



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:18 am GMT

PDB ID : 4WQ1
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with C-A mismatch in the first position in the A-site.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-21
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28972

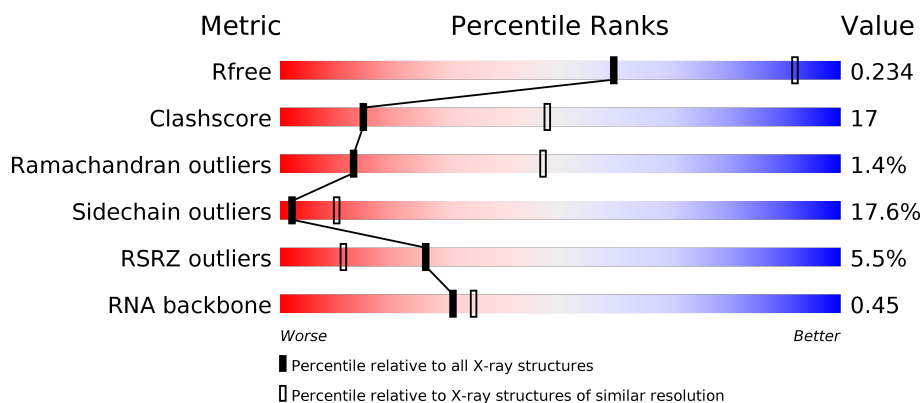
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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	<div> <div>30%</div> <div>45%</div> <div>20%</div> <div>• •</div> </div>
2	12	256	<div> <div>5%</div> <div>48%</div> <div>38%</div> <div>7%</div> <div>7%</div> </div>
2	1E	256	<div> <div>47%</div> <div>39%</div> <div>5%</div> <div>7%</div> </div>
3	22	239	<div> <div>12%</div> <div>49%</div> <div>31%</div> <div>6%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	2E	239	
4	32	208	
4	3E	208	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	
15	6I	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	85	
22	1L	85	
22	3K	85	
22	3L	85	
23	2K	77	
23	2L	77	
24	4K	30	
24	4L	30	
25	14	2912	
25	1H	2912	
26	16	122	
26	1J	122	
27	11	272	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	21	205	
28	29	205	
29	31	202	
30	41	181	
30	49	181	
31	51	180	
31	59	180	
32	61	146	
32	69	146	
33	15	138	
33	58	138	
34	25	122	
34	68	122	
35	35	150	
35	78	150	
36	45	141	
36	88	141	
37	55	118	
37	98	118	
38	65	111	
38	A8	111	
39	75	137	
39	B8	137	
40	85	117	
40	C8	117	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	95	101	
41	D8	101	
42	A5	113	
42	E8	113	
43	B5	94	
43	F8	94	
44	C5	110	
44	G8	110	
45	H8	175	
46	E5	85	
46	I8	85	
47	F5	98	
47	J8	98	
48	G5	66	
48	K8	66	
49	H5	59	
49	L8	59	
50	I5	66	
50	M8	66	
51	J5	59	
51	N8	59	
52	K5	45	
52	O8	45	
53	L5	49	
53	P8	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Q8	65	
55	1G	1522	
56	19	276	
57	39	210	
58	D5	206	
59	M5	61	

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
60	MG	13	1604	-	-	-	X
60	MG	13	1605	-	-	-	X
60	MG	13	1608	-	-	-	X
60	MG	13	1617	-	-	-	X
60	MG	13	1621	-	-	-	X
60	MG	13	1627	-	-	-	X
60	MG	13	1642	-	-	-	X
60	MG	13	1648	-	-	-	X
60	MG	13	1650	-	-	-	X
60	MG	13	1651	-	-	-	X
60	MG	13	1660	-	-	-	X
60	MG	13	1664	-	-	-	X
60	MG	13	1668	-	-	-	X
60	MG	13	1672	-	-	-	X
60	MG	13	1692	-	-	-	X
60	MG	13	1710	-	-	-	X
60	MG	14	3004	-	-	-	X
60	MG	14	3010	-	-	-	X
60	MG	14	3011	-	-	-	X
60	MG	14	3012	-	-	-	X
60	MG	14	3023	-	-	-	X
60	MG	14	3028	-	-	-	X
60	MG	14	3034	-	-	-	X
60	MG	14	3035	-	-	-	X
60	MG	14	3036	-	-	-	X
60	MG	14	3042	-	-	-	X
60	MG	14	3052	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	14	3054	-	-	-	X
60	MG	14	3058	-	-	-	X
60	MG	14	3061	-	-	-	X
60	MG	14	3064	-	-	-	X
60	MG	14	3066	-	-	-	X
60	MG	14	3068	-	-	-	X
60	MG	14	3074	-	-	-	X
60	MG	14	3079	-	-	-	X
60	MG	14	3082	-	-	-	X
60	MG	14	3083	-	-	-	X
60	MG	14	3086	-	-	-	X
60	MG	14	3088	-	-	-	X
60	MG	14	3090	-	-	-	X
60	MG	14	3092	-	-	-	X
60	MG	14	3094	-	-	-	X
60	MG	14	3095	-	-	-	X
60	MG	14	3097	-	-	-	X
60	MG	14	3098	-	-	-	X
60	MG	14	3100	-	-	-	X
60	MG	14	3102	-	-	-	X
60	MG	14	3112	-	-	-	X
60	MG	14	3115	-	-	-	X
60	MG	14	3118	-	-	-	X
60	MG	14	3119	-	-	-	X
60	MG	14	3127	-	-	-	X
60	MG	14	3130	-	-	-	X
60	MG	14	3134	-	-	-	X
60	MG	14	3137	-	-	-	X
60	MG	14	3139	-	-	-	X
60	MG	14	3147	-	-	-	X
60	MG	14	3151	-	-	-	X
60	MG	14	3153	-	-	-	X
60	MG	14	3156	-	-	-	X
60	MG	14	3157	-	-	-	X
60	MG	14	3161	-	-	-	X
60	MG	14	3163	-	-	-	X
60	MG	14	3176	-	-	-	X
60	MG	14	3177	-	-	-	X
60	MG	14	3179	-	-	-	X
60	MG	14	3192	-	-	-	X
60	MG	14	3203	-	-	-	X
60	MG	14	3206	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	14	3208	-	-	-	X
60	MG	14	3214	-	-	-	X
60	MG	14	3219	-	-	-	X
60	MG	14	3221	-	-	-	X
60	MG	14	3223	-	-	-	X
60	MG	14	3225	-	-	-	X
60	MG	14	3229	-	-	-	X
60	MG	14	3231	-	-	-	X
60	MG	14	3232	-	-	-	X
60	MG	14	3233	-	-	-	X
60	MG	14	3235	-	-	-	X
60	MG	14	3237	-	-	-	X
60	MG	14	3238	-	-	-	X
60	MG	14	3245	-	-	-	X
60	MG	14	3246	-	-	-	X
60	MG	14	3258	-	-	-	X
60	MG	14	3270	-	-	-	X
60	MG	14	3279	-	-	-	X
60	MG	14	3281	-	-	-	X
60	MG	14	3284	-	-	-	X
60	MG	14	3286	-	-	-	X
60	MG	14	3288	-	-	-	X
60	MG	14	3289	-	-	-	X
60	MG	14	3290	-	-	-	X
60	MG	14	3294	-	-	-	X
60	MG	14	3299	-	-	-	X
60	MG	14	3305	-	-	-	X
60	MG	14	3306	-	-	-	X
60	MG	14	3386	-	-	-	X
60	MG	16	201	-	-	-	X
60	MG	16	204	-	-	-	X
60	MG	16	205	-	-	-	X
60	MG	1G	1601	-	-	-	X
60	MG	1G	1611	-	-	-	X
60	MG	1G	1614	-	-	-	X
60	MG	1G	1625	-	-	-	X
60	MG	1G	1631	-	-	-	X
60	MG	1G	1632	-	-	-	X
60	MG	1G	1644	-	-	-	X
60	MG	1G	1656	-	-	-	X
60	MG	1G	1657	-	-	-	X
60	MG	1G	1667	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	1G	1673	-	-	-	X
60	MG	1G	1674	-	-	-	X
60	MG	1G	1678	-	-	-	X
60	MG	1G	1684	-	-	-	X
60	MG	1G	1688	-	-	-	X
60	MG	1H	3002	-	-	-	X
60	MG	1H	3010	-	-	-	X
60	MG	1H	3012	-	-	-	X
60	MG	1H	3014	-	-	-	X
60	MG	1H	3016	-	-	-	X
60	MG	1H	3020	-	-	-	X
60	MG	1H	3021	-	-	-	X
60	MG	1H	3023	-	-	-	X
60	MG	1H	3024	-	-	-	X
60	MG	1H	3030	-	-	-	X
60	MG	1H	3033	-	-	-	X
60	MG	1H	3034	-	-	-	X
60	MG	1H	3037	-	-	-	X
60	MG	1H	3042	-	-	-	X
60	MG	1H	3044	-	-	-	X
60	MG	1H	3048	-	-	-	X
60	MG	1H	3050	-	-	-	X
60	MG	1H	3051	-	-	-	X
60	MG	1H	3054	-	-	-	X
60	MG	1H	3058	-	-	-	X
60	MG	1H	3060	-	-	-	X
60	MG	1H	3062	-	-	-	X
60	MG	1H	3066	-	-	-	X
60	MG	1H	3067	-	-	-	X
60	MG	1H	3069	-	-	-	X
60	MG	1H	3075	-	-	-	X
60	MG	1H	3076	-	-	-	X
60	MG	1H	3083	-	-	-	X
60	MG	1H	3087	-	-	-	X
60	MG	1H	3096	-	-	-	X
60	MG	1H	3099	-	-	-	X
60	MG	1H	3107	-	-	-	X
60	MG	1H	3110	-	-	-	X
60	MG	1H	3115	-	-	-	X
60	MG	1H	3122	-	-	-	X
60	MG	1H	3127	-	-	-	X
60	MG	1H	3132	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	1H	3142	-	-	-	X
60	MG	1H	3143	-	-	-	X
60	MG	1H	3147	-	-	-	X
60	MG	1H	3157	-	-	-	X
60	MG	1H	3164	-	-	-	X
60	MG	1H	3169	-	-	-	X
60	MG	1H	3173	-	-	-	X
60	MG	1H	3175	-	-	-	X
60	MG	1H	3184	-	-	-	X
60	MG	1H	3187	-	-	-	X
60	MG	1H	3191	-	-	-	X
60	MG	1H	3199	-	-	-	X
60	MG	1H	3202	-	-	-	X
60	MG	1H	3207	-	-	-	X
60	MG	1H	3221	-	-	-	X
60	MG	1H	3223	-	-	-	X
60	MG	1H	3229	-	-	-	X
60	MG	1H	3239	-	-	-	X
60	MG	1H	3242	-	-	-	X
60	MG	1H	3246	-	-	-	X
60	MG	1H	3256	-	-	-	X
60	MG	1H	3259	-	-	-	X
60	MG	1H	3265	-	-	-	X
60	MG	1H	3268	-	-	-	X
60	MG	1H	3270	-	-	-	X
60	MG	1H	3287	-	-	-	X
60	MG	1H	3294	-	-	-	X
60	MG	1H	3297	-	-	-	X
60	MG	1H	3298	-	-	-	X
60	MG	29	302	-	-	-	X
60	MG	2L	101	-	-	-	X
60	MG	85	201	-	-	-	X
61	ZN	32	301	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 299951 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	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			498	316	105	72	5			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	82	Total	C	N	O	S	0	0	0
			640	407	118	113	2			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			
22	3K	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	1L	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	3L	75	Total	C	N	O	P	S	0	0	0
			1615	728	288	522	75	2			

- 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
			1645	734	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675817920
2L	18	C	U	conflict	GB 675817920

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	15	Total	C	N	O	P	0	0	0
			325	147	68	95	15			
24	4L	16	Total	C	N	O	P	0	0	0
			347	157	73	101	16			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	14	2907	Total	C	N	O	P	0	0	0
			62605	27865	11708	20126	2906			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
30	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	59	171	Total	C	N	O	S	0	0	0
			1316	835	247	233	1			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	B8	136	Total	C	N	O	0	0	0
			1133	705	233	195			
39	75	137	Total	C	N	O	S	0	0
			1141	710	234	196	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
43	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	I8	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			
51	J5	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
53	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	62	Total	C	N	O	S	0	0	0
			442	281	83	76	2			

- Molecule 55 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

- Molecule 56 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 57 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 58 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 59 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	M5	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	98	2	Total	Mg	0	0
			2	2		
60	45	3	Total	Mg	0	0
			3	3		
60	P8	1	Total	Mg	0	0
			1	1		
60	85	1	Total	Mg	0	0
			1	1		
60	C5	1	Total	Mg	0	0
			1	1		
60	13	140	Total	Mg	0	0
			140	140		
60	B8	1	Total	Mg	0	0
			1	1		
60	K8	1	Total	Mg	0	0
			1	1		
60	5I	1	Total	Mg	0	0
			1	1		
60	C8	1	Total	Mg	0	0
			1	1		
60	16	12	Total	Mg	0	0
			12	12		
60	25	1	Total	Mg	0	0
			1	1		
60	3K	1	Total	Mg	0	0
			1	1		
60	21	2	Total	Mg	0	0
			2	2		
60	2K	4	Total	Mg	0	0
			4	4		
60	4I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	3I	1	Total 1	Mg 1	0	0
60	I8	2	Total 2	Mg 2	0	0
60	52	1	Total 1	Mg 1	0	0
60	68	1	Total 1	Mg 1	0	0
60	29	2	Total 2	Mg 2	0	0
60	78	3	Total 3	Mg 3	0	0
60	39	1	Total 1	Mg 1	0	0
60	1G	104	Total 104	Mg 104	0	0
60	11	2	Total 2	Mg 2	0	0
60	1H	438	Total 438	Mg 438	0	0
60	E5	1	Total 1	Mg 1	0	0
60	88	2	Total 2	Mg 2	0	0
60	49	1	Total 1	Mg 1	0	0
60	14	386	Total 386	Mg 386	0	0
60	19	1	Total 1	Mg 1	0	0
60	1J	7	Total 7	Mg 7	0	0
60	1K	1	Total 1	Mg 1	0	0
60	41	1	Total 1	Mg 1	0	0
60	2L	3	Total 3	Mg 3	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	32	1	Total 1	Zn 1	0	0
61	3E	1	Total 1	Zn 1	0	0
61	5I	1	Total 1	Zn 1	0	0
61	5A	1	Total 1	Zn 1	0	0
61	G8	1	Total 1	Zn 1	0	0
61	C5	1	Total 1	Zn 1	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	125	Total 125	O 125	0	0
62	3E	4	Total 4	O 4	0	0
62	3I	1	Total 1	O 1	0	0
62	5I	2	Total 2	O 2	0	0
62	7I	1	Total 1	O 1	0	0
62	1K	4	Total 4	O 4	0	0
62	3K	1	Total 1	O 1	0	0
62	4K	1	Total 1	O 1	0	0
62	1H	738	Total 738	O 738	0	0
62	16	15	Total 15	O 15	0	0
62	11	10	Total 10	O 10	0	0
62	21	4	Total 4	O 4	0	0
62	31	5	Total 5	O 5	0	0
62	78	3	Total 3	O 3	0	0

Continued on next page...

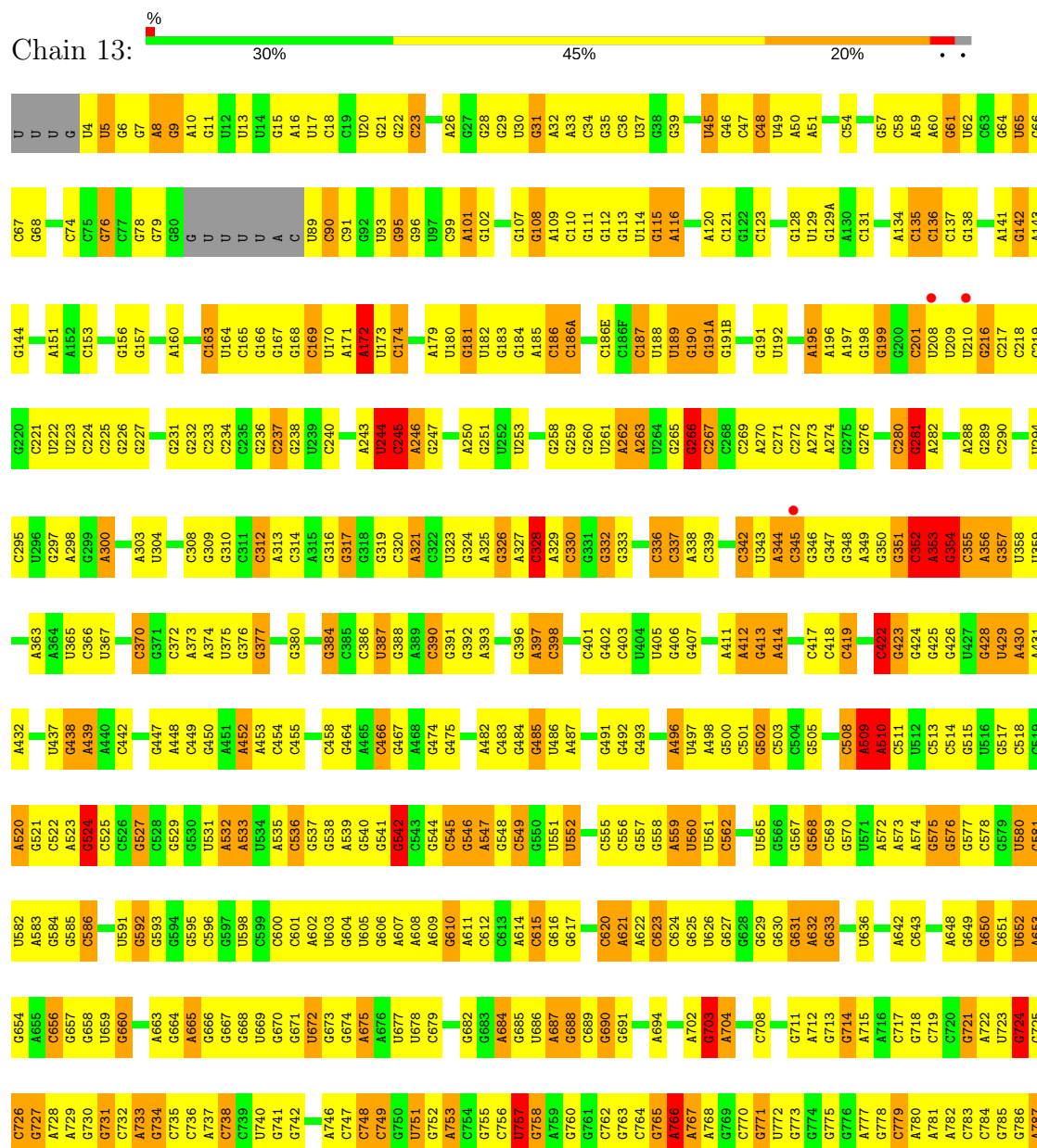
Continued from previous page...

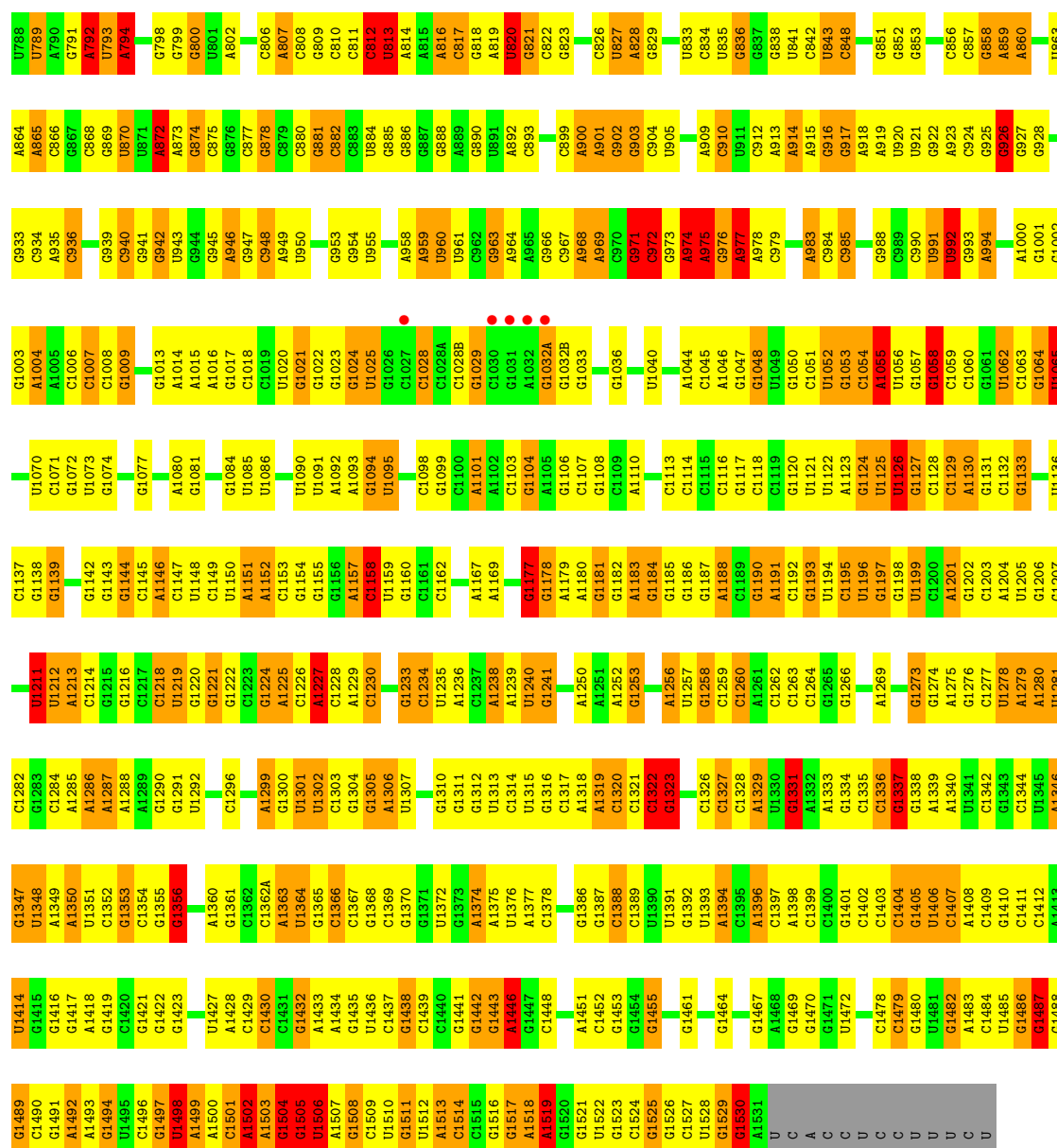
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	98	3	Total 3	O 3	0	0
62	B8	1	Total 1	O 1	0	0
62	C8	2	Total 2	O 2	0	0
62	D8	2	Total 2	O 2	0	0
62	G8	2	Total 2	O 2	0	0
62	L8	3	Total 3	O 3	0	0
62	Q8	1	Total 1	O 1	0	0
62	1G	74	Total 74	O 74	0	0
62	82	1	Total 1	O 1	0	0
62	BA	2	Total 2	O 2	0	0
62	4L	1	Total 1	O 1	0	0
62	14	446	Total 446	O 446	0	0
62	1J	12	Total 12	O 12	0	0
62	19	8	Total 8	O 8	0	0
62	39	1	Total 1	O 1	0	0
62	25	6	Total 6	O 6	0	0
62	85	2	Total 2	O 2	0	0
62	A5	1	Total 1	O 1	0	0
62	E5	1	Total 1	O 1	0	0
62	L5	1	Total 1	O 1	0	0
62	M5	2	Total 2	O 2	0	0

3 Residue-property plots

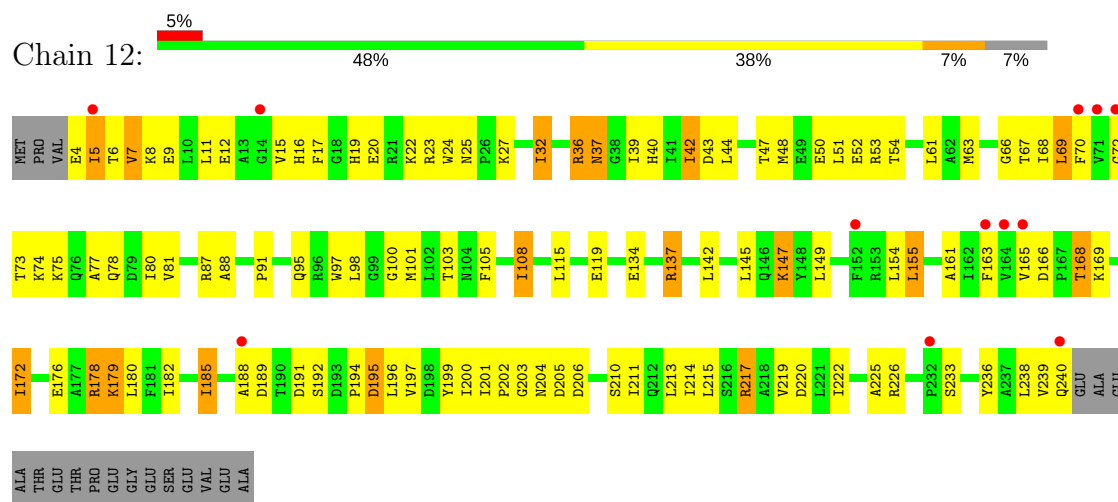
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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

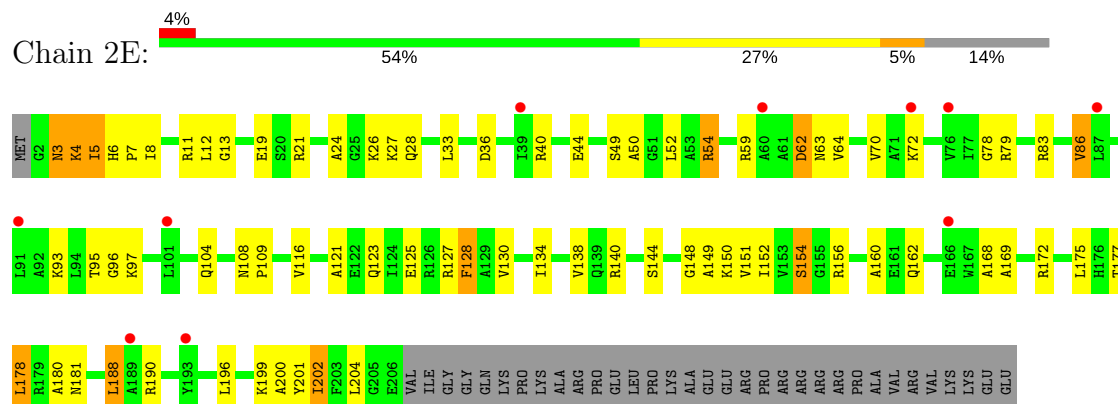




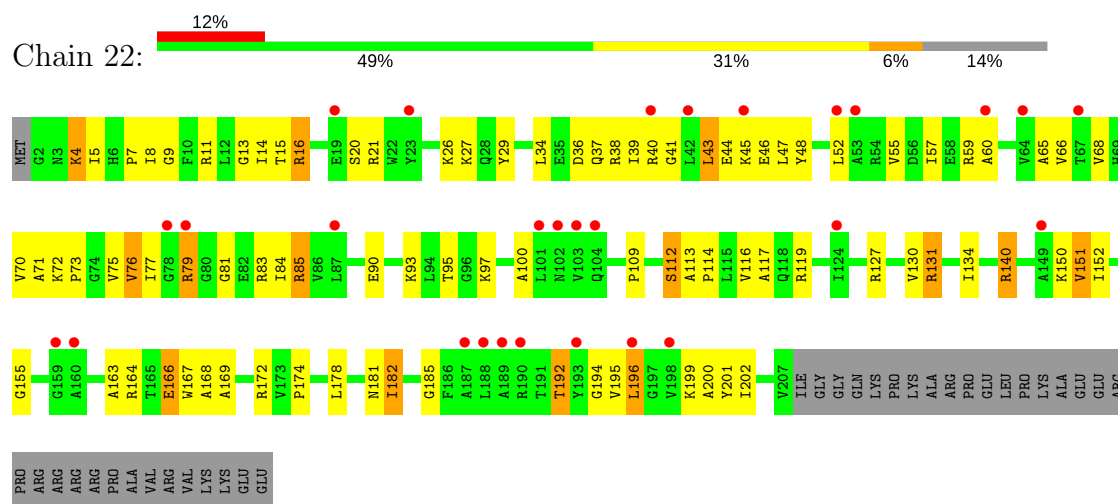
- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

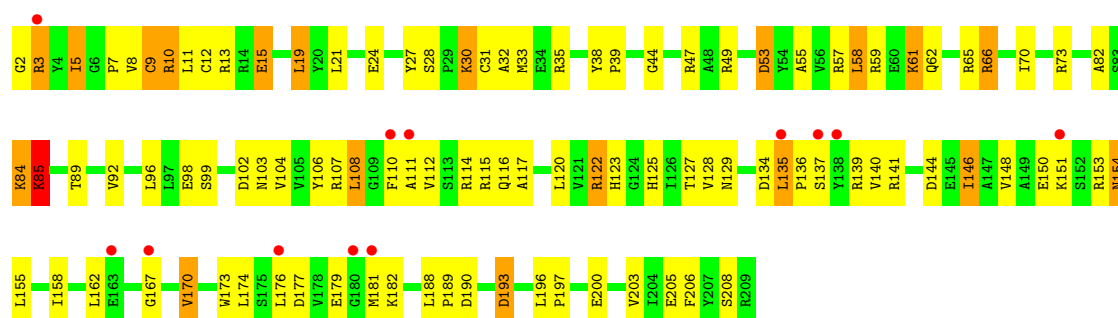


- Molecule 3: 30S ribosomal protein S3

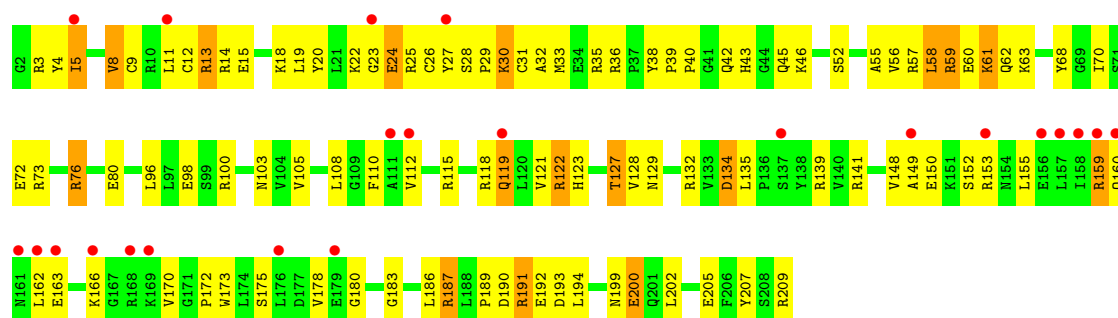


- Molecule 4: 30S ribosomal protein S4

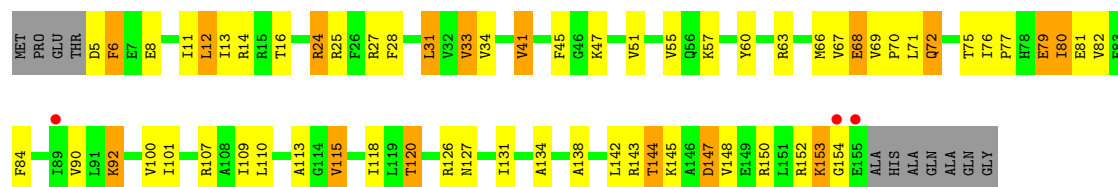




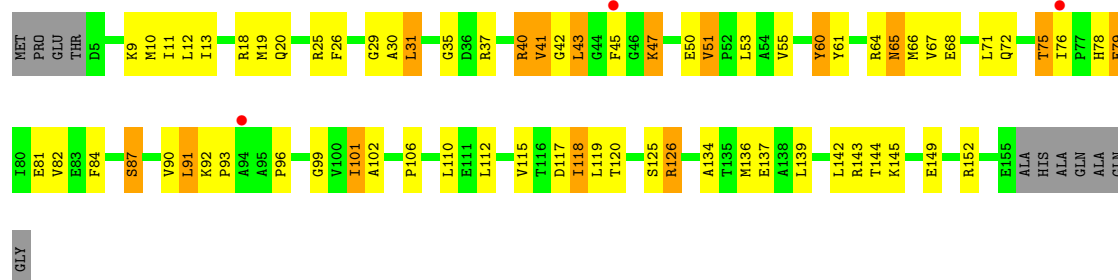
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

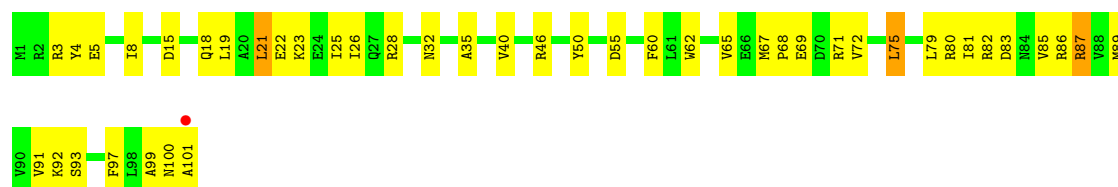


• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

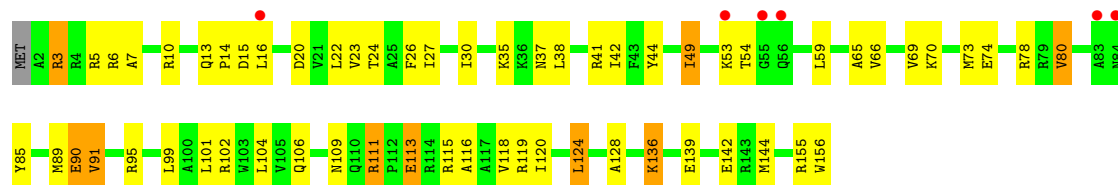




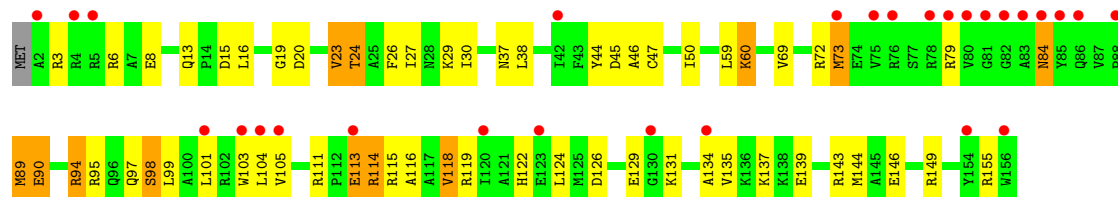
• Molecule 6: 30S ribosomal protein S6



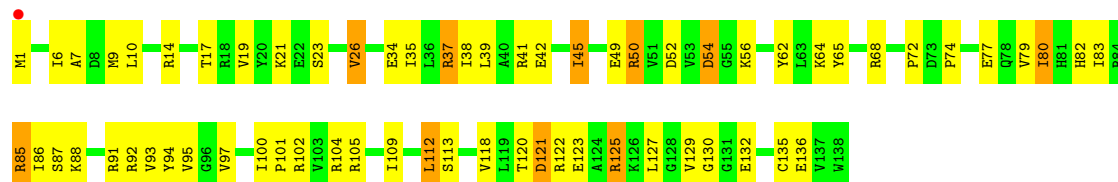
• Molecule 7: 30S ribosomal protein S7



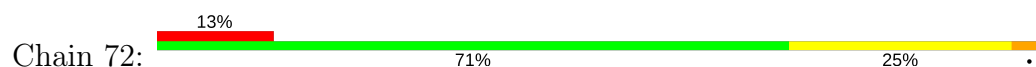
• Molecule 7: 30S ribosomal protein S7

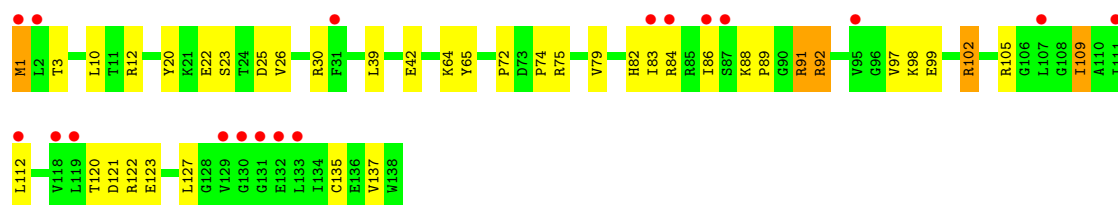


• Molecule 8: 30S ribosomal protein S8

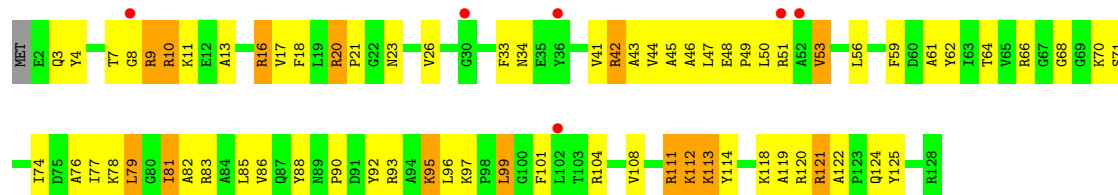


• Molecule 8: 30S ribosomal protein S8

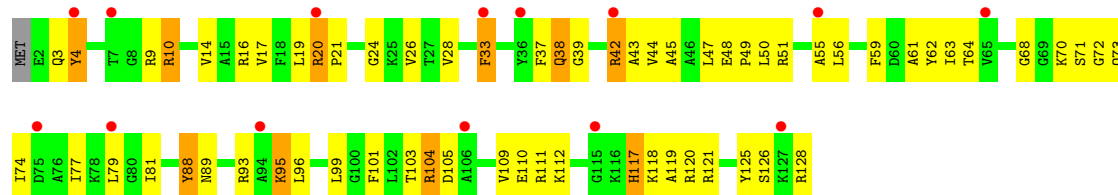




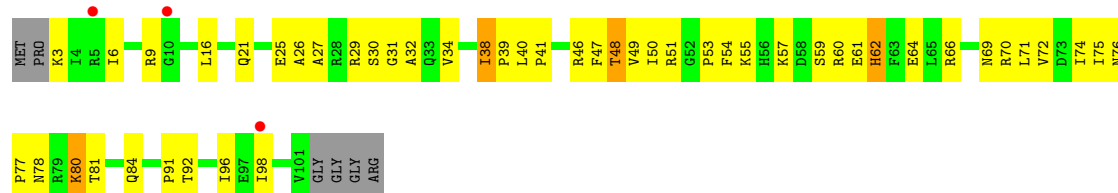
• Molecule 9: 30S ribosomal protein S9



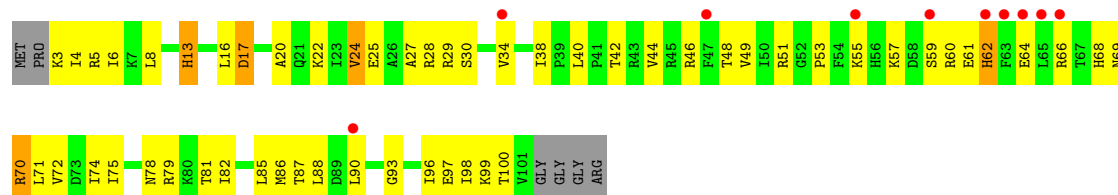
• Molecule 9: 30S ribosomal protein S9



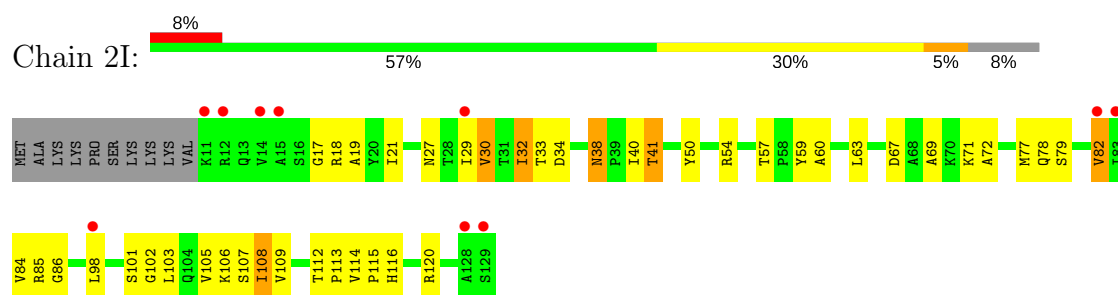
• Molecule 10: 30S ribosomal protein S10



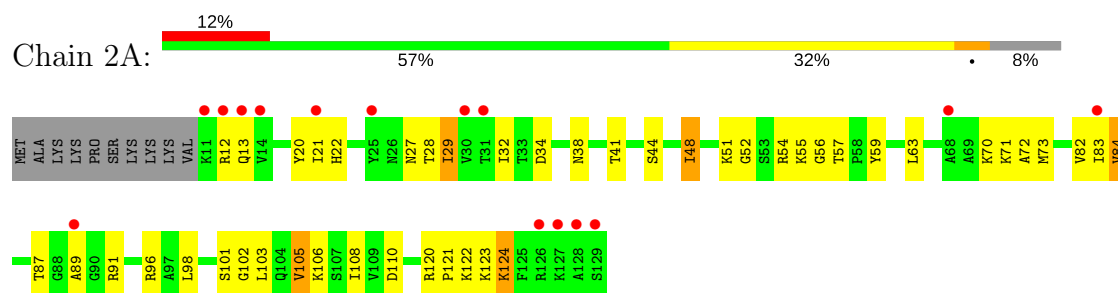
• Molecule 10: 30S ribosomal protein S10



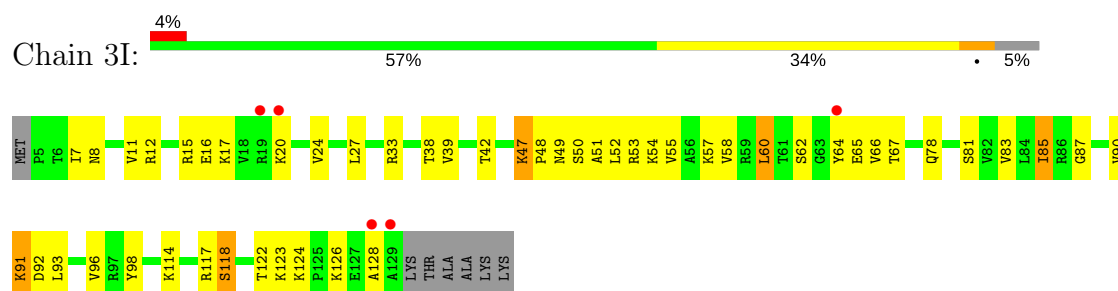
• Molecule 11: 30S ribosomal protein S11



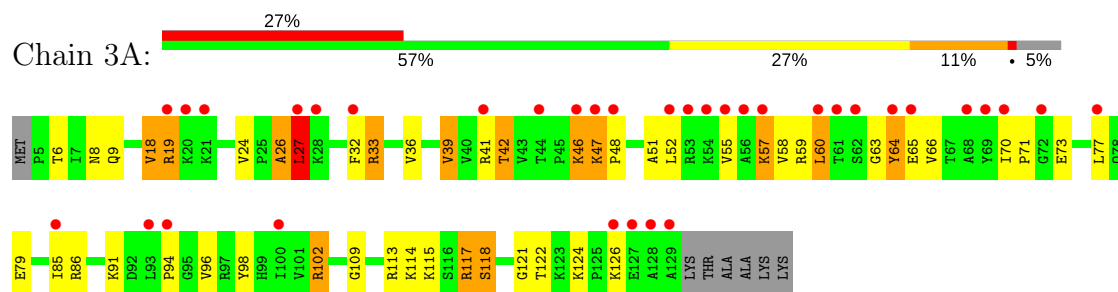
- Molecule 11: 30S ribosomal protein S11



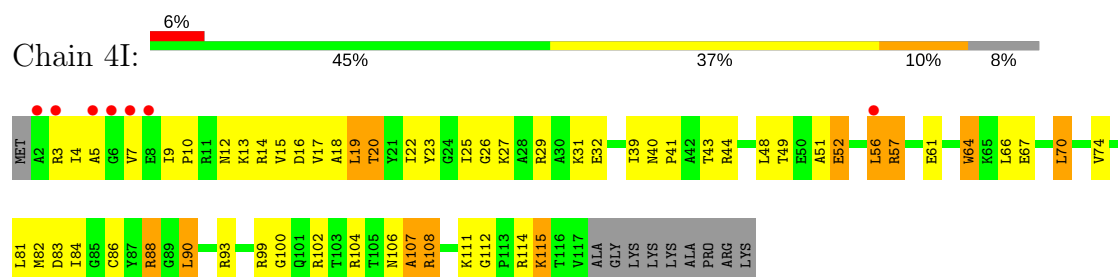
- Molecule 12: 30S ribosomal protein S12



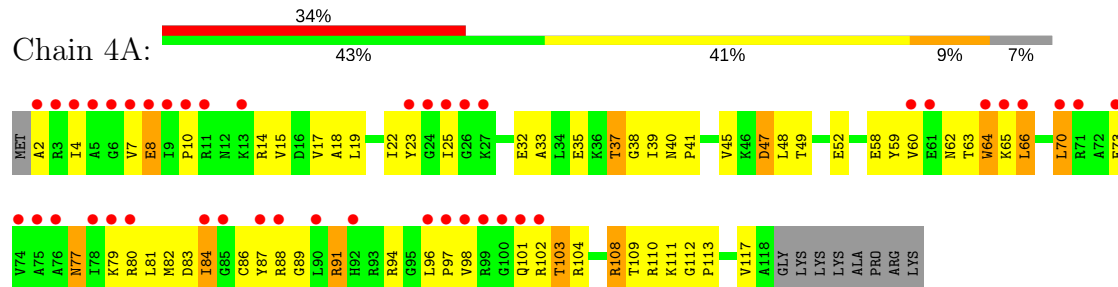
- Molecule 12: 30S ribosomal protein S12



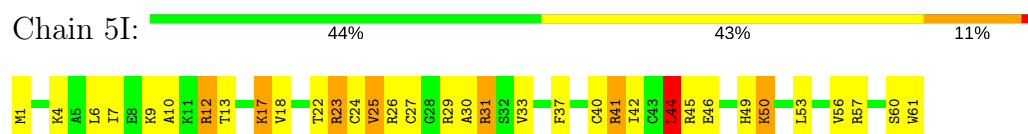
- Molecule 13: 30S ribosomal protein S13



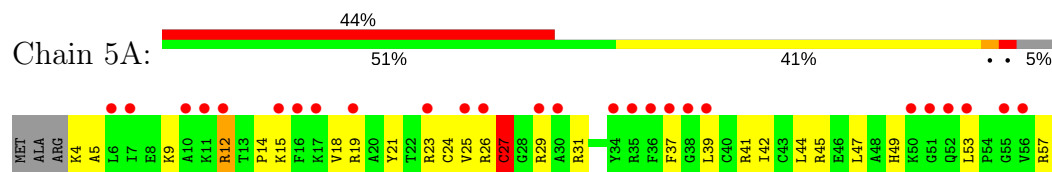
- Molecule 13: 30S ribosomal protein S13



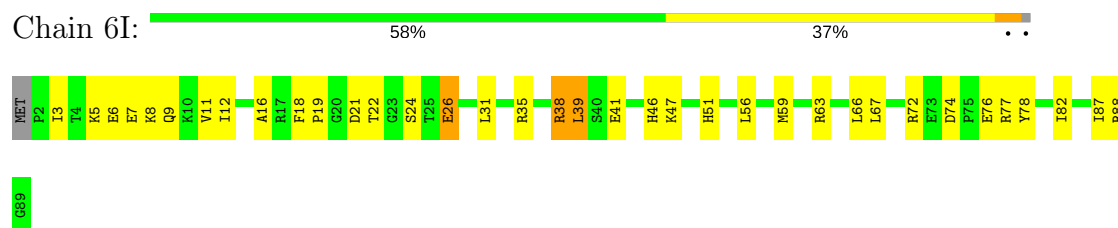
- Molecule 14: 30S ribosomal protein S14 type Z



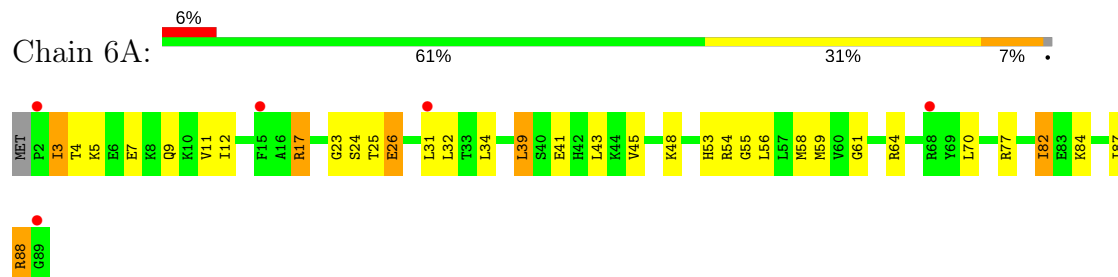
- Molecule 14: 30S ribosomal protein S14 type Z



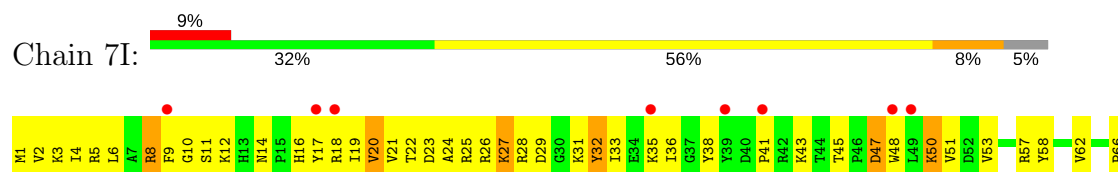
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

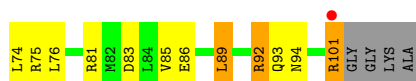
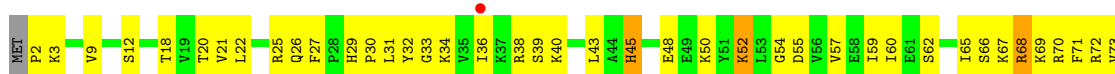




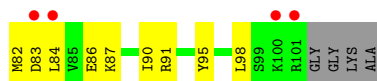
- Molecule 16: 30S ribosomal protein S16



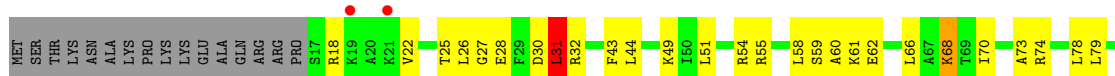
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



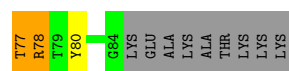
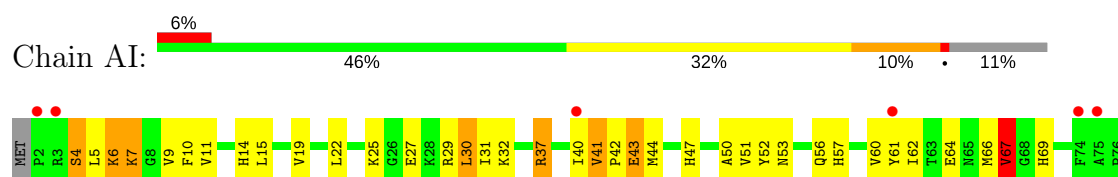
- Molecule 18: 30S ribosomal protein S18



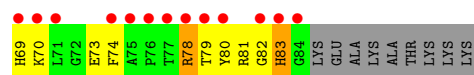
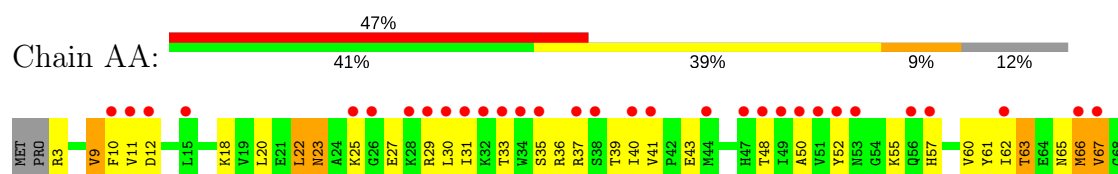
- Molecule 18: 30S ribosomal protein S18



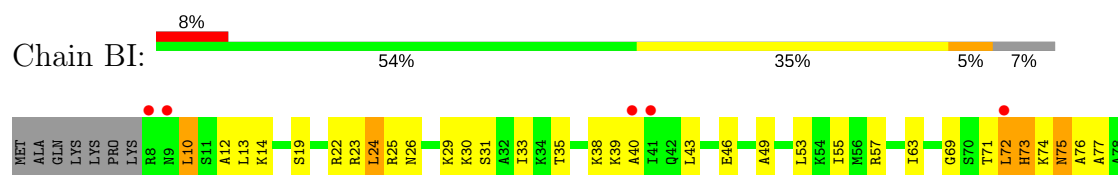
- Molecule 19: 30S ribosomal protein S19



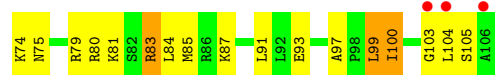
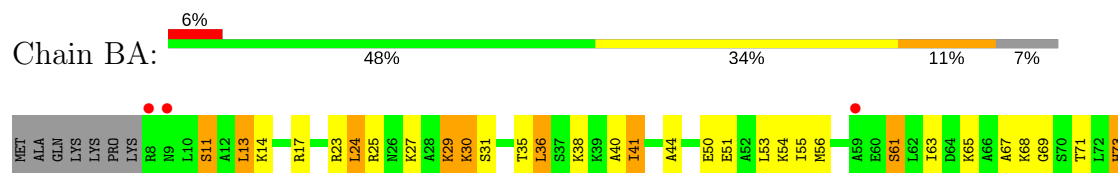
- Molecule 19: 30S ribosomal protein S19



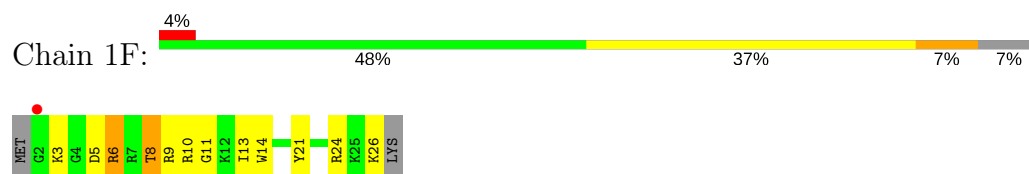
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx

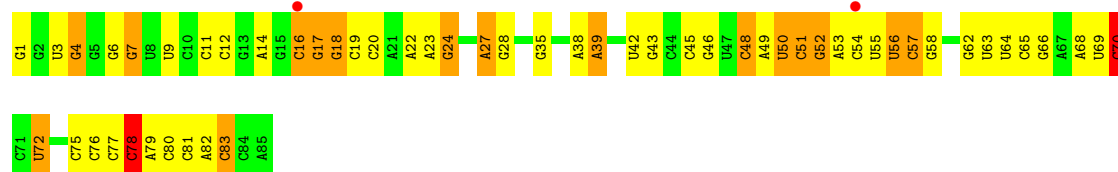


- Molecule 21: 30S ribosomal protein Thx

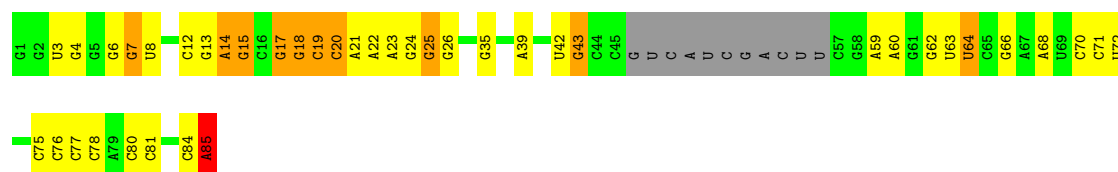




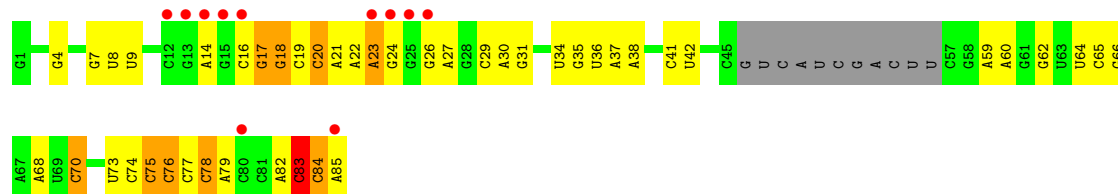
• Molecule 22: tRNA-Tyr



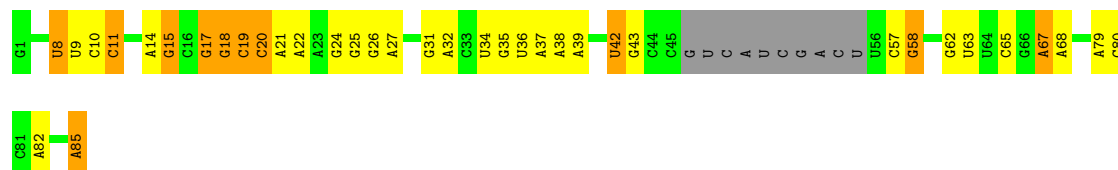
• Molecule 22: tRNA-Tyr



• Molecule 22: tRNA-Tyr



• Molecule 22: tRNA-Tyr



• Molecule 23: tRNA-fMET



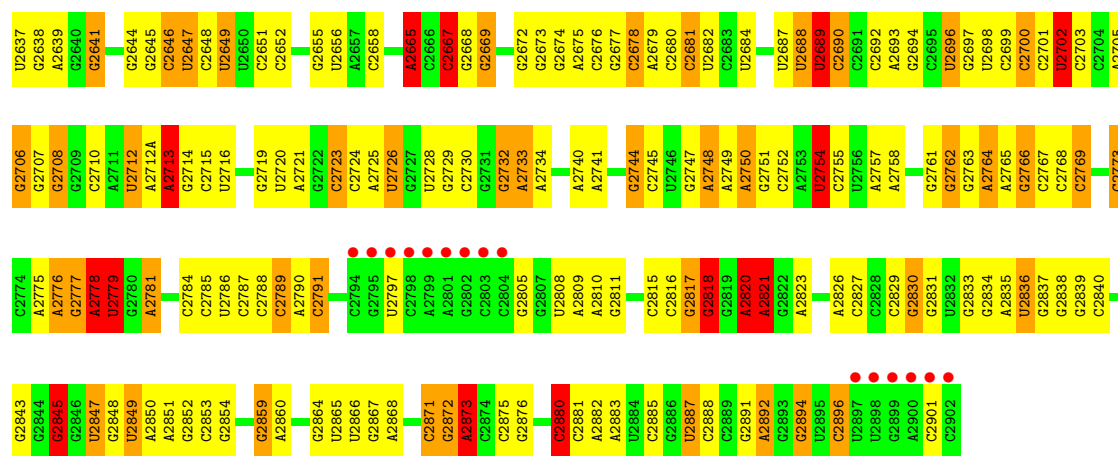
A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459																																																																																																																																																																																																																																																																																											
G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392																																																																																																																																																																																																																																																																																																	
C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392																																																																																																																																																																																																																																			
A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392																																																																																																																																																																	
U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392																																																																																																			
C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392																																
G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1

G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2461	G2462	G2466	G2467	G2468	G2469	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501																												
U2312	C2313	C2314	G2315	G2316	C2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372																							
U2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311																					
A2169	A2170	A2171	U2172	A2173	A2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248				
G2032	A2033	U2034	G2035	U2036	G2037	G2038	G2039	G2040	U2041	A2042	C2043	C2044	C2045	G2046	G2047	G2048	G2049	G2050	A2051	G2052	G2053	A2054	G2055	G2056	A2057	A2058	A2059	A2060	G2061	A2062	G2063	C2064	C2065	C2066	G2067	U2068	G2069	G2070	A2071	G2072	C2073	U2074	U2075	C2076	C2077	C2078	C2079	C2080	C2081	A2082	G2083	C2084	C2085	U2086	G2087	G2088	C2089	U2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	U2098	U2099	A2100															
G1968	A1969	A1970	A1971	A1972	G1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	A2021	U2022	G2023	G2024	C2025	G2026	G2027	U2028	G2029	A2030	A2031																				
U1898	G1899	A1900	A1901	C1902	G1903	G1904	G1905	G1906	G1907	G1908	G1909	G1910	G1911	G1912	G1913	C1914	G1915	A1916	G1917	G1918	G1919	G1920	G1921	G1922	G1923	G1924	G1925	U1926	A1927	G1928	G1929	U1930	A1931	A1932	G1933	G1934	G1935	A1936	A1937	A1938	U1939	U1940	C1941	C1942	U1943	U1944	G1945	U1946	G1947	G1948	G1949	G1950	U1951	U1952	U1953	U1954	U1955	U1956	C1957	A1958	A1959	A1960	G1961	C1962	U1963	G1964	C1965	A1966	C1967														
G1813	G1814	A1815	G1816	G1817	U1818	A1819	U1820	A1821	G1822	G1823	A1824	G1825	G1826	G1827	G1828	G1829	A1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	A1845	A1846	A1847	A1848	G1849	G1850	G1851	G1852	A1853	A1854	G1855	G1856	G1857	G1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	A1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893			
C1751	C1752	G1753	C1754	A1755	G1756	U1757	G1758	A1759	A1760	C1761	A1762	G1763	G1764	C1765	U1766	C1767	U1768	G1769	G1770	G1771	G1772	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	G1781	G1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	G1799	G1800	A1801	A1802	A1803	C1804	U1805	G1806	G1807	G1808	G1809	G1810	G1811	A1812																						
G1660	G1661	C1662	G1663	A1664	A1665	A1666	A1667	A1668	A1669	C1670	A1671	C1672	U1673	G1674	C1675	U1676	C1677	G1678	U1679	G1680	G1681	G1682	C1683	G1684	G1685	U1686	A1687	A1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	G1696	G1697	A1698	G1699	A1700	A1701	C1702	G1703	C1704	G1705	U1706	C1707	C1708	C1709	C1710	C1711	C1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743
C1598	C1599	C1600	C1601	U1602	A1603	C1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	C1612	C1613	A1614	C1615	A1616	C1617	A1618	G1619	G1620	U1621	G1622	G1623	G1624	G1625	G1626	C1627	C1628	C1629	C1630	A1631	A1632	G1633	A1634	G1635	C1636	A1637	C1638	U1639	C1640	A1641	G1642	G1643	C1644	G1645	C1646	G1647	C1648	G1649	C1650	C1651	A1652	U1653	C1654	A1655	C1656	C1657	A1658	A1659	C1660																					
G1534	U1535	A1536	C1537	G1538	G1539	U1540	U1541	G1542	C1543	A1544	A1545	A1546	C1547	C1548	C1549	C1550	C1551	A1552	A1553	C1554	C1555	A1556	A1557	A1558	A1559	A1560	A1561	C1562	C1563	C1564	C1565	A1566	A1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	C1575	C1576	U1577	C1578	A1579	A1580	C1581	C1582	C1583	A1584	A1585	A1586	A1587	C1588	C1589	U1590	C1591	C1592	A1593	G1594	A1595	A1596	A1597																				
G1459	A1460	G1461	C1462	G1463	G1464	G1465	G1466	G1467	C1468	A1469	A1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	U1481	G1482	G1483	A1484	A1485	A1486	G1487	G1488	U1489	C1490	C1491	C1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	A1510	A1511	C1512	C1513	U1514	C1515	C1516	C1517	C1518	A1519	U1520	G1521	G1522	C1523	C1524	C1525	C1526	G1527	A1528	A1529	A1530												

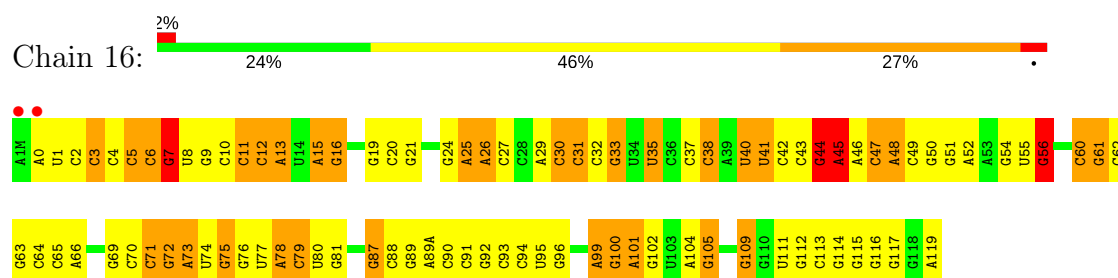


G1461	C1462	G1466	G1467		A1471	G1475	G1476	A1477	G1478	G1479	G1480	G1482	G1483	G1484	G1485	U1486	G1487	G1488	U1489	A1490		G1493	A1494	A1495	A1496		C1499	G1500	C1506	A1507	A1508	C1509	A1510	A1511	G1512	G1514	C1515	G1516	G1517	C1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	A1528	A1529	G1530		C1533	G1534																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G1388		U1391	A1392	G1393	U1394	A1395	G1396	U1397	C1398	G1399	G1400	G1401	C1402	C1403	C1404	U1405	U1406	C1407	G1408	C1409		G1416	G1417	A1418	A1419	U1420	G1421	G1422		G1425	G1426	C1427	G1428	G1429	C1430	U1431	A1432	A1433	A1434	G1435	G1436		U1438	G1441	G1442	G1443	G1444	A1444A	C1445		A1449	G1449A	C1450	C1451		C1458	G1459	A1460																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U1263	G1264	A1265	G1266	U1267	A1268	A1269	G1270	G1271	U1272	U1273	A1274	U1275	A1276	G1277	A1278	G1279	G1280	G1281	U1282	G1283	A1284	G1285	A1286	A1287	U1288	C1289	G1290	G1291	U1292	G1293		U1297	G1298	G1299	U1300	A1301	A1302	A1303	A1304	G1305	C1306	A1307	A1308	G1309	G1310	A1311	G1312	U1313	G1314	G1315	U1316	G1317	G1318	G1319	G1320	A1321	A1322	G1323	G1324	G1325	G1326	G1327	A1328	G1329	G1330	G1331	G1332	G1333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1183	G1184	G1187	C1188	U1189	G1190	G1191	G1192	G1197	U1198	U1199	C1200	C1201	G1202	G1203	A1204	U1205	C1208	G1209	A1210	U1211	G1212	A1213	C1217	A1220	G1224	C1225	G1226	A1227	G1228	G1236	A1237	A1241	G1242	G1243	A1247	U1248	U1249	G1250	G1251	G1252	A1253	A1254	U1255	G1256	G1257	G1258	G1259	G1260	C1261	A1262																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U1113	G1114	G1120	C1121	G1122	G1123	C1124	G1125	A1128	U1129	A1130	G1131	A1132	G1133	C1135	G1136	G1137	G1138	U1139	C1140	U1141	U1142	A1143	C1145	G1149	G1150	C1152	G1153	G1154	A1155	G1156	G1157	C1158	U1159	G1160	C1161	G1162		C1166	U1167	G1168	U1175	G1176	G1177	G1178	G1179	C1180	C1181	A1182																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G1047	A1048	G1051	C1052	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	A1073	G1074	C1075	G1076	A1077	U1078	C1079	A1085	A1086	G1087	A1088	G1089	U1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	U1104	U1105	G1106	C1109	G1110	A1111	G1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743	A1744	A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A1791	A1792	A1793	A1794	A1795	A1796	A1797	A1798	A1799	A1800	A1801	A1802	A1803	A1804	A1805	A1806	A1807	A1808	A1809	A1810	A1811	A1812	A1813	A1814	A1815	A1816	A1817	A1818	A1819	A1820	A1821	A1822	A1823	A1824	A1825	A1826	A1827	A1828	A1829	A1830	A1831	A1832	A1833	A1834	A1835	A1836	A1837	A1838	A1839	A1840	A1841	A1842	A1843	A1844	A1845	A1846	A1847	A1848	A1849	A1850	A1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A

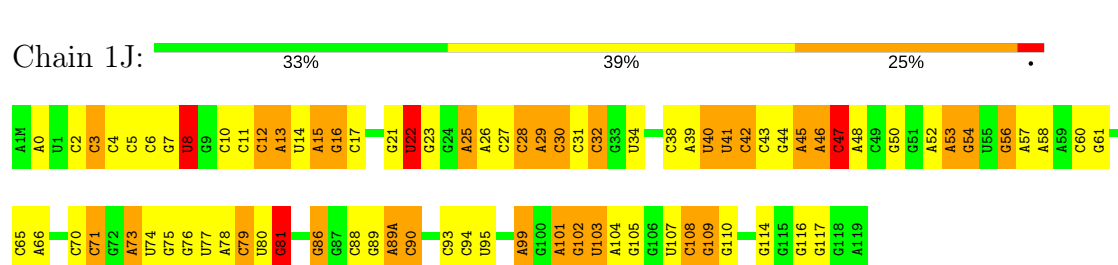




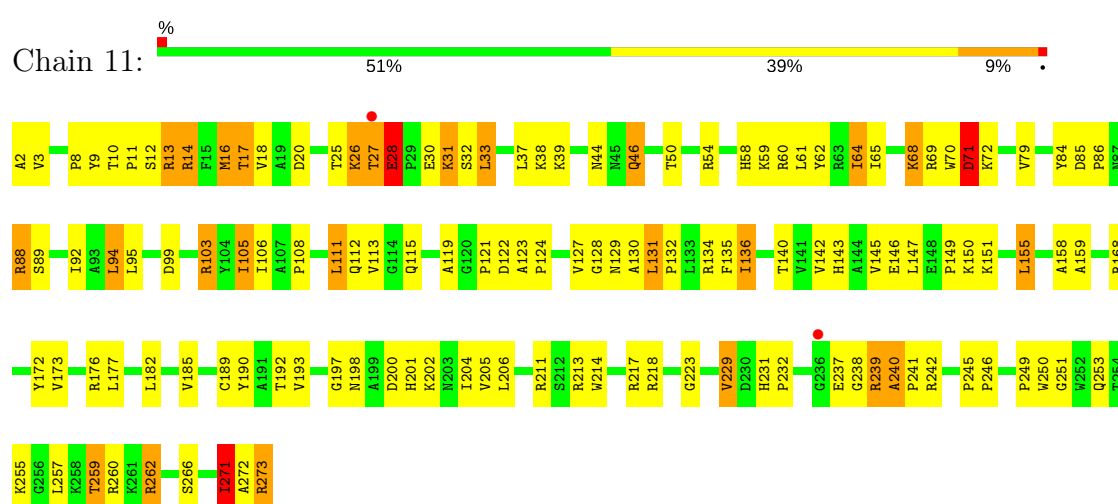
• Molecule 26: 5S ribosomal RNA



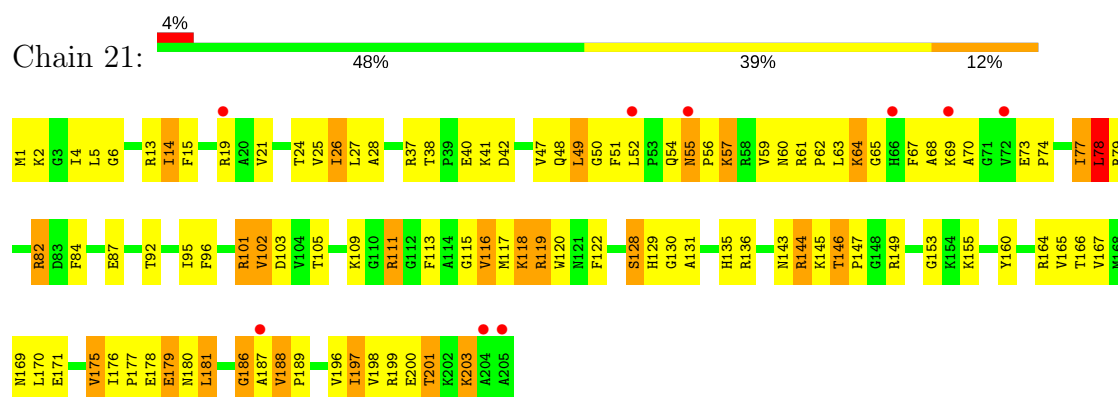
• Molecule 26: 5S ribosomal RNA



• Molecule 27: 50S ribosomal protein L2



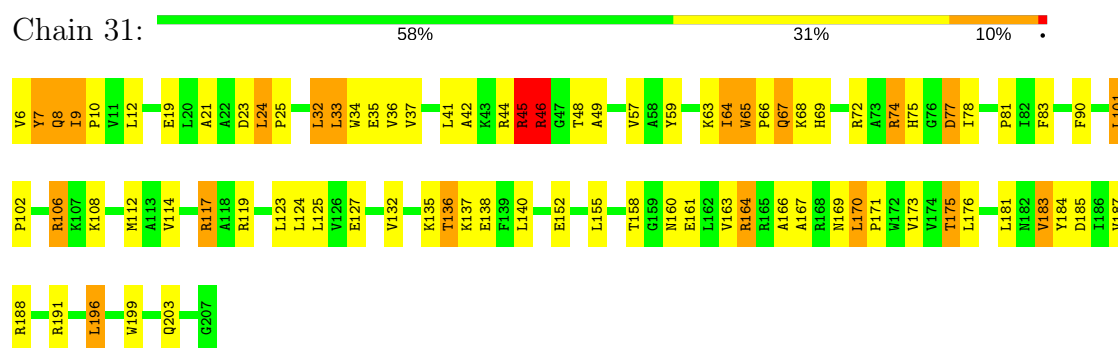
• Molecule 28: 50S ribosomal protein L3



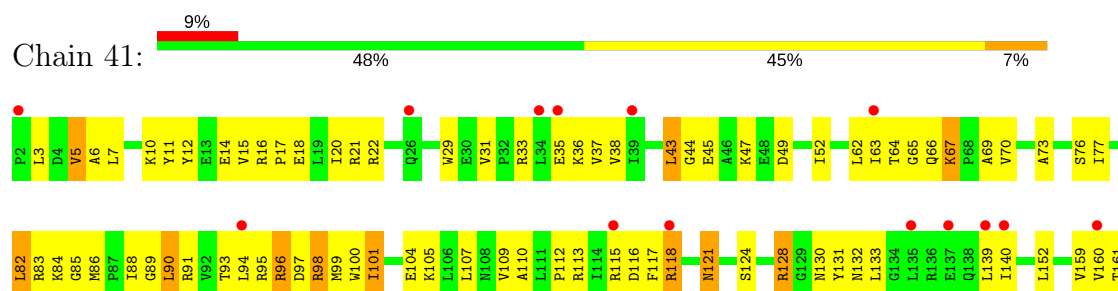
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

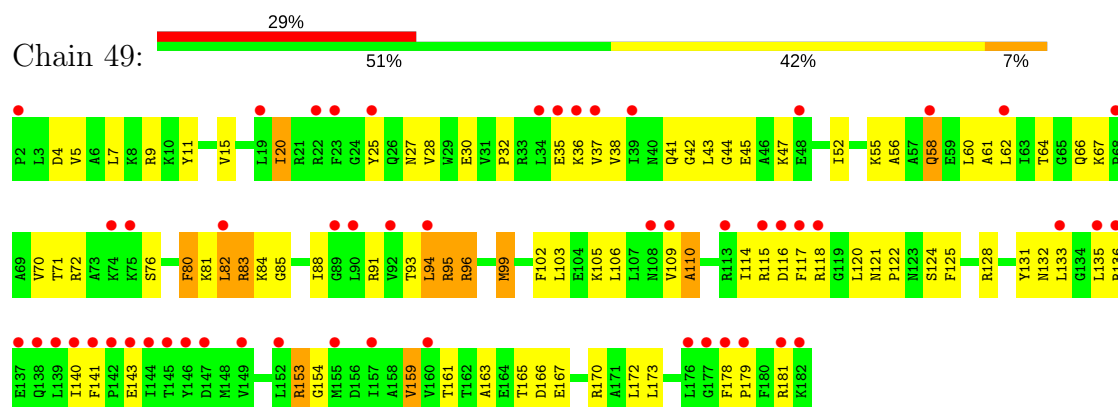


• Molecule 30: 50S ribosomal protein L5

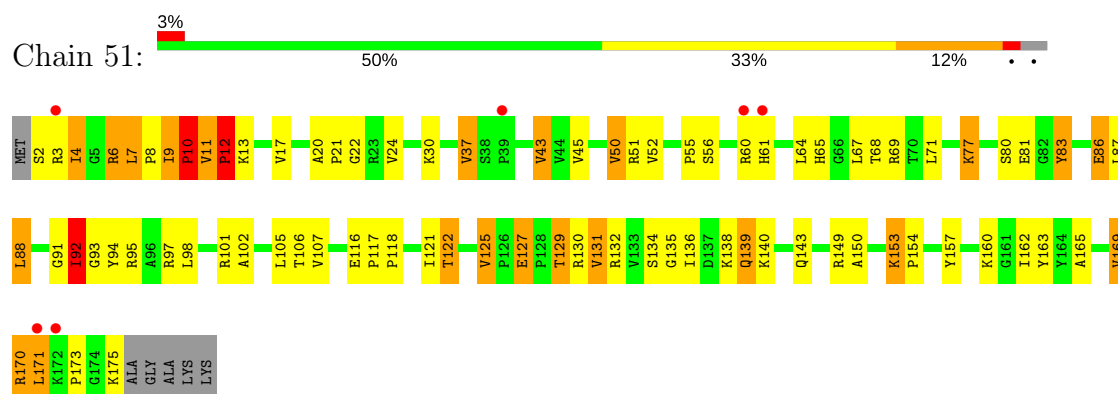




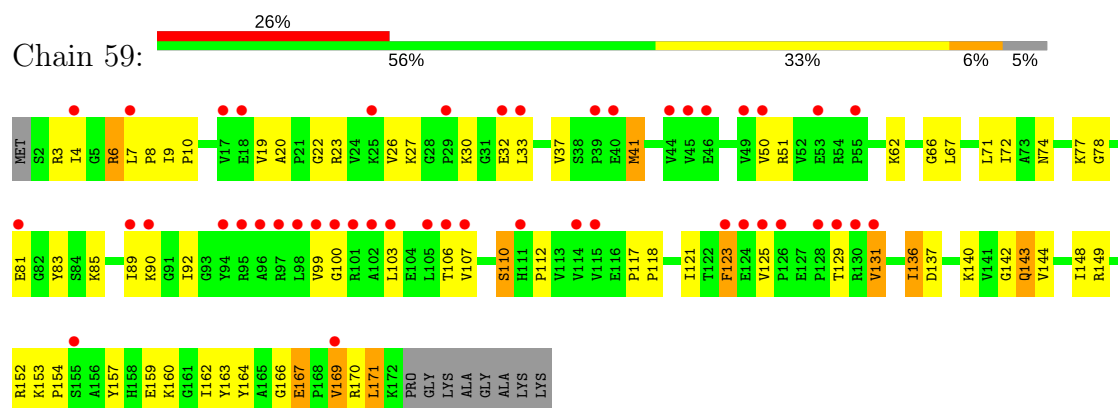
- Molecule 30: 50S ribosomal protein L5



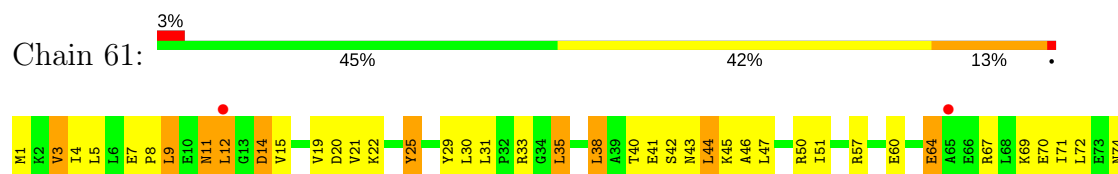
- Molecule 31: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L6

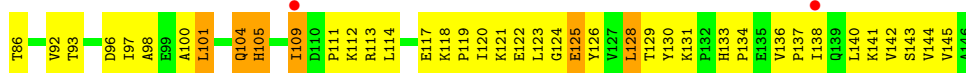
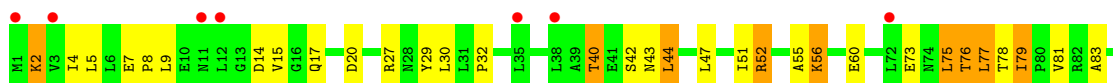


- Molecule 32: 50S ribosomal protein L9

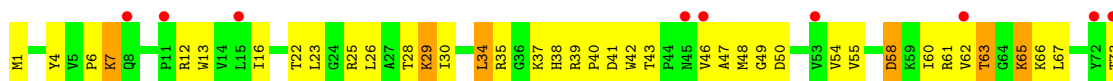




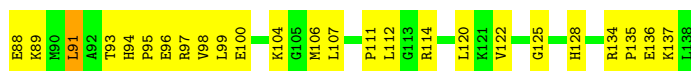
• Molecule 32: 50S ribosomal protein L9



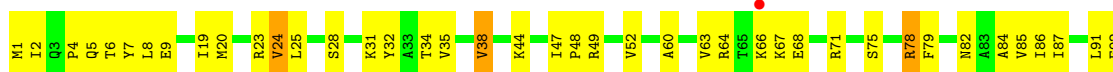
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

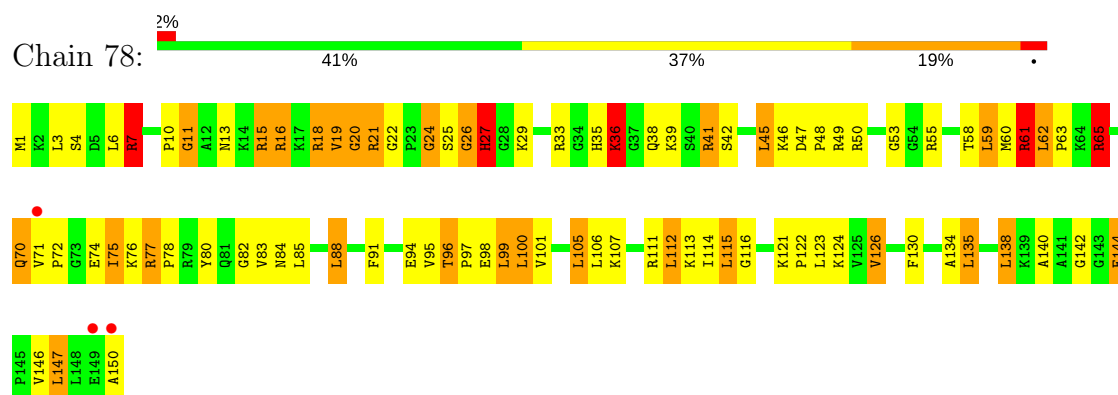


• Molecule 34: 50S ribosomal protein L14

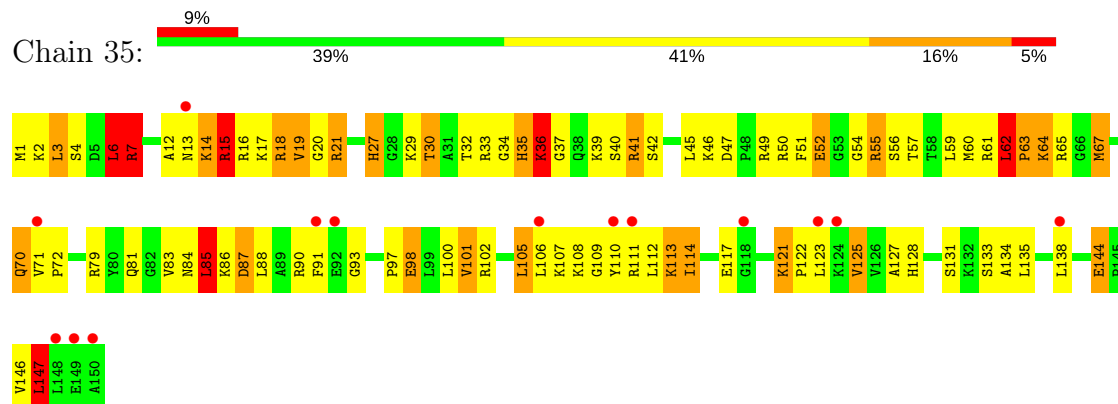




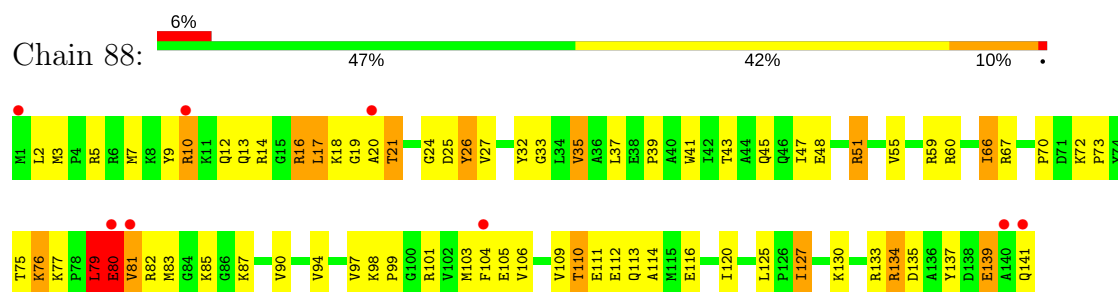
• Molecule 35: 50S ribosomal protein L15



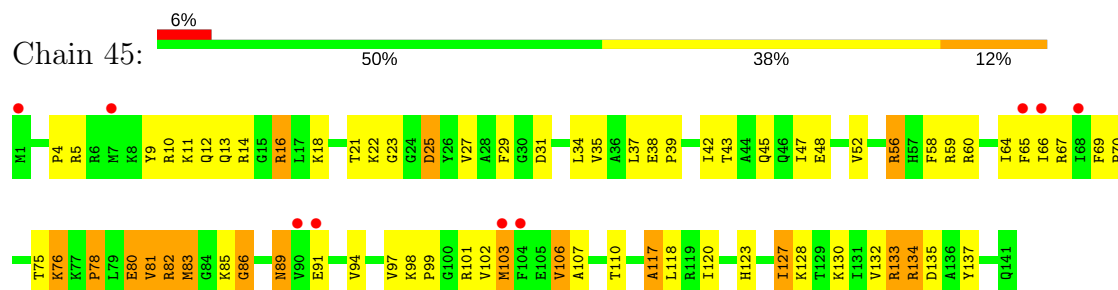
• Molecule 35: 50S ribosomal protein L15



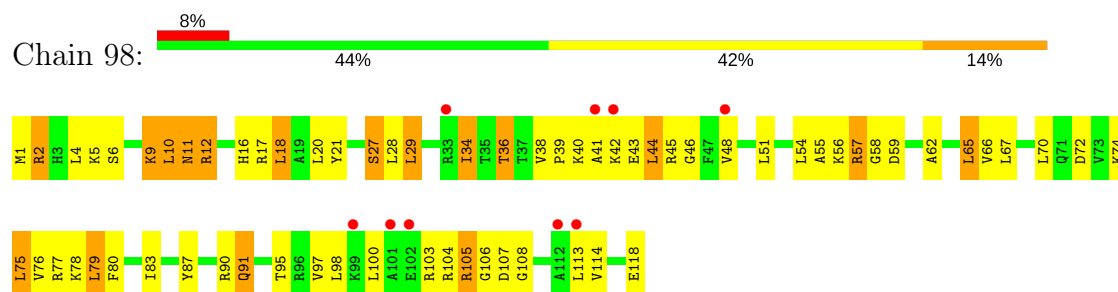
• Molecule 36: 50S ribosomal protein L16



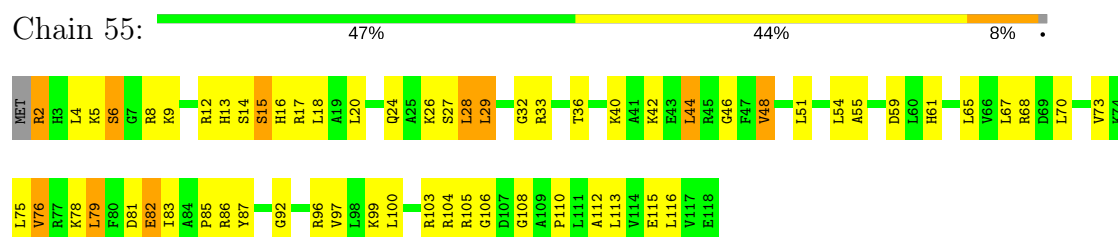
• Molecule 36: 50S ribosomal protein L16



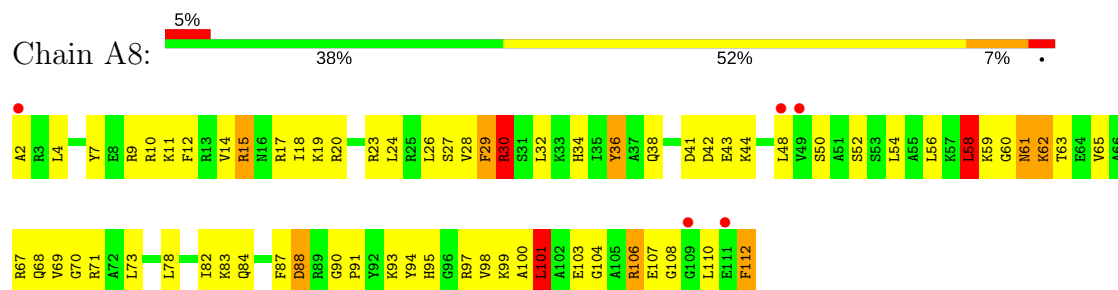
- Molecule 37: 50S ribosomal protein L17



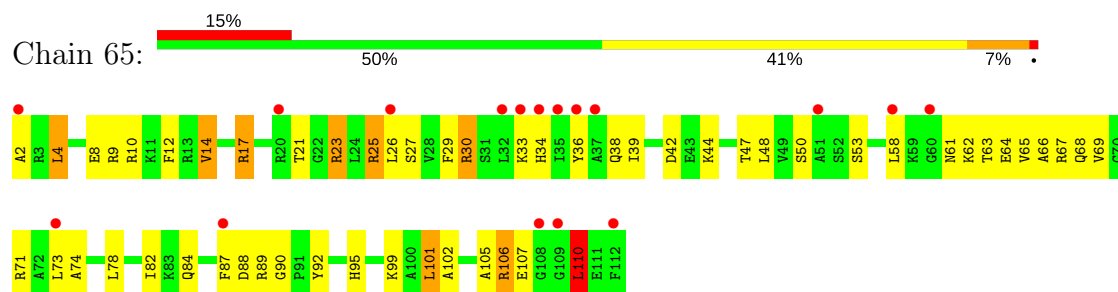
- Molecule 37: 50S ribosomal protein L17



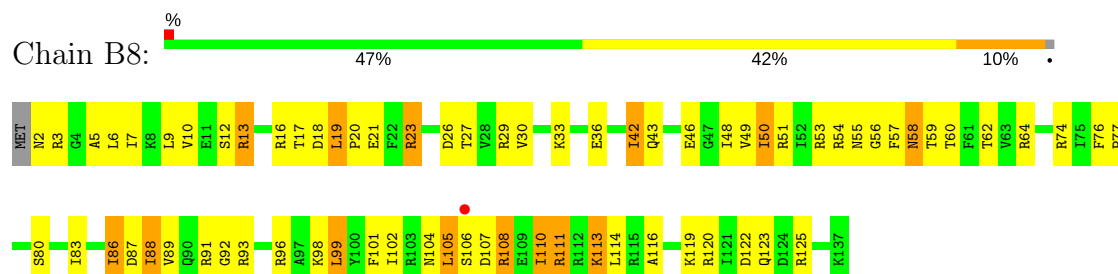
- Molecule 38: 50S ribosomal protein L18



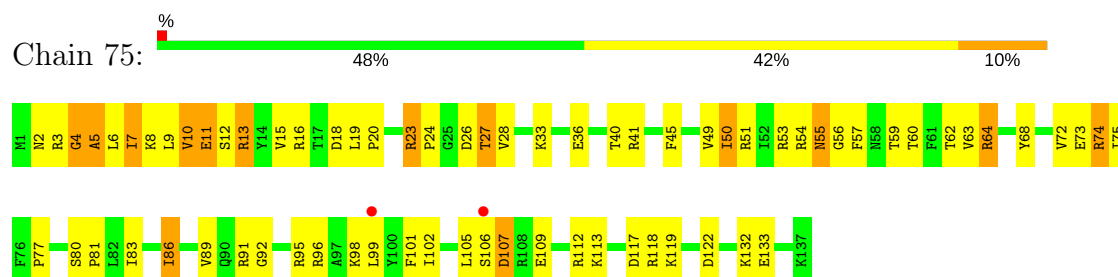
- Molecule 38: 50S ribosomal protein L18



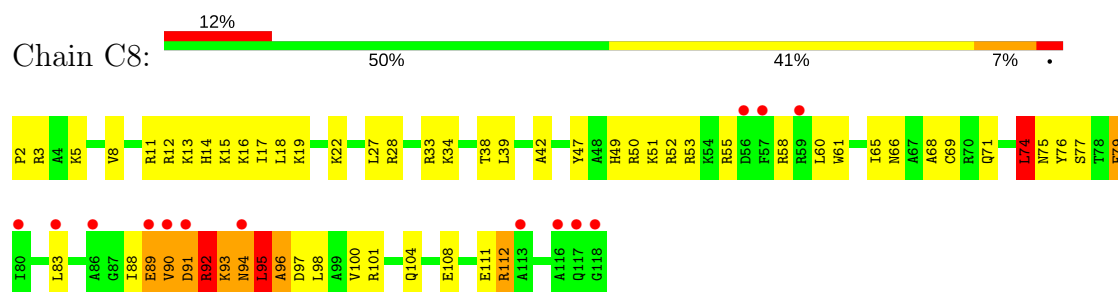
- Molecule 39: 50S ribosomal protein L19



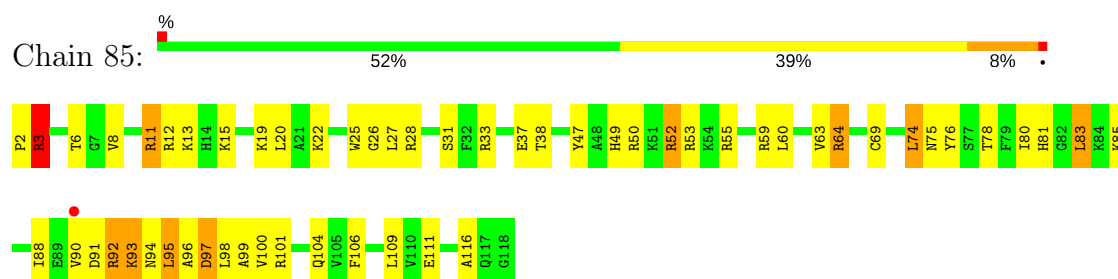
- Molecule 39: 50S ribosomal protein L19



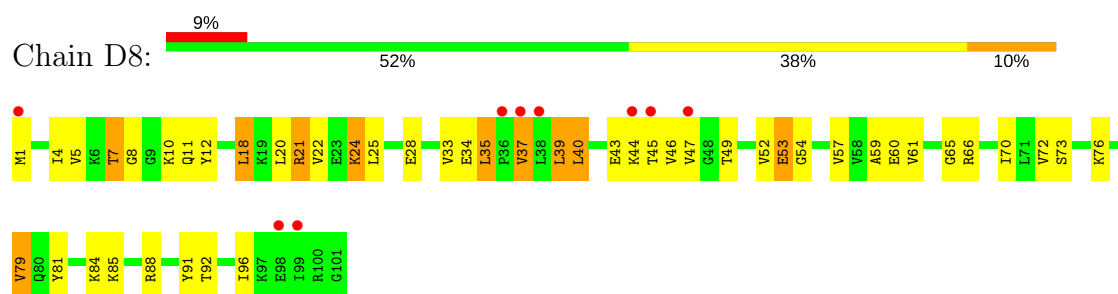
- Molecule 40: 50S ribosomal protein L20



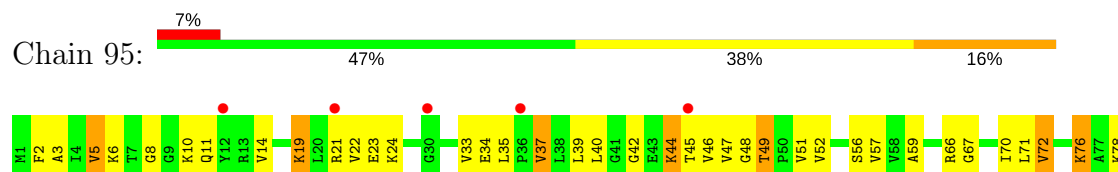
- Molecule 40: 50S ribosomal protein L20

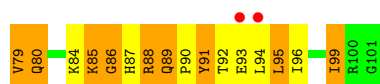


- Molecule 41: 50S ribosomal protein L21

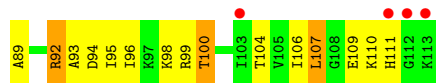


- Molecule 41: 50S ribosomal protein L21

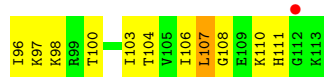
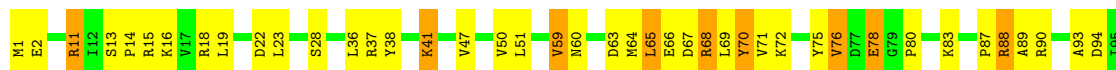




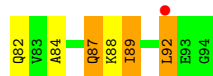
- Molecule 42: 50S ribosomal protein L22



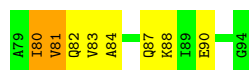
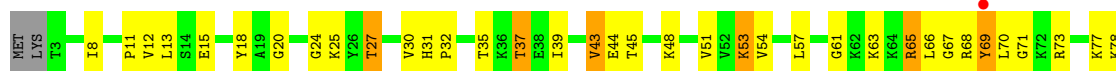
- Molecule 42: 50S ribosomal protein L22



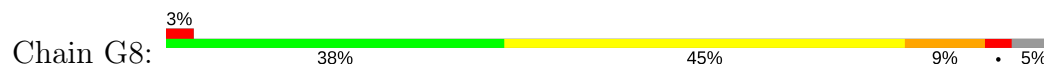
- Molecule 43: 50S ribosomal protein L23

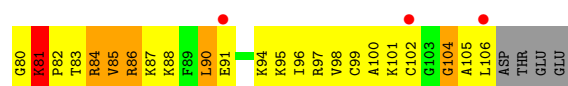


- Molecule 43: 50S ribosomal protein L23

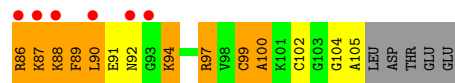
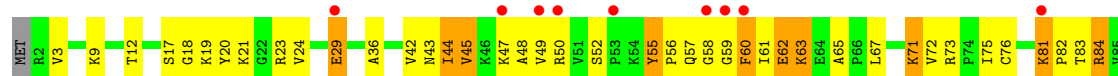


- Molecule 44: 50S ribosomal protein L24

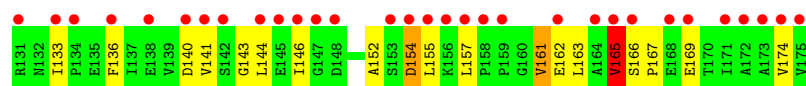
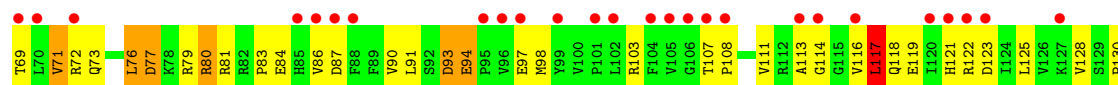
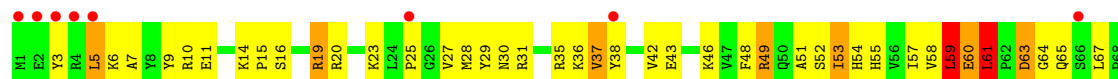
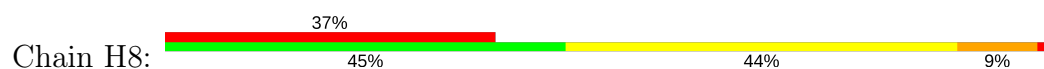




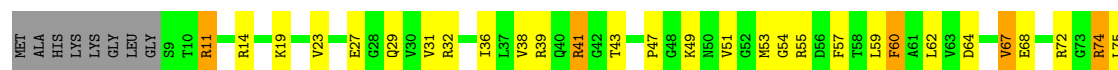
• Molecule 44: 50S ribosomal protein L24



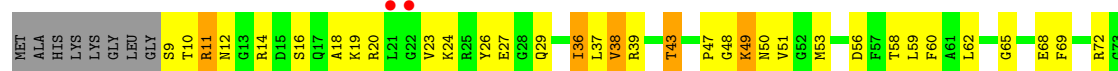
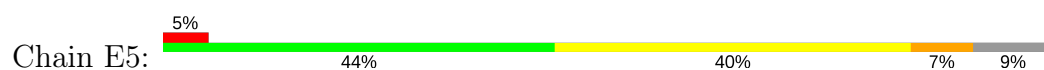
• Molecule 45: 50S ribosomal protein L25



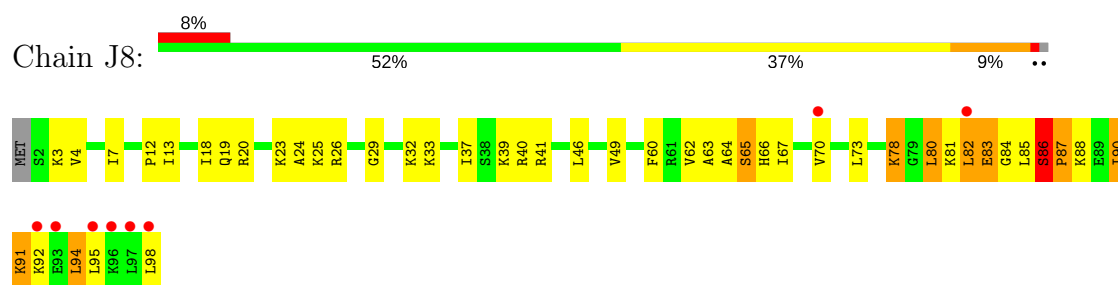
• Molecule 46: 50S ribosomal protein L27



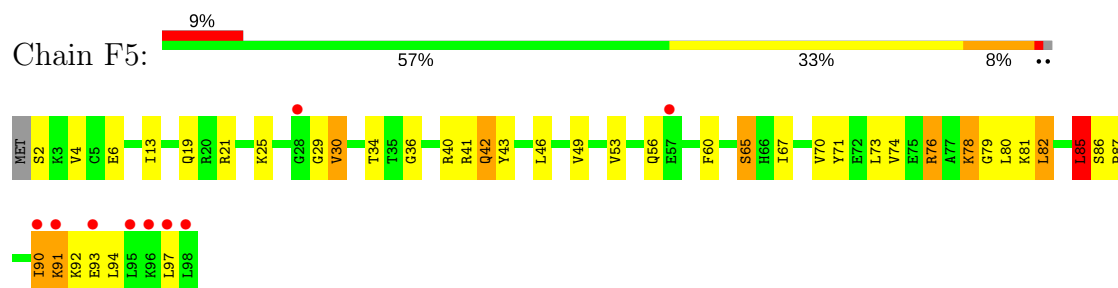
• Molecule 46: 50S ribosomal protein L27



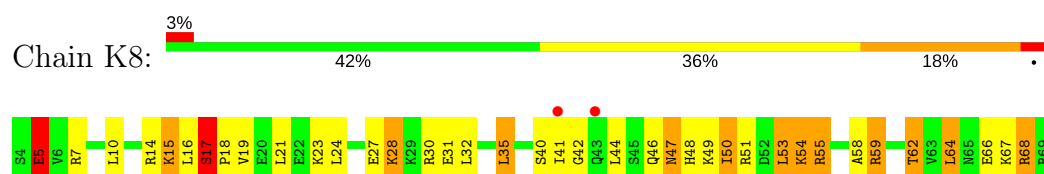
• Molecule 47: 50S ribosomal protein L28



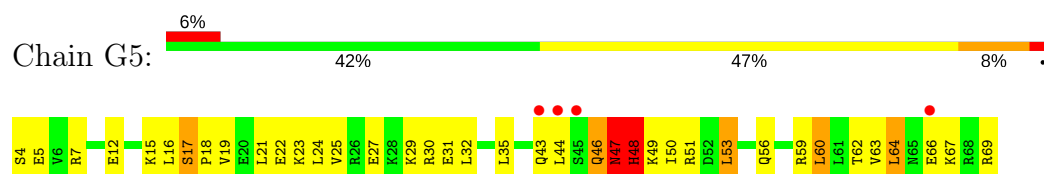
- Molecule 47: 50S ribosomal protein L28



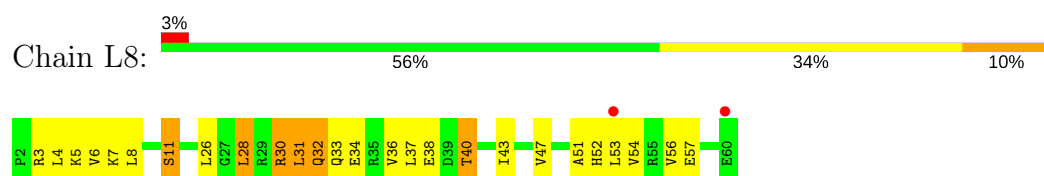
- Molecule 48: 50S ribosomal protein L29



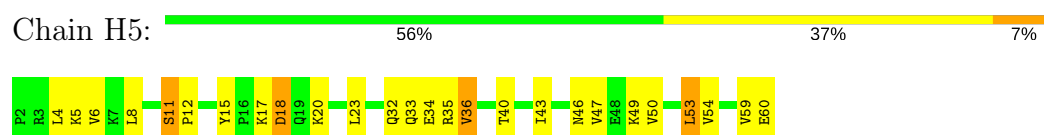
- Molecule 48: 50S ribosomal protein L29



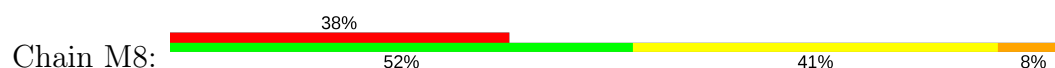
- Molecule 49: 50S ribosomal protein L30

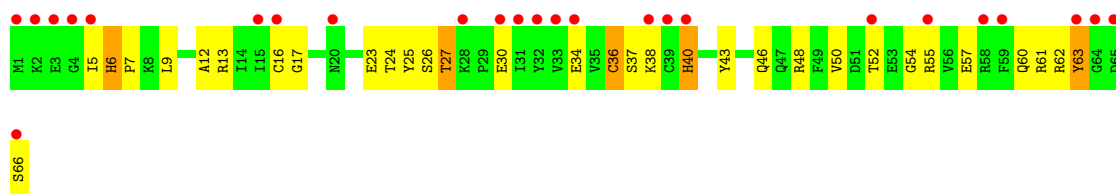


- Molecule 49: 50S ribosomal protein L30



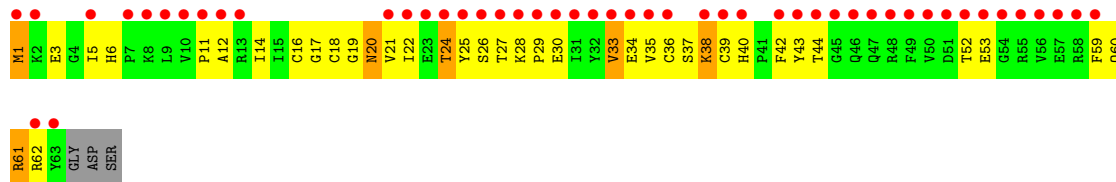
- Molecule 50: 50S ribosomal protein L31





- Molecule 50: 50S ribosomal protein L31

Chain I5: 74%
38% 48% 9% 5%



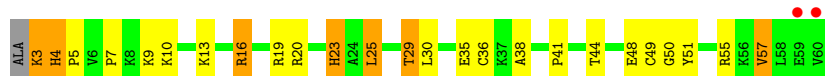
- Molecule 51: 50S ribosomal protein L32

Chain N8: 15%
49% 39% 12%



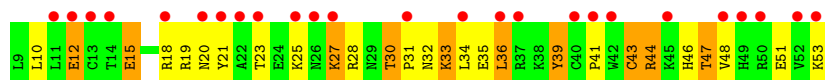
- Molecule 51: 50S ribosomal protein L32

Chain J5: 3%
56% 31% 12%



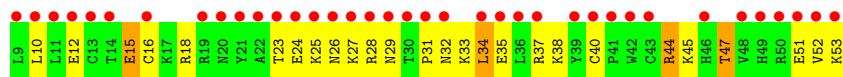
- Molecule 52: 50S ribosomal protein L33

Chain O8: 56%
40% 38% 22%



- Molecule 52: 50S ribosomal protein L33

Chain K5: 82%
42% 49% 9%



- Molecule 53: 50S ribosomal protein L34

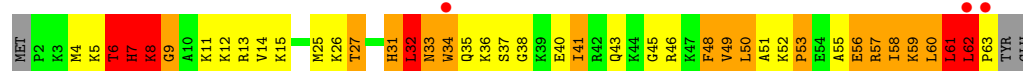
Chain P8: 43% 43% 6% 8%



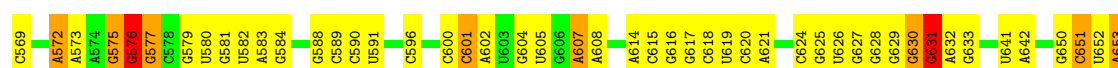
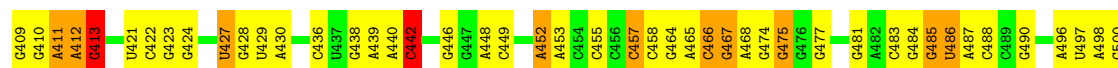
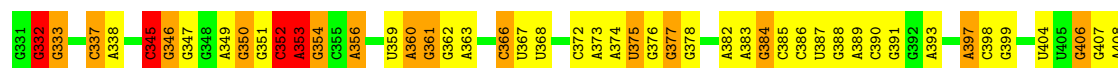
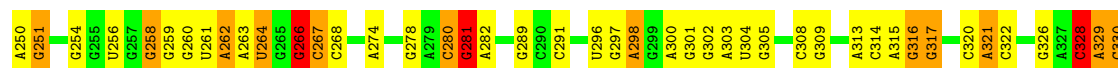
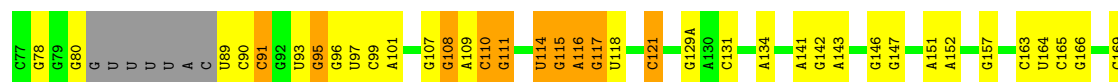
- Molecule 53: 50S ribosomal protein L34

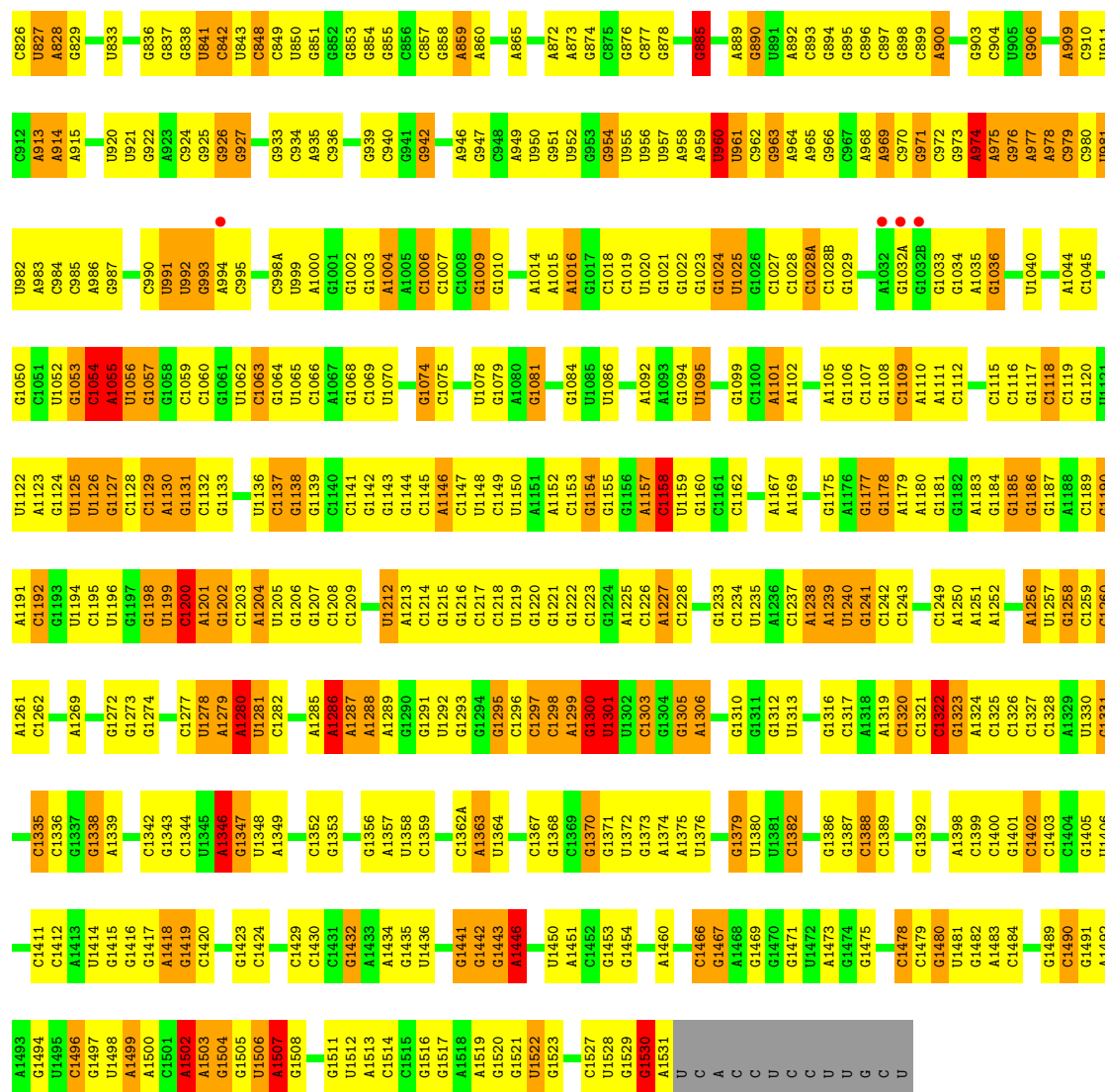


- Molecule 54: 50S ribosomal protein L35

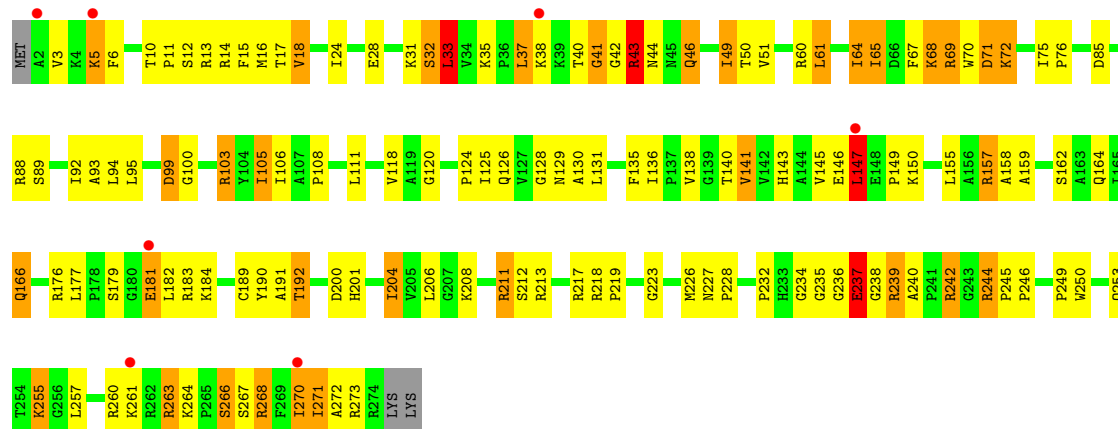


- Molecule 55: 16S ribosomal RNA

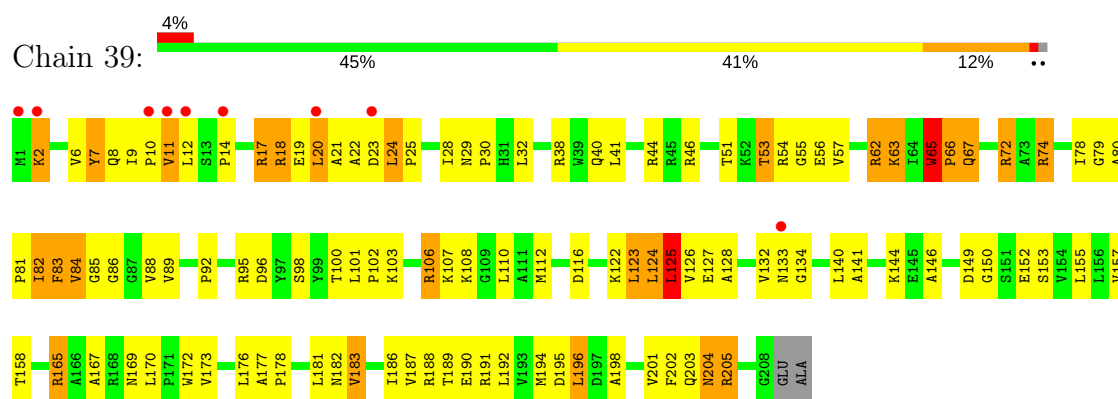




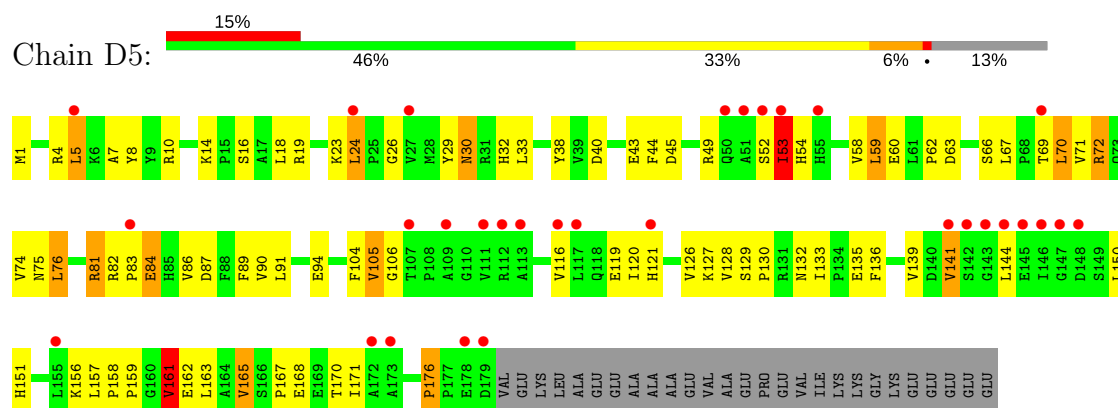
• Molecule 56: 50S ribosomal protein L2



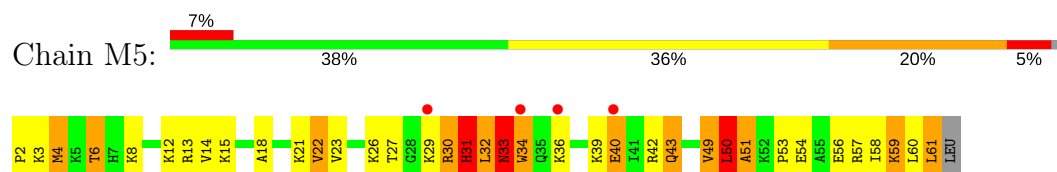
• Molecule 57: 50S ribosomal protein L4



• Molecule 58: 50S ribosomal protein L25



• Molecule 59: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 448.70Å 618.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.80 – 3.10 187.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.80-3.10) 94.5 (187.34-3.10)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.188 , 0.235 0.190 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	DCC
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299951	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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, OMG, MIA, MG, H2U, 4SU, QUO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.83	25/36053 (0.1%)	1.49	573/56270 (1.0%)
2	12	0.34	0/1959	0.57	0/2642
2	1E	0.42	0/1959	0.65	4/2642 (0.2%)
3	22	0.37	0/1636	0.56	0/2205
3	2E	0.49	0/1629	0.68	1/2195 (0.0%)
4	32	0.46	0/1732	0.66	0/2318
4	3E	0.61	2/1732 (0.1%)	0.73	1/2318 (0.0%)
5	42	0.43	0/1171	0.67	0/1576
5	4E	0.58	0/1171	0.75	1/1576 (0.1%)
6	52	0.54	0/855	0.68	0/1154
6	5E	0.54	0/855	0.75	0/1154
7	62	0.41	0/1275	0.58	0/1709
7	6E	0.46	0/1275	0.59	0/1709
8	72	0.42	0/1135	0.59	0/1527
8	7E	0.52	0/1135	0.70	0/1527
9	82	0.38	0/1028	0.60	0/1379
9	8E	0.41	0/1028	0.66	0/1379
10	1A	0.35	0/814	0.59	0/1095
10	1I	0.43	0/814	0.61	0/1095
11	2A	0.47	0/899	0.67	0/1213
11	2I	0.54	0/899	0.76	1/1213 (0.1%)
12	3A	0.52	0/991	0.78	2/1327 (0.2%)
12	3I	0.73	0/991	0.88	0/1327
13	4A	0.38	0/943	0.59	0/1265
13	4I	0.48	0/938	0.73	0/1258
14	5A	0.42	0/484	0.73	0/643
14	5I	0.63	0/507	0.88	1/672 (0.1%)
15	6A	0.48	0/744	0.63	0/992
15	6I	0.57	0/744	0.75	1/992 (0.1%)
16	7A	0.51	0/721	0.69	0/970
16	7I	0.48	0/721	0.74	0/970
17	8A	0.49	0/847	0.63	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8I	0.53	0/847	0.75	0/1131
18	9A	0.49	0/595	0.71	0/790
18	9I	0.50	0/595	0.71	1/790 (0.1%)
19	AA	0.37	0/654	0.61	0/884
19	AI	0.48	0/680	0.75	0/915
20	BA	0.47	0/764	0.73	1/1007 (0.1%)
20	BI	0.40	0/764	0.69	1/1007 (0.1%)
21	1B	0.43	0/221	0.66	0/288
21	1F	0.40	0/221	0.58	0/288
22	1K	0.44	0/1851	1.06	7/2877 (0.2%)
22	1L	0.38	0/1594	0.92	3/2475 (0.1%)
22	3K	0.46	0/1594	0.98	1/2475 (0.0%)
22	3L	0.41	0/1616	0.92	1/2509 (0.0%)
23	2K	0.94	1/1725 (0.1%)	1.60	30/2689 (1.1%)
23	2L	0.76	1/1725 (0.1%)	1.35	10/2689 (0.4%)
24	4K	0.87	0/366	1.25	1/568 (0.2%)
24	4L	0.60	0/391	1.19	2/607 (0.3%)
25	14	0.97	94/70119 (0.1%)	1.69	1912/109464 (1.7%)
25	1H	1.16	199/70233 (0.3%)	1.94	3139/109643 (2.9%)
26	16	0.91	0/2928	1.65	54/4568 (1.2%)
26	1J	0.78	0/2928	1.48	38/4568 (0.8%)
27	11	0.87	1/2165 (0.0%)	1.03	6/2919 (0.2%)
28	21	0.68	0/1601	0.93	1/2160 (0.0%)
28	29	0.66	0/1601	0.89	1/2160 (0.0%)
29	31	0.79	3/1620 (0.2%)	0.93	6/2194 (0.3%)
30	41	0.52	0/1498	0.73	0/2016
30	49	0.40	0/1498	0.66	0/2016
31	51	0.58	0/1362	0.87	1/1841 (0.1%)
31	59	0.34	0/1341	0.59	0/1813
32	61	0.49	0/1151	0.75	2/1558 (0.1%)
32	69	0.47	0/1151	0.71	1/1558 (0.1%)
33	15	0.48	0/1131	0.67	0/1525
33	58	0.60	0/1131	0.82	0/1525
34	25	0.65	0/942	0.80	1/1269 (0.1%)
34	68	0.70	0/942	0.78	0/1269
35	35	0.64	0/1161	1.05	4/1544 (0.3%)
35	78	0.75	0/1161	1.10	6/1544 (0.4%)
36	45	0.65	1/1142 (0.1%)	0.88	2/1527 (0.1%)
36	88	0.84	1/1142 (0.1%)	1.03	3/1527 (0.2%)
37	55	0.65	0/973	0.84	0/1302
37	98	0.69	0/981	0.92	1/1312 (0.1%)
38	65	0.55	0/891	0.84	2/1187 (0.2%)
38	A8	0.62	0/891	0.93	4/1187 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	75	0.61	0/1155	0.79	2/1542 (0.1%)
39	B8	0.65	0/1147	0.83	1/1532 (0.1%)
40	85	0.62	0/981	0.81	2/1306 (0.2%)
40	C8	0.72	0/981	0.96	3/1306 (0.2%)
41	95	0.58	0/789	0.81	0/1057
41	D8	0.64	0/789	0.82	1/1057 (0.1%)
42	A5	0.69	0/910	0.85	0/1220
42	E8	0.73	0/910	0.93	1/1220 (0.1%)
43	B5	0.75	0/739	0.81	0/993
43	F8	0.89	2/756 (0.3%)	0.96	1/1014 (0.1%)
44	C5	0.55	0/807	0.79	0/1076
44	G8	0.71	0/804	1.02	3/1073 (0.3%)
45	H8	0.48	0/1427	0.78	1/1935 (0.1%)
46	E5	0.68	0/620	0.90	0/827
46	I8	0.80	0/620	0.96	0/827
47	F5	0.64	0/769	0.93	1/1022 (0.1%)
47	J8	0.72	0/769	0.94	2/1022 (0.2%)
48	G5	0.58	0/560	0.81	1/741 (0.1%)
48	K8	0.82	2/560 (0.4%)	0.94	1/741 (0.1%)
49	H5	0.50	0/473	0.67	0/635
49	L8	0.64	0/473	0.78	0/635
50	I5	0.36	0/527	0.67	0/709
50	M8	0.38	0/545	0.62	0/733
51	J5	0.64	0/467	0.84	1/632 (0.2%)
51	N8	0.66	0/472	0.86	0/639
52	K5	0.46	0/396	0.78	0/529
52	O8	0.61	0/396	0.80	1/529 (0.2%)
53	L5	0.74	0/399	0.92	0/526
53	P8	0.99	0/399	1.07	2/526 (0.4%)
54	Q8	1.16	0/448	1.48	5/600 (0.8%)
55	1G	0.71	4/36049 (0.0%)	1.33	281/56262 (0.5%)
56	19	0.75	0/2170	0.96	5/2926 (0.2%)
57	39	0.63	1/1662 (0.1%)	0.87	2/2249 (0.1%)
58	D5	0.38	0/1460	0.62	0/1982
59	M5	0.74	0/486	1.13	2/638 (0.3%)
All	All	0.87	337/322487 (0.1%)	1.49	6146/482889 (1.3%)

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
4	3E	0	1
10	1A	0	1
12	3I	0	1
13	4I	0	1
14	5A	0	1
14	5I	0	1
19	AI	0	2
20	BA	0	1
27	11	0	3
28	21	0	4
28	29	0	5
30	41	0	1
31	51	0	1
31	59	0	1
32	61	0	4
32	69	0	1
33	58	0	1
35	35	0	3
35	78	0	6
36	45	0	3
36	88	0	2
37	98	0	1
39	75	0	1
39	B8	0	1
40	85	0	1
40	C8	0	2
41	95	0	1
43	B5	0	1
44	C5	0	2
44	G8	0	4
45	H8	0	3
47	F5	0	1
48	G5	0	3
48	K8	0	1
50	M8	0	1
52	K5	0	1
54	Q8	0	6
56	19	0	4
57	39	0	1
59	M5	0	3
All	All	0	82

The worst 5 of 337 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1H	1614	A	N9-C4	-12.72	1.30	1.37
25	1H	2430	A	N9-C4	-12.06	1.30	1.37
1	13	792	A	N9-C4	-11.71	1.30	1.37
25	1H	774	A	N9-C4	-11.62	1.30	1.37
25	1H	71	A	N9-C4	-11.59	1.30	1.37

The worst 5 of 6146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1899	G	N3-C4-N9	-25.74	110.56	126.00
25	1H	676	A	C2-N3-C4	-22.98	99.11	110.60
25	1H	1899	G	N3-C4-C5	22.06	139.63	128.60
25	14	1332	G	N3-C4-N9	-21.72	112.97	126.00
25	14	1332	G	N3-C4-C5	20.07	138.63	128.60

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3E	85	LYS	Peptide
12	3I	87	GLY	Peptide
13	4I	107	ALA	Peptide
14	5I	13	THR	Peptide
19	AI	4	SER	Peptide

5.2 Too-close contacts [i](#)

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	32207	0	16254	796	0
2	12	1924	0	1975	84	0
2	1E	1924	0	1975	77	0
3	22	1612	0	1677	69	0
3	2E	1605	0	1668	53	0
4	32	1702	0	1763	85	1
4	3E	1702	0	1763	84	0
5	42	1155	0	1213	42	0
5	4E	1155	0	1213	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	52	842	0	857	30	0
6	5E	842	0	857	33	1
7	62	1256	0	1296	53	0
7	6E	1256	0	1296	43	0
8	72	1115	0	1177	30	0
8	7E	1115	0	1177	46	0
9	82	1009	0	1037	66	0
9	8E	1009	0	1037	52	0
10	1A	801	0	849	53	0
10	1I	801	0	849	46	0
11	2A	884	0	904	39	0
11	2I	884	0	904	28	0
12	3A	975	0	1062	42	0
12	3I	975	0	1062	38	0
13	4A	933	0	992	49	0
13	4I	928	0	987	50	0
14	5A	475	0	511	27	0
14	5I	498	0	537	30	0
15	6A	733	0	771	27	0
15	6I	733	0	771	22	0
16	7A	705	0	725	21	0
16	7I	705	0	725	49	0
17	8A	834	0	904	27	0
17	8I	834	0	904	39	0
18	9A	590	0	662	13	0
18	9I	590	0	662	23	0
19	AA	640	0	633	38	0
19	AI	665	0	686	34	0
20	BA	762	0	861	35	0
20	BI	762	0	861	36	0
21	1B	217	0	234	11	0
21	1F	217	0	234	9	0
22	1K	1825	0	946	36	0
22	1L	1595	0	830	24	0
22	3K	1595	0	830	36	0
22	3L	1615	0	840	30	0
23	2K	1645	0	843	36	0
23	2L	1645	0	843	31	0
24	4K	325	0	165	6	0
24	4L	347	0	176	6	0
25	14	62605	0	31558	1370	0
25	1H	62707	0	31607	1469	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	16	2617	0	1328	79	0
26	1J	2617	0	1328	75	0
27	11	2115	0	2195	120	0
28	21	1568	0	1634	107	0
28	29	1568	0	1634	100	0
29	31	1585	0	1632	84	0
30	41	1473	0	1535	76	0
30	49	1473	0	1535	56	0
31	51	1336	0	1418	61	0
31	59	1316	0	1395	52	0
32	61	1136	0	1223	48	1
32	69	1136	0	1223	53	0
33	15	1104	0	1180	45	0
33	58	1104	0	1180	64	0
34	25	932	0	996	41	0
34	68	932	0	996	34	0
35	35	1144	0	1228	102	0
35	78	1144	0	1228	89	0
36	45	1121	0	1179	65	0
36	88	1121	0	1179	59	0
37	55	959	0	1021	47	0
37	98	967	0	1033	59	0
38	65	881	0	943	46	0
38	A8	881	0	943	53	0
39	75	1141	0	1202	47	0
39	B8	1133	0	1190	55	0
40	85	963	0	1022	46	0
40	C8	963	0	1022	60	0
41	95	778	0	852	56	0
41	D8	778	0	852	21	0
42	A5	899	0	964	32	0
42	E8	899	0	964	34	0
43	B5	725	0	778	29	0
43	F8	742	0	803	42	0
44	C5	794	0	883	47	0
44	G8	791	0	880	61	0
45	H8	1397	0	1430	71	0
46	E5	612	0	633	39	0
46	I8	612	0	633	28	0
47	F5	762	0	848	30	0
47	J8	762	0	848	29	0
48	G5	558	0	610	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	K8	558	0	610	31	0
49	H5	468	0	518	18	0
49	L8	468	0	518	15	0
50	I5	515	0	514	34	0
50	M8	533	0	526	22	0
51	J5	453	0	475	20	0
51	N8	458	0	480	25	0
52	K5	389	0	404	24	0
52	O8	389	0	404	23	0
53	L5	391	0	432	14	0
53	P8	391	0	432	15	0
54	Q8	442	0	452	59	0
55	1G	32204	0	16256	685	1
56	19	2120	0	2197	107	0
57	39	1627	0	1680	91	0
58	D5	1428	0	1454	51	0
59	M5	480	0	549	43	0
60	11	2	0	0	0	0
60	13	140	0	0	0	0
60	14	386	0	0	0	0
60	16	12	0	0	0	0
60	19	1	0	0	0	0
60	1G	104	0	0	0	0
60	1H	438	0	0	0	0
60	1J	7	0	0	0	0
60	1K	1	0	0	0	0
60	21	2	0	0	0	0
60	25	1	0	0	0	0
60	29	2	0	0	0	0
60	2K	4	0	0	0	0
60	2L	3	0	0	0	0
60	39	1	0	0	0	0
60	3I	1	0	0	0	0
60	3K	1	0	0	0	0
60	41	1	0	0	0	0
60	45	3	0	0	0	0
60	49	1	0	0	0	0
60	4I	1	0	0	0	0
60	52	1	0	0	0	0
60	5I	1	0	0	0	0
60	68	1	0	0	0	0
60	78	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	85	1	0	0	0	0
60	88	2	0	0	0	0
60	98	2	0	0	0	0
60	B8	1	0	0	0	0
60	C5	1	0	0	0	0
60	C8	1	0	0	0	0
60	E5	1	0	0	0	0
60	I8	2	0	0	0	0
60	K8	1	0	0	0	0
60	P8	1	0	0	0	0
61	32	1	0	0	0	0
61	3E	1	0	0	0	0
61	5A	1	0	0	0	0
61	5I	1	0	0	0	0
61	C5	1	0	0	0	0
61	G8	1	0	0	0	0
62	11	10	0	0	0	0
62	13	125	0	0	36	0
62	14	446	0	0	126	0
62	16	15	0	0	3	0
62	19	8	0	0	1	0
62	1G	74	0	0	23	0
62	1H	738	0	0	226	0
62	1J	12	0	0	5	0
62	1K	4	0	0	0	0
62	21	4	0	0	2	0
62	25	6	0	0	1	0
62	31	5	0	0	0	0
62	39	1	0	0	0	0
62	3E	4	0	0	0	0
62	3I	1	0	0	0	0
62	3K	1	0	0	0	0
62	4K	1	0	0	0	0
62	4L	1	0	0	0	0
62	5I	2	0	0	0	0
62	78	3	0	0	0	0
62	7I	1	0	0	0	0
62	82	1	0	0	0	0
62	85	2	0	0	1	0
62	98	3	0	0	1	0
62	A5	1	0	0	0	0
62	B8	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	BA	2	0	0	1	0
62	C8	2	0	0	0	0
62	D8	2	0	0	0	0
62	E5	1	0	0	0	0
62	G8	2	0	0	0	0
62	L5	1	0	0	0	0
62	L8	3	0	0	0	0
62	M5	2	0	0	0	0
62	Q8	1	0	0	0	0
All	All	299951	0	200664	8116	2

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

The worst 5 of 8116 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)
22:1L:35:QUO:C4	22:1L:35:QUO:N3	1.71	1.53
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.69	1.53
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.71	1.52
22:3L:35:QUO:N3	22:3L:35:QUO:C4	1.72	1.49
25:1H:973:A:OP2	62:1H:3767:HOH:O	1.69	1.10

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD2	4:32:27:TYR:OH[4_555]	2.10	0.10
32:61:91:SER:OG	55:1G:368:U:OP1[4_555]	2.18	0.02

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	235/256 (92%)	207 (88%)	25 (11%)	3 (1%)	14	48
2	1E	235/256 (92%)	202 (86%)	32 (14%)	1 (0%)	38	75
3	22	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
3	2E	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
4	32	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
4	3E	206/208 (99%)	193 (94%)	13 (6%)	0	100	100
5	42	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	4E	149/162 (92%)	145 (97%)	3 (2%)	1 (1%)	25	64
6	52	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
7	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	72	136/138 (99%)	127 (93%)	8 (6%)	1 (1%)	25	64
8	7E	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	82	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	8E	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	22	62
10	1A	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
10	1I	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
11	2A	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
11	2I	117/129 (91%)	102 (87%)	13 (11%)	2 (2%)	11	42
12	3A	123/132 (93%)	105 (85%)	14 (11%)	4 (3%)	4	25
12	3I	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
13	4A	115/126 (91%)	98 (85%)	16 (14%)	1 (1%)	20	60
13	4I	114/126 (90%)	97 (85%)	17 (15%)	0	100	100
14	5A	56/61 (92%)	48 (86%)	8 (14%)	0	100	100
14	5I	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	11	42
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	8A	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	13	47
19	AA	80/93 (86%)	65 (81%)	13 (16%)	2 (2%)	6	31
19	AI	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	6	31
20	BA	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	BI	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	1B	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	11	270/272 (99%)	251 (93%)	15 (6%)	4 (2%)	12	45
28	21	203/205 (99%)	172 (85%)	28 (14%)	3 (2%)	12	45
28	29	203/205 (99%)	162 (80%)	33 (16%)	8 (4%)	3	21
29	31	200/202 (99%)	185 (92%)	14 (7%)	1 (0%)	32	71
30	41	179/181 (99%)	159 (89%)	17 (10%)	3 (2%)	11	42
30	49	179/181 (99%)	160 (89%)	16 (9%)	3 (2%)	11	42
31	51	172/180 (96%)	150 (87%)	17 (10%)	5 (3%)	5	28
31	59	169/180 (94%)	138 (82%)	27 (16%)	4 (2%)	7	32
32	61	144/146 (99%)	120 (83%)	20 (14%)	4 (3%)	6	29
32	69	144/146 (99%)	120 (83%)	21 (15%)	3 (2%)	8	36
33	15	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	25	64
33	58	136/138 (99%)	121 (89%)	10 (7%)	5 (4%)	4	22
34	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	35	148/150 (99%)	109 (74%)	31 (21%)	8 (5%)	2	14
35	78	148/150 (99%)	116 (78%)	28 (19%)	4 (3%)	6	30
36	45	139/141 (99%)	115 (83%)	23 (16%)	1 (1%)	25	64
36	88	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	5	28
37	55	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
37	98	116/118 (98%)	105 (90%)	10 (9%)	1 (1%)	20	60
38	65	109/111 (98%)	89 (82%)	19 (17%)	1 (1%)	20	60
38	A8	109/111 (98%)	93 (85%)	15 (14%)	1 (1%)	20	60
39	75	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	8	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	B8	134/137 (98%)	123 (92%)	11 (8%)	0	100	100
40	85	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	20	60
40	C8	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	6	31
41	95	99/101 (98%)	78 (79%)	17 (17%)	4 (4%)	3	20
41	D8	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	9	37
42	A5	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
42	E8	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	20	60
43	B5	90/94 (96%)	83 (92%)	6 (7%)	1 (1%)	17	54
43	F8	92/94 (98%)	86 (94%)	4 (4%)	2 (2%)	8	35
44	C5	102/110 (93%)	76 (74%)	24 (24%)	2 (2%)	9	37
44	G8	102/110 (93%)	78 (76%)	18 (18%)	6 (6%)	2	12
45	H8	173/175 (99%)	146 (84%)	18 (10%)	9 (5%)	2	14
46	E5	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
46	I8	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	14	48
47	F5	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	8	36
47	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	8	36
48	G5	64/66 (97%)	60 (94%)	2 (3%)	2 (3%)	5	26
48	K8	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
49	H5	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
49	L8	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
50	I5	61/66 (92%)	36 (59%)	23 (38%)	2 (3%)	4	25
50	M8	64/66 (97%)	43 (67%)	19 (30%)	2 (3%)	5	26
51	J5	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	10	40
51	N8	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
52	K5	43/45 (96%)	27 (63%)	16 (37%)	0	100	100
52	O8	43/45 (96%)	32 (74%)	11 (26%)	0	100	100
53	L5	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
54	Q8	60/65 (92%)	39 (65%)	11 (18%)	10 (17%)	0	0
56	19	271/276 (98%)	258 (95%)	9 (3%)	4 (2%)	12	45
57	39	206/210 (98%)	175 (85%)	26 (13%)	5 (2%)	7	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	D5	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	3	17
59	M5	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	14
All	All	11344/11923 (95%)	10035 (88%)	1149 (10%)	160 (1%)	13	47

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	25	VAL
18	9I	22	VAL
36	88	80	GLU
44	G8	53	PRO
44	G8	81	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	181 (88%)	24 (12%)	6	26
2	1E	205/220 (93%)	176 (86%)	29 (14%)	4	18
3	22	160/188 (85%)	140 (88%)	20 (12%)	5	22
3	2E	159/188 (85%)	140 (88%)	19 (12%)	6	25
4	32	180/180 (100%)	153 (85%)	27 (15%)	3	15
4	3E	180/180 (100%)	148 (82%)	32 (18%)	2	9
5	42	116/123 (94%)	94 (81%)	22 (19%)	2	7
5	4E	116/123 (94%)	98 (84%)	18 (16%)	3	14
6	52	90/90 (100%)	79 (88%)	11 (12%)	6	23
6	5E	90/90 (100%)	81 (90%)	9 (10%)	9	33
7	62	126/127 (99%)	105 (83%)	21 (17%)	2	11
7	6E	126/127 (99%)	107 (85%)	19 (15%)	3	15
8	72	119/119 (100%)	106 (89%)	13 (11%)	7	30
8	7E	119/119 (100%)	96 (81%)	23 (19%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	82	98/99 (99%)	85 (87%)	13 (13%)	4	20
9	8E	98/99 (99%)	77 (79%)	21 (21%)	1	5
10	1A	89/92 (97%)	81 (91%)	8 (9%)	11	40
10	1I	89/92 (97%)	78 (88%)	11 (12%)	5	23
11	2A	90/99 (91%)	82 (91%)	8 (9%)	11	41
11	2I	90/99 (91%)	81 (90%)	9 (10%)	9	33
12	3A	104/109 (95%)	91 (88%)	13 (12%)	5	22
12	3I	104/109 (95%)	92 (88%)	12 (12%)	6	27
13	4A	94/101 (93%)	77 (82%)	17 (18%)	2	9
13	4I	94/101 (93%)	76 (81%)	18 (19%)	2	7
14	5A	48/50 (96%)	43 (90%)	5 (10%)	8	31
14	5I	50/50 (100%)	39 (78%)	11 (22%)	1	5
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9	33
15	6I	79/80 (99%)	67 (85%)	12 (15%)	3	14
16	7A	72/74 (97%)	63 (88%)	9 (12%)	5	22
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	95/97 (98%)	88 (93%)	7 (7%)	16	49
17	8I	95/97 (98%)	79 (83%)	16 (17%)	2	11
18	9A	63/77 (82%)	49 (78%)	14 (22%)	1	4
18	9I	63/77 (82%)	55 (87%)	8 (13%)	5	21
19	AA	66/80 (82%)	55 (83%)	11 (17%)	2	11
19	AI	72/80 (90%)	58 (81%)	14 (19%)	1	7
20	BA	76/82 (93%)	57 (75%)	19 (25%)	1	2
20	BI	76/82 (93%)	67 (88%)	9 (12%)	6	25
21	1B	20/22 (91%)	19 (95%)	1 (5%)	28	65
21	1F	20/22 (91%)	17 (85%)	3 (15%)	3	15
27	11	214/214 (100%)	174 (81%)	40 (19%)	2	8
28	21	165/165 (100%)	131 (79%)	34 (21%)	1	6
28	29	165/165 (100%)	131 (79%)	34 (21%)	1	6
29	31	161/161 (100%)	133 (83%)	28 (17%)	2	10
30	41	155/155 (100%)	133 (86%)	22 (14%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	49	155/155 (100%)	132 (85%)	23 (15%)	3	15
31	51	145/148 (98%)	112 (77%)	33 (23%)	1	4
31	59	143/148 (97%)	128 (90%)	15 (10%)	8	31
32	61	122/122 (100%)	97 (80%)	25 (20%)	1	6
32	69	122/122 (100%)	102 (84%)	20 (16%)	2	12
33	15	117/117 (100%)	96 (82%)	21 (18%)	2	9
33	58	117/117 (100%)	92 (79%)	25 (21%)	1	5
34	25	100/100 (100%)	83 (83%)	17 (17%)	2	11
34	68	100/100 (100%)	87 (87%)	13 (13%)	5	21
35	35	116/116 (100%)	82 (71%)	34 (29%)	0	1
35	78	116/116 (100%)	84 (72%)	32 (28%)	0	1
36	45	111/111 (100%)	92 (83%)	19 (17%)	2	11
36	88	111/111 (100%)	90 (81%)	21 (19%)	2	7
37	55	100/101 (99%)	79 (79%)	21 (21%)	1	5
37	98	101/101 (100%)	81 (80%)	20 (20%)	1	6
38	65	87/87 (100%)	69 (79%)	18 (21%)	1	6
38	A8	87/87 (100%)	66 (76%)	21 (24%)	1	3
39	75	120/120 (100%)	95 (79%)	25 (21%)	1	6
39	B8	119/120 (99%)	91 (76%)	28 (24%)	1	3
40	85	93/93 (100%)	78 (84%)	15 (16%)	3	12
40	C8	93/93 (100%)	78 (84%)	15 (16%)	3	12
41	95	82/82 (100%)	63 (77%)	19 (23%)	1	4
41	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1
42	A5	92/92 (100%)	70 (76%)	22 (24%)	1	3
42	E8	92/92 (100%)	74 (80%)	18 (20%)	1	7
43	B5	74/76 (97%)	56 (76%)	18 (24%)	1	3
43	F8	76/76 (100%)	62 (82%)	14 (18%)	2	9
44	C5	85/91 (93%)	64 (75%)	21 (25%)	1	2
44	G8	85/91 (93%)	69 (81%)	16 (19%)	2	8
45	H8	154/154 (100%)	129 (84%)	25 (16%)	3	12
46	E5	62/67 (92%)	54 (87%)	8 (13%)	5	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	I8	62/67 (92%)	54 (87%)	8 (13%)	5	21
47	F5	82/83 (99%)	68 (83%)	14 (17%)	2	11
47	J8	82/83 (99%)	67 (82%)	15 (18%)	2	9
48	G5	62/62 (100%)	46 (74%)	16 (26%)	0	2
48	K8	62/62 (100%)	44 (71%)	18 (29%)	0	1
49	H5	51/51 (100%)	41 (80%)	10 (20%)	1	7
49	L8	51/51 (100%)	41 (80%)	10 (20%)	1	7
50	I5	57/59 (97%)	47 (82%)	10 (18%)	2	10
50	M8	59/59 (100%)	50 (85%)	9 (15%)	3	14
51	J5	51/51 (100%)	42 (82%)	9 (18%)	2	10
51	N8	51/51 (100%)	41 (80%)	10 (20%)	1	7
52	K5	44/44 (100%)	38 (86%)	6 (14%)	4	19
52	O8	44/44 (100%)	32 (73%)	12 (27%)	0	1
53	L5	38/42 (90%)	31 (82%)	7 (18%)	2	9
53	P8	38/42 (90%)	31 (82%)	7 (18%)	2	9
54	Q8	41/55 (74%)	26 (63%)	15 (37%)	0	0
56	19	214/218 (98%)	165 (77%)	49 (23%)	1	4
57	39	165/166 (99%)	132 (80%)	33 (20%)	1	6
58	D5	158/179 (88%)	132 (84%)	26 (16%)	2	12
59	M5	50/51 (98%)	35 (70%)	15 (30%)	0	1
All	All	9568/9886 (97%)	7886 (82%)	1682 (18%)	2	10

5 of 1682 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	H8	154	ASP
5	42	41	VAL
44	C5	87	LYS
47	J8	94	LEU
54	Q8	11	LYS

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

Mol	Chain	Res	Type
43	F8	31	HIS
18	9A	63	GLN
41	95	87	HIS
42	E8	60	ASN
42	A5	60	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	320 (21%)	0
22	1K	82/85 (96%)	30 (36%)	0
22	1L	70/85 (82%)	26 (37%)	0
22	3K	70/85 (82%)	15 (21%)	0
22	3L	71/85 (83%)	16 (22%)	0
23	2K	76/77 (98%)	19 (25%)	0
23	2L	76/77 (98%)	14 (18%)	0
24	4K	14/30 (46%)	6 (42%)	0
24	4L	15/30 (50%)	6 (40%)	0
25	14	2905/2912 (99%)	646 (22%)	0
25	1H	2911/2912 (99%)	636 (21%)	0
26	16	121/122 (99%)	22 (18%)	0
26	1J	121/122 (99%)	35 (28%)	0
55	1G	1495/1522 (98%)	322 (21%)	0
All	All	9523/9666 (98%)	2113 (22%)	0

5 of 2113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	9	G
1	13	13	U
1	13	30	U
1	13	32	A

There are no RNA pucker outliers to report.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	OMG	1K	17	22	18,26,27	5.49	6 (33%)	22,38,41	5.16	7 (31%)
22	QUO	1K	35	24,22	28,35,36	5.45	9 (32%)	33,52,55	4.82	10 (30%)
22	MIA	1K	38	22	23,31,32	1.10	2 (8%)	25,44,47	2.45	7 (28%)
22	PSU	1K	40	22	16,21,22	1.01	2 (12%)	20,30,33	3.59	6 (30%)
22	5MU	1K	63	22	14,22,23	1.71	2 (14%)	16,32,35	1.80	2 (12%)
22	PSU	1K	64	22	16,21,22	1.24	3 (18%)	20,30,33	3.51	6 (30%)
22	4SU	1K	8	22	14,21,22	3.07	2 (14%)	15,30,33	1.29	2 (13%)
22	OMG	1L	17	22	18,26,27	5.60	6 (33%)	22,38,41	5.23	8 (36%)
22	QUO	1L	35	24,22	28,35,36	5.77	11 (39%)	33,52,55	5.10	12 (36%)
22	MIA	1L	38	22	23,31,32	1.15	1 (4%)	25,44,47	2.86	6 (24%)
22	PSU	1L	40	22	16,21,22	1.10	1 (6%)	20,30,33	3.78	6 (30%)
22	5MU	1L	63	22	14,22,23	1.75	2 (14%)	16,32,35	1.68	2 (12%)
22	PSU	1L	64	22	16,21,22	0.99	1 (6%)	20,30,33	3.84	7 (35%)
22	4SU	1L	8	22	14,21,22	3.05	2 (14%)	15,30,33	1.27	2 (13%)
23	H2U	2K	21	23	17,21,22	2.22	4 (23%)	21,30,33	2.89	5 (23%)
23	OMC	2K	33	23	15,22,23	2.14	4 (26%)	19,31,34	0.96	1 (5%)
23	5MU	2K	55	60,23	14,22,23	1.76	3 (21%)	16,32,35	2.00	2 (12%)
23	PSU	2K	56	23	16,21,22	1.22	2 (12%)	20,30,33	3.48	5 (25%)
23	4SU	2K	8	23	14,21,22	3.23	2 (14%)	15,30,33	0.98	1 (6%)
23	H2U	2L	21	23	17,21,22	2.37	5 (29%)	21,30,33	2.99	4 (19%)
23	OMC	2L	33	23	15,22,23	2.11	4 (26%)	19,31,34	0.86	1 (5%)
23	5MU	2L	55	23	14,22,23	1.75	2 (14%)	16,32,35	1.88	2 (12%)
23	PSU	2L	56	23	16,21,22	1.15	2 (12%)	20,30,33	3.67	6 (30%)
23	4SU	2L	8	23	14,21,22	3.17	2 (14%)	15,30,33	0.82	1 (6%)
22	OMG	3K	17	22	18,26,27	5.71	6 (33%)	22,38,41	5.27	7 (31%)
22	QUO	3K	35	22	28,35,36	5.72	9 (32%)	33,52,55	4.80	12 (36%)
22	MIA	3K	38	22	23,31,32	1.34	2 (8%)	25,44,47	1.34	4 (16%)
22	PSU	3K	40	22	16,21,22	1.00	1 (6%)	20,30,33	3.95	7 (35%)
22	5MU	3K	63	22	14,22,23	1.72	2 (14%)	16,32,35	1.69	2 (12%)
22	PSU	3K	64	22	16,21,22	1.22	3 (18%)	20,30,33	3.72	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	4SU	3K	8	22	14,21,22	3.01	2 (14%)	15,30,33	1.25	2 (13%)
22	OMG	3L	17	22	18,26,27	5.75	6 (33%)	22,38,41	5.29	7 (31%)
22	QUO	3L	35	22	28,35,36	5.76	9 (32%)	33,52,55	5.21	14 (42%)
22	MIA	3L	38	22	23,31,32	1.05	2 (8%)	25,44,47	1.36	4 (16%)
22	PSU	3L	40	22	16,21,22	1.21	1 (6%)	20,30,33	4.01	6 (30%)
22	5MU	3L	63	22	14,22,23	1.72	2 (14%)	16,32,35	1.68	2 (12%)
22	PSU	3L	64	22	16,21,22	1.01	1 (6%)	20,30,33	3.47	6 (30%)
22	4SU	3L	8	22	14,21,22	3.19	2 (14%)	15,30,33	1.27	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	1K	17	22	-	0/5/27/28	0/3/3/3
22	QUO	1K	35	24,22	-	0/6/43/44	0/4/4/4
22	MIA	1K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	1K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	1L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	1L	35	24,22	-	0/6/43/44	0/4/4/4
22	MIA	1L	38	22	-	2/11/33/34	0/3/3/3
22	PSU	1L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	1L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	1L	8	22	-	0/3/25/26	0/2/2/2
23	H2U	2K	21	23	-	0/7/38/39	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	5MU	2K	55	60,23	-	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	H2U	2L	21	23	-	0/7/38/39	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
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
22	OMG	3K	17	22	-	0/5/27/28	0/3/3/3
22	QUO	3K	35	22	-	0/6/43/44	0/4/4/4

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3L	17	OMG	C8-N7	-14.02	1.08	1.34
22	3K	17	OMG	C8-N7	-13.94	1.08	1.34
22	1K	17	OMG	C8-N7	-13.81	1.08	1.34
22	1L	17	OMG	C8-N7	-13.66	1.09	1.34
22	1L	35	QUO	C6-N1	-10.37	1.14	1.33

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	17	OMG	C6-C5-C4	-14.26	106.66	120.84
22	3L	35	QUO	C8-N9-C1'	-14.17	113.07	125.49
22	3L	40	PSU	N1-C2-N3	-14.00	118.33	128.40
22	3L	17	OMG	C6-C5-C4	-13.74	107.18	120.84
22	1L	17	OMG	C6-C5-C4	-13.62	107.30	120.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	38	MIA	N3-C2-S10-C11
22	1L	38	MIA	N1-C2-S10-C11

There are no ring outliers.

26 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	17	OMG	2	0
22	1K	35	QUO	4	0
22	1K	38	MIA	3	0
22	1K	63	5MU	1	0
22	1K	64	PSU	1	0
22	1L	17	OMG	1	0
22	1L	35	QUO	2	0
22	1L	38	MIA	1	0
22	1L	64	PSU	1	0
23	2K	21	H2U	6	0
23	2K	33	OMC	1	0
23	2K	55	5MU	2	0
23	2K	8	4SU	2	0
23	2L	21	H2U	1	0
23	2L	33	OMC	2	0
23	2L	55	5MU	2	0
23	2L	8	4SU	2	0
22	3K	17	OMG	3	0
22	3K	35	QUO	3	0
22	3K	64	PSU	1	0
22	3K	8	4SU	1	0
22	3L	17	OMG	1	0
22	3L	35	QUO	2	0
22	3L	38	MIA	1	0
22	3L	63	5MU	2	0
22	3L	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1137 ligands modelled in this entry, 1137 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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
55	1G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1G	1530:G	O3'	1531:A	P	3.01

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1498/1522 (98%)	-0.47	8 (0%) 90 80	52, 95, 191, 430	0
2	12	237/256 (92%)	0.24	12 (5%) 29 13	115, 168, 226, 251	0
2	1E	237/256 (92%)	-0.08	3 (1%) 77 59	104, 142, 195, 252	0
3	22	206/239 (86%)	0.83	28 (13%) 3 1	124, 151, 185, 240	0
3	2E	205/239 (85%)	0.29	10 (4%) 30 14	83, 109, 154, 191	0
4	32	208/208 (100%)	0.70	23 (11%) 6 2	90, 116, 161, 199	0
4	3E	208/208 (100%)	0.44	12 (5%) 24 10	75, 106, 145, 171	0
5	42	151/162 (93%)	0.32	3 (1%) 65 44	98, 124, 157, 188	0
5	4E	151/162 (93%)	0.09	3 (1%) 65 44	73, 98, 129, 175	0
6	52	101/101 (100%)	0.14	1 (0%) 82 67	78, 101, 133, 177	0
6	5E	101/101 (100%)	0.07	1 (0%) 82 67	75, 102, 131, 171	0
7	62	155/156 (99%)	1.02	28 (18%) 1 1	101, 128, 163, 204	0
7	6E	155/156 (99%)	0.28	6 (3%) 40 19	95, 117, 154, 199	0
8	72	138/138 (100%)	0.76	18 (13%) 4 2	93, 127, 152, 171	0
8	7E	138/138 (100%)	0.15	1 (0%) 87 75	81, 106, 133, 157	0
9	82	127/128 (99%)	0.77	14 (11%) 6 2	110, 159, 203, 214	0
9	8E	127/128 (99%)	0.12	6 (4%) 32 14	86, 139, 183, 217	0
10	1A	99/105 (94%)	0.64	10 (10%) 8 2	120, 162, 202, 221	0
10	1I	99/105 (94%)	0.06	3 (3%) 51 27	84, 134, 180, 197	0
11	2A	119/129 (92%)	1.16	15 (12%) 4 2	85, 111, 149, 259	0
11	2I	119/129 (92%)	0.45	10 (8%) 12 4	68, 101, 158, 186	0
12	3A	125/132 (94%)	1.43	35 (28%) 1 0	78, 103, 165, 208	0
12	3I	125/132 (94%)	0.13	5 (4%) 39 19	60, 72, 138, 239	0
13	4A	117/126 (92%)	1.75	43 (36%) 0 0	107, 146, 182, 217	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4I	116/126 (92%)	0.36	7 (6%) 23 9	85, 122, 159, 196	0
14	5A	58/61 (95%)	1.91	27 (46%) 0 0	120, 150, 175, 199	0
14	5I	61/61 (100%)	0.04	0 100 100	83, 100, 131, 187	0
15	6A	88/89 (98%)	0.62	5 (5%) 24 11	78, 110, 141, 162	0
15	6I	88/89 (98%)	-0.23	0 100 100	75, 99, 133, 167	0
16	7A	84/88 (95%)	0.65	3 (3%) 43 21	87, 101, 148, 183	0
16	7I	84/88 (95%)	0.57	8 (9%) 9 3	95, 115, 160, 193	0
17	8A	100/105 (95%)	1.27	24 (24%) 1 0	88, 111, 142, 212	0
17	8I	100/105 (95%)	-0.08	2 (2%) 65 44	85, 108, 137, 174	0
18	9A	72/88 (81%)	0.93	8 (11%) 6 2	90, 117, 165, 216	0
18	9I	72/88 (81%)	0.24	3 (4%) 37 18	81, 106, 165, 192	0
19	AA	82/93 (88%)	2.10	44 (53%) 0 0	120, 163, 207, 254	0
19	AI	83/93 (89%)	0.23	6 (7%) 16 6	91, 122, 184, 229	0
20	BA	99/106 (93%)	0.55	6 (6%) 22 9	85, 110, 159, 210	0
20	BI	99/106 (93%)	0.51	9 (9%) 10 4	101, 123, 179, 208	0
21	1B	25/27 (92%)	1.85	11 (44%) 0 0	109, 131, 161, 194	0
21	1F	25/27 (92%)	0.46	1 (4%) 39 19	88, 106, 144, 196	0
22	1K	78/85 (91%)	-0.06	2 (2%) 56 33	78, 184, 302, 353	0
22	1L	67/85 (78%)	0.85	11 (16%) 2 1	118, 208, 263, 287	0
22	3K	67/85 (78%)	-0.51	0 100 100	64, 176, 247, 292	0
22	3L	68/85 (80%)	-0.27	0 100 100	72, 188, 243, 285	0
23	2K	72/77 (93%)	-0.53	0 100 100	61, 89, 126, 155	0
23	2L	72/77 (93%)	-0.39	0 100 100	72, 104, 146, 163	0
24	4K	15/30 (50%)	-0.33	0 100 100	64, 95, 185, 192	0
24	4L	16/30 (53%)	0.59	1 (6%) 21 8	84, 129, 213, 234	0
25	14	2907/2912 (99%)	-0.22	53 (1%) 69 47	48, 80, 246, 500	0
25	1H	2912/2912 (100%)	-0.13	35 (1%) 79 61	37, 68, 231, 416	0
26	16	122/122 (100%)	-0.33	2 (1%) 72 51	65, 88, 112, 273	0
26	1J	122/122 (100%)	-0.56	0 100 100	79, 111, 139, 235	0
27	11	272/272 (100%)	0.05	2 (0%) 87 75	39, 60, 90, 171	0
28	21	205/205 (100%)	0.52	9 (4%) 35 17	47, 86, 159, 217	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	29	205/205 (100%)	0.21	10 (4%) 30 14	55, 92, 186, 254	0
29	31	202/202 (100%)	-0.13	0 100 100	44, 75, 130, 195	0
30	41	181/181 (100%)	0.51	16 (8%) 11 4	80, 104, 155, 203	0
30	49	181/181 (100%)	1.51	53 (29%) 1 0	99, 133, 183, 213	0
31	51	174/180 (96%)	0.25	6 (3%) 46 23	74, 108, 142, 187	0
31	59	171/180 (95%)	1.28	46 (26%) 1 0	129, 194, 264, 306	0
32	61	146/146 (100%)	0.30	5 (3%) 46 23	71, 128, 164, 189	0
32	69	146/146 (100%)	0.43	9 (6%) 21 8	78, 126, 180, 217	0
33	15	138/138 (100%)	-0.30	0 100 100	73, 104, 157, 174	0
33	58	138/138 (100%)	0.80	12 (8%) 11 4	60, 90, 143, 192	0
34	25	122/122 (100%)	0.34	4 (3%) 47 24	64, 84, 113, 129	0
34	68	122/122 (100%)	0.40	1 (0%) 86 71	54, 72, 94, 105	0
35	35	150/150 (100%)	0.45	14 (9%) 9 3	55, 107, 169, 217	0
35	78	150/150 (100%)	-0.18	3 (2%) 65 44	45, 82, 117, 215	0
36	45	141/141 (100%)	0.35	9 (6%) 20 7	73, 107, 152, 190	0
36	88	141/141 (100%)	0.39	8 (5%) 24 11	55, 79, 127, 152	0
37	55	117/118 (99%)	-0.21	0 100 100	54, 77, 104, 141	0
37	98	118/118 (100%)	0.69	9 (7%) 15 5	55, 79, 105, 134	0
38	65	111/111 (100%)	0.97	17 (15%) 2 1	87, 113, 162, 235	0
38	A8	111/111 (100%)	0.35	5 (4%) 34 16	72, 90, 136, 206	0
39	75	137/137 (100%)	-0.14	2 (1%) 74 54	75, 95, 162, 229	0
39	B8	136/137 (99%)	0.08	1 (0%) 87 75	67, 90, 153, 191	0
40	85	117/117 (100%)	-0.07	1 (0%) 84 69	65, 89, 142, 206	0
40	C8	117/117 (100%)	0.67	14 (11%) 5 2	51, 79, 131, 184	0
41	95	101/101 (100%)	0.51	7 (6%) 18 7	61, 129, 158, 199	0
41	D8	101/101 (100%)	0.96	9 (8%) 10 4	53, 105, 180, 251	0
42	A5	113/113 (100%)	-0.02	1 (0%) 84 69	57, 72, 119, 205	0
42	E8	113/113 (100%)	0.83	6 (5%) 27 12	54, 69, 115, 197	0
43	B5	92/94 (97%)	0.02	1 (1%) 80 65	60, 80, 115, 161	0
43	F8	94/94 (100%)	0.50	3 (3%) 48 25	51, 66, 102, 137	0
44	C5	104/110 (94%)	0.83	15 (14%) 3 1	88, 130, 215, 257	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	G8	104/110 (94%)	0.22	3 (2%) 52 28	67, 98, 165, 204	0
45	H8	175/175 (100%)	1.85	65 (37%) 0 0	83, 136, 224, 250	0
46	E5	77/85 (90%)	0.45	4 (5%) 28 12	61, 85, 112, 202	0
46	I8	77/85 (90%)	0.30	1 (1%) 77 59	52, 69, 99, 223	0
47	F5	97/98 (98%)	0.75	9 (9%) 9 3	55, 80, 162, 236	0
47	J8	97/98 (98%)	0.39	8 (8%) 12 5	46, 69, 184, 208	0
48	G5	66/66 (100%)	0.38	4 (6%) 22 9	77, 102, 150, 231	0
48	K8	66/66 (100%)	0.25	2 (3%) 51 27	58, 77, 117, 208	0
49	H5	59/59 (100%)	0.09	0 100 100	76, 98, 151, 172	0
49	L8	59/59 (100%)	0.50	2 (3%) 46 23	59, 77, 114, 147	0
50	I5	63/66 (95%)	4.55	49 (77%) 0 0	165, 220, 260, 276	0
50	M8	66/66 (100%)	1.75	25 (37%) 0 0	114, 177, 241, 262	0
51	J5	58/59 (98%)	-0.07	2 (3%) 46 23	56, 81, 192, 229	0
51	N8	59/59 (100%)	1.43	9 (15%) 2 1	46, 82, 212, 227	0
52	K5	45/45 (100%)	4.29	37 (82%) 0 0	136, 199, 245, 278	0
52	O8	45/45 (100%)	2.50	25 (55%) 0 0	111, 162, 201, 227	0
53	L5	45/49 (91%)	-0.02	0 100 100	47, 56, 71, 90	0
53	P8	45/49 (91%)	-0.20	0 100 100	38, 46, 61, 76	0
54	Q8	62/65 (95%)	0.20	3 (4%) 31 14	56, 72, 111, 166	0
55	1G	1498/1522 (98%)	-0.28	5 (0%) 93 86	65, 110, 185, 415	0
56	19	273/276 (98%)	0.30	7 (2%) 56 33	47, 71, 97, 127	0
57	39	208/210 (99%)	0.31	9 (4%) 36 17	56, 99, 194, 251	0
58	D5	179/206 (86%)	0.89	31 (17%) 2 1	111, 162, 259, 295	0
59	M5	60/61 (98%)	0.45	4 (6%) 19 7	67, 81, 131, 191	0
All	All	21050/21589 (97%)	0.18	1168 (5%) 26 11	37, 98, 201, 500	0

The worst 5 of 1168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	I5	31	ILE	17.4
51	N8	59	GLU	16.3
12	3I	129	ALA	14.0
28	29	205	ALA	13.7
25	1H	2799	A	13.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	QUO	3L	35	32/33	0.91	0.31	-	124,129,153,158	0
22	5MU	1L	63	21/22	0.89	0.16	-	179,192,198,199	0
22	PSU	3K	40	20/21	0.95	0.12	-	101,110,114,118	0
22	QUO	1L	35	32/33	0.90	0.32	-	107,128,151,155	0
22	PSU	1L	64	20/21	0.87	0.13	-	160,190,212,217	0
22	4SU	1L	8	20/21	0.86	0.28	-	196,199,202,204	0
22	4SU	3K	8	20/21	0.81	0.14	-	175,183,197,200	0
22	PSU	1L	40	20/21	0.91	0.17	-	106,139,158,159	0
22	PSU	1K	64	20/21	0.91	0.17	-	119,139,152,156	0
23	OMC	2L	33	21/22	0.98	0.16	-	90,96,100,103	0
22	5MU	1K	63	21/22	0.91	0.22	-	137,144,151,152	0
22	MIA	3K	38	29/30	0.95	0.14	-	100,113,136,140	0
22	OMG	1L	17	24/25	0.67	0.38	-	214,233,260,267	0
22	OMG	3K	17	24/25	0.88	0.18	-	198,221,226,229	0
23	5MU	2K	55	21/22	0.95	0.14	-	93,103,114,118	0
22	PSU	3L	40	20/21	0.94	0.16	-	112,122,127,128	0
22	QUO	3K	35	32/33	0.94	0.14	-	109,116,133,141	0
23	PSU	2K	56	20/21	0.95	0.09	-	92,99,106,110	0
23	H2U	2K	21	20/21	0.87	0.23	-	133,176,266,270	0
22	5MU	3L	63	21/22	0.88	0.20	-	184,193,204,205	0
22	PSU	3K	64	20/21	0.78	0.17	-	204,248,266,281	0
22	OMG	3L	17	24/25	0.74	0.22	-	197,218,241,244	0
23	H2U	2L	21	20/21	0.81	0.21	-	165,170,178,179	0
22	4SU	3L	8	20/21	0.74	0.13	-	189,200,212,215	0
22	PSU	1K	40	20/21	0.95	0.12	-	81,102,111,111	0
23	OMC	2K	33	21/22	0.97	0.17	-	72,75,81,86	0
23	4SU	2L	8	20/21	0.92	0.12	-	103,112,116,121	0
22	MIA	1K	38	29/30	0.95	0.18	-	64,83,97,102	0
22	5MU	3K	63	21/22	0.85	0.17	-	197,231,241,247	0
22	4SU	1K	8	20/21	0.79	0.16	-	149,171,199,201	0
23	4SU	2K	8	20/21	0.95	0.14	-	87,91,98,101	0
22	MIA	1L	38	29/30	0.93	0.29	-	102,126,149,151	0
23	5MU	2L	55	21/22	0.95	0.12	-	118,122,133,134	0
22	PSU	3L	64	20/21	0.71	0.22	-	190,201,215,215	0
22	MIA	3L	38	29/30	0.93	0.18	-	112,126,138,143	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	OMG	1K	17	24/25	0.86	0.16	-	148,195,234,241	0
22	QUO	1K	35	32/33	0.94	0.18	-	73,84,105,108	0
23	PSU	2L	56	20/21	0.94	0.08	-	107,113,120,121	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(\AA^2)	Q<0.9
60	MG	14	3286	1/1	0.86	0.93	69.03	60,60,60,60	0
60	MG	14	3232	1/1	0.83	0.66	46.70	92,92,92,92	0
60	MG	1H	3030	1/1	0.72	0.58	32.61	70,70,70,70	0
60	MG	1H	3107	1/1	0.94	0.47	29.17	63,63,63,63	0
60	MG	1H	3298	1/1	0.74	0.43	27.02	56,56,56,56	0
60	MG	14	3246	1/1	0.96	0.45	26.55	81,81,81,81	0
60	MG	1H	3012	1/1	0.95	0.52	25.73	49,49,49,49	0
60	MG	14	3094	1/1	0.98	0.40	25.52	58,58,58,58	0
60	MG	14	3066	1/1	0.94	0.43	24.89	47,47,47,47	0
60	MG	1G	1656	1/1	0.69	0.38	23.93	86,86,86,86	0
60	MG	14	3058	1/1	0.97	0.35	23.26	64,64,64,64	0
60	MG	14	3064	1/1	0.64	0.48	22.35	70,70,70,70	0
60	MG	13	1668	1/1	0.54	0.46	22.10	114,114,114,114	0
60	MG	1H	3050	1/1	0.92	0.32	20.80	54,54,54,54	0
60	MG	1H	3016	1/1	0.97	0.32	20.67	42,42,42,42	0
60	MG	14	3284	1/1	0.90	0.43	20.61	75,75,75,75	0
60	MG	14	3258	1/1	0.86	0.32	20.33	65,65,65,65	0
60	MG	14	3100	1/1	0.97	0.46	20.14	49,49,49,49	0
60	MG	14	3097	1/1	0.97	0.39	19.09	54,54,54,54	0
60	MG	1H	3202	1/1	0.95	0.46	18.94	43,43,43,43	0
60	MG	14	3036	1/1	0.96	0.37	18.49	66,66,66,66	0
60	MG	14	3290	1/1	0.96	0.33	18.46	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
60	MG	14	3305	1/1	0.83	0.28	18.38	94,94,94,94	0
60	MG	1H	3147	1/1	0.71	0.42	18.29	76,76,76,76	0
60	MG	13	1648	1/1	0.83	0.48	18.01	76,76,76,76	0
60	MG	14	3086	1/1	0.99	0.45	16.92	48,48,48,48	0
60	MG	1H	3270	1/1	0.88	0.42	16.51	58,58,58,58	0
60	MG	13	1710	1/1	0.65	0.34	16.49	104,104,104,104	0
60	MG	13	1660	1/1	0.94	0.37	16.27	70,70,70,70	0
60	MG	14	3082	1/1	0.95	0.44	15.72	65,65,65,65	0
60	MG	14	3115	1/1	0.97	0.34	15.53	39,39,39,39	0
60	MG	14	3061	1/1	0.93	0.34	15.39	49,49,49,49	0
60	MG	1H	3076	1/1	0.97	0.35	15.23	44,44,44,44	0
60	MG	1H	3010	1/1	0.98	0.38	15.03	50,50,50,50	0
60	MG	14	3010	1/1	0.98	0.38	14.99	54,54,54,54	0
60	MG	1H	3034	1/1	0.96	0.37	14.94	38,38,38,38	0
60	MG	1H	3256	1/1	0.77	0.42	14.75	93,93,93,93	0
60	MG	14	3179	1/1	0.99	0.30	14.73	51,51,51,51	0
60	MG	14	3028	1/1	0.71	0.35	14.58	77,77,77,77	0
60	MG	16	205	1/1	0.91	0.27	14.52	79,79,79,79	0
60	MG	1H	3115	1/1	0.92	0.41	13.94	52,52,52,52	0
60	MG	1H	3002	1/1	0.97	0.33	13.83	51,51,51,51	0
60	MG	1H	3287	1/1	0.93	0.28	13.52	54,54,54,54	0
60	MG	13	1621	1/1	0.98	0.43	13.34	62,62,62,62	0
60	MG	14	3079	1/1	0.97	0.35	13.22	68,68,68,68	0
60	MG	13	1664	1/1	0.93	0.27	13.13	68,68,68,68	0
60	MG	1H	3087	1/1	0.90	0.33	13.06	72,72,72,72	0
60	MG	13	1642	1/1	0.81	0.29	12.95	63,63,63,63	0
60	MG	85	201	1/1	0.83	0.42	12.86	71,71,71,71	0
60	MG	14	3068	1/1	0.98	0.37	12.85	53,53,53,53	0
60	MG	13	1627	1/1	0.97	0.39	12.72	50,50,50,50	0
60	MG	14	3306	1/1	0.89	0.31	12.57	67,67,67,67	0
60	MG	1H	3191	1/1	0.92	0.33	12.52	73,73,73,73	0
60	MG	14	3074	1/1	0.94	0.49	12.51	53,53,53,53	0
60	MG	1G	1631	1/1	0.96	0.32	11.79	83,83,83,83	0
60	MG	1G	1673	1/1	0.82	0.33	11.50	186,186,186,186	0
60	MG	1H	3042	1/1	0.91	0.29	11.47	54,54,54,54	0
60	MG	1H	3060	1/1	0.89	0.32	11.02	64,64,64,64	0
60	MG	1H	3142	1/1	0.94	0.26	11.01	57,57,57,57	0
60	MG	1H	3083	1/1	0.97	0.37	11.01	44,44,44,44	0
60	MG	1H	3014	1/1	0.97	0.33	10.95	52,52,52,52	0
60	MG	1H	3024	1/1	0.97	0.26	10.60	51,51,51,51	0
60	MG	1G	1632	1/1	0.88	0.41	10.60	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3075	1/1	0.99	0.28	10.33	41,41,41,41	0
60	MG	1H	3184	1/1	0.84	0.25	10.25	58,58,58,58	0
60	MG	14	3090	1/1	0.89	0.38	9.98	63,63,63,63	0
60	MG	14	3127	1/1	0.97	0.30	9.94	71,71,71,71	0
60	MG	1H	3164	1/1	0.85	0.25	9.89	60,60,60,60	0
60	MG	14	3192	1/1	0.72	0.20	9.68	80,80,80,80	0
60	MG	14	3161	1/1	0.95	0.31	9.44	69,69,69,69	0
60	MG	14	3054	1/1	0.97	0.45	9.43	64,64,64,64	0
60	MG	14	3156	1/1	0.91	0.26	9.22	54,54,54,54	0
60	MG	14	3214	1/1	0.98	0.34	9.08	84,84,84,84	0
60	MG	14	3270	1/1	0.94	0.31	8.80	57,57,57,57	0
60	MG	14	3294	1/1	0.59	0.42	8.75	91,91,91,91	0
60	MG	14	3225	1/1	0.96	0.24	8.68	53,53,53,53	0
60	MG	14	3012	1/1	0.98	0.32	8.67	59,59,59,59	0
60	MG	14	3235	1/1	0.97	0.31	8.61	78,78,78,78	0
60	MG	14	3151	1/1	0.89	0.23	8.51	55,55,55,55	0
60	MG	1H	3051	1/1	0.96	0.36	8.40	61,61,61,61	0
60	MG	1H	3175	1/1	0.97	0.32	8.23	81,81,81,81	0
60	MG	13	1672	1/1	0.98	0.28	8.21	63,63,63,63	0
60	MG	13	1650	1/1	0.89	0.28	8.14	77,77,77,77	0
60	MG	14	3004	1/1	0.99	0.25	8.09	53,53,53,53	0
60	MG	14	3035	1/1	0.99	0.33	8.08	57,57,57,57	0
60	MG	14	3083	1/1	0.96	0.30	8.03	56,56,56,56	0
60	MG	14	3206	1/1	0.92	0.26	8.00	63,63,63,63	0
60	MG	1H	3268	1/1	0.96	0.47	7.99	58,58,58,58	0
60	MG	13	1651	1/1	0.97	0.30	7.98	54,54,54,54	0
60	MG	14	3177	1/1	0.86	0.28	7.88	61,61,61,61	0
60	MG	1H	3066	1/1	0.98	0.34	7.68	36,36,36,36	0
60	MG	1H	3048	1/1	0.87	0.26	7.67	51,51,51,51	0
60	MG	14	3245	1/1	0.67	0.27	7.33	82,82,82,82	0
60	MG	13	1605	1/1	0.96	0.22	7.29	71,71,71,71	0
60	MG	14	3153	1/1	0.71	0.35	7.08	61,61,61,61	0
60	MG	14	3157	1/1	0.96	0.34	7.03	69,69,69,69	0
60	MG	14	3102	1/1	0.95	0.30	6.95	46,46,46,46	0
60	MG	1H	3229	1/1	0.91	0.27	6.93	56,56,56,56	0
60	MG	1G	1601	1/1	0.96	0.35	6.81	59,59,59,59	0
60	MG	1H	3297	1/1	0.89	0.48	6.74	63,63,63,63	0
60	MG	14	3237	1/1	0.74	0.21	6.68	66,66,66,66	0
60	MG	14	3288	1/1	0.72	0.26	6.67	61,61,61,61	0
60	MG	14	3147	1/1	0.73	0.32	6.50	99,99,99,99	0
60	MG	1H	3265	1/1	0.92	0.25	6.37	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1G	1667	1/1	0.95	0.31	6.35	66,66,66,66	0
60	MG	1G	1625	1/1	0.86	0.27	6.24	72,72,72,72	0
60	MG	14	3112	1/1	0.96	0.38	6.06	72,72,72,72	0
60	MG	14	3134	1/1	0.95	0.20	5.79	84,84,84,84	0
60	MG	1H	3020	1/1	0.89	0.26	5.74	59,59,59,59	0
60	MG	1G	1678	1/1	0.94	0.24	5.55	79,79,79,79	0
60	MG	1H	3187	1/1	0.91	0.26	5.47	60,60,60,60	0
60	MG	1H	3069	1/1	0.96	0.30	5.44	60,60,60,60	0
60	MG	14	3203	1/1	0.95	0.32	5.36	66,66,66,66	0
60	MG	1H	3207	1/1	0.75	0.24	5.31	63,63,63,63	0
60	MG	1H	3033	1/1	0.99	0.31	5.30	61,61,61,61	0
60	MG	14	3281	1/1	0.83	0.22	5.29	63,63,63,63	0
60	MG	1G	1674	1/1	0.91	0.24	5.23	84,84,84,84	0
60	MG	13	1617	1/1	0.84	0.17	5.08	99,99,99,99	0
60	MG	14	3223	1/1	0.81	0.30	5.07	67,67,67,67	0
60	MG	16	201	1/1	0.80	0.20	5.05	78,78,78,78	0
60	MG	14	3095	1/1	0.92	0.21	4.98	66,66,66,66	0
60	MG	1H	3054	1/1	0.95	0.27	4.93	56,56,56,56	0
60	MG	1H	3023	1/1	0.93	0.33	4.81	58,58,58,58	0
60	MG	1H	3259	1/1	0.91	0.18	4.76	59,59,59,59	0
60	MG	14	3137	1/1	0.91	0.36	4.70	69,69,69,69	0
60	MG	14	3118	1/1	0.88	0.23	4.63	60,60,60,60	0
60	MG	14	3208	1/1	0.87	0.24	4.57	66,66,66,66	0
60	MG	1H	3021	1/1	0.85	0.19	4.45	59,59,59,59	0
60	MG	14	3289	1/1	0.98	0.22	4.41	65,65,65,65	0
60	MG	14	3042	1/1	0.94	0.27	4.41	44,44,44,44	0
60	MG	1H	3110	1/1	0.75	0.24	4.32	43,43,43,43	0
60	MG	1G	1688	1/1	0.93	0.34	4.25	105,105,105,105	0
60	MG	14	3023	1/1	0.97	0.26	4.23	74,74,74,74	0
60	MG	14	3279	1/1	0.88	0.15	4.16	76,76,76,76	0
60	MG	1H	3223	1/1	0.85	0.21	4.09	44,44,44,44	0
60	MG	14	3233	1/1	0.93	0.27	4.02	69,69,69,69	0
60	MG	14	3176	1/1	0.97	0.28	4.01	67,67,67,67	0
60	MG	14	3098	1/1	0.93	0.47	3.98	59,59,59,59	0
60	MG	1H	3099	1/1	0.84	0.20	3.98	49,49,49,49	0
60	MG	14	3130	1/1	0.96	0.25	3.73	53,53,53,53	0
60	MG	14	3119	1/1	0.98	0.22	3.71	65,65,65,65	0
60	MG	1H	3294	1/1	0.82	0.22	3.68	66,66,66,66	0
60	MG	14	3011	1/1	0.97	0.21	3.63	58,58,58,58	0
60	MG	1H	3067	1/1	0.97	0.26	3.54	46,46,46,46	0
60	MG	29	302	1/1	0.85	0.23	3.53	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3199	1/1	0.93	0.27	3.51	74,74,74,74	0
60	MG	1H	3157	1/1	0.94	0.22	3.42	58,58,58,58	0
60	MG	14	3139	1/1	0.97	0.23	3.39	53,53,53,53	0
60	MG	14	3034	1/1	0.98	0.28	3.24	62,62,62,62	0
60	MG	13	1604	1/1	0.97	0.29	3.24	74,74,74,74	0
60	MG	1G	1657	1/1	0.75	0.30	3.23	102,102,102,102	0
60	MG	1G	1611	1/1	0.95	0.24	3.23	103,103,103,103	0
60	MG	1H	3239	1/1	0.63	0.25	3.17	48,48,48,48	0
61	ZN	32	301	1/1	0.98	0.35	3.13	108,108,108,108	0
60	MG	1G	1684	1/1	0.87	0.23	3.10	91,91,91,91	0
60	MG	2L	101	1/1	0.97	0.25	3.08	72,72,72,72	0
60	MG	14	3386	1/1	0.97	0.33	3.07	57,57,57,57	0
60	MG	1H	3242	1/1	0.86	0.21	3.06	74,74,74,74	0
60	MG	14	3052	1/1	0.97	0.31	3.00	55,55,55,55	0
60	MG	16	204	1/1	0.71	0.18	2.98	83,83,83,83	0
60	MG	1H	3122	1/1	0.88	0.20	2.92	56,56,56,56	0
60	MG	1H	3246	1/1	0.68	0.20	2.89	73,73,73,73	0
60	MG	1H	3096	1/1	0.95	0.32	2.89	53,53,53,53	0
60	MG	1G	1614	1/1	0.97	0.19	2.88	109,109,109,109	0
60	MG	14	3092	1/1	0.91	0.27	2.86	62,62,62,62	0
60	MG	1H	3169	1/1	0.88	0.21	2.84	63,63,63,63	0
60	MG	1H	3173	1/1	0.90	0.18	2.82	72,72,72,72	0
60	MG	13	1608	1/1	0.96	0.20	2.82	70,70,70,70	0
60	MG	1H	3058	1/1	0.90	0.20	2.80	57,57,57,57	0
60	MG	14	3229	1/1	0.95	0.24	2.80	84,84,84,84	0
60	MG	1G	1644	1/1	0.98	0.24	2.79	85,85,85,85	0
60	MG	14	3299	1/1	0.83	0.18	2.68	60,60,60,60	0
60	MG	14	3163	1/1	0.45	0.21	2.65	80,80,80,80	0
60	MG	13	1692	1/1	0.72	0.25	2.58	78,78,78,78	0
60	MG	1H	3221	1/1	0.96	0.37	2.46	58,58,58,58	0
60	MG	14	3219	1/1	0.97	0.20	2.45	48,48,48,48	0
60	MG	14	3238	1/1	0.95	0.20	2.37	56,56,56,56	0
60	MG	1H	3062	1/1	0.99	0.21	2.36	39,39,39,39	0
60	MG	14	3221	1/1	0.96	0.27	2.31	56,56,56,56	0
60	MG	14	3088	1/1	0.95	0.29	2.29	64,64,64,64	0
60	MG	14	3231	1/1	0.98	0.26	2.19	79,79,79,79	0
60	MG	1H	3037	1/1	0.97	0.24	2.17	53,53,53,53	0
60	MG	1H	3127	1/1	0.85	0.18	2.16	44,44,44,44	0
60	MG	1H	3044	1/1	0.97	0.21	2.16	73,73,73,73	0
60	MG	1H	3132	1/1	0.98	0.34	2.16	73,73,73,73	0
60	MG	1H	3143	1/1	0.89	0.27	2.03	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
60	MG	14	3217	1/1	0.93	0.20	1.87	71,71,71,71	0
60	MG	14	3045	1/1	0.97	0.34	1.84	45,45,45,45	0
60	MG	13	1698	1/1	0.91	0.19	1.84	86,86,86,86	0
60	MG	1G	1602	1/1	0.94	0.23	1.82	69,69,69,69	0
60	MG	14	3273	1/1	0.83	0.21	1.77	65,65,65,65	0
61	ZN	3E	301	1/1	0.97	0.39	1.76	90,90,90,90	0
60	MG	13	1700	1/1	0.88	0.16	1.75	102,102,102,102	0
60	MG	1H	3063	1/1	0.99	0.20	1.68	43,43,43,43	0
60	MG	13	1649	1/1	0.87	0.20	1.67	75,75,75,75	0
60	MG	13	1696	1/1	0.64	0.17	1.54	82,82,82,82	0
60	MG	1H	3337	1/1	0.93	0.15	1.52	66,66,66,66	0
60	MG	1H	3092	1/1	0.99	0.22	1.51	44,44,44,44	0
60	MG	16	203	1/1	0.80	0.24	1.51	77,77,77,77	0
60	MG	2K	104	1/1	0.96	0.28	1.51	54,54,54,54	0
60	MG	13	1713	1/1	0.82	0.25	1.51	96,96,96,96	0
60	MG	1H	3111	1/1	0.90	0.18	1.47	49,49,49,49	0
60	MG	14	3152	1/1	0.69	0.14	1.47	96,96,96,96	0
60	MG	14	3209	1/1	0.84	0.21	1.42	77,77,77,77	0
60	MG	14	3263	1/1	0.88	0.18	1.39	63,63,63,63	0
60	MG	1H	3176	1/1	0.94	0.21	1.39	73,73,73,73	0
60	MG	1H	3053	1/1	0.98	0.23	1.37	51,51,51,51	0
60	MG	13	1679	1/1	0.95	0.18	1.31	70,70,70,70	0
60	MG	1H	3005	1/1	0.98	0.23	1.23	47,47,47,47	0
60	MG	1H	3009	1/1	0.96	0.23	1.22	48,48,48,48	0
60	MG	14	3260	1/1	0.81	0.14	1.21	73,73,73,73	0
60	MG	1H	3282	1/1	0.93	0.17	1.19	56,56,56,56	0
60	MG	1H	3007	1/1	0.96	0.26	1.12	33,33,33,33	0
60	MG	14	3234	1/1	0.94	0.18	1.03	57,57,57,57	0
60	MG	13	1658	1/1	0.84	0.16	0.95	57,57,57,57	0
60	MG	1H	3436	1/1	0.99	0.22	0.93	63,63,63,63	0
60	MG	14	3213	1/1	0.97	0.29	0.90	69,69,69,69	0
60	MG	1H	3149	1/1	0.77	0.18	0.85	56,56,56,56	0
60	MG	14	3172	1/1	0.98	0.20	0.84	57,57,57,57	0
60	MG	1H	3086	1/1	0.86	0.18	0.84	53,53,53,53	0
60	MG	1H	3235	1/1	0.95	0.17	0.74	59,59,59,59	0
60	MG	13	1662	1/1	0.89	0.17	0.71	89,89,89,89	0
60	MG	1H	3095	1/1	0.98	0.21	0.67	49,49,49,49	0
60	MG	3I	201	1/1	0.95	0.16	0.67	59,59,59,59	0
60	MG	1H	3437	1/1	0.98	0.25	0.61	52,52,52,52	0
60	MG	13	1632	1/1	0.95	0.17	0.54	55,55,55,55	0
61	ZN	G8	201	1/1	0.74	0.30	0.50	209,209,209,209	0
60	MG	14	3026	1/1	0.94	0.17	0.48	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	13	1678	1/1	0.78	0.24	0.45	163,163,163,163	0
60	MG	13	1681	1/1	0.79	0.19	0.34	88,88,88,88	0
60	MG	1G	1669	1/1	0.93	0.23	0.30	84,84,84,84	0
60	MG	1H	3088	1/1	0.96	0.25	0.28	66,66,66,66	0
60	MG	1H	3227	1/1	0.93	0.24	0.18	65,65,65,65	0
60	MG	13	1616	1/1	0.92	0.23	0.18	100,100,100,100	0
60	MG	45	201	1/1	0.93	0.20	0.12	81,81,81,81	0
60	MG	14	3030	1/1	0.88	0.13	0.12	71,71,71,71	0
60	MG	13	1674	1/1	0.93	0.23	0.10	184,184,184,184	0
60	MG	14	3049	1/1	0.97	0.17	0.04	53,53,53,53	0
60	MG	1H	3253	1/1	0.81	0.17	0.03	56,56,56,56	0
60	MG	1G	1671	1/1	0.88	0.18	0.01	77,77,77,77	0
60	MG	1H	3081	1/1	0.94	0.21	-0.04	34,34,34,34	0
60	MG	1H	3281	1/1	0.94	0.15	-0.14	69,69,69,69	0
60	MG	14	3169	1/1	0.93	0.18	-0.14	46,46,46,46	0
60	MG	13	1703	1/1	0.78	0.22	-0.14	111,111,111,111	0
60	MG	14	3031	1/1	0.85	0.14	-0.15	75,75,75,75	0
60	MG	13	1646	1/1	0.95	0.13	-0.17	111,111,111,111	0
60	MG	88	201	1/1	0.98	0.30	-0.23	81,81,81,81	0
60	MG	14	3044	1/1	0.97	0.19	-0.30	39,39,39,39	0
60	MG	1H	3192	1/1	0.88	0.16	-0.38	84,84,84,84	0
60	MG	1H	3361	1/1	0.94	0.16	-0.47	78,78,78,78	0
60	MG	1H	3404	1/1	0.99	0.18	-0.53	79,79,79,79	0
60	MG	14	3025	1/1	0.90	0.14	-0.54	81,81,81,81	0
60	MG	1G	1613	1/1	0.82	0.15	-0.57	116,116,116,116	0
60	MG	1G	1642	1/1	0.93	0.16	-0.57	87,87,87,87	0
60	MG	B8	201	1/1	0.95	0.19	-0.61	97,97,97,97	0
60	MG	1H	3025	1/1	0.95	0.18	-0.63	51,51,51,51	0
60	MG	1G	1629	1/1	0.93	0.15	-0.65	99,99,99,99	0
60	MG	14	3344	1/1	0.95	0.15	-0.71	54,54,54,54	0
60	MG	13	1680	1/1	0.86	0.16	-0.72	68,68,68,68	0
60	MG	1H	3271	1/1	0.95	0.15	-0.73	62,62,62,62	0
60	MG	16	209	1/1	0.99	0.12	-0.75	81,81,81,81	0
60	MG	14	3361	1/1	0.93	0.16	-0.79	60,60,60,60	0
60	MG	1G	1610	1/1	0.89	0.15	-0.81	78,78,78,78	0
61	ZN	5A	101	1/1	0.92	0.12	-0.91	129,129,129,129	0
60	MG	13	1739	1/1	0.94	0.13	-0.94	68,68,68,68	0
61	ZN	5I	102	1/1	0.99	0.14	-0.98	90,90,90,90	0
60	MG	1H	3379	1/1	0.89	0.18	-0.98	75,75,75,75	0
60	MG	1G	1704	1/1	0.94	0.15	-0.98	91,91,91,91	0
60	MG	1H	3438	1/1	0.91	0.12	-0.98	78,78,78,78	0
60	MG	1H	3390	1/1	0.77	0.14	-0.99	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	11	301	1/1	0.92	0.17	-1.00	42,42,42,42	0
60	MG	5I	101	1/1	0.86	0.13	-1.01	83,83,83,83	0
60	MG	1H	3094	1/1	0.97	0.13	-1.02	35,35,35,35	0
60	MG	13	1677	1/1	0.79	0.12	-1.07	67,67,67,67	0
60	MG	1G	1616	1/1	0.89	0.14	-1.15	125,125,125,125	0
60	MG	14	3256	1/1	0.78	0.14	-1.17	64,64,64,64	0
60	MG	88	202	1/1	0.74	0.17	-1.19	78,78,78,78	0
60	MG	14	3313	1/1	0.94	0.17	-1.19	53,53,53,53	0
60	MG	13	1719	1/1	0.97	0.11	-1.20	74,74,74,74	0
60	MG	14	3293	1/1	0.98	0.11	-1.24	85,85,85,85	0
60	MG	19	301	1/1	0.95	0.15	-1.24	87,87,87,87	0
61	ZN	C5	202	1/1	0.65	0.18	-1.28	197,197,197,197	0
60	MG	1H	3156	1/1	0.89	0.15	-1.28	62,62,62,62	0
60	MG	14	3257	1/1	0.80	0.14	-1.36	69,69,69,69	0
60	MG	1H	3022	1/1	0.94	0.14	-1.37	51,51,51,51	0
60	MG	14	3268	1/1	0.95	0.13	-1.43	74,74,74,74	0
60	MG	13	1630	1/1	0.78	0.15	-1.46	51,51,51,51	0
60	MG	13	1740	1/1	0.93	0.12	-1.50	54,54,54,54	0
60	MG	1J	201	1/1	0.89	0.10	-1.54	105,105,105,105	0
60	MG	1G	1698	1/1	0.91	0.10	-1.56	113,113,113,113	0
60	MG	21	302	1/1	0.94	0.13	-1.57	64,64,64,64	0
60	MG	1G	1628	1/1	0.97	0.12	-1.60	78,78,78,78	0
60	MG	13	1671	1/1	0.93	0.13	-1.61	64,64,64,64	0
60	MG	45	202	1/1	0.95	0.06	-1.63	94,94,94,94	0
60	MG	1H	3266	1/1	0.98	0.15	-1.64	65,65,65,65	0
60	MG	14	3032	1/1	0.94	0.10	-1.68	103,103,103,103	0
60	MG	14	3347	1/1	0.92	0.15	-1.73	83,83,83,83	0
60	MG	1H	3355	1/1	0.91	0.11	-1.76	51,51,51,51	0
60	MG	41	201	1/1	0.83	0.10	-1.77	75,75,75,75	0
60	MG	14	3331	1/1	0.97	0.10	-1.78	51,51,51,51	0
60	MG	1H	3335	1/1	0.86	0.10	-1.89	74,74,74,74	0
60	MG	13	1691	1/1	0.93	0.13	-1.90	96,96,96,96	0
60	MG	14	3227	1/1	0.89	0.13	-1.91	69,69,69,69	0
60	MG	98	202	1/1	0.96	0.11	-1.93	69,69,69,69	0
60	MG	1H	3362	1/1	0.94	0.15	-1.93	47,47,47,47	0
60	MG	4I	201	1/1	0.85	0.07	-1.95	86,86,86,86	0
60	MG	1H	3344	1/1	0.97	0.17	-2.00	47,47,47,47	0
60	MG	1H	3406	1/1	0.95	0.11	-2.09	44,44,44,44	0
60	MG	1H	3261	1/1	0.97	0.14	-2.12	44,44,44,44	0
60	MG	49	201	1/1	0.78	0.12	-2.12	93,93,93,93	0
60	MG	39	301	1/1	0.88	0.13	-2.15	86,86,86,86	0
60	MG	1H	3325	1/1	0.98	0.11	-2.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	1H	3331	1/1	0.93	0.09	-2.18	44,44,44,44	0
60	MG	1G	1691	1/1	0.97	0.11	-2.18	85,85,85,85	0
60	MG	14	3345	1/1	0.99	0.15	-2.25	69,69,69,69	0
60	MG	1H	3118	1/1	0.86	0.13	-2.25	56,56,56,56	0
60	MG	14	3015	1/1	0.91	0.11	-2.25	50,50,50,50	0
60	MG	1H	3084	1/1	0.98	0.14	-2.26	43,43,43,43	0
60	MG	14	3343	1/1	0.98	0.14	-2.35	46,46,46,46	0
60	MG	1J	206	1/1	0.83	0.10	-2.37	125,125,125,125	0
60	MG	1G	1606	1/1	0.97	0.08	-2.38	85,85,85,85	0
60	MG	1G	1620	1/1	0.95	0.14	-2.38	83,83,83,83	0
60	MG	14	3311	1/1	0.95	0.12	-2.39	58,58,58,58	0
60	MG	13	1731	1/1	0.97	0.08	-2.39	63,63,63,63	0
60	MG	16	207	1/1	0.80	0.09	-2.49	62,62,62,62	0
60	MG	13	1639	1/1	0.96	0.12	-2.49	93,93,93,93	0
60	MG	14	3230	1/1	0.94	0.16	-2.52	51,51,51,51	0
60	MG	14	3021	1/1	0.95	0.12	-2.52	68,68,68,68	0
60	MG	1H	3324	1/1	0.95	0.09	-2.52	45,45,45,45	0
60	MG	1H	3314	1/1	0.95	0.14	-2.58	38,38,38,38	0
60	MG	1G	1692	1/1	0.99	0.12	-2.59	67,67,67,67	0
60	MG	1H	3327	1/1	0.99	0.15	-2.62	45,45,45,45	0
60	MG	1H	3315	1/1	0.98	0.12	-2.69	59,59,59,59	0
60	MG	1H	3408	1/1	0.97	0.10	-2.69	50,50,50,50	0
60	MG	1H	3364	1/1	0.92	0.15	-2.70	51,51,51,51	0
60	MG	14	3287	1/1	0.99	0.15	-2.72	57,57,57,57	0
60	MG	14	3350	1/1	0.96	0.09	-2.76	65,65,65,65	0
60	MG	13	1673	1/1	0.79	0.09	-2.77	69,69,69,69	0
60	MG	1H	3377	1/1	0.89	0.12	-2.81	60,60,60,60	0
60	MG	1H	3139	1/1	0.99	0.14	-2.82	39,39,39,39	0
60	MG	13	1720	1/1	0.96	0.06	-2.85	96,96,96,96	0
60	MG	1G	1699	1/1	0.91	0.12	-2.87	108,108,108,108	0
60	MG	1H	3226	1/1	0.98	0.08	-3.04	41,41,41,41	0
60	MG	13	1721	1/1	0.98	0.10	-3.10	80,80,80,80	0
60	MG	1H	3347	1/1	0.99	0.10	-3.17	70,70,70,70	0
60	MG	1G	1679	1/1	0.95	0.11	-3.18	71,71,71,71	0
60	MG	1H	3369	1/1	0.96	0.16	-3.20	46,46,46,46	0
60	MG	1H	3380	1/1	0.98	0.13	-3.23	53,53,53,53	0
60	MG	1H	3308	1/1	0.97	0.11	-3.38	39,39,39,39	0
60	MG	14	3316	1/1	0.99	0.12	-3.43	58,58,58,58	0
60	MG	14	3335	1/1	0.96	0.15	-3.46	60,60,60,60	0
60	MG	1H	3225	1/1	0.97	0.16	-3.47	38,38,38,38	0
60	MG	1H	3257	1/1	0.96	0.08	-3.49	52,52,52,52	0
60	MG	13	1611	1/1	0.98	0.08	-3.55	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
60	MG	14	3325	1/1	0.81	0.10	-3.59	50,50,50,50	0
60	MG	1H	3392	1/1	0.94	0.14	-3.66	53,53,53,53	0
60	MG	13	1718	1/1	0.97	0.13	-3.67	54,54,54,54	0
60	MG	13	1730	1/1	0.93	0.08	-3.72	103,103,103,103	0
60	MG	14	3385	1/1	0.97	0.07	-3.76	44,44,44,44	0
60	MG	13	1717	1/1	0.95	0.10	-3.78	63,63,63,63	0
60	MG	14	3377	1/1	0.93	0.09	-3.81	71,71,71,71	0
60	MG	13	1643	1/1	0.93	0.06	-3.81	75,75,75,75	0
60	MG	1H	3329	1/1	0.90	0.08	-3.82	51,51,51,51	0
60	MG	14	3368	1/1	0.95	0.07	-3.83	83,83,83,83	0
60	MG	1H	3321	1/1	0.97	0.12	-3.89	57,57,57,57	0
60	MG	14	3339	1/1	0.92	0.13	-3.92	62,62,62,62	0
60	MG	14	3340	1/1	0.97	0.10	-4.00	50,50,50,50	0
60	MG	1G	1695	1/1	0.89	0.10	-4.01	83,83,83,83	0
60	MG	14	3342	1/1	0.98	0.11	-4.06	48,48,48,48	0
60	MG	1G	1626	1/1	0.90	0.10	-4.07	87,87,87,87	0
60	MG	1H	3312	1/1	0.90	0.12	-4.13	45,45,45,45	0
60	MG	1H	3435	1/1	0.98	0.09	-4.23	36,36,36,36	0
60	MG	14	3362	1/1	0.94	0.08	-4.27	74,74,74,74	0
60	MG	14	3320	1/1	0.95	0.10	-4.31	52,52,52,52	0
60	MG	14	3321	1/1	0.96	0.10	-4.41	78,78,78,78	0
60	MG	14	3332	1/1	0.92	0.14	-4.47	71,71,71,71	0
60	MG	13	1685	1/1	0.98	0.06	-4.47	80,80,80,80	0
60	MG	1H	3341	1/1	0.99	0.06	-4.63	77,77,77,77	0
60	MG	14	3280	1/1	0.80	0.13	-4.68	55,55,55,55	0
60	MG	1G	1693	1/1	0.97	0.09	-4.71	76,76,76,76	0
60	MG	1H	3230	1/1	0.94	0.11	-4.72	39,39,39,39	0
60	MG	14	3103	1/1	0.98	0.13	-4.74	55,55,55,55	0
60	MG	1H	3264	1/1	0.93	0.13	-4.81	66,66,66,66	0
60	MG	13	1727	1/1	0.93	0.07	-4.82	86,86,86,86	0
60	MG	1H	3396	1/1	0.94	0.10	-4.84	56,56,56,56	0
60	MG	1H	3363	1/1	0.96	0.11	-4.88	52,52,52,52	0
60	MG	14	3326	1/1	0.95	0.11	-4.96	54,54,54,54	0
60	MG	14	3329	1/1	0.92	0.12	-5.07	65,65,65,65	0
60	MG	13	1738	1/1	0.86	0.08	-5.19	81,81,81,81	0
60	MG	1H	3422	1/1	0.97	0.04	-5.22	87,87,87,87	0
60	MG	14	3349	1/1	0.97	0.07	-5.26	61,61,61,61	0
60	MG	1H	3353	1/1	0.96	0.12	-5.32	51,51,51,51	0
60	MG	1H	3416	1/1	0.96	0.07	-5.41	55,55,55,55	0
60	MG	1H	3342	1/1	0.94	0.10	-5.46	59,59,59,59	0
60	MG	1H	3343	1/1	0.99	0.11	-5.48	44,44,44,44	0
60	MG	1H	3309	1/1	0.89	0.10	-5.51	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
60	MG	14	3324	1/1	0.94	0.08	-5.52	63,63,63,63	0
60	MG	14	3019	1/1	0.97	0.07	-5.57	44,44,44,44	0
60	MG	1H	3318	1/1	0.93	0.08	-5.60	45,45,45,45	0
60	MG	1H	3332	1/1	0.88	0.10	-5.62	49,49,49,49	0
60	MG	1H	3368	1/1	0.99	0.08	-5.66	46,46,46,46	0
60	MG	1H	3370	1/1	0.97	0.12	-5.66	45,45,45,45	0
60	MG	1H	3372	1/1	0.97	0.10	-5.81	61,61,61,61	0
60	MG	14	3357	1/1	0.86	0.06	-5.86	96,96,96,96	0
60	MG	14	3355	1/1	0.90	0.08	-5.89	68,68,68,68	0
60	MG	1H	3311	1/1	0.95	0.11	-6.06	42,42,42,42	0
60	MG	1G	1621	1/1	0.93	0.09	-6.11	68,68,68,68	0
60	MG	14	3356	1/1	0.77	0.08	-6.20	66,66,66,66	0
60	MG	1H	3429	1/1	0.95	0.11	-6.26	61,61,61,61	0
60	MG	1H	3397	1/1	0.99	0.10	-6.44	50,50,50,50	0
60	MG	1H	3065	1/1	0.96	0.11	-6.58	39,39,39,39	0
60	MG	1H	3399	1/1	0.96	0.11	-6.58	60,60,60,60	0
60	MG	1H	3394	1/1	0.99	0.10	-6.62	43,43,43,43	0
60	MG	14	3315	1/1	0.98	0.10	-6.71	52,52,52,52	0
60	MG	14	3314	1/1	0.96	0.12	-6.71	63,63,63,63	0
60	MG	1H	3405	1/1	0.92	0.06	-6.95	73,73,73,73	0
60	MG	1H	3367	1/1	0.95	0.06	-7.24	56,56,56,56	0
60	MG	1H	3381	1/1	0.96	0.12	-7.33	41,41,41,41	0
60	MG	1H	3401	1/1	0.94	0.11	-7.65	61,61,61,61	0
60	MG	14	3360	1/1	0.94	0.10	-7.99	103,103,103,103	0
60	MG	1H	3105	1/1	0.94	0.09	-8.36	59,59,59,59	0
60	MG	14	3337	1/1	0.97	0.08	-8.62	59,59,59,59	0
60	MG	1H	3349	1/1	0.91	0.09	-8.69	58,58,58,58	0
60	MG	14	3318	1/1	0.86	0.11	-9.80	76,76,76,76	0
60	MG	13	1724	1/1	0.94	0.05	-10.58	82,82,82,82	0
60	MG	14	3367	1/1	0.94	0.08	-11.67	90,90,90,90	0
60	MG	14	3373	1/1	0.98	0.10	-11.98	65,65,65,65	0
60	MG	13	1723	1/1	0.96	0.06	-12.28	85,85,85,85	0
60	MG	1H	3354	1/1	0.99	0.07	-14.01	39,39,39,39	0
60	MG	1H	3319	1/1	0.98	0.11	-16.00	46,46,46,46	0
60	MG	14	3382	1/1	0.95	0.11	-17.25	100,100,100,100	0
60	MG	14	3376	1/1	0.96	0.04	-	91,91,91,91	0
60	MG	1H	3154	1/1	0.77	0.30	-	89,89,89,89	0
60	MG	1H	3102	1/1	0.94	0.32	-	61,61,61,61	0
60	MG	14	3300	1/1	0.90	0.44	-	76,76,76,76	0
60	MG	14	3363	1/1	0.81	0.07	-	73,73,73,73	0
60	MG	14	3144	1/1	0.76	0.45	-	80,80,80,80	0
60	MG	14	3307	1/1	0.84	0.43	-	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
60	MG	13	1683	1/1	0.86	0.32	-	89,89,89,89	0
60	MG	1H	3409	1/1	0.84	0.16	-	99,99,99,99	0
60	MG	1H	3350	1/1	0.93	0.14	-	47,47,47,47	0
60	MG	1H	3004	1/1	0.97	0.35	-	45,45,45,45	0
60	MG	14	3166	1/1	0.92	0.38	-	73,73,73,73	0
60	MG	1H	3357	1/1	0.92	0.10	-	69,69,69,69	0
60	MG	E5	101	1/1	0.58	0.20	-	80,80,80,80	0
60	MG	1H	3190	1/1	0.95	0.42	-	61,61,61,61	0
60	MG	13	1709	1/1	0.49	0.23	-	81,81,81,81	0
60	MG	1G	1694	1/1	0.92	0.09	-	110,110,110,110	0
60	MG	14	3336	1/1	0.94	0.06	-	80,80,80,80	0
60	MG	1H	3241	1/1	0.89	0.31	-	61,61,61,61	0
60	MG	78	203	1/1	0.83	0.39	-	87,87,87,87	0
60	MG	1G	1681	1/1	0.81	0.73	-	107,107,107,107	0
60	MG	1G	1630	1/1	0.93	0.26	-	80,80,80,80	0
60	MG	1H	3293	1/1	0.64	0.39	-	80,80,80,80	0
60	MG	1H	3304	1/1	0.89	0.18	-	69,69,69,69	0
60	MG	13	1689	1/1	0.74	0.15	-	83,83,83,83	0
60	MG	14	3013	1/1	0.96	0.33	-	61,61,61,61	0
60	MG	1H	3236	1/1	0.95	0.19	-	55,55,55,55	0
60	MG	14	3309	1/1	0.80	0.34	-	72,72,72,72	0
60	MG	13	1619	1/1	0.92	0.30	-	70,70,70,70	0
60	MG	14	3080	1/1	0.97	0.27	-	78,78,78,78	0
60	MG	1H	3402	1/1	0.96	0.11	-	109,109,109,109	0
60	MG	14	3071	1/1	0.98	0.48	-	68,68,68,68	0
60	MG	1H	3064	1/1	0.96	0.20	-	51,51,51,51	0
60	MG	1G	1619	1/1	0.91	0.25	-	82,82,82,82	0
60	MG	1H	3136	1/1	0.61	0.26	-	72,72,72,72	0
60	MG	1H	3032	1/1	0.98	0.38	-	41,41,41,41	0
60	MG	1H	3348	1/1	0.94	0.07	-	82,82,82,82	0
60	MG	1H	3204	1/1	0.80	0.30	-	62,62,62,62	0
60	MG	1G	1685	1/1	0.89	0.27	-	136,136,136,136	0
60	MG	13	1705	1/1	0.72	0.20	-	83,83,83,83	0
60	MG	14	3101	1/1	0.89	0.52	-	65,65,65,65	0
60	MG	14	3312	1/1	0.94	0.16	-	57,57,57,57	0
60	MG	14	3029	1/1	0.95	0.20	-	75,75,75,75	0
60	MG	1H	3254	1/1	0.81	0.41	-	57,57,57,57	0
60	MG	1H	3300	1/1	0.95	0.28	-	52,52,52,52	0
60	MG	1H	3431	1/1	0.95	0.07	-	73,73,73,73	0
60	MG	1H	3276	1/1	0.82	0.57	-	76,76,76,76	0
60	MG	14	3039	1/1	0.58	0.23	-	75,75,75,75	0
60	MG	1H	3112	1/1	0.95	0.14	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	13	1704	1/1	0.92	0.20	-	71,71,71,71	0
60	MG	1H	3289	1/1	0.96	0.48	-	71,71,71,71	0
60	MG	1G	1634	1/1	0.95	0.19	-	112,112,112,112	0
60	MG	14	3359	1/1	0.97	0.11	-	69,69,69,69	0
60	MG	1H	3424	1/1	0.83	0.08	-	115,115,115,115	0
60	MG	1H	3046	1/1	0.97	0.17	-	90,90,90,90	0
60	MG	1H	3365	1/1	0.82	0.12	-	88,88,88,88	0
60	MG	14	3274	1/1	0.84	0.33	-	79,79,79,79	0
60	MG	1H	3307	1/1	0.93	0.33	-	74,74,74,74	0
60	MG	1H	3427	1/1	0.77	0.11	-	92,92,92,92	0
60	MG	1G	1660	1/1	0.89	0.36	-	78,78,78,78	0
60	MG	13	1736	1/1	0.54	0.08	-	141,141,141,141	0
60	MG	1H	3378	1/1	0.86	0.13	-	67,67,67,67	0
60	MG	14	3366	1/1	0.92	0.06	-	102,102,102,102	0
60	MG	1G	1624	1/1	0.98	0.38	-	70,70,70,70	0
60	MG	1H	3232	1/1	0.94	0.20	-	71,71,71,71	0
60	MG	1G	1677	1/1	0.97	0.22	-	88,88,88,88	0
60	MG	14	3236	1/1	0.97	0.30	-	66,66,66,66	0
60	MG	14	3009	1/1	0.98	0.23	-	50,50,50,50	0
60	MG	1H	3302	1/1	0.82	0.27	-	67,67,67,67	0
60	MG	1H	3305	1/1	0.91	0.31	-	99,99,99,99	0
60	MG	1H	3278	1/1	0.84	0.30	-	64,64,64,64	0
60	MG	13	1601	1/1	0.97	0.26	-	66,66,66,66	0
60	MG	13	1676	1/1	0.92	0.23	-	63,63,63,63	0
60	MG	1G	1703	1/1	0.43	0.12	-	128,128,128,128	0
60	MG	1H	3205	1/1	0.86	0.37	-	60,60,60,60	0
60	MG	1H	3162	1/1	0.81	0.14	-	67,67,67,67	0
60	MG	14	3087	1/1	0.95	0.30	-	78,78,78,78	0
60	MG	1H	3194	1/1	0.72	0.31	-	71,71,71,71	0
60	MG	1G	1639	1/1	0.75	0.34	-	82,82,82,82	0
60	MG	14	3283	1/1	0.89	0.60	-	79,79,79,79	0
60	MG	14	3148	1/1	0.81	0.32	-	86,86,86,86	0
60	MG	1H	3072	1/1	0.91	0.45	-	70,70,70,70	0
60	MG	14	3024	1/1	0.98	0.33	-	81,81,81,81	0
60	MG	1H	3269	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	1H	3426	1/1	0.87	0.08	-	112,112,112,112	0
60	MG	1H	3326	1/1	0.91	0.16	-	57,57,57,57	0
60	MG	14	3218	1/1	0.94	0.27	-	67,67,67,67	0
60	MG	13	1607	1/1	0.98	0.09	-	75,75,75,75	0
60	MG	14	3250	1/1	0.90	0.33	-	65,65,65,65	0
60	MG	14	3171	1/1	0.92	0.38	-	78,78,78,78	0
60	MG	98	201	1/1	0.98	0.26	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	13	1722	1/1	0.89	0.18	-	82,82,82,82	0
60	MG	14	3164	1/1	0.90	0.44	-	75,75,75,75	0
60	MG	1H	3129	1/1	0.89	0.61	-	72,72,72,72	0
60	MG	1G	1680	1/1	0.83	0.37	-	162,162,162,162	0
60	MG	1H	3277	1/1	0.95	0.20	-	59,59,59,59	0
60	MG	1H	3077	1/1	0.89	0.39	-	70,70,70,70	0
60	MG	14	3059	1/1	0.86	0.38	-	72,72,72,72	0
60	MG	1H	3043	1/1	0.97	0.22	-	70,70,70,70	0
60	MG	1K	101	1/1	0.97	0.04	-	93,93,93,93	0
60	MG	1H	3218	1/1	0.84	0.39	-	84,84,84,84	0
60	MG	1H	3210	1/1	0.97	0.29	-	72,72,72,72	0
60	MG	1H	3090	1/1	0.85	0.30	-	67,67,67,67	0
60	MG	1H	3200	1/1	0.98	0.44	-	69,69,69,69	0
60	MG	1H	3356	1/1	0.90	0.16	-	54,54,54,54	0
60	MG	1H	3070	1/1	0.96	0.47	-	45,45,45,45	0
60	MG	1G	1687	1/1	0.85	0.15	-	83,83,83,83	0
60	MG	1H	3283	1/1	0.95	0.30	-	64,64,64,64	0
60	MG	14	3055	1/1	0.99	0.40	-	60,60,60,60	0
60	MG	1H	3049	1/1	0.93	0.29	-	66,66,66,66	0
60	MG	14	3187	1/1	0.83	0.58	-	84,84,84,84	0
60	MG	16	212	1/1	0.94	0.10	-	71,71,71,71	0
60	MG	1G	1658	1/1	0.91	0.33	-	71,71,71,71	0
60	MG	1G	1627	1/1	0.80	0.31	-	66,66,66,66	0
60	MG	1H	3216	1/1	0.86	0.24	-	73,73,73,73	0
60	MG	14	3073	1/1	0.99	0.43	-	40,40,40,40	0
60	MG	1H	3038	1/1	0.94	0.61	-	59,59,59,59	0
60	MG	1H	3240	1/1	0.91	0.28	-	109,109,109,109	0
60	MG	14	3063	1/1	0.90	0.51	-	70,70,70,70	0
60	MG	14	3338	1/1	0.91	0.16	-	52,52,52,52	0
60	MG	1H	3393	1/1	0.97	0.08	-	68,68,68,68	0
60	MG	1H	3414	1/1	0.96	0.07	-	75,75,75,75	0
60	MG	1H	3359	1/1	0.94	0.09	-	83,83,83,83	0
60	MG	14	3244	1/1	0.84	0.29	-	75,75,75,75	0
60	MG	1H	3267	1/1	0.65	0.26	-	83,83,83,83	0
60	MG	14	3253	1/1	0.59	0.58	-	71,71,71,71	0
60	MG	1H	3415	1/1	0.88	0.10	-	75,75,75,75	0
60	MG	1H	3040	1/1	0.96	0.12	-	58,58,58,58	0
60	MG	13	1635	1/1	0.95	0.34	-	63,63,63,63	0
60	MG	1H	3163	1/1	0.95	0.48	-	64,64,64,64	0
60	MG	14	3351	1/1	0.93	0.14	-	93,93,93,93	0
60	MG	13	1609	1/1	0.85	0.41	-	64,64,64,64	0
60	MG	14	3372	1/1	0.93	0.05	-	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	14	3155	1/1	0.98	0.12	-	63,63,63,63	0
60	MG	13	1641	1/1	0.75	0.24	-	74,74,74,74	0
60	MG	13	1625	1/1	0.94	0.49	-	75,75,75,75	0
60	MG	13	1633	1/1	0.98	0.21	-	46,46,46,46	0
60	MG	1H	3179	1/1	0.94	0.33	-	57,57,57,57	0
60	MG	14	3264	1/1	0.87	0.39	-	91,91,91,91	0
60	MG	14	3183	1/1	0.97	0.24	-	84,84,84,84	0
60	MG	13	1708	1/1	0.86	0.36	-	167,167,167,167	0
60	MG	14	3141	1/1	0.74	0.30	-	85,85,85,85	0
60	MG	14	3210	1/1	0.86	0.44	-	79,79,79,79	0
60	MG	13	1734	1/1	0.96	0.10	-	108,108,108,108	0
60	MG	14	3211	1/1	0.77	0.48	-	108,108,108,108	0
60	MG	14	3303	1/1	0.87	0.59	-	93,93,93,93	0
60	MG	1G	1645	1/1	0.83	0.17	-	78,78,78,78	0
60	MG	1H	3336	1/1	0.97	0.11	-	88,88,88,88	0
60	MG	1H	3243	1/1	0.95	0.22	-	60,60,60,60	0
60	MG	1H	3093	1/1	0.81	0.20	-	64,64,64,64	0
60	MG	14	3008	1/1	0.98	0.45	-	53,53,53,53	0
60	MG	14	3165	1/1	0.82	0.24	-	84,84,84,84	0
60	MG	13	1622	1/1	0.95	0.48	-	86,86,86,86	0
60	MG	14	3259	1/1	0.85	0.20	-	76,76,76,76	0
60	MG	13	1603	1/1	0.93	0.25	-	57,57,57,57	0
60	MG	1H	3151	1/1	0.94	0.43	-	77,77,77,77	0
60	MG	1H	3383	1/1	0.98	0.13	-	64,64,64,64	0
60	MG	1H	3385	1/1	0.97	0.10	-	66,66,66,66	0
60	MG	14	3051	1/1	0.98	0.26	-	61,61,61,61	0
60	MG	1H	3376	1/1	0.97	0.10	-	43,43,43,43	0
60	MG	1H	3417	1/1	0.95	0.08	-	98,98,98,98	0
60	MG	13	1654	1/1	0.91	0.30	-	69,69,69,69	0
60	MG	P8	101	1/1	0.81	0.55	-	70,70,70,70	0
60	MG	14	3358	1/1	0.73	0.27	-	86,86,86,86	0
60	MG	1H	3137	1/1	0.92	0.26	-	72,72,72,72	0
60	MG	1H	3073	1/1	0.98	0.35	-	53,53,53,53	0
60	MG	13	1693	1/1	0.86	0.17	-	89,89,89,89	0
60	MG	14	3174	1/1	0.89	0.45	-	77,77,77,77	0
60	MG	14	3330	1/1	0.94	0.13	-	58,58,58,58	0
60	MG	1H	3109	1/1	0.96	0.31	-	50,50,50,50	0
60	MG	14	3379	1/1	0.89	0.09	-	104,104,104,104	0
60	MG	1H	3172	1/1	0.80	0.18	-	71,71,71,71	0
60	MG	1H	3209	1/1	0.85	0.44	-	81,81,81,81	0
60	MG	14	3380	1/1	0.87	0.09	-	92,92,92,92	0
60	MG	14	3180	1/1	0.88	0.30	-	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
60	MG	13	1712	1/1	0.98	0.13	-	112,112,112,112	0
60	MG	1H	3250	1/1	0.86	0.41	-	68,68,68,68	0
60	MG	1H	3185	1/1	0.82	0.30	-	65,65,65,65	0
60	MG	14	3005	1/1	0.95	0.34	-	46,46,46,46	0
60	MG	14	3091	1/1	0.74	0.40	-	67,67,67,67	0
60	MG	13	1653	1/1	0.51	0.32	-	83,83,83,83	0
60	MG	1H	3145	1/1	0.85	0.33	-	63,63,63,63	0
60	MG	16	202	1/1	0.89	0.51	-	82,82,82,82	0
60	MG	16	206	1/1	0.95	0.32	-	70,70,70,70	0
60	MG	14	3348	1/1	0.93	0.10	-	83,83,83,83	0
60	MG	14	3222	1/1	0.97	0.30	-	43,43,43,43	0
60	MG	1H	3133	1/1	0.94	0.52	-	83,83,83,83	0
60	MG	1G	1617	1/1	0.89	0.08	-	83,83,83,83	0
60	MG	1H	3352	1/1	0.95	0.09	-	46,46,46,46	0
60	MG	1H	3252	1/1	0.81	0.43	-	66,66,66,66	0
60	MG	1G	1659	1/1	0.54	0.26	-	118,118,118,118	0
60	MG	13	1656	1/1	0.63	0.32	-	84,84,84,84	0
60	MG	1H	3101	1/1	0.93	0.45	-	77,77,77,77	0
60	MG	14	3189	1/1	0.78	0.73	-	73,73,73,73	0
60	MG	1H	3303	1/1	0.94	0.66	-	90,90,90,90	0
60	MG	13	1728	1/1	0.76	0.08	-	88,88,88,88	0
60	MG	14	3037	1/1	0.84	0.42	-	79,79,79,79	0
60	MG	1H	3126	1/1	0.94	0.12	-	79,79,79,79	0
60	MG	14	3160	1/1	0.96	0.34	-	56,56,56,56	0
60	MG	13	1690	1/1	0.77	0.32	-	86,86,86,86	0
60	MG	1H	3421	1/1	0.74	0.14	-	138,138,138,138	0
60	MG	14	3128	1/1	0.67	0.31	-	86,86,86,86	0
60	MG	1G	1661	1/1	0.87	0.32	-	69,69,69,69	0
60	MG	13	1624	1/1	0.97	0.41	-	77,77,77,77	0
60	MG	1H	3419	1/1	0.90	0.09	-	99,99,99,99	0
60	MG	14	3191	1/1	0.92	0.33	-	69,69,69,69	0
60	MG	25	201	1/1	0.81	0.04	-	125,125,125,125	0
60	MG	14	3093	1/1	0.73	0.46	-	70,70,70,70	0
60	MG	78	201	1/1	0.92	0.21	-	66,66,66,66	0
60	MG	1H	3388	1/1	0.98	0.10	-	57,57,57,57	0
60	MG	1H	3288	1/1	0.78	0.45	-	92,92,92,92	0
60	MG	1H	3333	1/1	0.97	0.10	-	55,55,55,55	0
60	MG	1H	3374	1/1	0.90	0.11	-	86,86,86,86	0
60	MG	13	1699	1/1	0.47	0.25	-	89,89,89,89	0
60	MG	1H	3384	1/1	0.94	0.08	-	85,85,85,85	0
60	MG	14	3215	1/1	0.82	0.48	-	69,69,69,69	0
60	MG	13	1602	1/1	0.99	0.21	-	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
60	MG	14	3168	1/1	0.96	0.49	-	77,77,77,77	0
60	MG	1H	3340	1/1	0.98	0.14	-	65,65,65,65	0
60	MG	1H	3279	1/1	0.80	0.38	-	71,71,71,71	0
60	MG	1G	1668	1/1	0.83	0.49	-	95,95,95,95	0
60	MG	1H	3338	1/1	0.90	0.06	-	83,83,83,83	0
60	MG	13	1629	1/1	0.89	0.34	-	62,62,62,62	0
60	MG	13	1634	1/1	0.91	0.39	-	67,67,67,67	0
60	MG	14	3072	1/1	0.96	0.34	-	66,66,66,66	0
60	MG	1H	3231	1/1	0.89	0.30	-	91,91,91,91	0
60	MG	1H	3003	1/1	0.91	0.33	-	45,45,45,45	0
60	MG	13	1682	1/1	0.85	0.33	-	85,85,85,85	0
60	MG	1H	3217	1/1	0.95	0.39	-	75,75,75,75	0
60	MG	1H	3222	1/1	0.69	0.44	-	77,77,77,77	0
60	MG	14	3167	1/1	0.71	0.22	-	93,93,93,93	0
60	MG	14	3266	1/1	0.95	0.46	-	81,81,81,81	0
60	MG	1H	3113	1/1	0.91	0.35	-	53,53,53,53	0
60	MG	1H	3296	1/1	0.83	0.17	-	69,69,69,69	0
60	MG	1G	1676	1/1	0.82	0.30	-	90,90,90,90	0
60	MG	14	3200	1/1	0.86	0.80	-	91,91,91,91	0
60	MG	14	3085	1/1	0.90	0.23	-	52,52,52,52	0
60	MG	1G	1663	1/1	0.84	0.14	-	93,93,93,93	0
60	MG	1H	3195	1/1	0.93	0.52	-	75,75,75,75	0
60	MG	14	3135	1/1	0.80	0.36	-	78,78,78,78	0
60	MG	1H	3262	1/1	0.83	0.39	-	80,80,80,80	0
60	MG	14	3184	1/1	0.84	0.57	-	75,75,75,75	0
60	MG	1G	1641	1/1	0.59	0.14	-	130,130,130,130	0
60	MG	1H	3211	1/1	0.93	0.26	-	84,84,84,84	0
60	MG	14	3084	1/1	0.96	0.27	-	60,60,60,60	0
60	MG	13	1638	1/1	0.88	0.35	-	80,80,80,80	0
60	MG	1J	203	1/1	0.78	0.26	-	91,91,91,91	0
60	MG	11	302	1/1	0.87	0.21	-	54,54,54,54	0
60	MG	14	3375	1/1	0.86	0.04	-	90,90,90,90	0
60	MG	1H	3104	1/1	0.97	0.40	-	63,63,63,63	0
60	MG	1G	1654	1/1	0.91	0.27	-	66,66,66,66	0
60	MG	1G	1651	1/1	0.85	0.43	-	87,87,87,87	0
60	MG	13	1675	1/1	0.90	0.29	-	67,67,67,67	0
60	MG	1H	3119	1/1	0.97	0.46	-	67,67,67,67	0
60	MG	13	1714	1/1	0.88	0.22	-	89,89,89,89	0
60	MG	1H	3418	1/1	0.91	0.08	-	81,81,81,81	0
60	MG	14	3327	1/1	0.94	0.15	-	58,58,58,58	0
60	MG	14	3370	1/1	0.89	0.07	-	116,116,116,116	0
60	MG	1H	3238	1/1	0.97	0.35	-	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
60	MG	1H	3423	1/1	0.91	0.08	-	60,60,60,60	0
60	MG	13	1702	1/1	0.83	0.21	-	80,80,80,80	0
60	MG	1H	3295	1/1	0.50	0.32	-	87,87,87,87	0
60	MG	1G	1683	1/1	0.91	0.25	-	109,109,109,109	0
60	MG	1H	3248	1/1	0.89	0.25	-	97,97,97,97	0
60	MG	14	3014	1/1	0.95	0.31	-	79,79,79,79	0
60	MG	1H	3019	1/1	0.97	0.23	-	33,33,33,33	0
60	MG	1H	3100	1/1	0.91	0.58	-	74,74,74,74	0
60	MG	14	3003	1/1	0.94	0.34	-	45,45,45,45	0
60	MG	1H	3159	1/1	0.82	0.35	-	77,77,77,77	0
60	MG	14	3251	1/1	0.98	0.31	-	69,69,69,69	0
60	MG	1H	3258	1/1	0.92	0.43	-	64,64,64,64	0
60	MG	14	3104	1/1	0.81	0.33	-	70,70,70,70	0
60	MG	1H	3103	1/1	0.54	0.36	-	88,88,88,88	0
60	MG	K8	101	1/1	0.96	0.34	-	69,69,69,69	0
60	MG	13	1729	1/1	0.96	0.04	-	76,76,76,76	0
60	MG	1G	1603	1/1	0.96	0.11	-	79,79,79,79	0
60	MG	1H	3186	1/1	0.79	0.32	-	79,79,79,79	0
60	MG	1H	3360	1/1	0.92	0.14	-	99,99,99,99	0
60	MG	14	3188	1/1	0.83	0.23	-	93,93,93,93	0
60	MG	14	3304	1/1	0.91	0.44	-	66,66,66,66	0
60	MG	1H	3150	1/1	0.88	0.29	-	63,63,63,63	0
60	MG	1H	3290	1/1	0.94	0.15	-	76,76,76,76	0
60	MG	1G	1648	1/1	0.89	0.29	-	78,78,78,78	0
60	MG	14	3076	1/1	0.96	0.34	-	44,44,44,44	0
60	MG	14	3323	1/1	0.98	0.09	-	57,57,57,57	0
60	MG	1H	3011	1/1	0.99	0.20	-	37,37,37,37	0
60	MG	1H	3214	1/1	0.85	0.26	-	62,62,62,62	0
60	MG	14	3109	1/1	0.90	0.51	-	82,82,82,82	0
60	MG	14	3150	1/1	0.85	0.23	-	92,92,92,92	0
60	MG	1J	204	1/1	0.93	0.33	-	92,92,92,92	0
60	MG	1G	1653	1/1	0.74	0.25	-	73,73,73,73	0
60	MG	1H	3301	1/1	0.95	0.29	-	70,70,70,70	0
60	MG	1H	3196	1/1	0.81	0.70	-	91,91,91,91	0
60	MG	14	3220	1/1	0.94	0.12	-	44,44,44,44	0
60	MG	1H	3346	1/1	0.98	0.05	-	67,67,67,67	0
60	MG	14	3048	1/1	0.88	0.27	-	59,59,59,59	0
60	MG	14	3297	1/1	0.84	0.41	-	100,100,100,100	0
60	MG	1H	3171	1/1	0.92	0.49	-	69,69,69,69	0
60	MG	13	1640	1/1	0.88	0.32	-	76,76,76,76	0
60	MG	1H	3387	1/1	0.95	0.11	-	53,53,53,53	0
60	MG	1G	1664	1/1	0.94	0.20	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	14	3114	1/1	0.92	0.68	-	91,91,91,91	0
60	MG	C8	201	1/1	0.96	0.23	-	89,89,89,89	0
60	MG	14	3075	1/1	0.94	0.40	-	49,49,49,49	0
60	MG	45	203	1/1	0.88	0.17	-	66,66,66,66	0
60	MG	1H	3310	1/1	0.94	0.15	-	50,50,50,50	0
60	MG	1G	1607	1/1	0.97	0.20	-	98,98,98,98	0
60	MG	1G	1615	1/1	0.94	0.30	-	87,87,87,87	0
60	MG	1H	3373	1/1	0.98	0.09	-	70,70,70,70	0
60	MG	13	1687	1/1	0.97	0.12	-	73,73,73,73	0
60	MG	1G	1633	1/1	0.87	0.41	-	95,95,95,95	0
60	MG	1H	3108	1/1	0.64	0.49	-	77,77,77,77	0
60	MG	14	3271	1/1	0.99	0.15	-	67,67,67,67	0
60	MG	1G	1604	1/1	0.91	0.17	-	78,78,78,78	0
60	MG	1G	1605	1/1	0.94	0.21	-	81,81,81,81	0
60	MG	14	3106	1/1	0.90	0.47	-	62,62,62,62	0
60	MG	1G	1689	1/1	0.83	0.38	-	86,86,86,86	0
60	MG	1H	3018	1/1	0.97	0.28	-	53,53,53,53	0
60	MG	1H	3140	1/1	0.87	0.28	-	59,59,59,59	0
60	MG	14	3277	1/1	0.76	0.14	-	81,81,81,81	0
60	MG	52	201	1/1	0.89	0.12	-	77,77,77,77	0
60	MG	14	3158	1/1	0.90	0.19	-	54,54,54,54	0
60	MG	1G	1636	1/1	0.98	0.24	-	89,89,89,89	0
60	MG	14	3269	1/1	0.83	0.23	-	60,60,60,60	0
60	MG	2K	101	1/1	0.86	0.15	-	81,81,81,81	0
60	MG	14	3053	1/1	0.92	0.61	-	66,66,66,66	0
60	MG	1G	1701	1/1	0.76	0.08	-	106,106,106,106	0
60	MG	1H	3183	1/1	0.96	0.30	-	61,61,61,61	0
60	MG	14	3275	1/1	0.89	0.53	-	76,76,76,76	0
60	MG	14	3067	1/1	0.96	0.51	-	48,48,48,48	0
60	MG	14	3132	1/1	0.94	0.37	-	84,84,84,84	0
60	MG	1G	1637	1/1	0.97	0.22	-	67,67,67,67	0
60	MG	14	3081	1/1	0.78	0.40	-	86,86,86,86	0
60	MG	14	3122	1/1	0.95	0.39	-	66,66,66,66	0
60	MG	14	3131	1/1	0.95	0.39	-	39,39,39,39	0
60	MG	14	3296	1/1	0.98	0.23	-	135,135,135,135	0
60	MG	14	3204	1/1	0.92	0.29	-	105,105,105,105	0
60	MG	1H	3339	1/1	0.89	0.15	-	75,75,75,75	0
60	MG	14	3105	1/1	0.82	0.23	-	82,82,82,82	0
60	MG	1H	3158	1/1	0.96	0.49	-	65,65,65,65	0
60	MG	1H	3079	1/1	0.97	0.37	-	39,39,39,39	0
60	MG	13	1707	1/1	0.85	0.46	-	114,114,114,114	0
60	MG	1H	3161	1/1	0.97	0.23	-	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
60	MG	14	3124	1/1	0.92	0.32	-	82,82,82,82	0
60	MG	1H	3116	1/1	0.63	0.20	-	69,69,69,69	0
60	MG	1H	3323	1/1	0.97	0.10	-	58,58,58,58	0
60	MG	2L	102	1/1	0.38	0.36	-	95,95,95,95	0
60	MG	1H	3028	1/1	0.88	0.32	-	51,51,51,51	0
60	MG	14	3267	1/1	0.98	0.26	-	71,71,71,71	0
60	MG	13	1670	1/1	0.97	0.07	-	66,66,66,66	0
60	MG	14	3060	1/1	0.96	0.29	-	63,63,63,63	0
60	MG	14	3352	1/1	0.98	0.12	-	77,77,77,77	0
60	MG	1H	3074	1/1	0.95	0.40	-	57,57,57,57	0
60	MG	14	3282	1/1	0.89	0.17	-	73,73,73,73	0
60	MG	13	1725	1/1	0.96	0.05	-	96,96,96,96	0
60	MG	14	3116	1/1	0.97	0.40	-	53,53,53,53	0
60	MG	1J	205	1/1	0.94	0.10	-	119,119,119,119	0
60	MG	14	3261	1/1	0.23	0.28	-	136,136,136,136	0
60	MG	14	3136	1/1	0.86	0.34	-	90,90,90,90	0
60	MG	13	1666	1/1	0.87	0.26	-	94,94,94,94	0
60	MG	14	3226	1/1	0.81	0.44	-	68,68,68,68	0
60	MG	1H	3284	1/1	0.87	0.15	-	66,66,66,66	0
60	MG	1H	3375	1/1	0.80	0.11	-	48,48,48,48	0
60	MG	1H	3035	1/1	0.94	0.26	-	63,63,63,63	0
60	MG	14	3149	1/1	0.92	0.36	-	73,73,73,73	0
60	MG	1H	3106	1/1	0.92	0.18	-	66,66,66,66	0
60	MG	1H	3071	1/1	0.88	0.31	-	57,57,57,57	0
60	MG	13	1711	1/1	0.64	0.41	-	83,83,83,83	0
60	MG	1H	3057	1/1	0.98	0.40	-	47,47,47,47	0
60	MG	14	3240	1/1	0.94	0.30	-	50,50,50,50	0
60	MG	14	3046	1/1	0.97	0.37	-	80,80,80,80	0
60	MG	14	3295	1/1	0.91	0.17	-	77,77,77,77	0
60	MG	14	3243	1/1	0.95	0.48	-	61,61,61,61	0
60	MG	14	3002	1/1	0.95	0.35	-	50,50,50,50	0
60	MG	1H	3244	1/1	0.96	0.29	-	56,56,56,56	0
60	MG	13	1686	1/1	0.91	0.19	-	76,76,76,76	0
60	MG	1H	3174	1/1	0.96	0.60	-	53,53,53,53	0
60	MG	I8	101	1/1	0.69	0.22	-	70,70,70,70	0
60	MG	1G	1618	1/1	0.94	0.49	-	86,86,86,86	0
60	MG	14	3333	1/1	0.95	0.11	-	55,55,55,55	0
60	MG	14	3242	1/1	0.96	0.34	-	53,53,53,53	0
60	MG	14	3018	1/1	0.24	0.31	-	103,103,103,103	0
60	MG	1H	3328	1/1	0.95	0.13	-	50,50,50,50	0
60	MG	13	1637	1/1	0.89	0.48	-	76,76,76,76	0
60	MG	1H	3316	1/1	0.95	0.16	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3167	1/1	0.62	0.38	-	83,83,83,83	0
60	MG	14	3173	1/1	0.93	0.43	-	61,61,61,61	0
60	MG	1G	1638	1/1	0.91	0.43	-	88,88,88,88	0
60	MG	14	3185	1/1	0.86	0.42	-	76,76,76,76	0
60	MG	16	208	1/1	0.92	0.13	-	84,84,84,84	0
60	MG	1H	3121	1/1	0.98	0.17	-	43,43,43,43	0
60	MG	2K	102	1/1	0.93	0.21	-	84,84,84,84	0
60	MG	13	1631	1/1	0.88	0.28	-	74,74,74,74	0
60	MG	1G	1702	1/1	0.79	0.08	-	124,124,124,124	0
60	MG	1H	3389	1/1	0.92	0.11	-	47,47,47,47	0
60	MG	14	3113	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	14	3317	1/1	0.88	0.10	-	54,54,54,54	0
60	MG	1H	3047	1/1	0.86	0.33	-	73,73,73,73	0
60	MG	13	1733	1/1	0.94	0.08	-	75,75,75,75	0
60	MG	14	3248	1/1	0.85	0.26	-	80,80,80,80	0
60	MG	14	3249	1/1	0.94	0.29	-	61,61,61,61	0
60	MG	1H	3306	1/1	0.85	0.48	-	77,77,77,77	0
60	MG	1G	1608	1/1	0.92	0.27	-	95,95,95,95	0
60	MG	14	3145	1/1	0.70	0.64	-	82,82,82,82	0
60	MG	14	3328	1/1	0.95	0.16	-	72,72,72,72	0
60	MG	14	3371	1/1	0.69	0.07	-	106,106,106,106	0
60	MG	1G	1665	1/1	0.77	0.39	-	75,75,75,75	0
60	MG	14	3308	1/1	0.85	0.57	-	66,66,66,66	0
60	MG	14	3069	1/1	0.79	0.61	-	78,78,78,78	0
60	MG	14	3365	1/1	0.92	0.07	-	90,90,90,90	0
60	MG	13	1645	1/1	0.98	0.39	-	57,57,57,57	0
60	MG	14	3384	1/1	0.86	0.04	-	122,122,122,122	0
60	MG	1H	3182	1/1	0.89	0.62	-	91,91,91,91	0
60	MG	1G	1666	1/1	0.94	0.39	-	113,113,113,113	0
60	MG	1G	1697	1/1	0.94	0.08	-	111,111,111,111	0
60	MG	13	1618	1/1	0.58	0.24	-	77,77,77,77	0
60	MG	1H	3134	1/1	0.94	0.51	-	64,64,64,64	0
60	MG	1H	3059	1/1	0.97	0.46	-	41,41,41,41	0
60	MG	1G	1662	1/1	0.83	0.44	-	84,84,84,84	0
60	MG	1H	3433	1/1	0.79	0.10	-	91,91,91,91	0
60	MG	1H	3153	1/1	0.80	0.36	-	59,59,59,59	0
60	MG	1H	3114	1/1	0.93	0.38	-	61,61,61,61	0
60	MG	1H	3272	1/1	0.91	0.30	-	72,72,72,72	0
60	MG	14	3123	1/1	0.77	0.34	-	81,81,81,81	0
60	MG	13	1644	1/1	0.93	0.32	-	55,55,55,55	0
60	MG	14	3089	1/1	0.97	0.34	-	52,52,52,52	0
60	MG	21	301	1/1	0.98	0.28	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3234	1/1	0.93	0.45	-	53,53,53,53	0
60	MG	1H	3237	1/1	0.94	0.12	-	63,63,63,63	0
60	MG	13	1688	1/1	0.82	0.34	-	66,66,66,66	0
60	MG	1H	3224	1/1	0.95	0.13	-	37,37,37,37	0
60	MG	1H	3219	1/1	0.97	0.25	-	123,123,123,123	0
60	MG	14	3125	1/1	0.90	0.17	-	63,63,63,63	0
60	MG	14	3195	1/1	0.70	0.38	-	90,90,90,90	0
60	MG	1H	3045	1/1	0.85	0.48	-	65,65,65,65	0
60	MG	1H	3395	1/1	0.93	0.09	-	69,69,69,69	0
60	MG	14	3181	1/1	0.95	0.18	-	73,73,73,73	0
60	MG	14	3194	1/1	0.96	0.33	-	63,63,63,63	0
60	MG	1J	202	1/1	0.67	0.30	-	85,85,85,85	0
60	MG	1G	1682	1/1	0.90	0.24	-	115,115,115,115	0
60	MG	1H	3061	1/1	0.90	0.27	-	56,56,56,56	0
60	MG	14	3202	1/1	0.96	0.43	-	72,72,72,72	0
60	MG	14	3285	1/1	0.77	0.15	-	62,62,62,62	0
60	MG	1H	3247	1/1	0.99	0.20	-	60,60,60,60	0
60	MG	1H	3041	1/1	0.91	0.48	-	58,58,58,58	0
60	MG	14	3062	1/1	0.92	0.48	-	66,66,66,66	0
60	MG	1H	3097	1/1	0.98	0.43	-	60,60,60,60	0
60	MG	14	3143	1/1	0.73	0.58	-	76,76,76,76	0
60	MG	C5	201	1/1	0.86	0.74	-	107,107,107,107	0
60	MG	14	3341	1/1	0.92	0.10	-	66,66,66,66	0
60	MG	14	3381	1/1	0.95	0.10	-	79,79,79,79	0
60	MG	13	1661	1/1	0.91	0.42	-	70,70,70,70	0
60	MG	14	3254	1/1	0.94	0.19	-	78,78,78,78	0
60	MG	1H	3371	1/1	0.77	0.07	-	91,91,91,91	0
60	MG	13	1665	1/1	0.84	0.32	-	91,91,91,91	0
60	MG	1H	3144	1/1	0.89	0.23	-	78,78,78,78	0
60	MG	1G	1652	1/1	0.90	0.37	-	72,72,72,72	0
60	MG	13	1626	1/1	0.95	0.34	-	50,50,50,50	0
60	MG	13	1694	1/1	0.98	0.09	-	115,115,115,115	0
60	MG	1H	3026	1/1	0.94	0.31	-	80,80,80,80	0
60	MG	1H	3420	1/1	0.94	0.12	-	111,111,111,111	0
60	MG	1H	3068	1/1	0.96	0.40	-	52,52,52,52	0
60	MG	14	3047	1/1	0.96	0.29	-	72,72,72,72	0
60	MG	1H	3017	1/1	0.96	0.18	-	54,54,54,54	0
60	MG	1H	3407	1/1	0.81	0.10	-	76,76,76,76	0
60	MG	13	1735	1/1	0.89	0.12	-	153,153,153,153	0
60	MG	14	3133	1/1	0.88	0.37	-	80,80,80,80	0
60	MG	14	3126	1/1	0.95	0.20	-	82,82,82,82	0
60	MG	14	3041	1/1	0.96	0.29	-	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3228	1/1	0.96	0.12	-	42,42,42,42	0
60	MG	14	3193	1/1	0.80	0.35	-	76,76,76,76	0
60	MG	1H	3260	1/1	0.97	0.15	-	62,62,62,62	0
60	MG	14	3056	1/1	0.95	0.32	-	65,65,65,65	0
60	MG	13	1623	1/1	0.95	0.45	-	76,76,76,76	0
60	MG	14	3043	1/1	0.96	0.33	-	64,64,64,64	0
60	MG	1H	3152	1/1	0.90	0.28	-	76,76,76,76	0
60	MG	1H	3285	1/1	0.88	0.17	-	61,61,61,61	0
60	MG	1G	1609	1/1	0.96	0.21	-	74,74,74,74	0
60	MG	1H	3181	1/1	0.73	0.36	-	81,81,81,81	0
60	MG	14	3369	1/1	0.96	0.11	-	79,79,79,79	0
60	MG	14	3186	1/1	0.88	0.53	-	62,62,62,62	0
60	MG	1H	3201	1/1	0.94	0.52	-	65,65,65,65	0
60	MG	1H	3203	1/1	0.89	0.38	-	91,91,91,91	0
60	MG	14	3190	1/1	0.96	0.28	-	68,68,68,68	0
60	MG	14	3197	1/1	0.90	0.28	-	79,79,79,79	0
60	MG	14	3196	1/1	0.93	0.82	-	82,82,82,82	0
60	MG	14	3022	1/1	0.92	0.24	-	48,48,48,48	0
60	MG	1G	1700	1/1	0.88	0.09	-	152,152,152,152	0
60	MG	1H	3006	1/1	0.95	0.27	-	42,42,42,42	0
60	MG	13	1706	1/1	0.89	0.35	-	85,85,85,85	0
60	MG	1H	3135	1/1	0.89	0.28	-	50,50,50,50	0
60	MG	14	3291	1/1	0.80	0.18	-	80,80,80,80	0
60	MG	13	1701	1/1	0.73	0.27	-	85,85,85,85	0
60	MG	14	3334	1/1	0.93	0.07	-	80,80,80,80	0
60	MG	1H	3039	1/1	0.95	0.33	-	46,46,46,46	0
60	MG	1H	3212	1/1	0.80	0.52	-	89,89,89,89	0
60	MG	1G	1622	1/1	0.96	0.43	-	52,52,52,52	0
60	MG	1H	3124	1/1	0.93	0.29	-	68,68,68,68	0
60	MG	1H	3131	1/1	0.92	0.46	-	76,76,76,76	0
60	MG	1H	3177	1/1	0.97	0.32	-	62,62,62,62	0
60	MG	14	3110	1/1	0.98	0.54	-	56,56,56,56	0
60	MG	14	3346	1/1	0.82	0.07	-	108,108,108,108	0
60	MG	1J	207	1/1	0.81	0.10	-	92,92,92,92	0
60	MG	1H	3056	1/1	0.92	0.21	-	67,67,67,67	0
60	MG	1H	3117	1/1	0.96	0.31	-	57,57,57,57	0
60	MG	14	3162	1/1	0.91	0.30	-	83,83,83,83	0
60	MG	1H	3188	1/1	0.94	0.22	-	63,63,63,63	0
60	MG	14	3374	1/1	0.94	0.05	-	107,107,107,107	0
60	MG	14	3301	1/1	0.87	0.21	-	75,75,75,75	0
60	MG	14	3040	1/1	0.93	0.29	-	66,66,66,66	0
60	MG	1H	3197	1/1	0.89	0.30	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1H	3286	1/1	0.90	0.29	-	72,72,72,72	0
60	MG	1H	3130	1/1	0.93	0.38	-	73,73,73,73	0
60	MG	13	1726	1/1	0.94	0.09	-	97,97,97,97	0
60	MG	1H	3138	1/1	0.96	0.52	-	81,81,81,81	0
60	MG	14	3298	1/1	0.95	0.33	-	64,64,64,64	0
60	MG	14	3170	1/1	0.97	0.37	-	81,81,81,81	0
60	MG	14	3159	1/1	0.94	0.37	-	64,64,64,64	0
60	MG	13	1716	1/1	0.88	0.19	-	77,77,77,77	0
60	MG	13	1606	1/1	0.97	0.30	-	78,78,78,78	0
60	MG	14	3383	1/1	0.79	0.08	-	101,101,101,101	0
60	MG	78	202	1/1	0.89	0.20	-	46,46,46,46	0
60	MG	14	3378	1/1	0.74	0.10	-	75,75,75,75	0
60	MG	13	1613	1/1	0.94	0.28	-	66,66,66,66	0
60	MG	14	3111	1/1	0.95	0.49	-	72,72,72,72	0
60	MG	14	3077	1/1	0.97	0.30	-	49,49,49,49	0
60	MG	14	3252	1/1	0.79	0.38	-	76,76,76,76	0
60	MG	1H	3403	1/1	0.91	0.18	-	83,83,83,83	0
60	MG	1H	3233	1/1	0.86	0.38	-	69,69,69,69	0
60	MG	14	3146	1/1	0.97	0.25	-	74,74,74,74	0
60	MG	13	1636	1/1	0.95	0.25	-	66,66,66,66	0
60	MG	1H	3358	1/1	0.98	0.09	-	55,55,55,55	0
60	MG	14	3107	1/1	0.94	0.46	-	69,69,69,69	0
60	MG	14	3364	1/1	0.94	0.12	-	89,89,89,89	0
60	MG	1H	3430	1/1	0.83	0.05	-	95,95,95,95	0
60	MG	1H	3351	1/1	0.96	0.06	-	68,68,68,68	0
60	MG	14	3016	1/1	0.98	0.33	-	52,52,52,52	0
60	MG	14	3140	1/1	0.94	0.17	-	46,46,46,46	0
60	MG	1G	1670	1/1	0.93	0.08	-	93,93,93,93	0
60	MG	1H	3413	1/1	0.88	0.11	-	103,103,103,103	0
60	MG	2L	103	1/1	0.90	0.27	-	67,67,67,67	0
60	MG	1H	3170	1/1	0.95	0.33	-	76,76,76,76	0
60	MG	1H	3160	1/1	0.89	0.53	-	76,76,76,76	0
60	MG	1H	3251	1/1	0.41	0.28	-	73,73,73,73	0
60	MG	14	3262	1/1	0.84	0.23	-	63,63,63,63	0
60	MG	13	1663	1/1	0.81	0.34	-	93,93,93,93	0
60	MG	2K	103	1/1	0.85	0.34	-	76,76,76,76	0
60	MG	14	3292	1/1	0.97	0.14	-	77,77,77,77	0
60	MG	1H	3273	1/1	0.91	0.27	-	55,55,55,55	0
60	MG	14	3310	1/1	0.98	0.14	-	46,46,46,46	0
60	MG	13	1659	1/1	0.92	0.33	-	79,79,79,79	0
60	MG	1H	3398	1/1	0.88	0.04	-	71,71,71,71	0
60	MG	14	3027	1/1	0.96	0.25	-	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
60	MG	14	3001	1/1	0.95	0.11	-	44,44,44,44	0
60	MG	14	3117	1/1	0.88	0.32	-	74,74,74,74	0
60	MG	16	210	1/1	0.89	0.08	-	64,64,64,64	0
60	MG	1H	3434	1/1	0.94	0.08	-	44,44,44,44	0
60	MG	14	3129	1/1	0.93	0.28	-	56,56,56,56	0
60	MG	1H	3320	1/1	0.99	0.11	-	41,41,41,41	0
60	MG	13	1657	1/1	0.94	0.47	-	73,73,73,73	0
60	MG	1H	3029	1/1	0.91	0.39	-	65,65,65,65	0
60	MG	13	1697	1/1	0.92	0.07	-	95,95,95,95	0
60	MG	68	201	1/1	0.73	0.46	-	83,83,83,83	0
60	MG	1H	3085	1/1	0.95	0.26	-	47,47,47,47	0
60	MG	13	1669	1/1	0.98	0.40	-	84,84,84,84	0
60	MG	13	1684	1/1	0.96	0.34	-	66,66,66,66	0
60	MG	1G	1690	1/1	0.92	0.43	-	75,75,75,75	0
60	MG	13	1620	1/1	0.89	0.33	-	64,64,64,64	0
60	MG	1H	3078	1/1	0.95	0.16	-	46,46,46,46	0
60	MG	13	1667	1/1	0.35	0.41	-	102,102,102,102	0
60	MG	1G	1672	1/1	0.96	0.20	-	84,84,84,84	0
60	MG	1G	1646	1/1	0.84	0.27	-	77,77,77,77	0
60	MG	1H	3189	1/1	0.96	0.24	-	62,62,62,62	0
60	MG	13	1628	1/1	0.90	0.47	-	72,72,72,72	0
60	MG	14	3017	1/1	0.94	0.28	-	68,68,68,68	0
60	MG	14	3354	1/1	0.93	0.09	-	74,74,74,74	0
60	MG	14	3006	1/1	0.99	0.30	-	49,49,49,49	0
60	MG	1H	3098	1/1	0.96	0.37	-	69,69,69,69	0
60	MG	1H	3386	1/1	0.99	0.10	-	53,53,53,53	0
60	MG	1G	1686	1/1	0.97	0.18	-	115,115,115,115	0
60	MG	1G	1649	1/1	0.88	0.34	-	76,76,76,76	0
60	MG	1H	3317	1/1	0.93	0.16	-	74,74,74,74	0
60	MG	14	3070	1/1	0.95	0.42	-	61,61,61,61	0
60	MG	1H	3082	1/1	0.89	0.32	-	39,39,39,39	0
60	MG	14	3198	1/1	0.86	0.34	-	63,63,63,63	0
60	MG	1H	3146	1/1	0.92	0.35	-	84,84,84,84	0
60	MG	1H	3215	1/1	0.92	0.41	-	80,80,80,80	0
60	MG	14	3038	1/1	0.96	0.52	-	60,60,60,60	0
60	MG	14	3120	1/1	0.97	0.28	-	53,53,53,53	0
60	MG	1H	3036	1/1	0.98	0.34	-	52,52,52,52	0
60	MG	1H	3411	1/1	0.95	0.10	-	68,68,68,68	0
60	MG	14	3247	1/1	0.96	0.24	-	73,73,73,73	0
60	MG	1H	3425	1/1	0.96	0.10	-	60,60,60,60	0
60	MG	1H	3208	1/1	0.95	0.11	-	56,56,56,56	0
60	MG	14	3278	1/1	0.90	0.29	-	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
60	MG	1G	1655	1/1	0.90	0.26	-	96,96,96,96	0
60	MG	1G	1647	1/1	0.96	0.53	-	76,76,76,76	0
60	MG	3K	101	1/1	0.98	0.20	-	83,83,83,83	0
60	MG	1H	3412	1/1	0.87	0.08	-	93,93,93,93	0
60	MG	1H	3391	1/1	0.98	0.06	-	58,58,58,58	0
60	MG	14	3099	1/1	0.97	0.34	-	58,58,58,58	0
60	MG	1H	3128	1/1	0.96	0.42	-	49,49,49,49	0
60	MG	1H	3280	1/1	0.84	0.22	-	70,70,70,70	0
60	MG	13	1615	1/1	0.94	0.31	-	75,75,75,75	0
60	MG	1H	3330	1/1	0.94	0.11	-	51,51,51,51	0
60	MG	14	3138	1/1	0.95	0.50	-	50,50,50,50	0
60	MG	1H	3052	1/1	0.97	0.11	-	44,44,44,44	0
60	MG	13	1715	1/1	0.91	0.36	-	82,82,82,82	0
60	MG	14	3255	1/1	0.93	0.37	-	75,75,75,75	0
60	MG	1H	3245	1/1	0.91	0.17	-	50,50,50,50	0
60	MG	1G	1650	1/1	0.93	0.46	-	88,88,88,88	0
60	MG	13	1732	1/1	0.97	0.07	-	86,86,86,86	0
60	MG	14	3276	1/1	0.78	0.21	-	66,66,66,66	0
60	MG	14	3302	1/1	0.87	0.34	-	87,87,87,87	0
60	MG	1H	3055	1/1	0.97	0.20	-	45,45,45,45	0
60	MG	13	1614	1/1	0.94	0.27	-	82,82,82,82	0
60	MG	14	3212	1/1	0.93	0.47	-	106,106,106,106	0
60	MG	1H	3198	1/1	0.88	0.27	-	64,64,64,64	0
60	MG	1H	3274	1/1	0.98	0.18	-	71,71,71,71	0
60	MG	1H	3220	1/1	0.90	0.38	-	78,78,78,78	0
60	MG	1H	3166	1/1	0.93	0.36	-	83,83,83,83	0
60	MG	1H	3013	1/1	0.97	0.30	-	48,48,48,48	0
60	MG	1G	1640	1/1	0.96	0.59	-	105,105,105,105	0
60	MG	13	1647	1/1	0.93	0.42	-	83,83,83,83	0
60	MG	1H	3165	1/1	0.84	0.27	-	77,77,77,77	0
60	MG	14	3272	1/1	0.81	0.25	-	55,55,55,55	0
60	MG	14	3142	1/1	0.95	0.29	-	68,68,68,68	0
60	MG	14	3353	1/1	0.98	0.07	-	72,72,72,72	0
60	MG	1H	3089	1/1	0.86	0.24	-	69,69,69,69	0
60	MG	1H	3125	1/1	0.88	0.14	-	34,34,34,34	0
60	MG	1H	3292	1/1	0.95	0.38	-	89,89,89,89	0
60	MG	1H	3123	1/1	0.95	0.23	-	65,65,65,65	0
60	MG	1G	1643	1/1	0.88	0.21	-	80,80,80,80	0
60	MG	14	3078	1/1	0.94	0.27	-	59,59,59,59	0
60	MG	1H	3031	1/1	0.65	0.40	-	78,78,78,78	0
60	MG	13	1652	1/1	0.95	0.38	-	61,61,61,61	0
60	MG	14	3216	1/1	0.60	0.51	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	1G	1635	1/1	0.64	0.38	-	104,104,104,104	0
60	MG	14	3108	1/1	0.90	0.58	-	71,71,71,71	0
60	MG	14	3224	1/1	0.94	0.56	-	51,51,51,51	0
60	MG	14	3241	1/1	0.95	0.20	-	65,65,65,65	0
60	MG	1H	3334	1/1	0.95	0.14	-	59,59,59,59	0
60	MG	1H	3255	1/1	0.69	0.38	-	71,71,71,71	0
60	MG	14	3033	1/1	0.98	0.27	-	58,58,58,58	0
60	MG	1H	3080	1/1	0.95	0.29	-	59,59,59,59	0
60	MG	1H	3263	1/1	0.97	0.42	-	72,72,72,72	0
60	MG	14	3319	1/1	0.95	0.06	-	98,98,98,98	0
60	MG	1G	1696	1/1	0.97	0.07	-	108,108,108,108	0
60	MG	14	3201	1/1	0.89	0.58	-	81,81,81,81	0
60	MG	14	3175	1/1	0.90	0.38	-	80,80,80,80	0
60	MG	1H	3249	1/1	0.94	0.40	-	72,72,72,72	0
60	MG	1H	3206	1/1	0.94	0.22	-	58,58,58,58	0
60	MG	13	1610	1/1	0.95	0.16	-	67,67,67,67	0
60	MG	14	3020	1/1	0.98	0.25	-	57,57,57,57	0
60	MG	1H	3410	1/1	0.84	0.07	-	87,87,87,87	0
60	MG	14	3205	1/1	0.90	0.35	-	72,72,72,72	0
60	MG	13	1655	1/1	0.95	0.27	-	97,97,97,97	0
60	MG	1G	1612	1/1	0.91	0.31	-	84,84,84,84	0
60	MG	14	3096	1/1	0.69	0.22	-	60,60,60,60	0
60	MG	14	3182	1/1	0.93	0.52	-	81,81,81,81	0
60	MG	1H	3193	1/1	0.88	0.34	-	67,67,67,67	0
60	MG	1H	3015	1/1	0.96	0.22	-	56,56,56,56	0
60	MG	1H	3432	1/1	0.92	0.07	-	107,107,107,107	0
60	MG	29	301	1/1	0.98	0.30	-	48,48,48,48	0
60	MG	14	3199	1/1	0.92	0.59	-	66,66,66,66	0
60	MG	1H	3141	1/1	0.85	0.54	-	70,70,70,70	0
60	MG	14	3154	1/1	0.92	0.24	-	64,64,64,64	0
60	MG	1H	3213	1/1	0.83	0.38	-	95,95,95,95	0
60	MG	14	3007	1/1	0.96	0.41	-	54,54,54,54	0
60	MG	14	3057	1/1	0.94	0.41	-	62,62,62,62	0
60	MG	1H	3168	1/1	0.95	0.38	-	72,72,72,72	0
60	MG	1H	3180	1/1	0.86	0.26	-	87,87,87,87	0
60	MG	1G	1623	1/1	0.94	0.50	-	82,82,82,82	0
60	MG	14	3178	1/1	0.86	0.38	-	66,66,66,66	0
60	MG	14	3322	1/1	0.96	0.12	-	42,42,42,42	0
60	MG	14	3265	1/1	0.97	0.40	-	78,78,78,78	0
60	MG	1H	3400	1/1	0.83	0.07	-	82,82,82,82	0
60	MG	14	3065	1/1	0.87	0.57	-	71,71,71,71	0
60	MG	1H	3091	1/1	0.95	0.18	-	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	13	1737	1/1	0.95	0.10	-	91,91,91,91	0
60	MG	1H	3313	1/1	0.97	0.09	-	36,36,36,36	0
60	MG	14	3228	1/1	0.97	0.36	-	76,76,76,76	0
60	MG	1H	3001	1/1	0.95	0.31	-	36,36,36,36	0
60	MG	1H	3382	1/1	0.93	0.06	-	68,68,68,68	0
60	MG	1H	3027	1/1	0.95	0.40	-	79,79,79,79	0
60	MG	1H	3345	1/1	0.95	0.09	-	65,65,65,65	0
60	MG	1H	3299	1/1	0.83	0.24	-	72,72,72,72	0
60	MG	1H	3428	1/1	0.82	0.06	-	102,102,102,102	0
60	MG	14	3050	1/1	0.97	0.15	-	54,54,54,54	0
60	MG	1H	3322	1/1	0.90	0.15	-	48,48,48,48	0
60	MG	1H	3178	1/1	0.89	0.31	-	80,80,80,80	0
60	MG	1H	3148	1/1	0.92	0.65	-	67,67,67,67	0
60	MG	1H	3008	1/1	0.99	0.27	-	47,47,47,47	0
60	MG	1H	3155	1/1	0.69	0.50	-	60,60,60,60	0
60	MG	14	3207	1/1	0.84	0.25	-	74,74,74,74	0
60	MG	14	3121	1/1	0.83	0.43	-	64,64,64,64	0
60	MG	I8	102	1/1	0.78	0.23	-	56,56,56,56	0
60	MG	14	3239	1/1	0.97	0.37	-	83,83,83,83	0
60	MG	13	1695	1/1	0.91	0.21	-	90,90,90,90	0
60	MG	16	211	1/1	0.88	0.08	-	87,87,87,87	0
60	MG	1G	1675	1/1	0.80	0.19	-	86,86,86,86	0
60	MG	1H	3366	1/1	0.92	0.16	-	53,53,53,53	0
60	MG	1H	3275	1/1	0.93	0.26	-	58,58,58,58	0
60	MG	13	1612	1/1	0.98	0.18	-	67,67,67,67	0
60	MG	1H	3120	1/1	0.91	0.36	-	63,63,63,63	0
60	MG	1H	3291	1/1	0.80	0.28	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.