72,72,72,72	0
57	MG	1H	3394	1/1	0.89	0.20	3.23	83,83,83,83	0
60	SPE	14	3458	13/13	0.90	0.21	2.90	92,101,106,108	0
57	MG	1H	3126	1/1	0.86	0.20	2.87	71,71,71,71	0
57	MG	1G	1607	1/1	0.96	0.28	2.87	107,107,107,107	0
57	MG	1H	3432	1/1	0.60	0.16	2.80	116,116,116,116	0
57	MG	1H	3497	1/1	0.57	0.24	2.74	96,96,96,96	0
57	MG	1G	1606	1/1	0.87	0.25	2.69	87,87,87,87	0
57	MG	1G	1632	1/1	0.92	0.25	2.56	108,108,108,108	0
57	MG	14	3038	1/1	0.92	0.27	2.52	68,68,68,68	0
57	MG	14	3182	1/1	0.96	0.26	2.44	66,66,66,66	0
57	MG	1H	3019	1/1	0.97	0.29	2.44	53,53,53,53	0
57	MG	14	3170	1/1	0.90	0.25	2.36	76,76,76,76	0
57	MG	13	1649	1/1	0.79	0.19	2.33	83,83,83,83	0
57	MG	14	3032	1/1	0.96	0.25	2.28	72,72,72,72	0
57	MG	1H	3541	1/1	0.85	0.20	2.26	109,109,109,109	0
57	MG	13	1625	1/1	0.96	0.23	2.22	68,68,68,68	0
57	MG	14	3228	1/1	0.93	0.25	2.15	64,64,64,64	0
57	MG	1G	1679	1/1	0.94	0.17	2.07	105,105,105,105	0
57	MG	1H	3075	1/1	0.88	0.21	2.06	75,75,75,75	0
57	MG	14	3080	1/1	0.41	0.23	2.05	71,71,71,71	0
57	MG	14	3010	1/1	0.71	0.23	1.99	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3068	1/1	0.88	0.22	1.98	66,66,66,66	0
57	MG	2I	301	1/1	0.91	0.34	1.94	77,77,77,77	0
57	MG	1H	3181	1/1	0.77	0.35	1.93	98,98,98,98	0
57	MG	1H	3001	1/1	0.98	0.23	1.92	49,49,49,49	0
57	MG	13	1618	1/1	0.80	0.27	1.90	72,72,72,72	0
57	MG	14	3065	1/1	0.87	0.31	1.80	70,70,70,70	0
57	MG	14	3460	1/1	0.98	0.26	1.78	92,92,92,92	0
57	MG	14	3092	1/1	0.90	0.22	1.76	67,67,67,67	0
57	MG	14	3216	1/1	0.99	0.23	1.68	62,62,62,62	0
57	MG	14	3082	1/1	0.90	0.41	1.66	80,80,80,80	0
57	MG	14	3093	1/1	0.98	0.29	1.65	86,86,86,86	0
57	MG	1H	3034	1/1	0.98	0.15	1.51	74,74,74,74	0
57	MG	1H	3543	1/1	0.79	0.12	1.45	166,166,166,166	0
57	MG	14	3372	1/1	0.84	0.19	1.39	112,112,112,112	0
57	MG	1H	3100	1/1	0.94	0.27	1.32	77,77,77,77	0
57	MG	1G	1654	1/1	0.85	0.22	1.28	102,102,102,102	0
57	MG	14	3189	1/1	0.98	0.32	1.21	81,81,81,81	0
57	MG	13	1667	1/1	0.67	0.15	1.19	104,104,104,104	0
57	MG	14	3136	1/1	0.94	0.25	1.13	95,95,95,95	0
57	MG	14	3223	1/1	0.94	0.22	1.11	61,61,61,61	0
57	MG	14	3031	1/1	0.94	0.24	1.08	51,51,51,51	0
57	MG	14	3208	1/1	0.96	0.23	1.06	63,63,63,63	0
57	MG	1H	3485	1/1	0.88	0.18	1.03	102,102,102,102	0
57	MG	1G	1622	1/1	0.93	0.16	0.98	104,104,104,104	0
57	MG	1H	3047	1/1	0.96	0.21	0.97	64,64,64,64	0
57	MG	14	3087	1/1	0.78	0.18	0.95	75,75,75,75	0
57	MG	14	3356	1/1	0.81	0.21	0.84	78,78,78,78	0
57	MG	14	3311	1/1	0.91	0.18	0.74	84,84,84,84	0
57	MG	14	3120	1/1	0.95	0.14	0.74	84,84,84,84	0
57	MG	1H	3113	1/1	0.95	0.16	0.73	70,70,70,70	0
57	MG	14	3089	1/1	0.85	0.23	0.70	73,73,73,73	0
57	MG	1G	1667	1/1	0.79	0.21	0.64	111,111,111,111	0
57	MG	13	1652	1/1	0.98	0.18	0.59	82,82,82,82	0
57	MG	1H	3026	1/1	0.85	0.15	0.59	82,82,82,82	0
57	MG	1H	3205	1/1	0.97	0.18	0.58	71,71,71,71	0
57	MG	14	3020	1/1	0.90	0.21	0.55	69,69,69,69	0
57	MG	1H	3208	1/1	0.77	0.19	0.54	69,69,69,69	0
57	MG	1H	3066	1/1	0.98	0.23	0.54	65,65,65,65	0
57	MG	13	1637	1/1	0.93	0.18	0.54	90,90,90,90	0
57	MG	1G	1623	1/1	0.95	0.12	0.48	109,109,109,109	0
57	MG	14	3270	1/1	0.89	0.19	0.45	74,74,74,74	0
57	MG	14	3060	1/1	0.98	0.16	0.39	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3049	1/1	0.96	0.19	0.39	69,69,69,69	0
57	MG	1H	3115	1/1	0.97	0.19	0.37	64,64,64,64	0
58	SF4	3E	301	8/8	0.99	0.21	0.32	95,98,106,108	0
57	MG	1H	3029	1/1	0.96	0.21	0.20	59,59,59,59	0
57	MG	14	3083	1/1	0.93	0.20	0.17	58,58,58,58	0
57	MG	14	3007	1/1	0.87	0.27	0.16	61,61,61,61	0
57	MG	14	3044	1/1	0.96	0.23	0.15	71,71,71,71	0
57	MG	1G	1700	1/1	0.94	0.13	0.12	107,107,107,107	0
57	MG	1H	3171	1/1	0.96	0.18	0.11	88,88,88,88	0
58	SF4	32	302	8/8	0.99	0.20	0.10	115,120,128,136	0
57	MG	1G	1644	1/1	0.95	0.15	0.08	130,130,130,130	0
57	MG	1H	3132	1/1	0.96	0.19	0.01	55,55,55,55	0
57	MG	13	1678	1/1	0.74	0.17	0.01	114,114,114,114	0
57	MG	14	3394	1/1	0.87	0.30	-0.03	91,91,91,91	0
57	MG	13	1619	1/1	0.92	0.21	-0.04	54,54,54,54	0
57	MG	13	1644	1/1	0.93	0.12	-0.07	99,99,99,99	0
57	MG	1G	1630	1/1	0.93	0.14	-0.08	132,132,132,132	0
57	MG	14	3098	1/1	0.96	0.19	-0.11	63,63,63,63	0
57	MG	41	201	1/1	0.91	0.17	-0.13	81,81,81,81	0
57	MG	14	3288	1/1	0.93	0.20	-0.19	59,59,59,59	0
57	MG	1H	3103	1/1	0.84	0.15	-0.19	64,64,64,64	0
57	MG	1G	1603	1/1	0.97	0.16	-0.21	91,91,91,91	0
57	MG	1H	3396	1/1	0.95	0.17	-0.21	81,81,81,81	0
57	MG	13	1612	1/1	0.97	0.14	-0.23	111,111,111,111	0
57	MG	13	1673	1/1	0.94	0.11	-0.24	110,110,110,110	0
57	MG	14	3114	1/1	0.82	0.18	-0.26	77,77,77,77	0
57	MG	1H	3434	1/1	0.87	0.14	-0.27	96,96,96,96	0
57	MG	88	201	1/1	0.87	0.20	-0.27	83,83,83,83	0
57	MG	1H	3027	1/1	0.98	0.17	-0.32	60,60,60,60	0
57	MG	1G	1726	1/1	0.95	0.20	-0.35	94,94,94,94	0
57	MG	1H	3002	1/1	0.96	0.17	-0.36	51,51,51,51	0
57	MG	14	3029	1/1	0.98	0.15	-0.41	80,80,80,80	0
57	MG	14	3077	1/1	0.92	0.16	-0.42	85,85,85,85	0
57	MG	1H	3088	1/1	0.96	0.14	-0.42	87,87,87,87	0
57	MG	13	1606	1/1	0.97	0.16	-0.43	88,88,88,88	0
57	MG	1G	1699	1/1	0.87	0.16	-0.45	113,113,113,113	0
57	MG	1H	3065	1/1	0.81	0.16	-0.49	72,72,72,72	0
57	MG	1H	3377	1/1	0.94	0.13	-0.53	94,94,94,94	0
57	MG	1H	3101	1/1	0.90	0.19	-0.53	72,72,72,72	0
57	MG	14	3100	1/1	0.83	0.25	-0.54	77,77,77,77	0
57	MG	14	3164	1/1	0.93	0.19	-0.55	83,83,83,83	0
57	MG	1G	1610	1/1	0.92	0.16	-0.56	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3111	1/1	0.93	0.17	-0.57	83,83,83,83	0
57	MG	1H	3307	1/1	0.92	0.17	-0.62	56,56,56,56	0
57	MG	1H	3268	1/1	0.90	0.14	-0.63	70,70,70,70	0
57	MG	1H	3219	1/1	0.91	0.11	-0.72	83,83,83,83	0
57	MG	1H	3476	1/1	0.98	0.16	-0.74	94,94,94,94	0
57	MG	1H	3273	1/1	0.98	0.16	-0.74	56,56,56,56	0
57	MG	M5	101	1/1	0.93	0.36	-0.76	81,81,81,81	0
57	MG	14	3392	1/1	0.76	0.15	-0.76	98,98,98,98	0
57	MG	14	3286	1/1	0.93	0.19	-0.77	58,58,58,58	0
57	MG	1H	3125	1/1	0.91	0.14	-0.79	79,79,79,79	0
57	MG	14	3259	1/1	0.81	0.13	-0.83	97,97,97,97	0
59	ZN	5I	101	1/1	0.99	0.13	-0.84	94,94,94,94	0
57	MG	1G	1604	1/1	0.93	0.11	-0.85	132,132,132,132	0
57	MG	1G	1693	1/1	0.89	0.10	-0.86	121,121,121,121	0
57	MG	14	3391	1/1	0.87	0.15	-0.87	87,87,87,87	0
57	MG	1H	3028	1/1	0.97	0.16	-0.87	62,62,62,62	0
57	MG	1J	204	1/1	0.82	0.10	-0.89	102,102,102,102	0
57	MG	14	3278	1/1	0.96	0.13	-0.90	83,83,83,83	0
57	MG	1H	3046	1/1	0.95	0.17	-0.91	43,43,43,43	0
57	MG	1H	3127	1/1	0.88	0.18	-0.94	69,69,69,69	0
57	MG	1G	1680	1/1	0.93	0.14	-0.95	103,103,103,103	0
57	MG	1G	1720	1/1	0.77	0.10	-0.96	135,135,135,135	0
57	MG	1H	3098	1/1	0.90	0.17	-0.97	59,59,59,59	0
59	ZN	5A	101	1/1	0.98	0.09	-0.97	129,129,129,129	0
57	MG	13	1683	1/1	0.67	0.12	-0.98	119,119,119,119	0
57	MG	1H	3291	1/1	0.99	0.15	-1.01	57,57,57,57	0
57	MG	14	3209	1/1	0.98	0.18	-1.01	61,61,61,61	0
57	MG	Q8	101	1/1	0.93	0.23	-1.03	82,82,82,82	0
57	MG	13	1675	1/1	0.76	0.16	-1.03	91,91,91,91	0
57	MG	1H	3283	1/1	0.99	0.12	-1.04	59,59,59,59	0
57	MG	14	3222	1/1	0.71	0.18	-1.07	73,73,73,73	0
57	MG	1H	3488	1/1	0.85	0.19	-1.07	84,84,84,84	0
57	MG	1H	3266	1/1	0.97	0.15	-1.08	92,92,92,92	0
57	MG	1H	3317	1/1	0.90	0.15	-1.09	70,70,70,70	0
57	MG	1H	3048	1/1	0.80	0.14	-1.10	68,68,68,68	0
57	MG	1H	3461	1/1	0.93	0.08	-1.10	80,80,80,80	0
57	MG	14	3293	1/1	0.93	0.18	-1.12	70,70,70,70	0
57	MG	14	3245	1/1	0.95	0.16	-1.13	74,74,74,74	0
57	MG	1H	3144	1/1	0.93	0.15	-1.16	71,71,71,71	0
57	MG	1H	3279	1/1	0.75	0.12	-1.17	68,68,68,68	0
57	MG	2I	201	1/1	0.91	0.10	-1.23	97,97,97,97	0
57	MG	1H	3270	1/1	0.89	0.14	-1.23	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3280	1/1	0.98	0.16	-1.30	76,76,76,76	0
57	MG	13	1632	1/1	0.89	0.08	-1.30	95,95,95,95	0
57	MG	14	3326	1/1	0.97	0.10	-1.31	87,87,87,87	0
57	MG	1H	3518	1/1	0.97	0.11	-1.32	57,57,57,57	0
57	MG	13	1741	1/1	0.85	0.11	-1.34	95,95,95,95	0
57	MG	14	3319	1/1	0.98	0.13	-1.35	72,72,72,72	0
57	MG	1H	3306	1/1	0.89	0.11	-1.35	79,79,79,79	0
57	MG	1H	3261	1/1	0.95	0.16	-1.38	61,61,61,61	0
57	MG	1H	3149	1/1	0.92	0.18	-1.39	81,81,81,81	0
57	MG	1H	3329	1/1	0.97	0.13	-1.39	53,53,53,53	0
57	MG	1G	1687	1/1	0.87	0.14	-1.42	111,111,111,111	0
57	MG	1G	1643	1/1	0.72	0.10	-1.43	100,100,100,100	0
60	SPE	1G	1725	13/13	0.86	0.09	-1.44	110,113,117,118	0
57	MG	14	3275	1/1	0.88	0.14	-1.46	85,85,85,85	0
57	MG	14	3227	1/1	0.94	0.17	-1.46	52,52,52,52	0
57	MG	16	207	1/1	0.91	0.09	-1.51	91,91,91,91	0
57	MG	1H	3297	1/1	0.92	0.17	-1.53	56,56,56,56	0
57	MG	14	3399	1/1	0.69	0.09	-1.54	122,122,122,122	0
57	MG	13	1677	1/1	0.96	0.13	-1.57	90,90,90,90	0
57	MG	1H	3038	1/1	0.95	0.16	-1.58	61,61,61,61	0
57	MG	1H	3257	1/1	0.99	0.16	-1.59	49,49,49,49	0
57	MG	39	301	1/1	0.74	0.17	-1.62	80,80,80,80	0
57	MG	14	3309	1/1	0.93	0.13	-1.63	48,48,48,48	0
57	MG	13	1687	1/1	0.91	0.13	-1.64	89,89,89,89	0
57	MG	14	3285	1/1	0.94	0.11	-1.67	89,89,89,89	0
57	MG	14	3459	1/1	0.96	0.10	-1.67	68,68,68,68	0
57	MG	1H	3054	1/1	0.97	0.15	-1.67	63,63,63,63	0
57	MG	14	3252	1/1	0.93	0.14	-1.69	69,69,69,69	0
57	MG	14	3263	1/1	0.90	0.13	-1.75	86,86,86,86	0
57	MG	1H	3275	1/1	0.99	0.10	-1.77	72,72,72,72	0
57	MG	14	3169	1/1	0.88	0.14	-1.79	88,88,88,88	0
57	MG	1H	3033	1/1	0.98	0.18	-1.85	63,63,63,63	0
57	MG	14	3261	1/1	0.95	0.12	-1.86	64,64,64,64	0
57	MG	13	1703	1/1	0.92	0.14	-1.92	71,71,71,71	0
57	MG	1G	1658	1/1	0.81	0.08	-1.94	97,97,97,97	0
57	MG	14	3461	1/1	0.91	0.07	-1.94	108,108,108,108	0
57	MG	14	3377	1/1	0.73	0.12	-1.98	72,72,72,72	0
57	MG	14	3253	1/1	0.95	0.12	-2.02	79,79,79,79	0
57	MG	1G	1662	1/1	0.74	0.11	-2.06	118,118,118,118	0
57	MG	1H	3062	1/1	0.60	0.17	-2.09	64,64,64,64	0
57	MG	1H	3357	1/1	0.99	0.11	-2.14	64,64,64,64	0
57	MG	1G	1664	1/1	0.83	0.14	-2.15	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3442	1/1	0.94	0.08	-2.17	83,83,83,83	0
57	MG	1H	3102	1/1	0.90	0.14	-2.17	52,52,52,52	0
57	MG	14	3214	1/1	0.96	0.15	-2.23	83,83,83,83	0
57	MG	1H	3272	1/1	0.94	0.12	-2.24	79,79,79,79	0
57	MG	1H	3472	1/1	0.94	0.14	-2.26	63,63,63,63	0
57	MG	13	1686	1/1	0.97	0.10	-2.30	107,107,107,107	0
57	MG	14	3242	1/1	0.97	0.11	-2.36	82,82,82,82	0
57	MG	13	1674	1/1	0.91	0.07	-2.46	105,105,105,105	0
57	MG	1H	3296	1/1	0.93	0.16	-2.46	56,56,56,56	0
57	MG	1H	3053	1/1	0.84	0.14	-2.49	47,47,47,47	0
57	MG	14	3383	1/1	0.79	0.13	-2.50	91,91,91,91	0
57	MG	1H	3308	1/1	0.89	0.14	-2.55	62,62,62,62	0
57	MG	14	3017	1/1	0.95	0.14	-2.55	74,74,74,74	0
57	MG	14	3308	1/1	0.96	0.13	-2.56	64,64,64,64	0
57	MG	1H	3229	1/1	0.85	0.11	-2.58	84,84,84,84	0
57	MG	1G	1655	1/1	0.93	0.15	-2.61	90,90,90,90	0
57	MG	1H	3302	1/1	0.96	0.16	-2.62	54,54,54,54	0
57	MG	14	3192	1/1	0.99	0.14	-2.63	80,80,80,80	0
57	MG	13	1676	1/1	0.99	0.11	-2.72	67,67,67,67	0
57	MG	14	3027	1/1	0.70	0.08	-2.74	85,85,85,85	0
57	MG	1H	3382	1/1	0.95	0.16	-2.77	43,43,43,43	0
57	MG	14	3212	1/1	0.99	0.11	-2.83	60,60,60,60	0
57	MG	1H	3496	1/1	0.97	0.10	-2.85	89,89,89,89	0
57	MG	1H	3133	1/1	0.83	0.13	-2.86	72,72,72,72	0
57	MG	1H	3294	1/1	0.98	0.10	-2.87	68,68,68,68	0
57	MG	1H	3351	1/1	0.96	0.09	-2.89	66,66,66,66	0
57	MG	14	3320	1/1	0.97	0.15	-2.91	70,70,70,70	0
57	MG	1H	3383	1/1	0.81	0.16	-2.93	74,74,74,74	0
57	MG	1H	3292	1/1	0.98	0.07	-2.97	62,62,62,62	0
57	MG	1H	3330	1/1	0.98	0.09	-2.98	74,74,74,74	0
57	MG	1G	1671	1/1	0.95	0.10	-3.02	101,101,101,101	0
57	MG	1H	3043	1/1	0.92	0.15	-3.02	64,64,64,64	0
57	MG	1H	3118	1/1	0.96	0.13	-3.03	63,63,63,63	0
57	MG	14	3256	1/1	0.93	0.08	-3.03	99,99,99,99	0
57	MG	14	3241	1/1	0.98	0.14	-3.04	61,61,61,61	0
57	MG	1H	3319	1/1	0.96	0.11	-3.06	58,58,58,58	0
57	MG	1H	3263	1/1	0.98	0.10	-3.07	53,53,53,53	0
57	MG	1H	3401	1/1	0.80	0.14	-3.14	99,99,99,99	0
57	MG	13	1729	1/1	0.98	0.08	-3.14	110,110,110,110	0
57	MG	1H	3289	1/1	0.98	0.11	-3.20	91,91,91,91	0
57	MG	14	3022	1/1	0.92	0.13	-3.22	77,77,77,77	0
57	MG	1H	3242	1/1	0.96	0.13	-3.24	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1713	1/1	0.97	0.09	-3.27	96,96,96,96	0
57	MG	14	3281	1/1	0.93	0.07	-3.35	75,75,75,75	0
57	MG	14	3237	1/1	0.92	0.12	-3.41	67,67,67,67	0
57	MG	1H	3256	1/1	0.99	0.12	-3.46	48,48,48,48	0
57	MG	14	3266	1/1	0.95	0.10	-3.47	77,77,77,77	0
57	MG	14	3236	1/1	0.92	0.14	-3.52	69,69,69,69	0
57	MG	14	3305	1/1	0.87	0.17	-3.55	64,64,64,64	0
57	MG	14	3229	1/1	0.94	0.10	-3.61	74,74,74,74	0
57	MG	1G	1724	1/1	0.76	0.06	-3.62	126,126,126,126	0
57	MG	1H	3274	1/1	0.94	0.12	-3.63	48,48,48,48	0
57	MG	14	3416	1/1	0.95	0.06	-3.68	87,87,87,87	0
57	MG	14	3348	1/1	0.90	0.09	-3.74	102,102,102,102	0
57	MG	2K	101	1/1	0.84	0.13	-3.77	80,80,80,80	0
57	MG	1H	3463	1/1	0.89	0.13	-3.79	70,70,70,70	0
57	MG	13	1694	1/1	0.95	0.11	-3.82	92,92,92,92	0
57	MG	13	1640	1/1	0.87	0.10	-3.84	97,97,97,97	0
57	MG	1H	3265	1/1	0.98	0.11	-3.84	74,74,74,74	0
57	MG	1H	3372	1/1	0.95	0.14	-3.86	66,66,66,66	0
57	MG	1H	3259	1/1	0.97	0.12	-4.00	59,59,59,59	0
57	MG	1H	3230	1/1	0.99	0.09	-4.01	90,90,90,90	0
57	MG	1G	1641	1/1	0.95	0.10	-4.01	115,115,115,115	0
57	MG	14	3315	1/1	0.83	0.10	-4.03	83,83,83,83	0
57	MG	1H	3253	1/1	0.96	0.12	-4.03	58,58,58,58	0
57	MG	14	3217	1/1	0.92	0.09	-4.12	76,76,76,76	0
57	MG	1H	3247	1/1	0.99	0.07	-4.15	67,67,67,67	0
57	MG	13	1735	1/1	0.79	0.12	-4.18	105,105,105,105	0
57	MG	1H	3239	1/1	0.95	0.09	-4.23	97,97,97,97	0
57	MG	1H	3288	1/1	0.96	0.11	-4.25	58,58,58,58	0
57	MG	1H	3145	1/1	0.98	0.09	-4.26	74,74,74,74	0
57	MG	1G	1619	1/1	0.98	0.07	-4.28	118,118,118,118	0
57	MG	16	205	1/1	0.93	0.05	-4.31	84,84,84,84	0
57	MG	14	3384	1/1	0.79	0.09	-4.47	88,88,88,88	0
57	MG	14	3225	1/1	0.82	0.16	-4.51	79,79,79,79	0
57	MG	14	3405	1/1	0.86	0.05	-4.56	118,118,118,118	0
57	MG	1H	3335	1/1	0.67	0.09	-4.56	83,83,83,83	0
57	MG	1H	3243	1/1	0.89	0.10	-4.63	63,63,63,63	0
57	MG	14	3274	1/1	0.88	0.15	-4.64	62,62,62,62	0
57	MG	1H	3250	1/1	0.97	0.10	-4.67	54,54,54,54	0
57	MG	14	3396	1/1	0.96	0.07	-4.70	71,71,71,71	0
57	MG	14	3024	1/1	0.84	0.14	-4.86	88,88,88,88	0
57	MG	14	3127	1/1	0.96	0.06	-4.87	70,70,70,70	0
57	MG	14	3322	1/1	0.96	0.14	-4.92	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1622	1/1	0.93	0.05	-4.93	111,111,111,111	0
57	MG	1H	3072	1/1	0.85	0.12	-4.96	60,60,60,60	0
57	MG	14	3318	1/1	0.94	0.12	-5.02	65,65,65,65	0
57	MG	1G	1656	1/1	0.87	0.10	-5.04	89,89,89,89	0
57	MG	14	3350	1/1	0.95	0.09	-5.04	88,88,88,88	0
57	MG	1H	3058	1/1	0.88	0.07	-5.05	68,68,68,68	0
57	MG	14	3258	1/1	0.95	0.05	-5.06	97,97,97,97	0
57	MG	14	3420	1/1	0.93	0.11	-5.10	119,119,119,119	0
57	MG	14	3232	1/1	0.94	0.11	-5.30	75,75,75,75	0
57	MG	14	3234	1/1	0.97	0.09	-5.32	62,62,62,62	0
57	MG	14	3239	1/1	0.92	0.10	-5.34	60,60,60,60	0
57	MG	14	3210	1/1	0.81	0.09	-5.55	78,78,78,78	0
57	MG	14	3026	1/1	0.96	0.06	-5.57	74,74,74,74	0
57	MG	1H	3300	1/1	0.91	0.10	-5.60	73,73,73,73	0
57	MG	1H	3468	1/1	0.95	0.05	-5.70	82,82,82,82	0
57	MG	14	3313	1/1	0.97	0.09	-5.71	67,67,67,67	0
57	MG	1H	3438	1/1	0.95	0.07	-5.73	95,95,95,95	0
57	MG	14	3379	1/1	0.78	0.12	-5.78	107,107,107,107	0
57	MG	1H	3128	1/1	0.96	0.07	-5.93	66,66,66,66	0
57	MG	13	1663	1/1	0.82	0.12	-6.04	77,77,77,77	0
57	MG	1G	1665	1/1	0.97	0.10	-6.30	82,82,82,82	0
57	MG	13	1709	1/1	0.79	0.05	-6.49	128,128,128,128	0
57	MG	14	3097	1/1	0.87	0.09	-6.52	84,84,84,84	0
57	MG	1H	3368	1/1	0.96	0.06	-6.74	72,72,72,72	0
57	MG	14	3287	1/1	0.93	0.13	-6.80	74,74,74,74	0
57	MG	1H	3414	1/1	0.96	0.07	-7.10	52,52,52,52	0
57	MG	1H	3251	1/1	0.99	0.06	-7.11	49,49,49,49	0
57	MG	1H	3278	1/1	0.93	0.07	-7.17	86,86,86,86	0
57	MG	1H	3324	1/1	0.92	0.09	-7.27	69,69,69,69	0
57	MG	1H	3393	1/1	0.98	0.10	-7.53	63,63,63,63	0
57	MG	13	1728	1/1	0.57	0.09	-7.60	117,117,117,117	0
57	MG	14	3433	1/1	0.94	0.11	-7.65	90,90,90,90	0
57	MG	1H	3258	1/1	0.95	0.10	-7.68	56,56,56,56	0
57	MG	1H	3248	1/1	0.92	0.11	-7.73	57,57,57,57	0
57	MG	1H	3224	1/1	0.96	0.09	-8.57	72,72,72,72	0
57	MG	1H	3298	1/1	0.97	0.05	-8.79	52,52,52,52	0
57	MG	14	3299	1/1	0.97	0.06	-9.04	63,63,63,63	0
57	MG	1H	3281	1/1	0.84	0.07	-9.26	85,85,85,85	0
57	MG	14	3221	1/1	0.90	0.10	-9.55	65,65,65,65	0
57	MG	14	3125	1/1	0.97	0.10	-10.13	92,92,92,92	0
57	MG	13	1710	1/1	0.96	0.08	-10.24	73,73,73,73	0
57	MG	1H	3374	1/1	0.97	0.07	-10.52	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3451	1/1	1.00	0.07	-10.54	55,55,55,55	0
57	MG	1H	3293	1/1	0.95	0.10	-10.71	60,60,60,60	0
57	MG	1H	3284	1/1	0.88	0.10	-11.63	62,62,62,62	0
57	MG	14	3403	1/1	0.96	0.07	-11.96	78,78,78,78	0
57	MG	1H	3478	1/1	0.96	0.05	-12.49	79,79,79,79	0
57	MG	1H	3388	1/1	0.98	0.07	-12.65	49,49,49,49	0
57	MG	1H	3417	1/1	0.95	0.04	-13.91	100,100,100,100	0
57	MG	1H	3389	1/1	0.99	0.05	-14.89	63,63,63,63	0
57	MG	1H	3358	1/1	0.89	0.07	-24.84	100,100,100,100	0
57	MG	1H	3522	1/1	0.90	0.10	-	112,112,112,112	0
57	MG	1H	3425	1/1	0.95	0.04	-	81,81,81,81	0
57	MG	1H	3506	1/1	0.54	0.24	-	103,103,103,103	0
57	MG	14	3019	1/1	0.84	0.35	-	131,131,131,131	0
57	MG	14	3200	1/1	0.90	0.10	-	86,86,86,86	0
57	MG	2K	102	1/1	0.91	0.11	-	99,99,99,99	0
57	MG	14	3235	1/1	0.99	0.09	-	55,55,55,55	0
57	MG	1H	3045	1/1	0.92	0.36	-	63,63,63,63	0
57	MG	1H	3466	1/1	0.85	0.09	-	103,103,103,103	0
57	MG	13	1688	1/1	0.95	0.07	-	96,96,96,96	0
57	MG	1H	3008	1/1	0.69	0.28	-	81,81,81,81	0
57	MG	14	3296	1/1	0.90	0.10	-	76,76,76,76	0
57	MG	1H	3194	1/1	0.81	0.37	-	80,80,80,80	0
57	MG	1H	3529	1/1	0.93	0.10	-	110,110,110,110	0
57	MG	1H	3431	1/1	0.92	0.05	-	102,102,102,102	0
57	MG	13	1689	1/1	0.90	0.22	-	98,98,98,98	0
57	MG	14	3271	1/1	0.97	0.10	-	67,67,67,67	0
57	MG	14	3186	1/1	0.91	0.13	-	95,95,95,95	0
57	MG	1H	3010	1/1	0.80	0.36	-	87,87,87,87	0
57	MG	1H	3071	1/1	0.65	0.25	-	101,101,101,101	0
57	MG	14	3406	1/1	0.73	0.17	-	121,121,121,121	0
57	MG	14	3037	1/1	0.95	0.49	-	54,54,54,54	0
57	MG	1H	3303	1/1	0.97	0.11	-	49,49,49,49	0
57	MG	1H	3435	1/1	0.94	0.30	-	100,100,100,100	0
57	MG	1H	3092	1/1	0.86	0.19	-	67,67,67,67	0
57	MG	1H	3457	1/1	0.96	0.08	-	102,102,102,102	0
57	MG	14	3351	1/1	0.78	0.10	-	101,101,101,101	0
57	MG	1H	3385	1/1	0.89	0.19	-	94,94,94,94	0
57	MG	1G	1710	1/1	0.84	0.08	-	113,113,113,113	0
57	MG	1H	3501	1/1	0.84	0.07	-	108,108,108,108	0
57	MG	1H	3077	1/1	0.76	0.42	-	76,76,76,76	0
57	MG	1H	3480	1/1	0.91	0.28	-	90,90,90,90	0
57	MG	14	3131	1/1	0.91	0.12	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3418	1/1	0.84	0.15	-	122,122,122,122	0
57	MG	14	3282	1/1	0.93	0.10	-	82,82,82,82	0
57	MG	14	3162	1/1	0.82	0.26	-	91,91,91,91	0
57	MG	1H	3441	1/1	0.99	0.07	-	100,100,100,100	0
57	MG	14	3291	1/1	0.90	0.16	-	71,71,71,71	0
57	MG	14	3155	1/1	0.93	0.32	-	83,83,83,83	0
57	MG	14	3207	1/1	0.95	0.49	-	70,70,70,70	0
57	MG	1H	3080	1/1	0.96	0.18	-	75,75,75,75	0
57	MG	1H	3313	1/1	0.81	0.12	-	62,62,62,62	0
57	MG	14	3336	1/1	0.86	0.09	-	109,109,109,109	0
57	MG	1H	3216	1/1	0.85	0.36	-	79,79,79,79	0
57	MG	1G	1616	1/1	0.92	0.24	-	84,84,84,84	0
57	MG	13	1650	1/1	0.86	0.38	-	85,85,85,85	0
57	MG	1H	3223	1/1	0.91	0.27	-	79,79,79,79	0
57	MG	14	3378	1/1	0.92	0.14	-	101,101,101,101	0
57	MG	1H	3059	1/1	0.86	0.14	-	72,72,72,72	0
57	MG	14	3157	1/1	0.94	0.13	-	96,96,96,96	0
57	MG	14	3085	1/1	0.97	0.22	-	52,52,52,52	0
57	MG	13	1623	1/1	0.83	0.20	-	70,70,70,70	0
57	MG	14	3104	1/1	0.89	0.25	-	89,89,89,89	0
57	MG	14	3374	1/1	0.91	0.10	-	94,94,94,94	0
57	MG	14	3088	1/1	0.94	0.43	-	82,82,82,82	0
57	MG	1G	1624	1/1	0.83	0.22	-	103,103,103,103	0
57	MG	1H	3516	1/1	0.96	0.09	-	122,122,122,122	0
57	MG	14	3441	1/1	0.93	0.14	-	103,103,103,103	0
57	MG	1G	1634	1/1	0.71	0.39	-	98,98,98,98	0
57	MG	1H	3277	1/1	0.85	0.14	-	79,79,79,79	0
57	MG	1H	3159	1/1	0.81	0.40	-	95,95,95,95	0
57	MG	14	3367	1/1	0.86	0.10	-	101,101,101,101	0
57	MG	13	1651	1/1	0.89	0.21	-	118,118,118,118	0
57	MG	21	302	1/1	0.80	0.34	-	85,85,85,85	0
57	MG	1G	1698	1/1	0.54	0.07	-	138,138,138,138	0
57	MG	1G	1716	1/1	0.91	0.15	-	110,110,110,110	0
57	MG	14	3175	1/1	0.73	0.53	-	100,100,100,100	0
57	MG	1H	3202	1/1	0.95	0.21	-	80,80,80,80	0
57	MG	1H	3121	1/1	0.94	0.22	-	89,89,89,89	0
57	MG	14	3063	1/1	0.96	0.20	-	93,93,93,93	0
57	MG	14	3361	1/1	0.93	0.17	-	87,87,87,87	0
57	MG	1H	3429	1/1	0.95	0.08	-	87,87,87,87	0
57	MG	14	3250	1/1	0.82	0.11	-	84,84,84,84	0
57	MG	1H	3269	1/1	0.95	0.08	-	83,83,83,83	0
57	MG	1G	1650	1/1	0.80	0.24	-	111,111,111,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3428	1/1	0.82	0.05	-	110,110,110,110	0
57	MG	13	1626	1/1	0.97	0.11	-	96,96,96,96	0
57	MG	13	1608	1/1	0.98	0.07	-	93,93,93,93	0
57	MG	1H	3530	1/1	0.87	0.56	-	99,99,99,99	0
57	MG	1G	1663	1/1	0.88	0.21	-	112,112,112,112	0
57	MG	1H	3346	1/1	0.87	0.10	-	75,75,75,75	0
57	MG	1H	3185	1/1	0.86	0.29	-	76,76,76,76	0
57	MG	1H	3187	1/1	0.89	0.28	-	83,83,83,83	0
57	MG	1H	3310	1/1	0.95	0.06	-	76,76,76,76	0
57	MG	14	3203	1/1	0.85	0.31	-	95,95,95,95	0
57	MG	13	1737	1/1	0.91	0.10	-	107,107,107,107	0
57	MG	1G	1701	1/1	0.71	0.12	-	115,115,115,115	0
57	MG	14	3353	1/1	0.97	0.10	-	89,89,89,89	0
57	MG	25	301	1/1	0.69	0.21	-	120,120,120,120	0
57	MG	1G	1708	1/1	0.94	0.12	-	127,127,127,127	0
57	MG	1H	3153	1/1	0.92	0.34	-	71,71,71,71	0
57	MG	14	3376	1/1	0.90	0.13	-	82,82,82,82	0
57	MG	1H	3260	1/1	0.94	0.07	-	70,70,70,70	0
57	MG	1H	3482	1/1	0.95	0.10	-	107,107,107,107	0
57	MG	1H	3448	1/1	0.95	0.23	-	76,76,76,76	0
57	MG	13	1666	1/1	0.69	0.24	-	98,98,98,98	0
57	MG	14	3387	1/1	0.98	0.06	-	83,83,83,83	0
57	MG	13	1716	1/1	0.86	0.12	-	116,116,116,116	0
57	MG	13	1739	1/1	0.88	0.16	-	119,119,119,119	0
57	MG	14	3429	1/1	0.64	0.31	-	109,109,109,109	0
59	ZN	G8	201	1/1	0.96	0.09	-	150,150,150,150	0
57	MG	35	201	1/1	0.90	0.24	-	81,81,81,81	0
57	MG	1H	3489	1/1	0.61	0.15	-	107,107,107,107	0
57	MG	1H	3192	1/1	0.92	0.25	-	83,83,83,83	0
57	MG	1H	3391	1/1	0.81	0.41	-	90,90,90,90	0
57	MG	1H	3354	1/1	0.87	0.17	-	78,78,78,78	0
57	MG	1H	3513	1/1	0.80	0.14	-	104,104,104,104	0
57	MG	14	3219	1/1	0.98	0.14	-	59,59,59,59	0
57	MG	1H	3295	1/1	0.98	0.12	-	58,58,58,58	0
57	MG	13	1697	1/1	0.95	0.07	-	110,110,110,110	0
57	MG	1H	3363	1/1	0.95	0.14	-	73,73,73,73	0
57	MG	14	3290	1/1	0.91	0.17	-	71,71,71,71	0
57	MG	1H	3109	1/1	0.95	0.67	-	79,79,79,79	0
57	MG	14	3230	1/1	0.95	0.15	-	56,56,56,56	0
57	MG	1H	3037	1/1	0.98	0.11	-	57,57,57,57	0
57	MG	1G	1660	1/1	0.92	0.12	-	128,128,128,128	0
57	MG	13	1656	1/1	0.90	0.27	-	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3195	1/1	0.95	0.23	-	85,85,85,85	0
57	MG	1H	3095	1/1	0.96	0.17	-	76,76,76,76	0
57	MG	1H	3467	1/1	0.98	0.11	-	74,74,74,74	0
57	MG	14	3329	1/1	0.98	0.16	-	93,93,93,93	0
57	MG	13	1613	1/1	0.94	0.18	-	94,94,94,94	0
57	MG	1H	3392	1/1	0.91	0.16	-	74,74,74,74	0
57	MG	1H	3087	1/1	0.66	0.52	-	75,75,75,75	0
57	MG	1G	1631	1/1	0.83	0.10	-	103,103,103,103	0
57	MG	1G	1697	1/1	0.80	0.09	-	125,125,125,125	0
57	MG	1H	3356	1/1	0.95	0.15	-	79,79,79,79	0
57	MG	13	1603	1/1	0.97	0.22	-	92,92,92,92	0
57	MG	14	3393	1/1	0.95	0.08	-	89,89,89,89	0
57	MG	14	3451	1/1	0.78	0.34	-	110,110,110,110	0
57	MG	1H	3005	1/1	1.00	0.15	-	67,67,67,67	0
57	MG	14	3276	1/1	0.82	0.08	-	85,85,85,85	0
57	MG	31	301	1/1	0.87	0.15	-	70,70,70,70	0
57	MG	1H	3339	1/1	0.88	0.06	-	99,99,99,99	0
57	MG	1G	1652	1/1	0.89	0.18	-	105,105,105,105	0
57	MG	1H	3334	1/1	0.88	0.18	-	103,103,103,103	0
57	MG	1H	3085	1/1	0.66	0.34	-	79,79,79,79	0
57	MG	14	3380	1/1	0.86	0.12	-	106,106,106,106	0
57	MG	14	3173	1/1	0.71	0.26	-	90,90,90,90	0
57	MG	1G	1633	1/1	0.80	0.12	-	102,102,102,102	0
57	MG	13	1682	1/1	0.92	0.04	-	109,109,109,109	0
57	MG	1H	3445	1/1	0.89	0.32	-	87,87,87,87	0
57	MG	1H	3549	1/1	0.95	0.15	-	94,94,94,94	0
57	MG	14	3151	1/1	0.96	0.15	-	108,108,108,108	0
57	MG	1G	1723	1/1	0.45	0.19	-	127,127,127,127	0
57	MG	1G	1713	1/1	0.92	0.20	-	120,120,120,120	0
57	MG	1H	3412	1/1	0.84	0.07	-	90,90,90,90	0
57	MG	1H	3180	1/1	0.63	0.34	-	81,81,81,81	0
57	MG	1H	3170	1/1	0.77	0.23	-	80,80,80,80	0
57	MG	1H	3165	1/1	0.83	0.23	-	85,85,85,85	0
57	MG	13	1647	1/1	0.84	0.38	-	99,99,99,99	0
57	MG	14	3249	1/1	0.95	0.06	-	85,85,85,85	0
57	MG	14	3267	1/1	0.81	0.07	-	119,119,119,119	0
57	MG	14	3435	1/1	0.94	0.05	-	122,122,122,122	0
57	MG	14	3297	1/1	0.95	0.08	-	90,90,90,90	0
57	MG	14	3215	1/1	0.86	0.08	-	98,98,98,98	0
57	MG	1H	3378	1/1	0.98	0.08	-	54,54,54,54	0
57	MG	14	3099	1/1	0.97	0.55	-	101,101,101,101	0
57	MG	13	1701	1/1	0.94	0.09	-	124,124,124,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3452	1/1	0.47	0.10	-	115,115,115,115	0
57	MG	14	3422	1/1	0.80	0.12	-	104,104,104,104	0
57	MG	1G	1692	1/1	0.92	0.07	-	103,103,103,103	0
57	MG	14	3048	1/1	0.95	0.13	-	72,72,72,72	0
57	MG	1G	1676	1/1	0.96	0.14	-	104,104,104,104	0
57	MG	14	3277	1/1	0.97	0.06	-	64,64,64,64	0
57	MG	1H	3540	1/1	0.76	0.45	-	110,110,110,110	0
57	MG	14	3363	1/1	0.91	0.05	-	83,83,83,83	0
57	MG	1G	1695	1/1	0.88	0.13	-	126,126,126,126	0
57	MG	1J	207	1/1	0.77	0.09	-	119,119,119,119	0
57	MG	1H	3526	1/1	0.94	0.20	-	96,96,96,96	0
57	MG	14	3116	1/1	0.79	0.20	-	77,77,77,77	0
57	MG	1H	3290	1/1	0.96	0.09	-	87,87,87,87	0
57	MG	1H	3545	1/1	0.91	0.47	-	102,102,102,102	0
57	MG	1H	3106	1/1	0.97	0.09	-	73,73,73,73	0
57	MG	1H	3309	1/1	0.88	0.07	-	73,73,73,73	0
57	MG	16	210	1/1	0.87	0.36	-	86,86,86,86	0
57	MG	1H	3440	1/1	0.98	0.05	-	83,83,83,83	0
57	MG	1H	3379	1/1	0.89	0.13	-	87,87,87,87	0
57	MG	14	3301	1/1	0.76	0.11	-	89,89,89,89	0
57	MG	14	3012	1/1	0.95	0.32	-	69,69,69,69	0
57	MG	F8	101	1/1	0.94	0.14	-	85,85,85,85	0
57	MG	1H	3528	1/1	0.84	0.12	-	117,117,117,117	0
57	MG	13	1726	1/1	0.96	0.05	-	107,107,107,107	0
57	MG	1H	3078	1/1	0.91	0.34	-	85,85,85,85	0
57	MG	1H	3447	1/1	0.95	0.04	-	98,98,98,98	0
57	MG	1H	3342	1/1	0.91	0.10	-	83,83,83,83	0
57	MG	1H	3359	1/1	0.94	0.04	-	92,92,92,92	0
57	MG	1H	3345	1/1	0.96	0.06	-	85,85,85,85	0
57	MG	1H	3197	1/1	0.51	0.38	-	93,93,93,93	0
57	MG	1H	3552	1/1	0.74	0.22	-	113,113,113,113	0
57	MG	1H	3487	1/1	0.85	0.04	-	108,108,108,108	0
57	MG	1H	3011	1/1	0.97	0.21	-	79,79,79,79	0
57	MG	14	3355	1/1	0.62	0.20	-	99,99,99,99	0
57	MG	88	203	1/1	0.86	0.32	-	83,83,83,83	0
57	MG	1H	3117	1/1	0.66	0.18	-	96,96,96,96	0
57	MG	14	3028	1/1	0.95	0.24	-	67,67,67,67	0
57	MG	14	3390	1/1	0.87	0.09	-	73,73,73,73	0
57	MG	1H	3537	1/1	0.72	0.11	-	112,112,112,112	0
57	MG	1H	3366	1/1	0.96	0.12	-	56,56,56,56	0
57	MG	1H	3327	1/1	0.95	0.13	-	81,81,81,81	0
57	MG	14	3047	1/1	0.88	0.12	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3341	1/1	0.62	0.14	-	113,113,113,113	0
57	MG	1G	1618	1/1	0.92	0.12	-	91,91,91,91	0
57	MG	1H	3325	1/1	0.76	0.10	-	88,88,88,88	0
57	MG	1G	1620	1/1	0.46	0.62	-	93,93,93,93	0
57	MG	1H	3524	1/1	0.93	0.17	-	61,61,61,61	0
57	MG	14	3254	1/1	0.96	0.12	-	87,87,87,87	0
57	MG	13	1715	1/1	0.51	0.17	-	119,119,119,119	0
57	MG	14	3122	1/1	0.97	0.14	-	90,90,90,90	0
57	MG	14	3140	1/1	0.79	0.32	-	89,89,89,89	0
57	MG	14	3284	1/1	0.85	0.29	-	107,107,107,107	0
57	MG	1G	1645	1/1	0.96	0.21	-	124,124,124,124	0
57	MG	14	3231	1/1	0.91	0.13	-	78,78,78,78	0
57	MG	1H	3409	1/1	0.98	0.10	-	83,83,83,83	0
57	MG	14	3011	1/1	0.89	0.57	-	76,76,76,76	0
57	MG	1H	3114	1/1	0.93	0.16	-	71,71,71,71	0
57	MG	14	3199	1/1	0.52	0.55	-	99,99,99,99	0
57	MG	13	1664	1/1	0.94	0.24	-	91,91,91,91	0
57	MG	1H	3484	1/1	0.53	0.29	-	97,97,97,97	0
57	MG	1H	3204	1/1	0.91	0.28	-	80,80,80,80	0
57	MG	1H	3422	1/1	0.68	0.11	-	114,114,114,114	0
57	MG	1H	3322	1/1	0.98	0.10	-	59,59,59,59	0
57	MG	14	3330	1/1	0.92	0.06	-	94,94,94,94	0
57	MG	88	202	1/1	0.77	0.31	-	71,71,71,71	0
57	MG	1G	1666	1/1	0.95	0.17	-	110,110,110,110	0
57	MG	14	3262	1/1	0.84	0.10	-	104,104,104,104	0
57	MG	1G	1628	1/1	0.84	0.23	-	123,123,123,123	0
57	MG	1G	1657	1/1	0.94	0.10	-	114,114,114,114	0
57	MG	1G	1681	1/1	0.90	0.12	-	131,131,131,131	0
57	MG	1G	1661	1/1	0.98	0.23	-	118,118,118,118	0
57	MG	14	3371	1/1	0.85	0.10	-	108,108,108,108	0
57	MG	1H	3081	1/1	0.90	0.15	-	77,77,77,77	0
57	MG	14	3021	1/1	0.98	0.36	-	63,63,63,63	0
57	MG	1H	3424	1/1	0.95	0.15	-	84,84,84,84	0
57	MG	14	3139	1/1	0.93	0.84	-	88,88,88,88	0
57	MG	1H	3148	1/1	0.94	0.13	-	88,88,88,88	0
57	MG	1H	3076	1/1	0.95	0.37	-	75,75,75,75	0
57	MG	14	3146	1/1	0.96	0.09	-	62,62,62,62	0
57	MG	1H	3166	1/1	0.58	0.22	-	67,67,67,67	0
57	MG	4L	101	1/1	0.85	0.43	-	102,102,102,102	0
57	MG	14	3233	1/1	0.91	0.11	-	85,85,85,85	0
57	MG	1H	3016	1/1	0.97	0.35	-	52,52,52,52	0
57	MG	1H	3186	1/1	0.99	0.09	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3079	1/1	0.94	0.17	-	85,85,85,85	0
57	MG	1H	3415	1/1	0.79	0.12	-	95,95,95,95	0
57	MG	1H	3404	1/1	0.92	0.67	-	71,71,71,71	0
57	MG	14	3357	1/1	0.92	0.08	-	116,116,116,116	0
57	MG	1H	3042	1/1	0.80	0.28	-	67,67,67,67	0
57	MG	1H	3023	1/1	0.90	0.30	-	71,71,71,71	0
57	MG	14	3314	1/1	0.88	0.19	-	78,78,78,78	0
57	MG	13	1712	1/1	0.76	0.07	-	106,106,106,106	0
57	MG	1H	3108	1/1	0.88	0.36	-	68,68,68,68	0
57	MG	1H	3161	1/1	0.82	0.35	-	77,77,77,77	0
57	MG	13	1733	1/1	0.90	0.05	-	118,118,118,118	0
57	MG	1H	3515	1/1	0.95	0.12	-	78,78,78,78	0
57	MG	14	3188	1/1	0.98	0.23	-	69,69,69,69	0
57	MG	1G	1621	1/1	0.87	0.46	-	105,105,105,105	0
57	MG	32	301	1/1	0.62	0.12	-	137,137,137,137	0
57	MG	14	3090	1/1	0.94	0.27	-	77,77,77,77	0
57	MG	14	3283	1/1	0.95	0.06	-	105,105,105,105	0
57	MG	1H	3220	1/1	0.96	0.21	-	71,71,71,71	0
57	MG	1H	3094	1/1	0.88	0.23	-	64,64,64,64	0
57	MG	42	201	1/1	0.89	0.28	-	107,107,107,107	0
57	MG	1H	3331	1/1	0.95	0.06	-	88,88,88,88	0
57	MG	14	3323	1/1	0.96	0.10	-	84,84,84,84	0
57	MG	14	3389	1/1	0.90	0.18	-	72,72,72,72	0
57	MG	1H	3221	1/1	0.75	0.37	-	81,81,81,81	0
57	MG	1H	3196	1/1	0.89	0.22	-	103,103,103,103	0
57	MG	14	3334	1/1	0.91	0.09	-	83,83,83,83	0
57	MG	1H	3152	1/1	0.70	0.28	-	87,87,87,87	0
57	MG	1H	3164	1/1	0.96	0.44	-	85,85,85,85	0
57	MG	1H	3122	1/1	0.86	0.39	-	80,80,80,80	0
57	MG	1H	3473	1/1	0.89	0.13	-	98,98,98,98	0
57	MG	14	3354	1/1	0.95	0.12	-	80,80,80,80	0
57	MG	1G	1704	1/1	0.70	0.21	-	127,127,127,127	0
57	MG	45	201	1/1	0.90	0.69	-	84,84,84,84	0
57	MG	1J	210	1/1	0.80	0.08	-	135,135,135,135	0
57	MG	13	1633	1/1	0.89	0.13	-	82,82,82,82	0
57	MG	14	3144	1/1	0.76	0.39	-	84,84,84,84	0
57	MG	14	3430	1/1	0.79	0.23	-	102,102,102,102	0
57	MG	14	3333	1/1	0.63	0.19	-	97,97,97,97	0
57	MG	14	3220	1/1	0.96	0.08	-	65,65,65,65	0
57	MG	13	1704	1/1	0.93	0.38	-	111,111,111,111	0
57	MG	7A	101	1/1	0.97	0.32	-	110,110,110,110	0
57	MG	1H	3210	1/1	0.64	0.34	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3245	1/1	0.99	0.11	-	58,58,58,58	0
57	MG	14	3300	1/1	0.78	0.08	-	86,86,86,86	0
57	MG	1H	3419	1/1	0.92	0.26	-	73,73,73,73	0
57	MG	1G	1649	1/1	0.87	0.81	-	96,96,96,96	0
57	MG	14	3382	1/1	0.89	0.08	-	116,116,116,116	0
57	MG	1H	3199	1/1	0.92	0.14	-	81,81,81,81	0
57	MG	1H	3233	1/1	0.90	0.20	-	94,94,94,94	0
57	MG	1H	3504	1/1	0.74	0.29	-	104,104,104,104	0
57	MG	14	3197	1/1	0.92	0.42	-	92,92,92,92	0
57	MG	1H	3255	1/1	0.95	0.12	-	72,72,72,72	0
57	MG	14	3316	1/1	0.94	0.07	-	100,100,100,100	0
57	MG	1H	3444	1/1	0.88	0.24	-	72,72,72,72	0
57	MG	13	1680	1/1	0.88	0.12	-	89,89,89,89	0
57	MG	1G	1638	1/1	0.70	0.34	-	119,119,119,119	0
57	MG	1H	3371	1/1	0.63	0.15	-	88,88,88,88	0
57	MG	1H	3475	1/1	0.84	0.05	-	99,99,99,99	0
57	MG	1H	3241	1/1	0.73	0.20	-	82,82,82,82	0
57	MG	1H	3061	1/1	0.99	0.38	-	62,62,62,62	0
57	MG	13	1642	1/1	0.69	0.30	-	95,95,95,95	0
57	MG	1H	3361	1/1	0.97	0.07	-	53,53,53,53	0
57	MG	1H	3280	1/1	0.91	0.14	-	47,47,47,47	0
57	MG	14	3340	1/1	0.94	0.09	-	63,63,63,63	0
57	MG	1G	1642	1/1	0.85	0.69	-	100,100,100,100	0
57	MG	14	3195	1/1	0.89	0.35	-	98,98,98,98	0
57	MG	1G	1602	1/1	0.95	0.33	-	105,105,105,105	0
57	MG	14	3411	1/1	0.91	0.07	-	115,115,115,115	0
57	MG	14	3201	1/1	0.98	0.29	-	82,82,82,82	0
57	MG	1H	3352	1/1	0.97	0.08	-	70,70,70,70	0
57	MG	1H	3097	1/1	0.94	0.22	-	43,43,43,43	0
57	MG	1H	3349	1/1	0.96	0.06	-	61,61,61,61	0
57	MG	1H	3285	1/1	0.98	0.16	-	69,69,69,69	0
57	MG	14	3362	1/1	0.92	0.10	-	99,99,99,99	0
57	MG	13	1654	1/1	0.76	0.34	-	85,85,85,85	0
57	MG	1H	3433	1/1	0.69	0.10	-	98,98,98,98	0
57	MG	14	3331	1/1	0.97	0.14	-	56,56,56,56	0
57	MG	1H	3494	1/1	0.78	0.20	-	87,87,87,87	0
57	MG	14	3043	1/1	0.98	0.70	-	96,96,96,96	0
57	MG	13	1681	1/1	0.93	0.20	-	91,91,91,91	0
57	MG	1G	1678	1/1	0.88	0.16	-	98,98,98,98	0
57	MG	1H	3176	1/1	0.32	0.41	-	102,102,102,102	0
57	MG	1G	1686	1/1	0.93	0.08	-	113,113,113,113	0
57	MG	1H	3360	1/1	0.86	0.13	-	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3174	1/1	0.90	0.25	-	78,78,78,78	0
57	MG	1H	3305	1/1	0.94	0.15	-	72,72,72,72	0
57	MG	14	3257	1/1	0.82	0.19	-	118,118,118,118	0
57	MG	14	3226	1/1	0.97	0.17	-	54,54,54,54	0
57	MG	14	3202	1/1	0.94	0.15	-	106,106,106,106	0
57	MG	1H	3436	1/1	0.81	0.10	-	87,87,87,87	0
57	MG	14	3346	1/1	0.91	0.09	-	98,98,98,98	0
57	MG	1H	3517	1/1	0.93	0.30	-	85,85,85,85	0
57	MG	1H	3536	1/1	0.63	0.17	-	104,104,104,104	0
57	MG	1H	3246	1/1	0.81	0.17	-	54,54,54,54	0
57	MG	14	3117	1/1	0.84	0.34	-	69,69,69,69	0
57	MG	1H	3151	1/1	0.91	0.28	-	79,79,79,79	0
57	MG	1H	3442	1/1	0.90	0.12	-	107,107,107,107	0
57	MG	14	3167	1/1	0.89	0.07	-	95,95,95,95	0
57	MG	1H	3050	1/1	0.75	0.36	-	85,85,85,85	0
57	MG	1H	3184	1/1	0.85	0.64	-	100,100,100,100	0
57	MG	1G	1718	1/1	0.87	0.10	-	124,124,124,124	0
57	MG	1H	3499	1/1	0.90	0.27	-	89,89,89,89	0
57	MG	1H	3510	1/1	0.77	0.07	-	104,104,104,104	0
57	MG	1H	3490	1/1	0.88	0.08	-	95,95,95,95	0
57	MG	14	3101	1/1	0.95	0.21	-	87,87,87,87	0
57	MG	14	3014	1/1	0.99	0.36	-	72,72,72,72	0
57	MG	1H	3384	1/1	0.85	0.10	-	59,59,59,59	0
57	MG	1H	3211	1/1	0.88	0.36	-	69,69,69,69	0
57	MG	14	3450	1/1	0.79	0.31	-	116,116,116,116	0
57	MG	1H	3287	1/1	0.95	0.10	-	76,76,76,76	0
57	MG	14	3153	1/1	0.50	0.23	-	123,123,123,123	0
57	MG	14	3453	1/1	0.55	0.20	-	118,118,118,118	0
57	MG	13	1641	1/1	0.82	0.44	-	79,79,79,79	0
57	MG	1H	3146	1/1	0.86	0.41	-	85,85,85,85	0
57	MG	1H	3060	1/1	0.82	0.54	-	90,90,90,90	0
57	MG	1H	3236	1/1	0.95	0.16	-	93,93,93,93	0
57	MG	14	3446	1/1	0.71	0.07	-	118,118,118,118	0
57	MG	14	3292	1/1	0.98	0.06	-	71,71,71,71	0
57	MG	1H	3301	1/1	0.87	0.18	-	86,86,86,86	0
57	MG	14	3183	1/1	0.77	0.45	-	88,88,88,88	0
57	MG	42	202	1/1	0.85	0.26	-	115,115,115,115	0
57	MG	14	3386	1/1	0.92	0.12	-	65,65,65,65	0
57	MG	14	3342	1/1	0.91	0.12	-	105,105,105,105	0
57	MG	14	3015	1/1	0.97	0.14	-	65,65,65,65	0
57	MG	1H	3535	1/1	0.71	0.20	-	110,110,110,110	0
57	MG	1H	3402	1/1	0.54	0.20	-	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3129	1/1	0.94	0.21	-	90,90,90,90	0
57	MG	14	3448	1/1	0.81	0.10	-	120,120,120,120	0
57	MG	1H	3140	1/1	0.88	0.20	-	90,90,90,90	0
57	MG	1J	205	1/1	0.81	0.12	-	101,101,101,101	0
57	MG	1H	3175	1/1	0.68	0.38	-	73,73,73,73	0
57	MG	1H	3453	1/1	0.91	0.19	-	82,82,82,82	0
57	MG	1H	3502	1/1	0.79	0.12	-	90,90,90,90	0
57	MG	14	3141	1/1	0.69	0.20	-	85,85,85,85	0
57	MG	1H	3347	1/1	0.14	0.12	-	113,113,113,113	0
57	MG	14	3421	1/1	0.89	0.23	-	96,96,96,96	0
57	MG	1H	3013	1/1	0.60	0.18	-	94,94,94,94	0
57	MG	14	3115	1/1	0.76	0.45	-	78,78,78,78	0
57	MG	14	3073	1/1	0.88	0.42	-	61,61,61,61	0
57	MG	14	3426	1/1	0.91	0.06	-	99,99,99,99	0
57	MG	1H	3350	1/1	0.91	0.12	-	58,58,58,58	0
57	MG	14	3072	1/1	0.85	0.26	-	88,88,88,88	0
57	MG	1H	3423	1/1	0.91	0.08	-	115,115,115,115	0
57	MG	14	3185	1/1	0.73	0.25	-	93,93,93,93	0
57	MG	1H	3542	1/1	0.88	0.07	-	103,103,103,103	0
57	MG	1H	3129	1/1	0.86	0.12	-	85,85,85,85	0
57	MG	13	1707	1/1	0.91	0.06	-	88,88,88,88	0
57	MG	13	1702	1/1	0.96	0.08	-	70,70,70,70	0
57	MG	13	1621	1/1	0.80	0.47	-	94,94,94,94	0
57	MG	1H	3311	1/1	0.87	0.10	-	91,91,91,91	0
57	MG	21	303	1/1	0.88	0.12	-	61,61,61,61	0
57	MG	13	1691	1/1	0.89	0.09	-	107,107,107,107	0
57	MG	14	3317	1/1	0.97	0.05	-	100,100,100,100	0
57	MG	14	3187	1/1	0.73	0.46	-	106,106,106,106	0
57	MG	1H	3474	1/1	0.92	0.09	-	83,83,83,83	0
57	MG	1H	3523	1/1	0.86	0.17	-	102,102,102,102	0
57	MG	13	1604	1/1	0.98	0.12	-	79,79,79,79	0
57	MG	1G	1721	1/1	0.87	0.06	-	128,128,128,128	0
57	MG	1H	3405	1/1	0.94	0.10	-	75,75,75,75	0
57	MG	14	3053	1/1	0.85	0.92	-	82,82,82,82	0
57	MG	13	1617	1/1	0.84	0.37	-	69,69,69,69	0
57	MG	14	3417	1/1	0.87	0.07	-	117,117,117,117	0
57	MG	1G	1659	1/1	0.80	0.10	-	120,120,120,120	0
57	MG	13	1719	1/1	0.70	0.07	-	118,118,118,118	0
57	MG	14	3204	1/1	0.86	0.13	-	120,120,120,120	0
57	MG	1H	3018	1/1	0.96	0.34	-	63,63,63,63	0
57	MG	1H	3458	1/1	0.87	0.12	-	89,89,89,89	0
57	MG	1H	3411	1/1	0.77	0.17	-	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1718	1/1	0.80	0.04	-	130,130,130,130	0
57	MG	14	3410	1/1	0.96	0.14	-	107,107,107,107	0
57	MG	14	3419	1/1	0.95	0.27	-	119,119,119,119	0
57	MG	14	3414	1/1	0.82	0.11	-	99,99,99,99	0
57	MG	14	3205	1/1	0.92	0.11	-	102,102,102,102	0
57	MG	1H	3399	1/1	0.80	0.07	-	109,109,109,109	0
57	MG	14	3006	1/1	0.97	0.18	-	78,78,78,78	0
57	MG	1G	1637	1/1	0.94	0.38	-	106,106,106,106	0
57	MG	29	301	1/1	0.95	0.27	-	65,65,65,65	0
57	MG	1H	3340	1/1	0.91	0.05	-	109,109,109,109	0
57	MG	14	3434	1/1	0.86	0.32	-	110,110,110,110	0
57	MG	1G	1609	1/1	0.69	0.65	-	96,96,96,96	0
57	MG	1H	3089	1/1	0.67	0.43	-	88,88,88,88	0
57	MG	14	3148	1/1	0.89	0.18	-	113,113,113,113	0
57	MG	14	3041	1/1	0.97	0.29	-	66,66,66,66	0
57	MG	1G	1705	1/1	0.92	0.03	-	117,117,117,117	0
57	MG	1H	3271	1/1	0.86	0.14	-	84,84,84,84	0
57	MG	14	3432	1/1	0.96	0.25	-	103,103,103,103	0
57	MG	14	3457	1/1	0.73	0.09	-	134,134,134,134	0
57	MG	14	3412	1/1	0.94	0.16	-	106,106,106,106	0
57	MG	14	3070	1/1	0.96	0.64	-	66,66,66,66	0
57	MG	13	1627	1/1	0.87	0.17	-	94,94,94,94	0
57	MG	13	1672	1/1	0.89	0.30	-	92,92,92,92	0
57	MG	1H	3493	1/1	0.47	0.17	-	106,106,106,106	0
57	MG	1H	3323	1/1	0.91	0.06	-	78,78,78,78	0
57	MG	1H	3507	1/1	0.94	0.16	-	90,90,90,90	0
57	MG	1H	3381	1/1	0.97	0.14	-	58,58,58,58	0
57	MG	13	1655	1/1	0.62	0.41	-	83,83,83,83	0
57	MG	14	3407	1/1	0.94	0.19	-	111,111,111,111	0
57	MG	13	1685	1/1	0.90	0.07	-	79,79,79,79	0
57	MG	1H	3481	1/1	0.69	0.15	-	92,92,92,92	0
57	MG	13	1720	1/1	0.83	0.06	-	121,121,121,121	0
57	MG	14	3279	1/1	0.92	0.10	-	93,93,93,93	0
57	MG	3I	201	1/1	0.95	0.24	-	75,75,75,75	0
57	MG	1H	3235	1/1	0.78	0.22	-	96,96,96,96	0
57	MG	1G	1683	1/1	0.90	0.09	-	132,132,132,132	0
57	MG	13	1740	1/1	0.70	0.14	-	162,162,162,162	0
57	MG	1G	1668	1/1	0.94	0.10	-	106,106,106,106	0
57	MG	14	3264	1/1	0.84	0.14	-	88,88,88,88	0
57	MG	1H	3032	1/1	0.98	0.36	-	68,68,68,68	0
57	MG	1H	3387	1/1	0.92	0.08	-	87,87,87,87	0
57	MG	13	1636	1/1	0.94	0.25	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3260	1/1	0.91	0.16	-	77,77,77,77	0
57	MG	P8	101	1/1	0.72	0.46	-	76,76,76,76	0
57	MG	1H	3376	1/1	0.96	0.10	-	71,71,71,71	0
57	MG	1H	3533	1/1	0.83	0.34	-	99,99,99,99	0
57	MG	1G	1615	1/1	0.84	0.15	-	89,89,89,89	0
57	MG	1H	3400	1/1	0.88	0.10	-	79,79,79,79	0
57	MG	14	3408	1/1	0.98	0.07	-	77,77,77,77	0
57	MG	13	1657	1/1	0.94	0.58	-	75,75,75,75	0
57	MG	14	3327	1/1	0.92	0.07	-	108,108,108,108	0
57	MG	14	3244	1/1	0.97	0.06	-	68,68,68,68	0
57	MG	1H	3004	1/1	0.95	0.26	-	64,64,64,64	0
57	MG	1H	3173	1/1	0.67	0.32	-	77,77,77,77	0
57	MG	14	3107	1/1	0.96	0.58	-	94,94,94,94	0
57	MG	14	3196	1/1	0.88	0.46	-	85,85,85,85	0
57	MG	14	3366	1/1	0.98	0.04	-	99,99,99,99	0
57	MG	1H	3477	1/1	0.83	0.18	-	91,91,91,91	0
57	MG	14	3056	1/1	0.97	0.37	-	74,74,74,74	0
57	MG	1G	1672	1/1	0.86	0.04	-	117,117,117,117	0
57	MG	1G	1635	1/1	0.91	0.29	-	94,94,94,94	0
57	MG	1H	3370	1/1	0.87	0.15	-	80,80,80,80	0
57	MG	1H	3547	1/1	0.90	0.07	-	131,131,131,131	0
57	MG	1H	3024	1/1	0.98	0.17	-	64,64,64,64	0
57	MG	13	1736	1/1	0.66	0.12	-	129,129,129,129	0
57	MG	1G	1684	1/1	0.76	0.07	-	109,109,109,109	0
57	MG	1H	3521	1/1	0.95	0.09	-	65,65,65,65	0
57	MG	14	3401	1/1	0.96	0.20	-	89,89,89,89	0
57	MG	1H	3135	1/1	0.87	0.31	-	73,73,73,73	0
57	MG	1H	3449	1/1	0.98	0.25	-	92,92,92,92	0
57	MG	1H	3353	1/1	0.91	0.12	-	62,62,62,62	0
57	MG	1H	3214	1/1	0.99	0.17	-	77,77,77,77	0
57	MG	1H	3083	1/1	0.91	0.44	-	80,80,80,80	0
57	MG	1H	3344	1/1	0.97	0.09	-	60,60,60,60	0
57	MG	1H	3254	1/1	0.97	0.14	-	49,49,49,49	0
57	MG	14	3138	1/1	0.68	0.45	-	91,91,91,91	0
57	MG	14	3003	1/1	0.97	0.17	-	68,68,68,68	0
57	MG	1H	3064	1/1	0.89	0.28	-	82,82,82,82	0
57	MG	1H	3395	1/1	0.93	0.07	-	92,92,92,92	0
57	MG	14	3255	1/1	0.76	0.12	-	110,110,110,110	0
57	MG	1H	3337	1/1	0.68	0.07	-	98,98,98,98	0
57	MG	14	3171	1/1	0.95	0.47	-	86,86,86,86	0
57	MG	1H	3465	1/1	0.91	0.09	-	112,112,112,112	0
57	MG	1H	3031	1/1	0.96	0.33	-	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3188	1/1	0.83	0.35	-	88,88,88,88	0
57	MG	14	3067	1/1	0.91	0.22	-	77,77,77,77	0
57	MG	1G	1612	1/1	0.84	0.11	-	103,103,103,103	0
57	MG	1G	1706	1/1	0.74	0.05	-	138,138,138,138	0
57	MG	1H	3483	1/1	0.95	0.06	-	99,99,99,99	0
57	MG	1H	3147	1/1	0.76	0.39	-	125,125,125,125	0
57	MG	14	3324	1/1	0.81	0.10	-	90,90,90,90	0
57	MG	1H	3091	1/1	0.83	0.64	-	77,77,77,77	0
57	MG	14	3112	1/1	0.93	0.46	-	68,68,68,68	0
57	MG	13	1684	1/1	0.72	0.10	-	105,105,105,105	0
57	MG	14	3084	1/1	0.97	0.27	-	67,67,67,67	0
57	MG	1H	3386	1/1	0.95	0.21	-	72,72,72,72	0
57	MG	1G	1613	1/1	0.81	0.95	-	93,93,93,93	0
57	MG	1J	201	1/1	0.91	0.22	-	97,97,97,97	0
57	MG	1H	3332	1/1	0.96	0.10	-	84,84,84,84	0
57	MG	1H	3304	1/1	0.92	0.20	-	64,64,64,64	0
57	MG	1G	1696	1/1	0.80	0.10	-	109,109,109,109	0
57	MG	1H	3104	1/1	0.94	0.16	-	68,68,68,68	0
57	MG	1H	3096	1/1	0.94	0.39	-	83,83,83,83	0
57	MG	14	3306	1/1	0.86	0.17	-	93,93,93,93	0
57	MG	2K	103	1/1	0.68	0.18	-	88,88,88,88	0
57	MG	1H	3105	1/1	0.91	0.18	-	78,78,78,78	0
57	MG	1H	3252	1/1	0.97	0.07	-	52,52,52,52	0
57	MG	1G	1639	1/1	0.89	0.69	-	90,90,90,90	0
57	MG	14	3344	1/1	0.89	0.07	-	104,104,104,104	0
57	MG	1H	3212	1/1	0.90	0.09	-	87,87,87,87	0
57	MG	1G	1640	1/1	0.95	0.39	-	80,80,80,80	0
57	MG	14	3158	1/1	0.79	0.25	-	84,84,84,84	0
57	MG	14	3193	1/1	0.93	0.44	-	96,96,96,96	0
57	MG	13	1727	1/1	0.80	0.07	-	124,124,124,124	0
57	MG	1H	3143	1/1	0.91	0.24	-	79,79,79,79	0
57	MG	14	3211	1/1	0.85	0.09	-	67,67,67,67	0
57	MG	13	1738	1/1	0.84	0.05	-	138,138,138,138	0
57	MG	14	3358	1/1	0.94	0.04	-	78,78,78,78	0
57	MG	1H	3312	1/1	0.93	0.21	-	69,69,69,69	0
57	MG	14	3449	1/1	0.93	0.06	-	105,105,105,105	0
57	MG	1H	3213	1/1	0.68	0.22	-	83,83,83,83	0
57	MG	1G	1611	1/1	0.79	0.62	-	84,84,84,84	0
57	MG	14	3332	1/1	0.97	0.16	-	63,63,63,63	0
57	MG	14	3400	1/1	0.80	0.08	-	135,135,135,135	0
57	MG	14	3025	1/1	0.84	0.24	-	78,78,78,78	0
57	MG	14	3110	1/1	0.93	0.24	-	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3349	1/1	0.91	0.07	-	99,99,99,99	0
57	MG	14	3341	1/1	0.76	0.32	-	78,78,78,78	0
57	MG	14	3431	1/1	0.69	0.17	-	107,107,107,107	0
57	MG	1H	3014	1/1	0.85	0.42	-	86,86,86,86	0
57	MG	14	3347	1/1	0.88	0.14	-	97,97,97,97	0
57	MG	13	1653	1/1	0.89	0.12	-	95,95,95,95	0
59	ZN	C5	201	1/1	0.96	0.05	-	167,167,167,167	0
57	MG	14	3321	1/1	0.90	0.12	-	89,89,89,89	0
57	MG	1H	3479	1/1	0.98	0.05	-	95,95,95,95	0
57	MG	14	3172	1/1	0.98	0.21	-	82,82,82,82	0
57	MG	13	1700	1/1	0.80	0.06	-	110,110,110,110	0
57	MG	14	3128	1/1	0.76	0.35	-	88,88,88,88	0
57	MG	1G	1711	1/1	0.59	0.06	-	156,156,156,156	0
57	MG	1H	3469	1/1	0.93	0.05	-	84,84,84,84	0
57	MG	14	3373	1/1	0.84	0.19	-	94,94,94,94	0
57	MG	1H	3495	1/1	0.90	0.08	-	87,87,87,87	0
57	MG	1H	3139	1/1	0.91	0.50	-	90,90,90,90	0
57	MG	14	3295	1/1	0.88	0.11	-	88,88,88,88	0
57	MG	1H	3227	1/1	0.76	0.19	-	90,90,90,90	0
57	MG	1H	3314	1/1	0.94	0.15	-	65,65,65,65	0
57	MG	14	3163	1/1	0.45	0.45	-	104,104,104,104	0
57	MG	1H	3217	1/1	0.80	0.39	-	79,79,79,79	0
57	MG	14	3312	1/1	0.90	0.09	-	109,109,109,109	0
57	MG	1H	3222	1/1	0.81	0.45	-	86,86,86,86	0
57	MG	14	3001	1/1	0.94	0.16	-	51,51,51,51	0
57	MG	1H	3367	1/1	0.93	0.09	-	69,69,69,69	0
57	MG	14	3154	1/1	0.75	0.33	-	78,78,78,78	0
57	MG	13	1725	1/1	0.85	0.05	-	99,99,99,99	0
57	MG	1H	3022	1/1	0.97	0.17	-	56,56,56,56	0
57	MG	1H	3056	1/1	0.84	0.47	-	86,86,86,86	0
57	MG	1G	1719	1/1	0.95	0.09	-	115,115,115,115	0
57	MG	1H	3267	1/1	0.93	0.06	-	103,103,103,103	0
57	MG	1H	3262	1/1	0.94	0.13	-	59,59,59,59	0
57	MG	16	203	1/1	0.95	0.28	-	84,84,84,84	0
57	MG	14	3176	1/1	0.94	0.51	-	90,90,90,90	0
57	MG	1H	3232	1/1	0.74	0.38	-	100,100,100,100	0
57	MG	14	3345	1/1	0.86	0.15	-	100,100,100,100	0
57	MG	14	3438	1/1	0.90	0.13	-	111,111,111,111	0
57	MG	14	3447	1/1	0.94	0.07	-	107,107,107,107	0
57	MG	14	3004	1/1	0.94	0.35	-	81,81,81,81	0
57	MG	1G	1707	1/1	0.83	0.08	-	115,115,115,115	0
57	MG	1G	1717	1/1	0.95	0.06	-	126,126,126,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3413	1/1	0.52	0.17	-	125,125,125,125	0
57	MG	1H	3491	1/1	0.84	0.23	-	100,100,100,100	0
57	MG	1H	3355	1/1	0.93	0.18	-	58,58,58,58	0
57	MG	1H	3362	1/1	0.87	0.13	-	78,78,78,78	0
57	MG	14	3213	1/1	0.98	0.12	-	70,70,70,70	0
57	MG	1H	3120	1/1	0.96	0.37	-	69,69,69,69	0
57	MG	14	3272	1/1	0.96	0.14	-	71,71,71,71	0
57	MG	14	3310	1/1	0.95	0.10	-	71,71,71,71	0
57	MG	1H	3365	1/1	0.65	0.10	-	82,82,82,82	0
57	MG	1H	3137	1/1	0.83	0.36	-	67,67,67,67	0
57	MG	1G	1703	1/1	0.87	0.10	-	107,107,107,107	0
57	MG	14	3218	1/1	0.99	0.10	-	55,55,55,55	0
57	MG	1H	3492	1/1	0.82	0.16	-	107,107,107,107	0
57	MG	14	3452	1/1	0.85	0.23	-	122,122,122,122	0
57	MG	14	3191	1/1	0.91	0.46	-	76,76,76,76	0
57	MG	1H	3511	1/1	0.92	0.07	-	113,113,113,113	0
57	MG	14	3206	1/1	0.95	0.27	-	97,97,97,97	0
57	MG	1H	3454	1/1	0.84	0.14	-	104,104,104,104	0
57	MG	14	3166	1/1	0.81	0.34	-	95,95,95,95	0
57	MG	1H	3012	1/1	0.81	0.23	-	81,81,81,81	0
57	MG	1H	3328	1/1	0.96	0.15	-	81,81,81,81	0
57	MG	1H	3509	1/1	0.67	0.36	-	114,114,114,114	0
57	MG	1G	1617	1/1	0.91	0.12	-	89,89,89,89	0
57	MG	1H	3446	1/1	0.92	0.07	-	100,100,100,100	0
57	MG	14	3135	1/1	0.59	0.38	-	112,112,112,112	0
57	MG	14	3352	1/1	0.93	0.11	-	95,95,95,95	0
57	MG	14	3455	1/1	0.72	0.36	-	115,115,115,115	0
57	MG	1H	3326	1/1	0.72	0.10	-	109,109,109,109	0
57	MG	1H	3006	1/1	0.94	0.21	-	77,77,77,77	0
57	MG	13	1668	1/1	0.63	0.29	-	112,112,112,112	0
57	MG	1H	3057	1/1	0.85	0.43	-	71,71,71,71	0
57	MG	1H	3110	1/1	0.80	0.33	-	86,86,86,86	0
57	MG	1H	3039	1/1	0.98	0.17	-	56,56,56,56	0
57	MG	14	3335	1/1	0.88	0.09	-	94,94,94,94	0
57	MG	1H	3025	1/1	0.97	0.24	-	52,52,52,52	0
57	MG	14	3018	1/1	0.90	0.24	-	82,82,82,82	0
57	MG	14	3152	1/1	0.90	0.37	-	99,99,99,99	0
57	MG	14	3243	1/1	0.88	0.18	-	93,93,93,93	0
57	MG	1G	1627	1/1	0.96	0.13	-	122,122,122,122	0
57	MG	B5	101	1/1	0.97	0.10	-	99,99,99,99	0
57	MG	13	1724	1/1	0.86	0.17	-	116,116,116,116	0
57	MG	1H	3459	1/1	0.73	0.16	-	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3416	1/1	0.96	0.07	-	80,80,80,80	0
57	MG	I8	101	1/1	0.90	0.06	-	95,95,95,95	0
57	MG	13	1671	1/1	0.94	0.07	-	108,108,108,108	0
57	MG	1H	3249	1/1	0.92	0.14	-	61,61,61,61	0
57	MG	14	3359	1/1	0.87	0.11	-	122,122,122,122	0
57	MG	1H	3190	1/1	0.90	0.13	-	73,73,73,73	0
57	MG	14	3337	1/1	0.86	0.06	-	116,116,116,116	0
57	MG	13	1661	1/1	0.93	0.16	-	101,101,101,101	0
57	MG	13	1645	1/1	0.84	0.21	-	117,117,117,117	0
57	MG	14	3364	1/1	0.82	0.08	-	98,98,98,98	0
57	MG	1H	3508	1/1	0.92	0.11	-	144,144,144,144	0
57	MG	14	3439	1/1	0.84	0.24	-	100,100,100,100	0
57	MG	14	3150	1/1	0.96	0.16	-	75,75,75,75	0
57	MG	1H	3155	1/1	0.91	0.27	-	106,106,106,106	0
57	MG	13	1706	1/1	0.90	0.15	-	88,88,88,88	0
57	MG	14	3126	1/1	0.86	0.18	-	89,89,89,89	0
57	MG	1H	3150	1/1	0.94	0.34	-	81,81,81,81	0
57	MG	14	3424	1/1	0.83	0.12	-	117,117,117,117	0
57	MG	14	3440	1/1	0.97	0.20	-	87,87,87,87	0
57	MG	1H	3500	1/1	0.85	0.10	-	90,90,90,90	0
57	MG	1H	3174	1/1	0.95	0.30	-	73,73,73,73	0
57	MG	1H	3201	1/1	0.98	0.26	-	80,80,80,80	0
57	MG	1H	3398	1/1	0.88	0.07	-	86,86,86,86	0
57	MG	14	3076	1/1	0.90	0.18	-	80,80,80,80	0
57	MG	1H	3234	1/1	0.95	0.28	-	84,84,84,84	0
57	MG	1H	3316	1/1	0.96	0.07	-	76,76,76,76	0
57	MG	1H	3462	1/1	0.83	0.06	-	99,99,99,99	0
57	MG	1H	3321	1/1	0.96	0.11	-	55,55,55,55	0
57	MG	13	1708	1/1	0.90	0.07	-	91,91,91,91	0
57	MG	1H	3464	1/1	0.97	0.17	-	57,57,57,57	0
57	MG	16	201	1/1	0.90	0.27	-	73,73,73,73	0
57	MG	1H	3525	1/1	0.53	0.19	-	99,99,99,99	0
57	MG	14	3039	1/1	0.99	0.27	-	85,85,85,85	0
57	MG	1G	1674	1/1	0.93	0.18	-	106,106,106,106	0
57	MG	1J	202	1/1	0.92	0.20	-	106,106,106,106	0
57	MG	1H	3156	1/1	0.82	0.33	-	106,106,106,106	0
57	MG	1J	208	1/1	0.78	0.17	-	124,124,124,124	0
57	MG	13	1660	1/1	0.90	0.50	-	91,91,91,91	0
57	MG	13	1639	1/1	0.91	0.44	-	80,80,80,80	0
57	MG	1H	3460	1/1	0.84	0.28	-	85,85,85,85	0
57	MG	1G	1685	1/1	0.84	0.08	-	129,129,129,129	0
57	MG	14	3444	1/1	0.90	0.48	-	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3397	1/1	0.78	0.07	-	162,162,162,162	0
57	MG	1H	3193	1/1	0.87	0.71	-	89,89,89,89	0
57	MG	14	3273	1/1	0.96	0.11	-	61,61,61,61	0
57	MG	1G	1601	1/1	0.95	0.21	-	92,92,92,92	0
57	MG	1H	3333	1/1	0.67	0.09	-	98,98,98,98	0
57	MG	14	3013	1/1	0.98	0.30	-	56,56,56,56	0
57	MG	14	3437	1/1	0.75	0.11	-	111,111,111,111	0
57	MG	14	3298	1/1	0.96	0.07	-	95,95,95,95	0
57	MG	14	3109	1/1	0.69	0.31	-	94,94,94,94	0
57	MG	14	3023	1/1	0.92	0.35	-	58,58,58,58	0
57	MG	1G	1646	1/1	0.91	0.31	-	78,78,78,78	0
57	MG	1H	3343	1/1	0.91	0.09	-	115,115,115,115	0
57	MG	14	3325	1/1	0.96	0.08	-	88,88,88,88	0
57	MG	1G	1714	1/1	0.94	0.11	-	126,126,126,126	0
57	MG	1G	1653	1/1	0.96	0.07	-	125,125,125,125	0
57	MG	1H	3527	1/1	0.93	0.10	-	97,97,97,97	0
57	MG	1H	3069	1/1	0.91	0.27	-	76,76,76,76	0
57	MG	1H	3124	1/1	0.70	0.36	-	90,90,90,90	0
57	MG	1G	1694	1/1	0.93	0.10	-	105,105,105,105	0
57	MG	14	3328	1/1	0.81	0.10	-	95,95,95,95	0
57	MG	E5	101	1/1	0.67	0.66	-	99,99,99,99	0
57	MG	13	1714	1/1	0.90	0.06	-	94,94,94,94	0
57	MG	1H	3020	1/1	0.97	0.24	-	60,60,60,60	0
57	MG	1H	3369	1/1	0.77	0.27	-	90,90,90,90	0
57	MG	13	1631	1/1	0.98	0.35	-	106,106,106,106	0
57	MG	1H	3420	1/1	0.89	0.22	-	94,94,94,94	0
57	MG	13	1665	1/1	0.92	0.20	-	128,128,128,128	0
57	MG	1G	1625	1/1	0.93	0.61	-	89,89,89,89	0
57	MG	14	3443	1/1	0.87	0.34	-	115,115,115,115	0
57	MG	1H	3183	1/1	0.92	0.29	-	75,75,75,75	0
57	MG	13	1669	1/1	0.56	0.14	-	111,111,111,111	0
57	MG	1H	3426	1/1	0.96	0.17	-	82,82,82,82	0
57	MG	14	3198	1/1	0.77	0.30	-	88,88,88,88	0
57	MG	16	209	1/1	0.88	0.07	-	86,86,86,86	0
57	MG	1G	1689	1/1	0.95	0.07	-	92,92,92,92	0
57	MG	14	3304	1/1	0.98	0.07	-	61,61,61,61	0
57	MG	14	3161	1/1	0.62	0.25	-	94,94,94,94	0
57	MG	1H	3373	1/1	0.83	0.22	-	79,79,79,79	0
57	MG	14	3008	1/1	0.80	0.14	-	73,73,73,73	0
57	MG	13	1730	1/1	0.95	0.07	-	110,110,110,110	0
57	MG	14	3108	1/1	0.95	0.53	-	103,103,103,103	0
57	MG	14	3071	1/1	0.85	0.16	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3238	1/1	0.81	0.10	-	67,67,67,67	0
57	MG	1H	3512	1/1	0.82	0.29	-	100,100,100,100	0
57	MG	14	3404	1/1	0.83	0.07	-	121,121,121,121	0
57	MG	14	3265	1/1	0.85	0.07	-	100,100,100,100	0
57	MG	1H	3226	1/1	0.95	0.50	-	92,92,92,92	0
57	MG	1H	3111	1/1	0.81	0.33	-	94,94,94,94	0
57	MG	1G	1691	1/1	0.91	0.07	-	104,104,104,104	0
57	MG	1G	1677	1/1	0.97	0.09	-	83,83,83,83	0
57	MG	1H	3544	1/1	0.90	0.14	-	105,105,105,105	0
57	MG	13	1602	1/1	0.90	0.12	-	130,130,130,130	0
57	MG	1H	3403	1/1	0.82	0.07	-	68,68,68,68	0
57	MG	14	3179	1/1	0.74	0.30	-	103,103,103,103	0
57	MG	1G	1675	1/1	0.88	0.12	-	86,86,86,86	0
57	MG	14	3030	1/1	0.94	0.40	-	90,90,90,90	0
57	MG	14	3057	1/1	0.92	0.05	-	93,93,93,93	0
57	MG	14	3064	1/1	0.95	0.23	-	99,99,99,99	0
57	MG	1H	3141	1/1	0.88	0.15	-	75,75,75,75	0
57	MG	1G	1722	1/1	0.84	0.20	-	116,116,116,116	0
57	MG	1H	3318	1/1	0.97	0.04	-	74,74,74,74	0
57	MG	1H	3380	1/1	0.90	0.15	-	76,76,76,76	0
57	MG	1H	3044	1/1	0.87	0.48	-	80,80,80,80	0
57	MG	14	3343	1/1	0.90	0.11	-	84,84,84,84	0
57	MG	14	3294	1/1	0.92	0.14	-	66,66,66,66	0
57	MG	14	3436	1/1	0.87	0.04	-	136,136,136,136	0
57	MG	1H	3040	1/1	0.93	0.20	-	76,76,76,76	0
57	MG	1H	3009	1/1	0.92	0.16	-	82,82,82,82	0
57	MG	13	1616	1/1	0.96	0.30	-	101,101,101,101	0
57	MG	14	3247	1/1	0.96	0.11	-	87,87,87,87	0
57	MG	1H	3546	1/1	0.97	0.10	-	105,105,105,105	0
57	MG	1H	3172	1/1	0.81	0.23	-	64,64,64,64	0
57	MG	14	3055	1/1	0.97	0.25	-	64,64,64,64	0
57	MG	1H	3498	1/1	0.76	0.08	-	113,113,113,113	0
57	MG	1H	3471	1/1	0.95	0.17	-	83,83,83,83	0
57	MG	13	1699	1/1	0.79	0.19	-	114,114,114,114	0
57	MG	1H	3051	1/1	0.97	0.29	-	74,74,74,74	0
57	MG	I8	102	1/1	0.98	0.06	-	70,70,70,70	0
57	MG	14	3454	1/1	0.81	0.12	-	108,108,108,108	0
57	MG	1J	209	1/1	0.60	0.07	-	131,131,131,131	0
57	MG	1H	3200	1/1	0.92	0.69	-	82,82,82,82	0
57	MG	14	3398	1/1	0.97	0.05	-	86,86,86,86	0
57	MG	14	3375	1/1	0.80	0.40	-	116,116,116,116	0
57	MG	14	3409	1/1	0.90	0.11	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3121	1/1	0.90	0.72	-	92,92,92,92	0
57	MG	13	1698	1/1	0.95	0.12	-	93,93,93,93	0
57	MG	1H	3410	1/1	0.86	0.17	-	108,108,108,108	0
57	MG	1H	3456	1/1	0.80	0.15	-	92,92,92,92	0
57	MG	1G	1702	1/1	0.62	0.08	-	117,117,117,117	0
57	MG	14	3415	1/1	0.89	0.27	-	93,93,93,93	0
57	MG	14	3061	1/1	0.96	0.35	-	60,60,60,60	0
57	MG	1H	3505	1/1	0.85	0.17	-	112,112,112,112	0
57	MG	1H	3123	1/1	0.90	0.26	-	68,68,68,68	0
57	MG	1H	3397	1/1	0.92	0.14	-	87,87,87,87	0
57	MG	1H	3390	1/1	0.95	0.13	-	48,48,48,48	0
57	MG	14	3178	1/1	0.94	0.13	-	83,83,83,83	0
57	MG	1H	3003	1/1	0.99	0.12	-	67,67,67,67	0
57	MG	14	3445	1/1	0.84	0.12	-	119,119,119,119	0
57	MG	1H	3364	1/1	0.73	0.12	-	85,85,85,85	0
57	MG	1H	3163	1/1	0.96	0.19	-	86,86,86,86	0
57	MG	1H	3551	1/1	0.80	0.11	-	86,86,86,86	0
57	MG	14	3360	1/1	0.83	0.16	-	107,107,107,107	0
57	MG	1H	3167	1/1	0.61	0.48	-	86,86,86,86	0
57	MG	14	3303	1/1	0.97	0.11	-	52,52,52,52	0
57	MG	1H	3514	1/1	0.56	0.13	-	112,112,112,112	0
57	MG	16	206	1/1	0.65	0.24	-	83,83,83,83	0
57	MG	14	3456	1/1	0.12	0.16	-	118,118,118,118	0
57	MG	52	300	1/1	0.81	0.13	-	133,133,133,133	0
57	MG	1H	3299	1/1	0.88	0.19	-	105,105,105,105	0
57	MG	14	3033	1/1	0.92	0.32	-	57,57,57,57	0
57	MG	13	1734	1/1	0.80	0.10	-	143,143,143,143	0
57	MG	14	3385	1/1	0.92	0.20	-	82,82,82,82	0
57	MG	14	3338	1/1	0.93	0.18	-	112,112,112,112	0
57	MG	1G	1629	1/1	0.47	0.19	-	129,129,129,129	0
57	MG	1H	3168	1/1	0.84	0.18	-	89,89,89,89	0
57	MG	1J	203	1/1	0.89	0.23	-	92,92,92,92	0
57	MG	14	3307	1/1	0.93	0.15	-	80,80,80,80	0
57	MG	1H	3486	1/1	0.92	0.30	-	99,99,99,99	0
57	MG	13	1695	1/1	0.97	0.07	-	91,91,91,91	0
57	MG	1H	3534	1/1	0.47	0.11	-	113,113,113,113	0
57	MG	1H	3049	1/1	0.94	0.27	-	79,79,79,79	0
57	MG	1H	3338	1/1	0.67	0.10	-	99,99,99,99	0
57	MG	14	3251	1/1	0.94	0.18	-	113,113,113,113	0
57	MG	13	1711	1/1	0.96	0.09	-	70,70,70,70	0
57	MG	1H	3209	1/1	0.96	0.17	-	92,92,92,92	0
57	MG	1G	1605	1/1	0.79	0.32	-	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3189	1/1	0.94	0.27	-	83,83,83,83	0
57	MG	1H	3315	1/1	0.95	0.13	-	61,61,61,61	0
57	MG	2L	102	1/1	0.78	0.16	-	126,126,126,126	0
57	MG	14	3156	1/1	0.88	0.29	-	81,81,81,81	0
57	MG	1H	3348	1/1	0.94	0.11	-	66,66,66,66	0
57	MG	14	3118	1/1	0.92	0.14	-	96,96,96,96	0
57	MG	1H	3439	1/1	0.97	0.04	-	76,76,76,76	0
57	MG	1H	3375	1/1	0.94	0.10	-	80,80,80,80	0
57	MG	1H	3406	1/1	0.90	0.08	-	95,95,95,95	0
57	MG	14	3074	1/1	0.45	0.59	-	95,95,95,95	0
57	MG	13	1705	1/1	0.87	0.12	-	108,108,108,108	0
57	MG	1H	3177	1/1	0.62	0.20	-	143,143,143,143	0
57	MG	14	3143	1/1	0.88	0.31	-	93,93,93,93	0
57	MG	14	3168	1/1	0.98	0.18	-	70,70,70,70	0
57	MG	14	3368	1/1	0.94	0.37	-	92,92,92,92	0
57	MG	1H	3550	1/1	0.92	0.66	-	111,111,111,111	0
57	MG	14	3339	1/1	0.77	0.05	-	106,106,106,106	0
57	MG	1G	1688	1/1	0.86	0.09	-	123,123,123,123	0
57	MG	13	1731	1/1	0.90	0.14	-	109,109,109,109	0
57	MG	14	3370	1/1	0.92	0.14	-	90,90,90,90	0
57	MG	1G	1669	1/1	0.91	0.08	-	114,114,114,114	0
57	MG	14	3051	1/1	0.98	0.30	-	70,70,70,70	0
57	MG	1H	3035	1/1	0.94	0.36	-	83,83,83,83	0
57	MG	1H	3138	1/1	0.87	0.18	-	98,98,98,98	0
57	MG	1H	3142	1/1	0.79	0.48	-	87,87,87,87	0
57	MG	13	1605	1/1	0.94	0.18	-	88,88,88,88	0
57	MG	1H	3286	1/1	0.91	0.22	-	65,65,65,65	0
57	MG	13	1670	1/1	0.92	0.60	-	85,85,85,85	0
57	MG	13	1646	1/1	0.85	0.52	-	91,91,91,91	0
57	MG	1H	3228	1/1	0.92	0.15	-	81,81,81,81	0
57	MG	14	3180	1/1	0.97	0.34	-	86,86,86,86	0
57	MG	1G	1712	1/1	0.75	0.29	-	110,110,110,110	0
57	MG	1G	1715	1/1	0.90	0.07	-	110,110,110,110	0
57	MG	14	3079	1/1	0.60	0.46	-	86,86,86,86	0
57	MG	14	3395	1/1	0.81	0.21	-	98,98,98,98	0
57	MG	1G	1673	1/1	0.97	0.11	-	80,80,80,80	0
57	MG	1H	3407	1/1	0.97	0.07	-	69,69,69,69	0
57	MG	1H	3136	1/1	0.89	0.19	-	63,63,63,63	0
57	MG	1H	3203	1/1	0.92	0.24	-	78,78,78,78	0
57	MG	14	3177	1/1	0.61	0.46	-	81,81,81,81	0
57	MG	1H	3178	1/1	0.94	0.45	-	80,80,80,80	0
57	MG	1J	206	1/1	0.91	0.07	-	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3190	1/1	0.95	0.33	-	89,89,89,89	0
57	MG	14	3002	1/1	0.96	0.35	-	63,63,63,63	0
57	MG	14	3365	1/1	0.96	0.10	-	93,93,93,93	0
57	MG	13	1610	1/1	0.73	0.55	-	81,81,81,81	0
57	MG	1H	3282	1/1	0.95	0.05	-	54,54,54,54	0
57	MG	1H	3131	1/1	0.86	0.14	-	101,101,101,101	0
57	MG	13	1679	1/1	0.96	0.06	-	89,89,89,89	0
57	MG	1H	3070	1/1	0.95	0.15	-	51,51,51,51	0
57	MG	14	3224	1/1	0.94	0.15	-	76,76,76,76	0
57	MG	1H	3162	1/1	0.78	0.61	-	92,92,92,92	0
57	MG	13	1658	1/1	0.99	0.29	-	83,83,83,83	0
57	MG	1H	3238	1/1	0.85	0.38	-	102,102,102,102	0
57	MG	13	1732	1/1	0.92	0.06	-	108,108,108,108	0
57	MG	1H	3231	1/1	0.88	0.08	-	103,103,103,103	0
57	MG	14	3184	1/1	0.93	0.38	-	78,78,78,78	0
57	MG	14	3423	1/1	0.72	0.18	-	118,118,118,118	0
57	MG	14	3269	1/1	0.94	0.07	-	104,104,104,104	0
57	MG	1H	3408	1/1	0.73	0.10	-	87,87,87,87	0
57	MG	1H	3244	1/1	0.98	0.11	-	47,47,47,47	0
57	MG	14	3040	1/1	0.98	0.26	-	80,80,80,80	0
57	MG	13	1690	1/1	0.88	0.10	-	117,117,117,117	0
57	MG	14	3059	1/1	0.95	0.21	-	58,58,58,58	0
57	MG	1H	3134	1/1	0.96	0.50	-	77,77,77,77	0
57	MG	1G	1709	1/1	0.91	0.12	-	119,119,119,119	0
57	MG	1H	3430	1/1	0.97	0.19	-	94,94,94,94	0
57	MG	1H	3067	1/1	0.88	0.12	-	55,55,55,55	0
57	MG	1H	3428	1/1	0.96	0.05	-	93,93,93,93	0
57	MG	35	202	1/1	0.94	0.17	-	80,80,80,80	0
57	MG	1H	3538	1/1	0.89	0.07	-	107,107,107,107	0
57	MG	13	1648	1/1	0.38	0.49	-	117,117,117,117	0
57	MG	1H	3437	1/1	0.96	0.15	-	76,76,76,76	0
57	MG	1H	3503	1/1	0.93	0.12	-	104,104,104,104	0
57	MG	13	1721	1/1	0.95	0.18	-	77,77,77,77	0
57	MG	1H	3539	1/1	0.91	0.23	-	95,95,95,95	0
57	MG	14	3036	1/1	0.97	0.28	-	85,85,85,85	0
57	MG	14	3289	1/1	0.90	0.16	-	89,89,89,89	0
57	MG	1H	3470	1/1	0.93	0.24	-	105,105,105,105	0
57	MG	14	3369	1/1	0.91	0.11	-	90,90,90,90	0
57	MG	14	3418	1/1	0.90	0.16	-	97,97,97,97	0
57	MG	1H	3443	1/1	0.92	0.08	-	112,112,112,112	0
57	MG	1H	3073	1/1	0.86	0.35	-	84,84,84,84	0
57	MG	1H	3158	1/1	0.87	0.24	-	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3030	1/1	0.91	0.17	-	89,89,89,89	0
57	MG	1H	3455	1/1	0.85	0.08	-	120,120,120,120	0
57	MG	14	3134	1/1	0.79	0.70	-	99,99,99,99	0
57	MG	1G	1682	1/1	0.84	0.09	-	123,123,123,123	0
57	MG	1H	3450	1/1	0.93	0.06	-	87,87,87,87	0
57	MG	1H	3531	1/1	0.82	0.13	-	114,114,114,114	0
57	MG	1G	1690	1/1	0.95	0.06	-	113,113,113,113	0
57	MG	1H	3421	1/1	0.47	0.38	-	93,93,93,93	0
57	MG	1H	3520	1/1	0.91	0.10	-	88,88,88,88	0
57	MG	1H	3182	1/1	0.76	0.17	-	108,108,108,108	0
57	MG	13	1722	1/1	0.95	0.18	-	99,99,99,99	0
57	MG	14	3425	1/1	0.77	0.28	-	106,106,106,106	0
57	MG	14	3402	1/1	0.94	0.07	-	111,111,111,111	0
57	MG	14	3246	1/1	0.94	0.10	-	93,93,93,93	0
57	MG	14	3268	1/1	0.88	0.16	-	89,89,89,89	0
57	MG	1H	3099	1/1	0.95	0.15	-	53,53,53,53	0
57	MG	1H	3264	1/1	0.82	0.19	-	55,55,55,55	0
57	MG	14	3137	1/1	0.81	0.34	-	76,76,76,76	0
57	MG	13	1693	1/1	0.96	0.10	-	95,95,95,95	0
57	MG	16	208	1/1	0.95	0.27	-	86,86,86,86	0
57	MG	14	3181	1/1	0.86	0.45	-	91,91,91,91	0
57	MG	14	3081	1/1	0.76	0.17	-	79,79,79,79	0
57	MG	13	1620	1/1	0.99	0.16	-	68,68,68,68	0
57	MG	14	3427	1/1	0.69	0.15	-	121,121,121,121	0
57	MG	13	1611	1/1	0.96	0.23	-	78,78,78,78	0
57	MG	1G	1636	1/1	0.89	0.35	-	87,87,87,87	0
57	MG	13	1717	1/1	0.94	0.10	-	93,93,93,93	0
57	MG	1H	3276	1/1	0.93	0.06	-	80,80,80,80	0
57	MG	14	3381	1/1	0.81	0.07	-	136,136,136,136	0
57	MG	E5	102	1/1	0.87	0.27	-	68,68,68,68	0
57	MG	16	212	1/1	0.94	0.07	-	78,78,78,78	0
57	MG	1H	3336	1/1	0.98	0.07	-	88,88,88,88	0
57	MG	13	1723	1/1	0.77	0.12	-	118,118,118,118	0
57	MG	13	1692	1/1	0.55	0.15	-	110,110,110,110	0
57	MG	14	3388	1/1	0.74	0.13	-	72,72,72,72	0
57	MG	1H	3519	1/1	0.74	0.15	-	104,104,104,104	0
57	MG	14	3062	1/1	0.94	0.24	-	97,97,97,97	0
57	MG	14	3103	1/1	0.69	0.53	-	80,80,80,80	0
57	MG	1H	3157	1/1	0.80	0.44	-	89,89,89,89	0
57	MG	16	211	1/1	0.91	0.08	-	93,93,93,93	0
57	MG	1G	1608	1/1	0.96	0.34	-	100,100,100,100	0
57	MG	14	3248	1/1	0.91	0.13	-	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3320	1/1	0.96	0.08	-	71,71,71,71	0
57	MG	14	3035	1/1	0.95	0.27	-	69,69,69,69	0
57	MG	13	1662	1/1	0.88	0.43	-	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.