



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 07:07 pm BST

PDB ID : 4WRA
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in the first position in the A-site and with antibiotic paromomycin.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-23
Resolution : 3.05 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

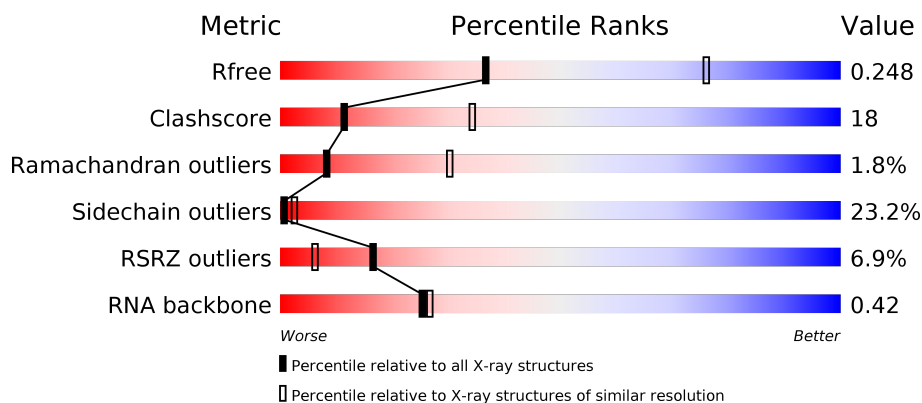
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

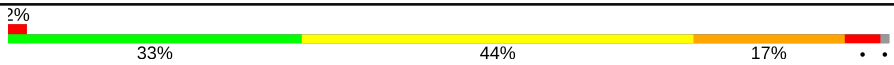



The reported resolution of this entry is 3.05 Å.

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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	85	
23	2K	77	
23	2L	77	
24	1L	85	
24	3K	85	
25	4K	30	
25	4L	30	
26	14	2918	
26	1H	2918	
27	16	122	
27	1J	122	
28	11	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	19	276	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	
40	B8	146	


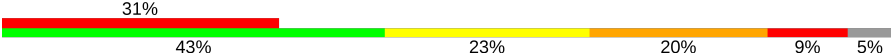
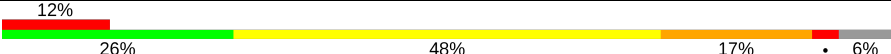
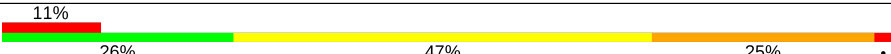
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	
53	L5	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	P8	49	
54	M5	65	
54	Q8	65	
55	3L	85	

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
56	MG	13	1623	-	-	-	X
56	MG	14	3118	-	-	-	X
56	MG	14	3158	-	-	-	X
56	MG	14	3280	-	-	-	X
56	MG	14	3293	-	-	-	X
56	MG	14	3298	-	-	-	X
56	MG	1G	1648	-	-	-	X
56	MG	1H	3076	-	-	-	X
56	MG	1H	3101	-	-	-	X
56	MG	1H	3211	-	-	-	X
56	MG	1H	3217	-	-	-	X
56	MG	1H	3223	-	-	-	X
56	MG	1H	3228	-	-	-	X
56	MG	1H	3273	-	-	-	X
56	MG	1H	3274	-	-	-	X
56	MG	1H	3275	-	-	-	X
56	MG	1H	3293	-	-	-	X
56	MG	1H	3319	-	-	-	X
56	MG	1H	3323	-	-	-	X
56	MG	1H	3326	-	-	-	X
56	MG	1H	3328	-	-	-	X
56	MG	1H	3332	-	-	-	X

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 299607 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	1505	Total	C	N	O	P	0	0	0
			32352	14399	5994	10454	1505			
1	1G	1504	Total	C	N	O	P	0	0	0
			32327	14389	5989	10446	1503			

- 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			
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	152	Total	C	N	O	S	0	0	0
			1243	774	249	214	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	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			
9	82	122	Total	C	N	O	0	0	0
			971	616	189	166			

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	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	59	Total	C	N	O	S	0	0	0
			480	306	100	70	4			
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	71	Total	C	N	O	0	0	0
			581	370	115	96			

- 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	78	Total	C	N	O	S	0	0	0
			624	398	115	109	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			
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
			1824	821	323	594	85	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			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 723229079
2L	18	C	U	conflict	GB 723229079

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			
24	1L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	12	Total	C	N	O	P	0	1	0
			283	128	60	82	13			
25	4L	12	Total	C	N	O	P	0	0	0
			261	118	55	76	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total 62707	C 27911	N 11722	O 20163	P 2911	0	0	0
26	14	2909	Total 62647	C 27884	N 11716	O 20139	P 2908	0	0	0

There are 18 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	654A	A	G	conflict	GB 48268
1H	654E	C	G	conflict	GB 48268
1H	654P	G	C	conflict	GB 48268
1H	654T	A	C	conflict	GB 48268
1H	1058	U	G	conflict	GB 48268
1H	1080	A	C	conflict	GB 48268
1H	1228	G	-	insertion	GB 48268
14	158	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	654A	A	G	conflict	GB 48268
14	654E	C	G	conflict	GB 48268
14	654P	G	C	conflict	GB 48268
14	654T	A	C	conflict	GB 48268
14	1058	U	G	conflict	GB 48268
14	1080	A	C	conflict	GB 48268
14	1228	G	-	insertion	GB 48268

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

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0
28	19	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	173	Total	C	N	O	S	0	0	0
			1321	837	248	235	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
33	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
35	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			
36	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
37	45	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
38	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	110	Total	C	N	O	0	0	0
			876	553	175	148			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
40	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
41	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
42	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	F8	93	Total	C	N	O	0	0	0
			730	474	132	124			
44	B5	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
46	D5	138	Total	C	N	O	S	0	0	0
			1139	732	205	199	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
47	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L31.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			
52	J5	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	46	Total	C	N	O	S	0	0	0
			396	243	98	53	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	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	M5	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			

- Molecule 55 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	3L	85	Total	C	N	O	P	S	0	0
			1814	813	323	592	85	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

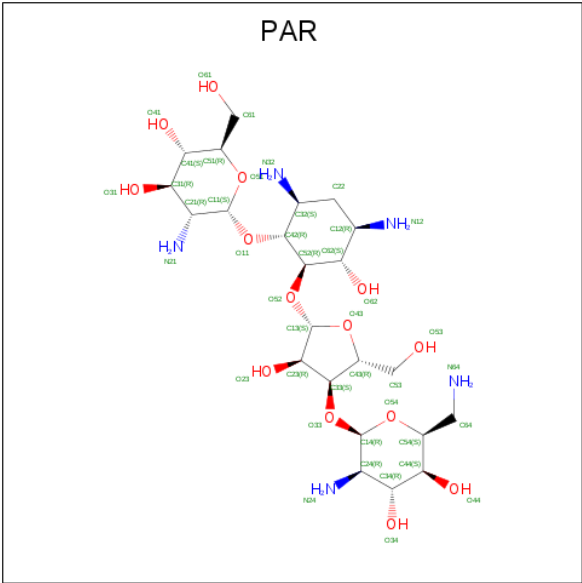
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	45	1	Total 1	Mg 1	0	0
56	P8	1	Total 1	Mg 1	0	0
56	85	1	Total 1	Mg 1	0	0
56	C5	1	Total 1	Mg 1	0	0
56	13	146	Total 146	Mg 146	0	0
56	1J	6	Total 6	Mg 6	0	0
56	35	1	Total 1	Mg 1	0	0
56	16	12	Total 12	Mg 12	0	0
56	25	1	Total 1	Mg 1	0	0
56	21	2	Total 2	Mg 2	0	0
56	31	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0
56	3I	1	Total 1	Mg 1	0	0
56	I8	1	Total 1	Mg 1	0	0
56	L5	1	Total 1	Mg 1	0	0
56	5E	1	Total 1	Mg 1	0	0
56	29	3	Total 3	Mg 3	0	0
56	2K	7	Total 7	Mg 7	0	0
56	39	1	Total 1	Mg 1	0	0
56	1G	86	Total 86	Mg 86	0	0
56	11	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1H	481	Total	Mg	0	0
			481	481		
56	88	1	Total	Mg	0	0
			1	1		
56	14	391	Total	Mg	0	0
			391	391		
56	78	1	Total	Mg	0	0
			1	1		
56	3E	1	Total	Mg	0	0
			1	1		
56	1K	1	Total	Mg	0	0
			1	1		
56	41	1	Total	Mg	0	0
			1	1		
56	2L	4	Total	Mg	0	0
			4	4		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	13	1	Total	C	N	O	0	0
			42	23	5	14		
57	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	32	1	Total Zn 1 1	0	0
58	3E	1	Total Zn 1 1	0	0
58	5I	1	Total Zn 1 1	0	0
58	5A	1	Total Zn 1 1	0	0
58	G8	1	Total Zn 1 1	0	0
58	C5	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	141	Total O 141 141	0	0
59	3E	1	Total O 1 1	0	0
59	1I	1	Total O 1 1	0	0
59	3I	2	Total O 2 2	0	0
59	5I	1	Total O 1 1	0	0
59	1K	1	Total O 1 1	0	0
59	2K	6	Total O 6 6	0	0
59	4K	3	Total O 3 3	0	0
59	1H	633	Total O 633 633	0	0
59	16	11	Total O 11 11	0	0
59	11	10	Total O 10 10	0	0
59	21	5	Total O 5 5	0	0
59	31	5	Total O 5 5	0	0
59	78	4	Total O 4 4	0	0

Continued on next page...

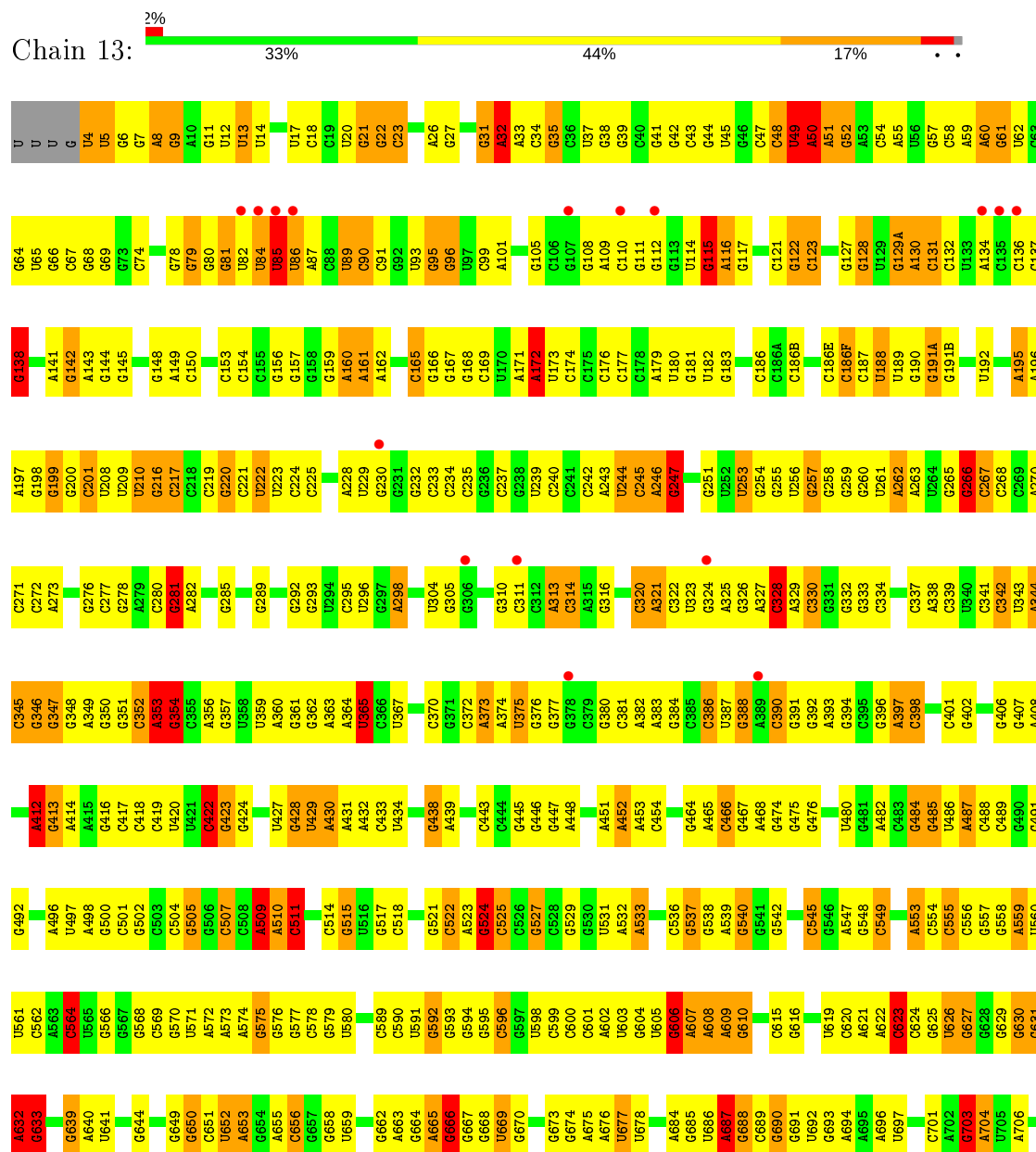
Continued from previous page...

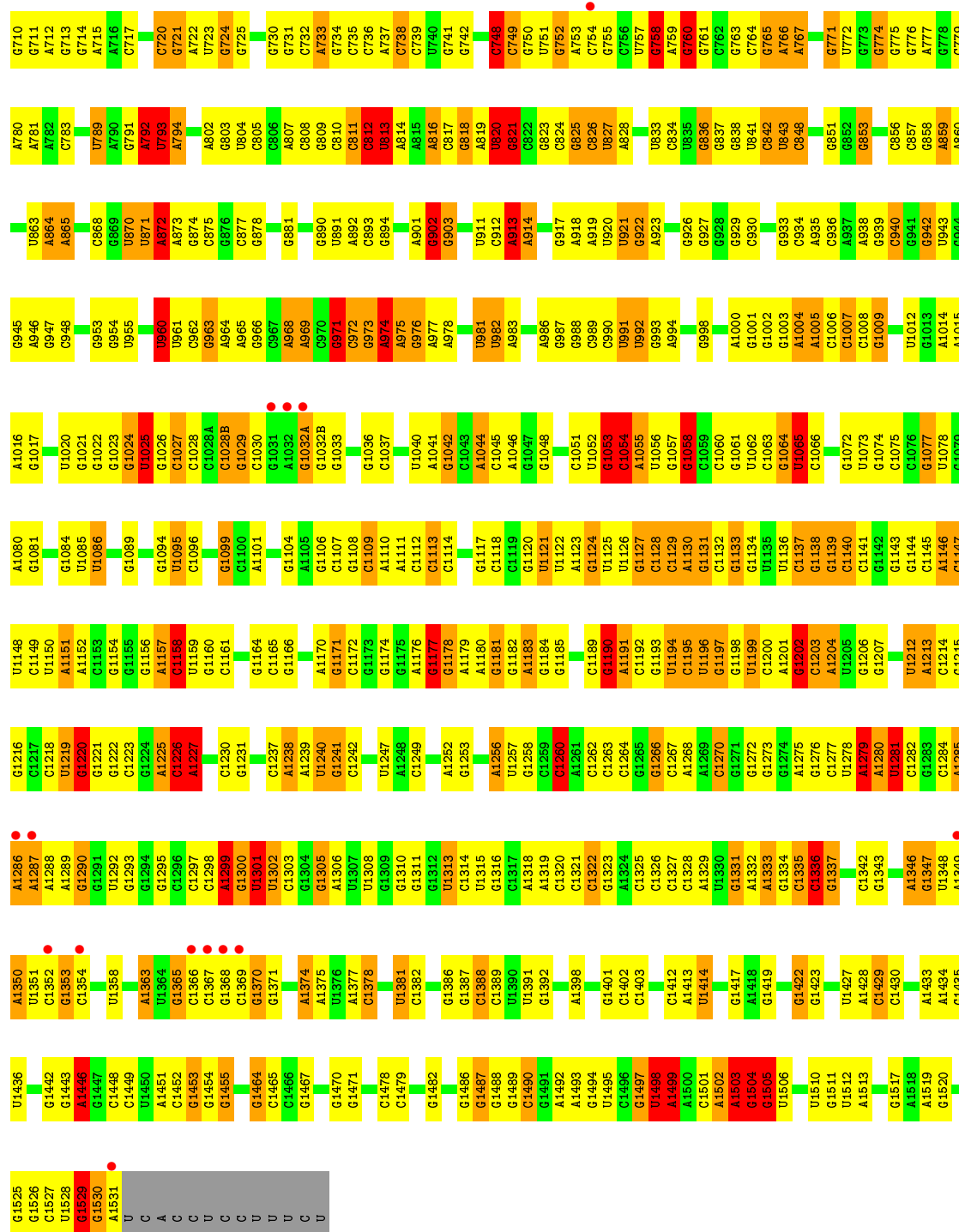
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	F8	1	Total 1	O 1	0	0
59	G8	2	Total 2	O 2	0	0
59	J8	1	Total 1	O 1	0	0
59	L8	2	Total 2	O 2	0	0
59	1G	87	Total 87	O 87	0	0
59	5A	1	Total 1	O 1	0	0
59	6A	1	Total 1	O 1	0	0
59	BA	1	Total 1	O 1	0	0
59	14	474	Total 474	O 474	0	0
59	1J	6	Total 6	O 6	0	0
59	19	9	Total 9	O 9	0	0
59	29	3	Total 3	O 3	0	0
59	39	5	Total 5	O 5	0	0
59	55	1	Total 1	O 1	0	0
59	75	1	Total 1	O 1	0	0
59	85	1	Total 1	O 1	0	0
59	A5	1	Total 1	O 1	0	0
59	M5	2	Total 2	O 2	0	0

3 Residue-property plots

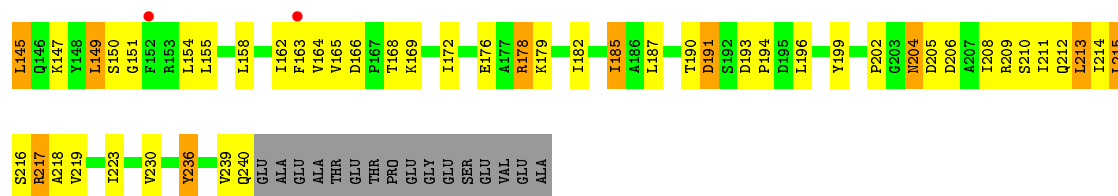
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

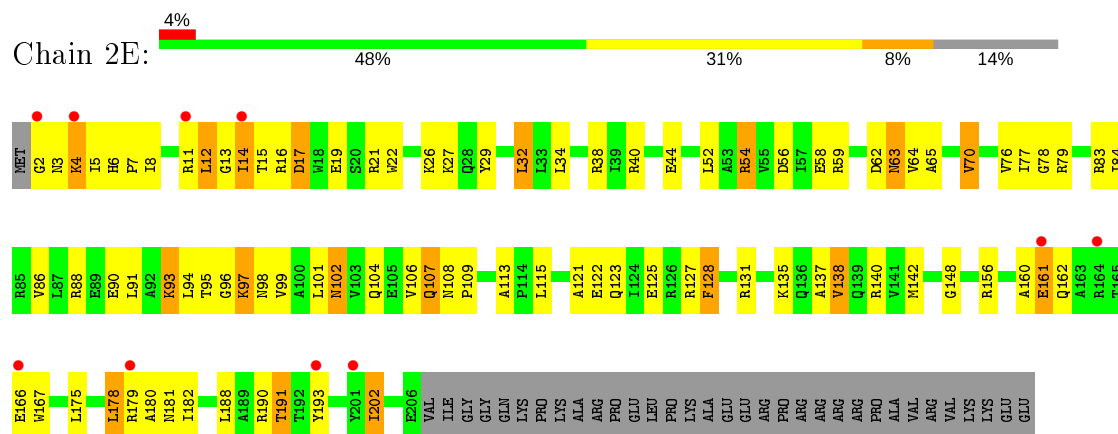




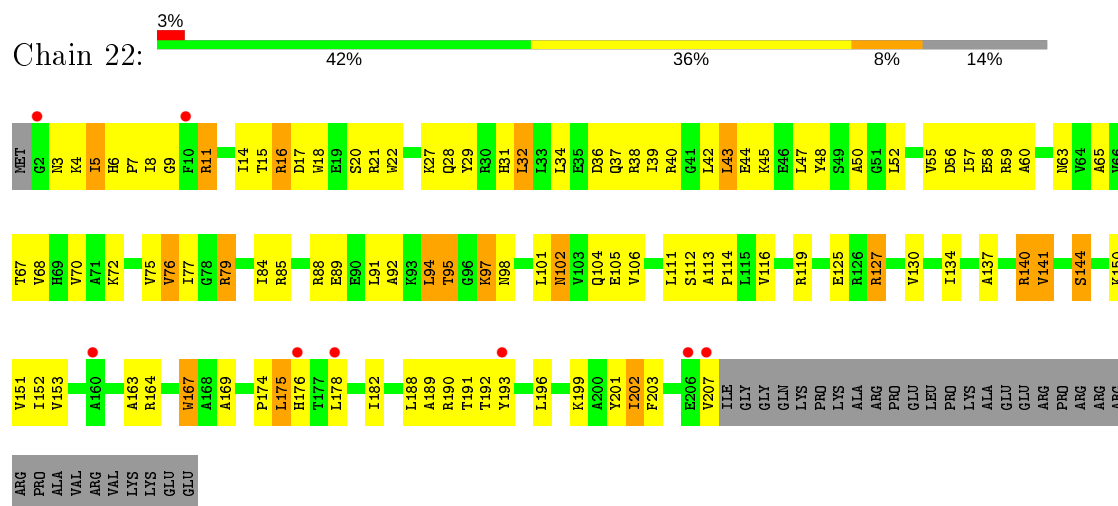
G1087	A1015	G947	G886	G765	G691	C543	A478	A397	C322	C235	A182	G79
G1088	A1016	C948	G887	A766	A696	G544	C479	C398	U323	G236	C163	G80
G1089	G1017	G951	U870	A767	U697	G545	U480	G406	G326	C237	C164	G81
A1092	C1019	G954	U871	G771	A702	A547	G481	G407	G327	A243	G166	U82
A1093	G1020	U955	A872	U772	G703	G550	G484	A408	C328	U244	G167	U84
G1094	G1021	U956	A873	U773	A704	G553	G485	G409	A329	G245	G168	U85
U1095	G1022	U957	G874	A777	U705	A553	U486	G410	C330	A246	U86	U86
C1096	G1023	U958	G875	A778	G706	C554	A487	G411	G331	G247	C174	C88
C1097	G1024	A958	G876	G779	A707	C555	C488	A412	G332	A412	C175	U89
A1101	U1025	A959	C877	C779	C707	C556	C489	G413	G333	A413	C176	C90
	G1026	U960	G878	A780	G708	C556	G490	G414	C337	A250	C177	C91
	C1027	U961	G879	G784	G709	A559	G491	G415	A338	U252	C178	
	G1028	C962	C880	C784	G710	U560	G492	C417	C339	U253	A179	G95
G1104	C1028B	G963	G881	G785	G713	U561	G493	C418	G344	G254	U180	G96
A1105	G1028B	G964	C882	G786	G714	C562	U494	C419	U345	G255	G181	
G1106	G1029	A965	A787	A787	G715	G563	A495	C345	U346	U256	U182	A101
C1107	C1030	G966	G885		G716	C564	A496	U421	G346	G257	G183	
C1108	G1031	C967	G886	G791	G718	U565	U497	C422	G347		G184	C106
C1109	A1032	A968	G888	G792	G721	U566	A498	G423	G350	U261	A185	G107
A1110	G1032A	A969	A889	A792	A722	A572	G500	G424	G351	A262	C186	G108
A1111	G1032B	C970	G890	A793	U723	A573	C501	G425	C352	U264	C186A	A109
C1112	G1033	G971	U891	A794	U724	G576	G502	G426	C353	G265	C187	C110
C1113	G1034	G972	A892	G799	G725	C569	C503	U427	A353	G266	G187	G111
C1114	A1035	C973	C893	G800	G726	A572	C504	U428	G354	C267	U188	G112
C1115	G1036	A974	G894	U801	C726	A573	G505	U429	U359		U189	G113
C1116	C1037	A975	G895	A802	G727	A574	G506	A430	A360	C272	U190	U114
G1117	G1038	G976	G896	G803	A728	G575	G507	A431	G361	A273	G191A	A116
C1118	C1039	A977	G898	A804	A729	G576	C508	A432	G362		U191D	
G1119	U1040	A978	C899	G805	G730	G577	A509	C433	A363	C277	G191E	G126
U1121	A1041	C979	A900	G806	G731	C578	A510	C434	U365	G278	G127	G128
U1122	G1042	C980		G807	G732	C579	A511	C435	U366	C280	C192	C193
A1123		U981	C904	A816	C735	G581	U512	U437	U367	G281	C194	U129
U1124	G1050	U982	G905	G826	A736	G582	C513	G438	U368		A195	G129A
U1125	G1051	A983	G906	G827	A737	G583	U516	A440	C369	G289	A196	A130
G1126	C1054	C984	A907	G828	C738	G584	G517	C442	C370		A197	C131
G1127	A1055	G985	A908	G829	C739	G585	G518	G445	G371	G297	C198	C132
C1128	U1056	A986	A909	C822	U740	G586	C519	G446	C372	A298	G199	U133
C1129		G987			G741	G587	A520	G447	A373	G299	G200	A134
A1130	C1059	C990	A913	G825	G742	G588	A521	A448	A374	A300	C201	
G1131	C1060	U991	A914	C826	G743	G589	G522	C449	U375	G301	U208	A141
G1132	G1061	G992	A918	U827	U744	G590	C523	G450	G376	G305	U209	G142
C1133	U1062	G993	A919	A828	C747	G591	A523	A451	G377	G306	U210	A143
U1135	C1063	A994	U920	G836	C748	G592	C526	A452	G378	C307	G216	G144
U1136	G1064		U921	G837	C749	G593	G527	A453	A382		C219	G145
C1137		C998A	A923	G838	G750	G594	C528	A454	C386	G310	G220	G147
G1138	C1069	U999	A924	U841	U751	G595	G529	A455	U387	C312	G221	G148
C1139		A1000	G926	U842	G752	G596	G530	C456	G388	A313	U222	A149
G1140	G1072	G1001	G927	U843	A753	G597	U531	C457	G389	C314	U223	C150
C1141	U1073	G1002	G928	C848	C754	G600	A533	C458	C390	A315		A151
G1142	G1074	G1003	G929	U850	G755	G601	C536	C459	G391	G316	U229	A152
G1143	C1075	A1004	G933	G853	G756	G602	G537	G467	G392	G317	G230	
G1144	U1078	A1005	G934	U854	C757	G603	G538	G468	A393	G318	G231	G157
C1145	G1079	C1006	A935	G855	A759	G604	G539	G474	G394	G319	G232	
A1146		G1009	C936	G856	G760	G605	A539	G475	C395		C233	A160
C1147	A1080		A937	G857	G761	G606	G540	G476	G396	A321	C234	
U1148	G1081	G1013	G942	A859	C762	A614	G541	G477				
C1149		A1014		A865			G542					
U1150												



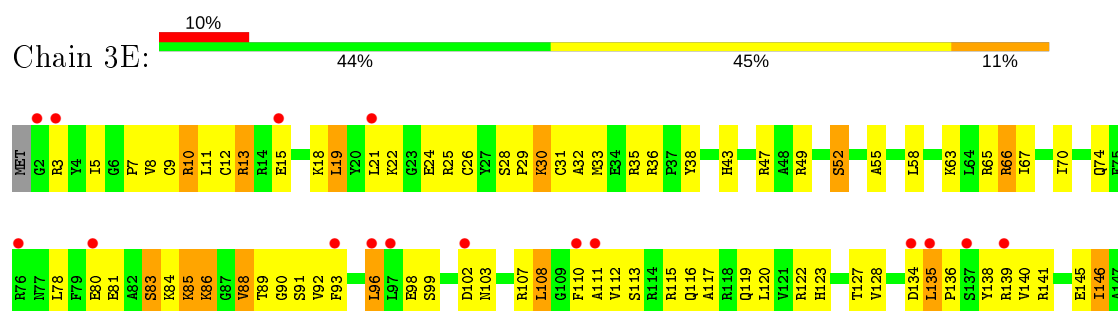
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

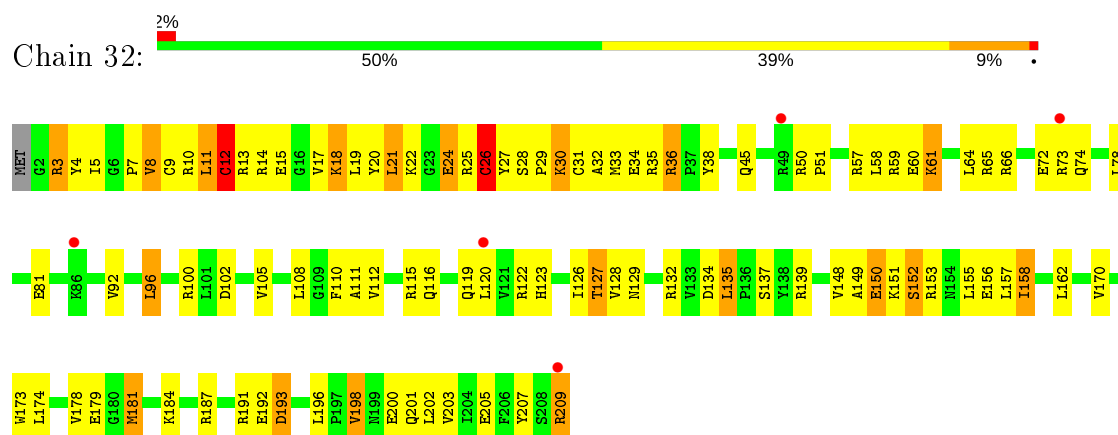


• Molecule 4: 30S ribosomal protein S4

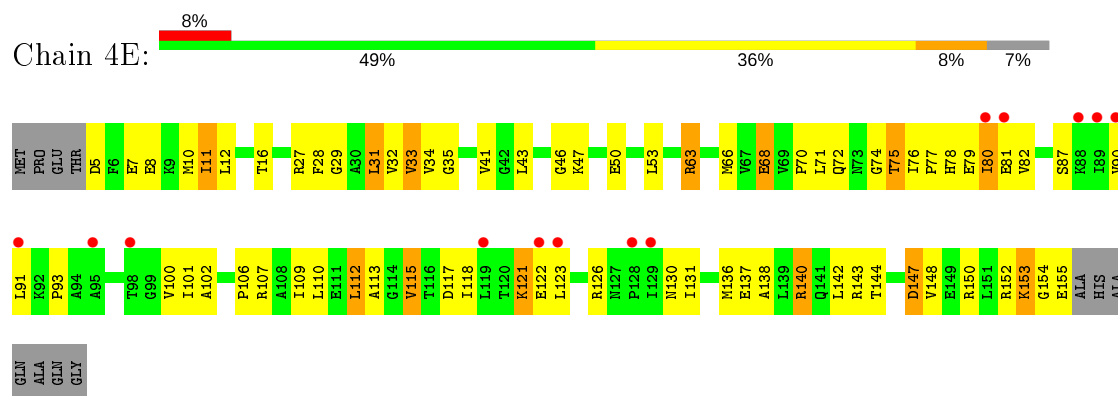




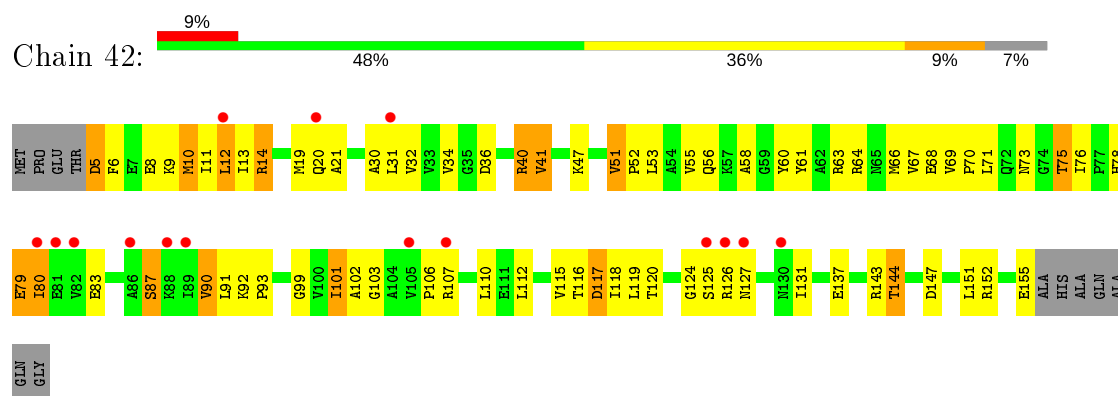
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

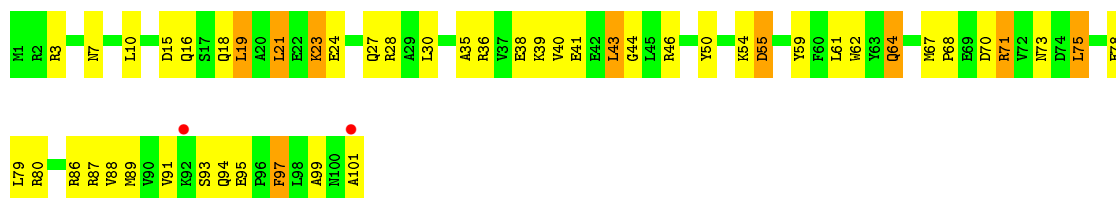


• Molecule 5: 30S ribosomal protein S5



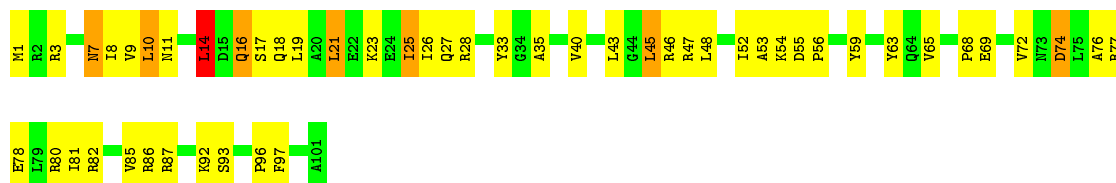
• Molecule 6: 30S ribosomal protein S6





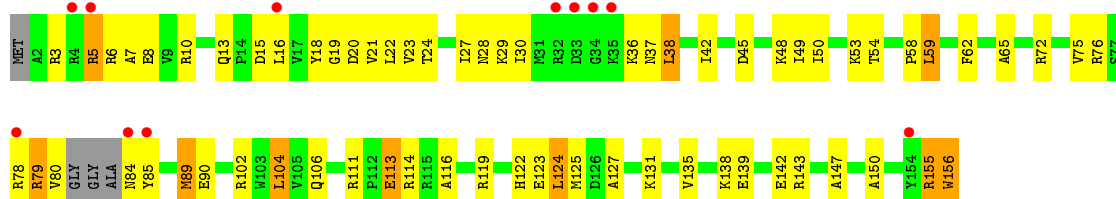
• Molecule 6: 30S ribosomal protein S6

Chain 52: 50% 43% 7% .



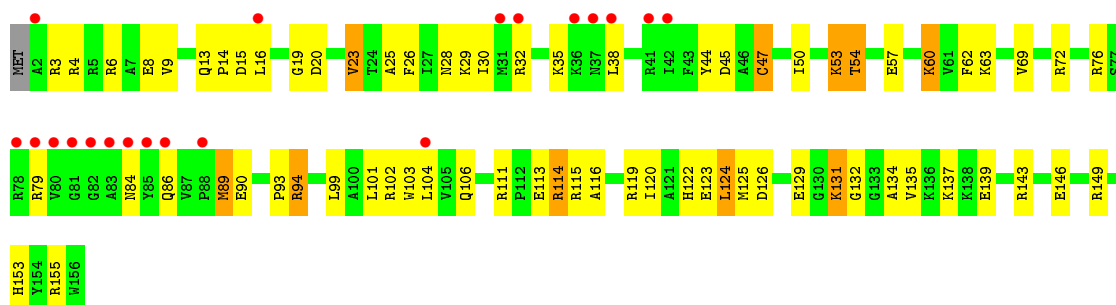
• Molecule 7: 30S ribosomal protein S7

Chain 6E: 7% 54% 37% 6% .



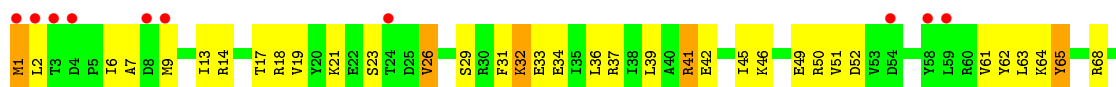
• Molecule 7: 30S ribosomal protein S7

Chain 62: 13% 54% 38% 6% .



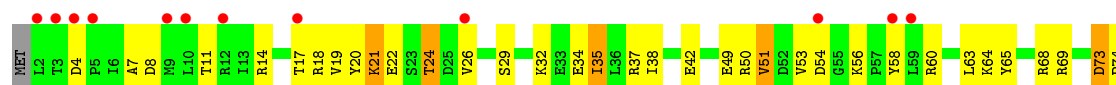
• Molecule 8: 30S ribosomal protein S8

Chain 7E: 20% 43% 46% 10% .

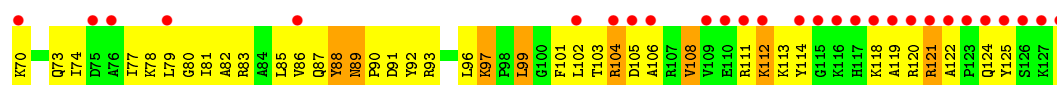
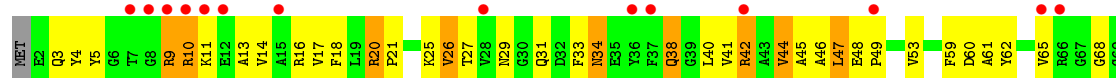




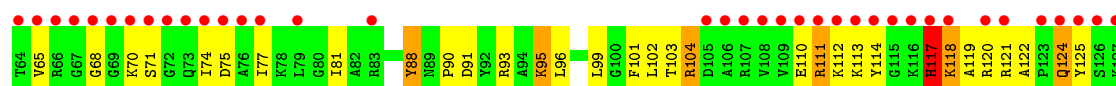
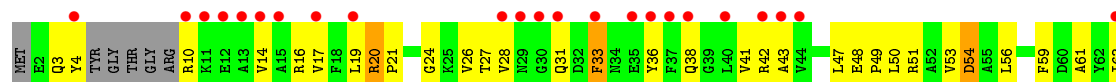
• Molecule 8: 30S ribosomal protein S8



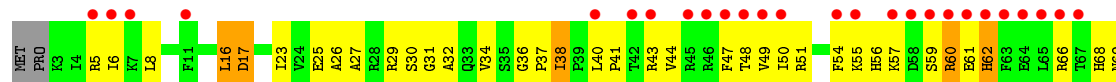
• Molecule 9: 30S ribosomal protein S9



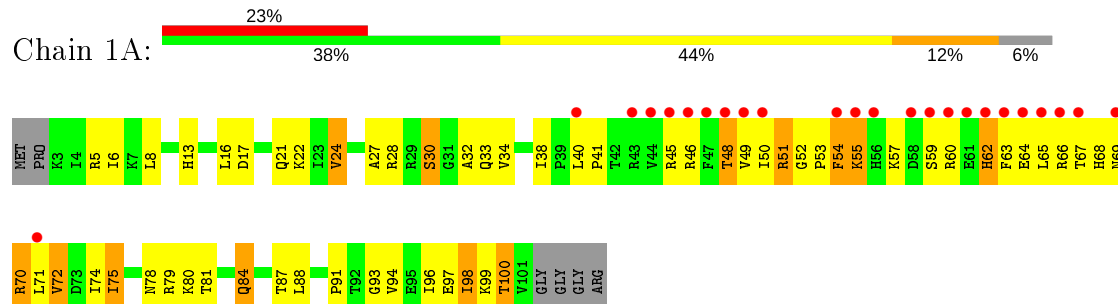
• Molecule 9: 30S ribosomal protein S9



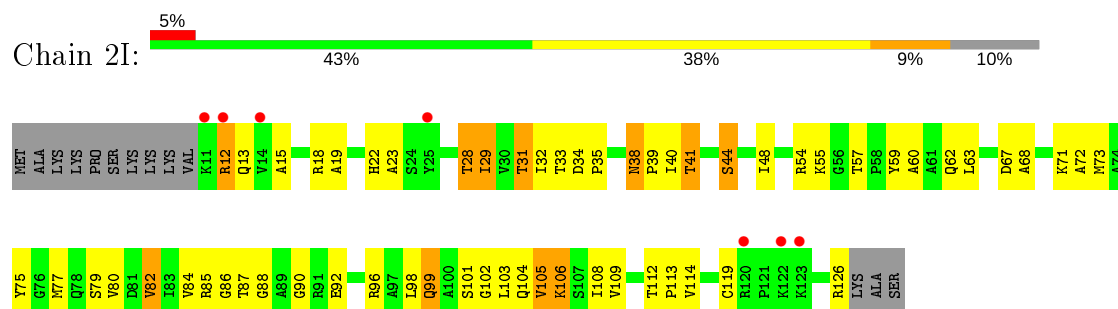
• Molecule 10: 30S ribosomal protein S10



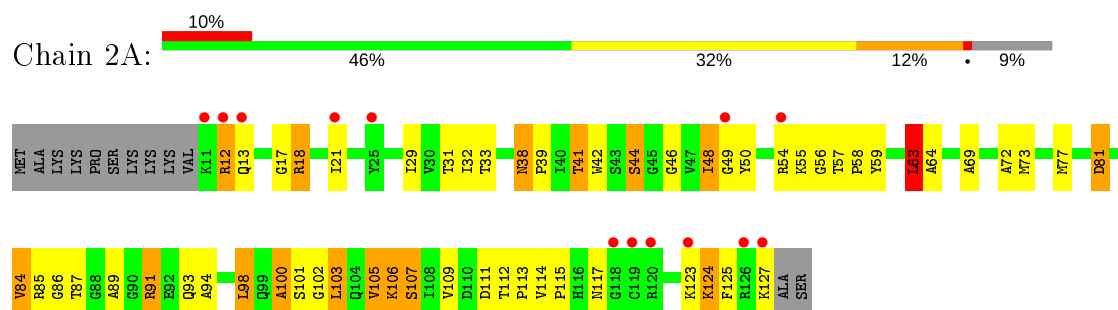
- Molecule 10: 30S ribosomal protein S10



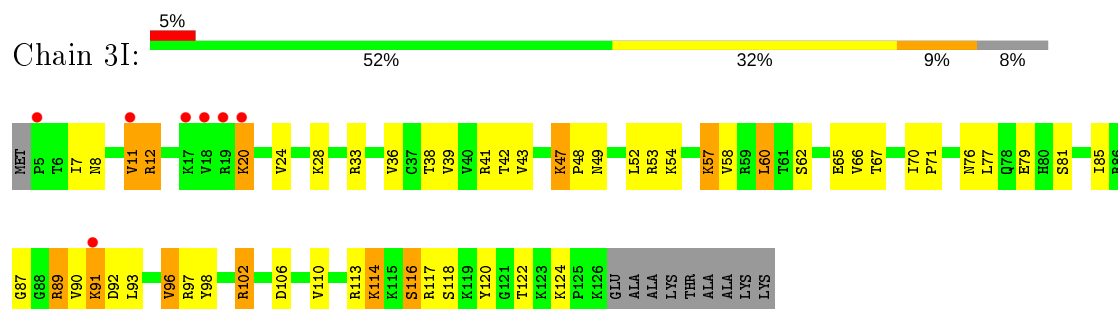
- Molecule 11: 30S ribosomal protein S11



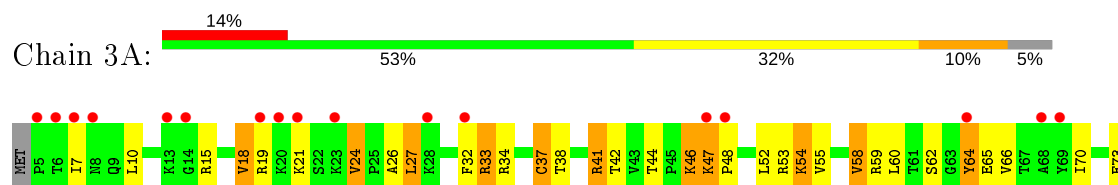
- Molecule 11: 30S ribosomal protein S11



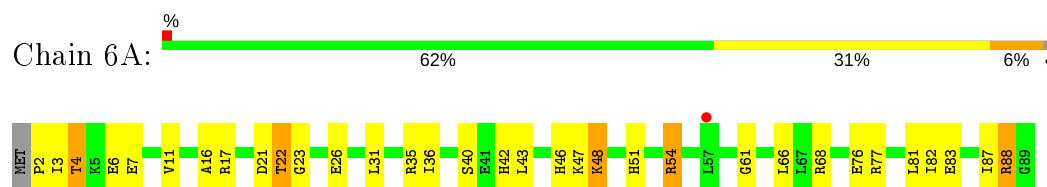
- Molecule 12: 30S ribosomal protein S12



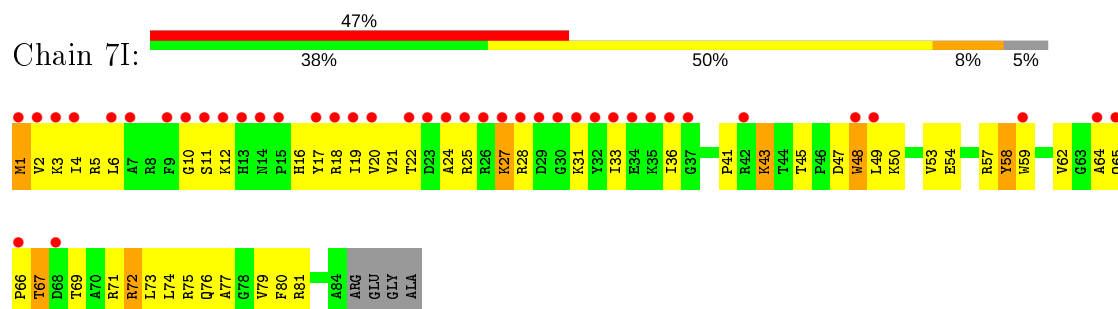
- Molecule 12: 30S ribosomal protein S12



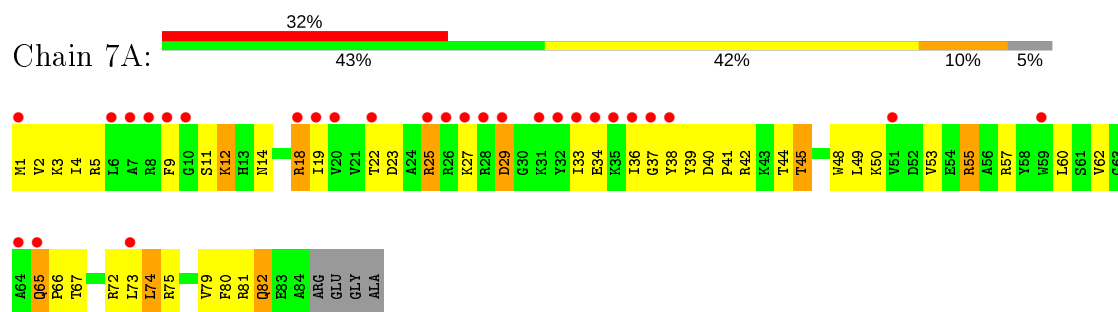
- Molecule 15: 30S ribosomal protein S15



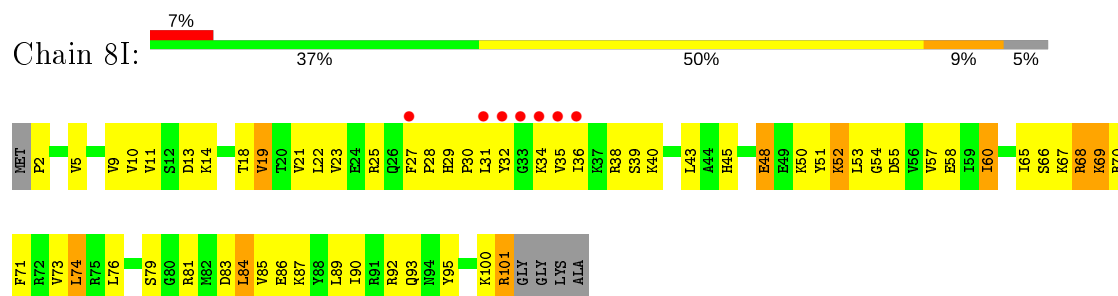
- Molecule 16: 30S ribosomal protein S16



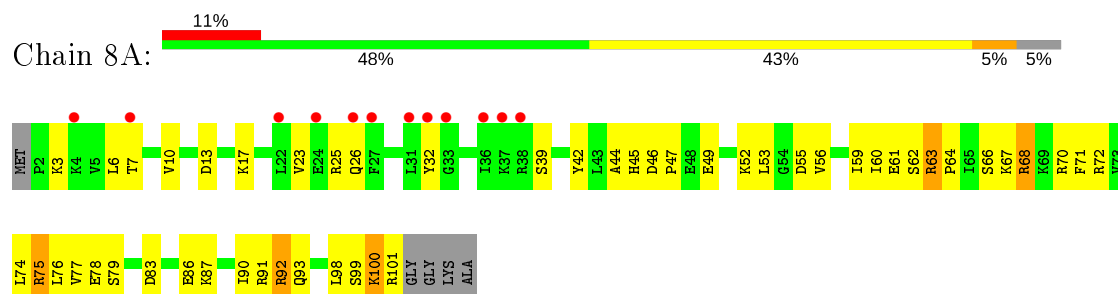
- Molecule 16: 30S ribosomal protein S16



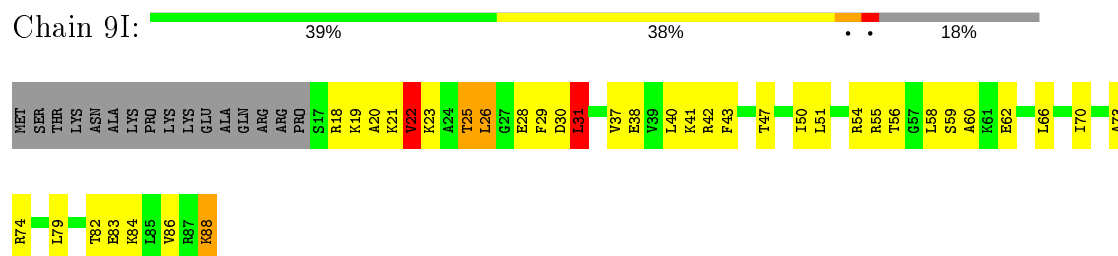
- Molecule 17: 30S ribosomal protein S17



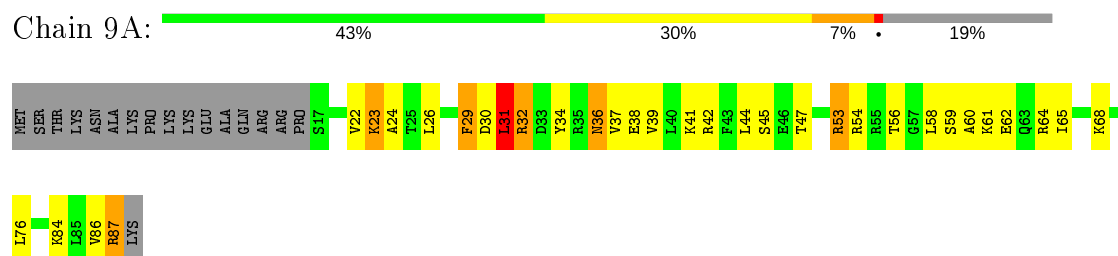
- Molecule 17: 30S ribosomal protein S17



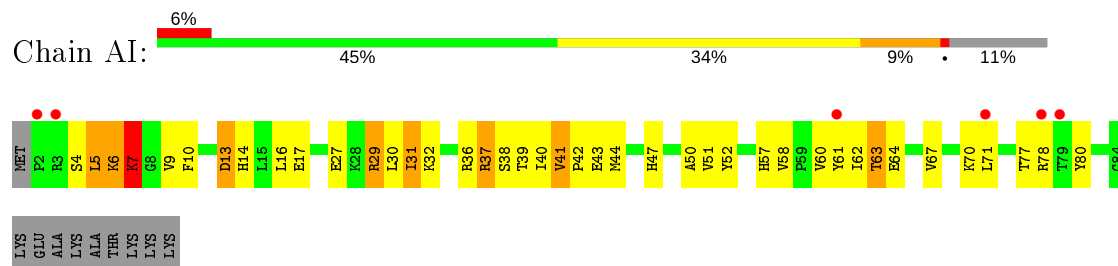
- Molecule 18: 30S ribosomal protein S18



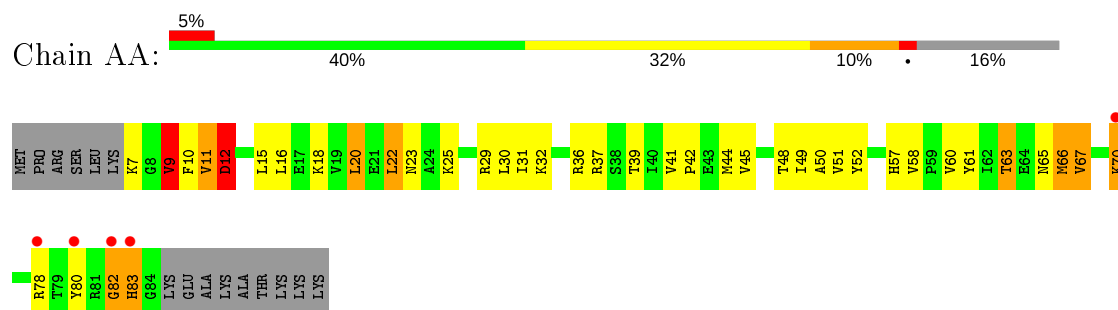
- Molecule 18: 30S ribosomal protein S18



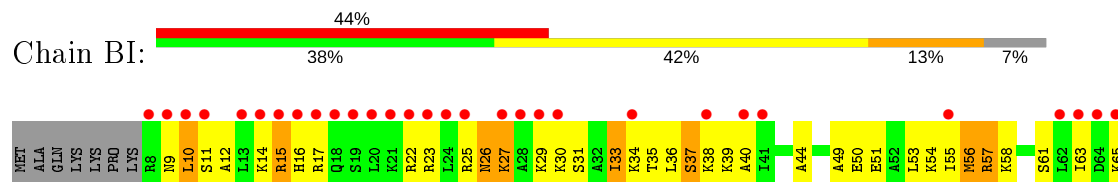
- Molecule 19: 30S ribosomal protein S19

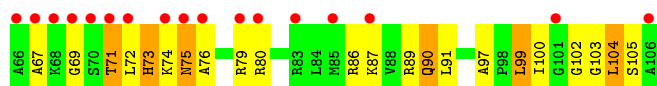


- Molecule 19: 30S ribosomal protein S19

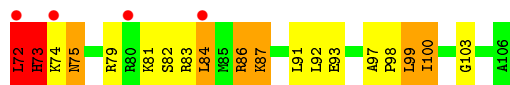
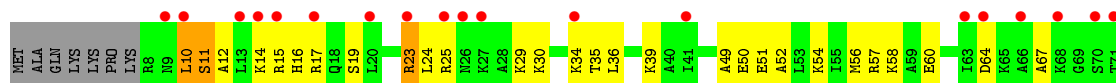


- Molecule 20: 30S ribosomal protein S20

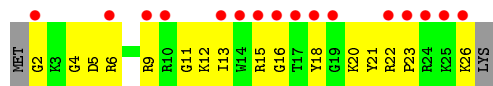




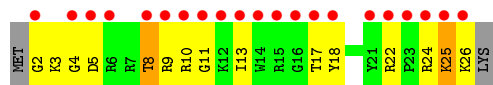
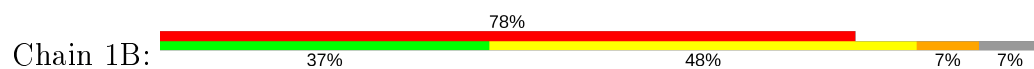
- Molecule 20: 30S ribosomal protein S20



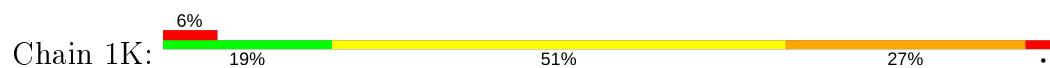
- Molecule 21: 30S ribosomal protein Thx



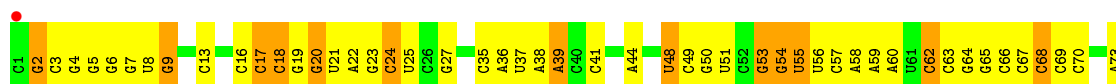
- Molecule 21: 30S ribosomal protein Thx



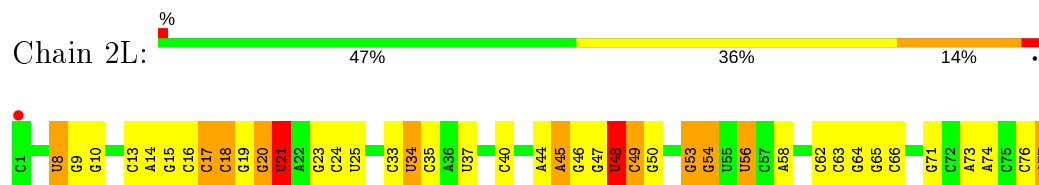
- Molecule 22: tRNA-Tyr



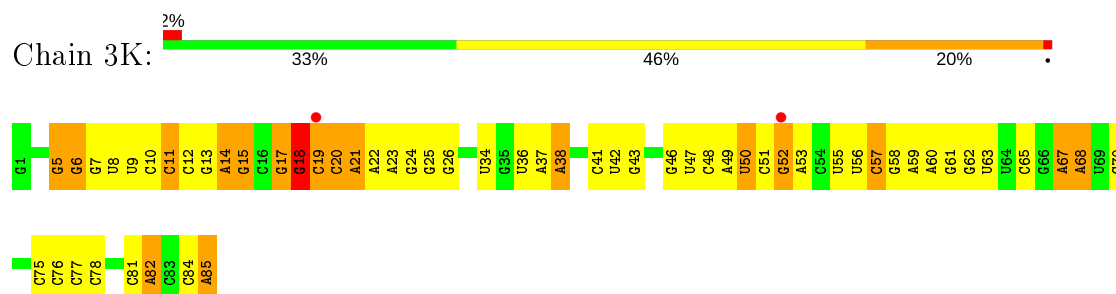
- Molecule 23: tRNA-fMet



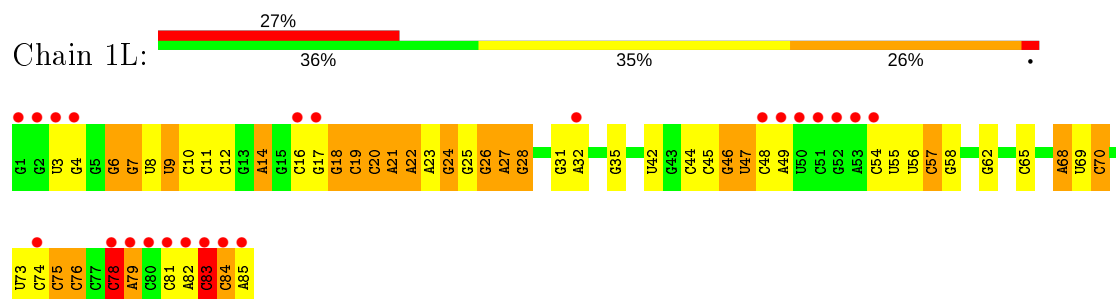
- Molecule 23: tRNA-fMet



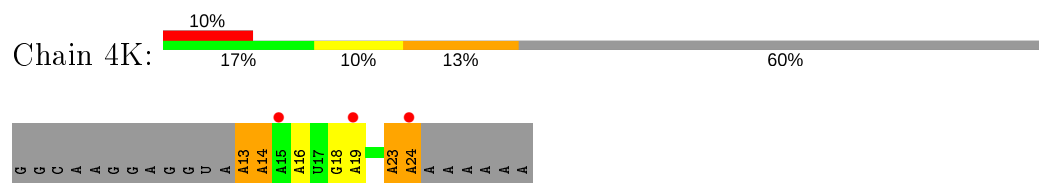
- Molecule 24: tRNA-Tyr



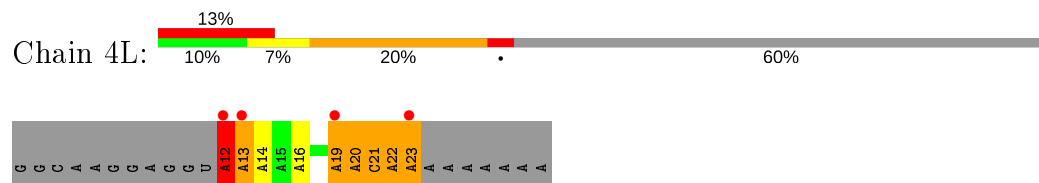
- Molecule 24: tRNA-Tyr



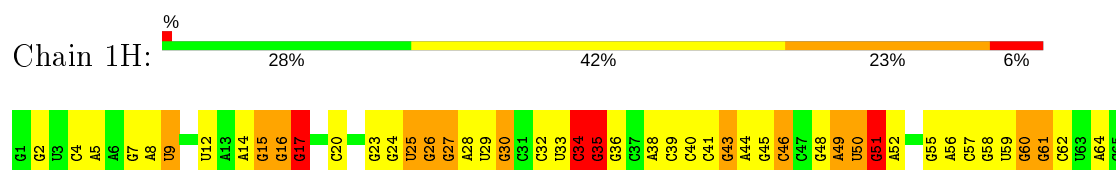
- Molecule 25: mRNA



- Molecule 25: mRNA

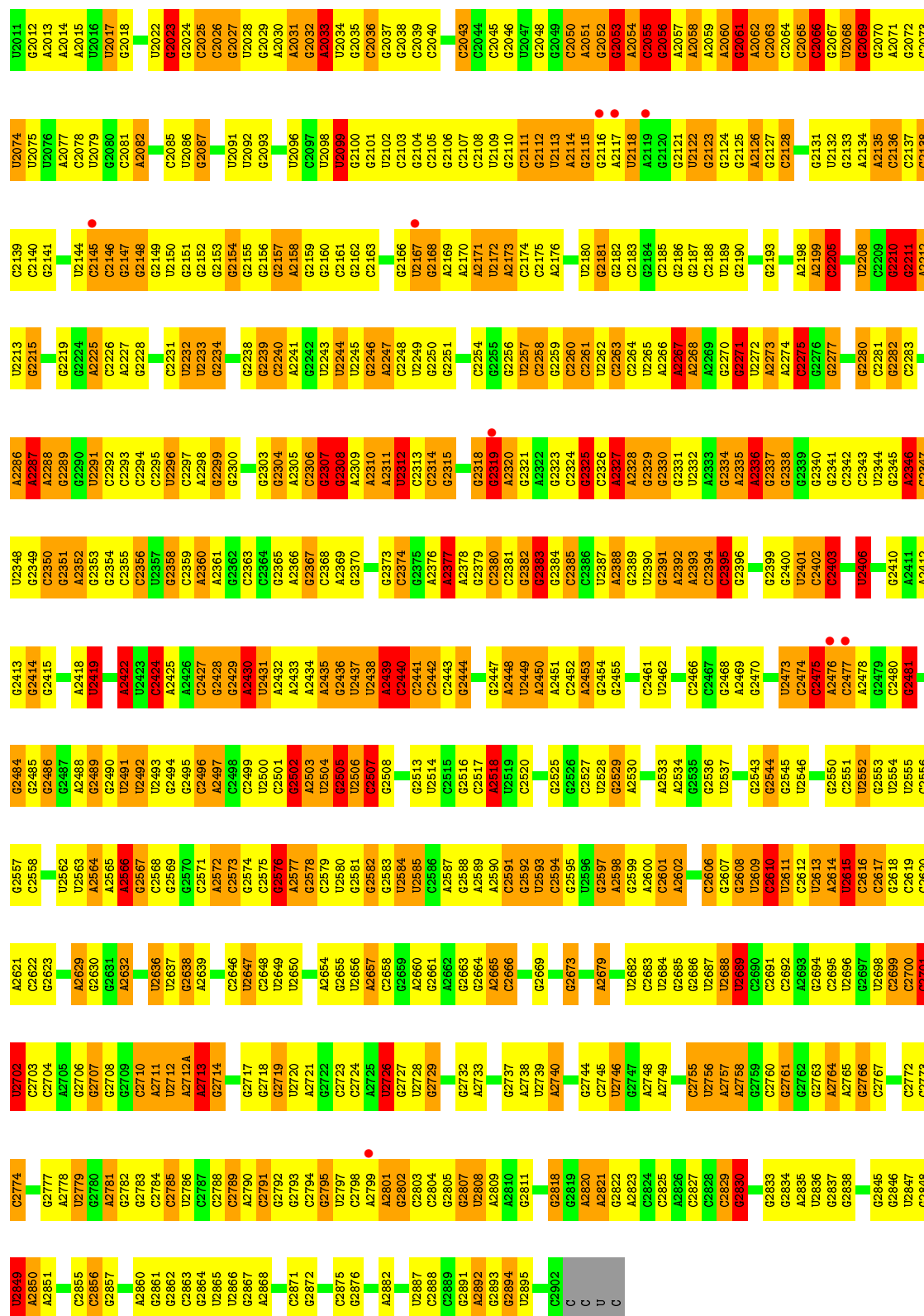


- Molecule 26: 23S ribosomal RNA



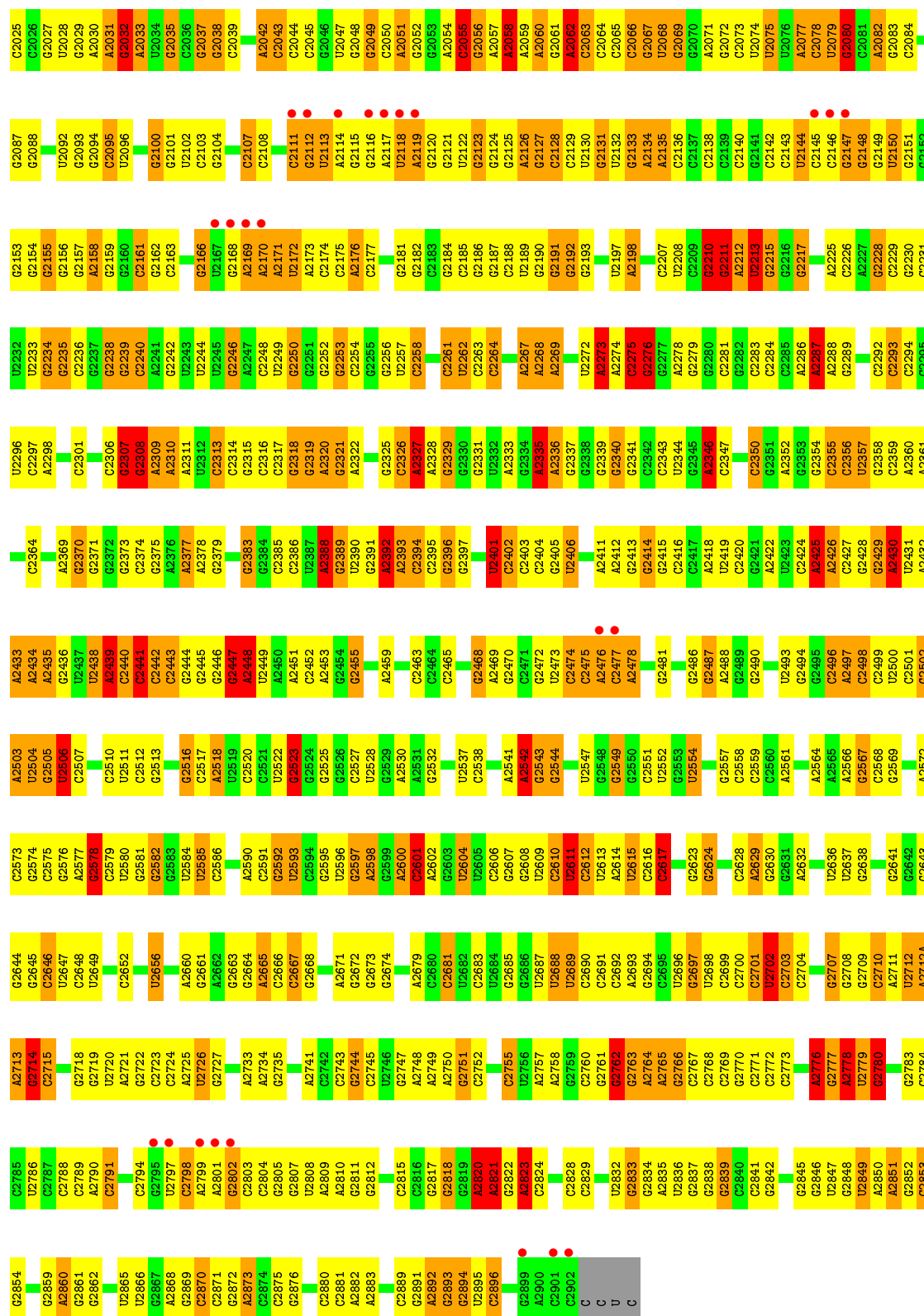
A884	U913	G845	A783	G654D	U607	U534	U459	G387	G321	C270H	C209	G134	G66
C985	G914	C946	A784	G654P	A608	C535	A460	G388	A322	C270K	C210	G138	U67
C986	G915	U947	G785	G654Q	G609	A536	C461	G389	G323	U270L	G214	G139	G68
G987	G916	G948	C786	G609A	C537	C537	C462	G390	G324	U270M	G215	A140	C69
A988	A917	A949	C787	A654T	G539	G539	C463	C392	G216	G270N	A216	A141	A71
A890	G919	G852	A788	A655	C611	C543	U464	G396	U328	G270O	A217	A142	U72
C991	G920	G853	C790	G656	U612	C544	A465	G397	G329	G270P	A218	C141A	A73
C992	C925	G854	C791	G657	U613	G545	A466	G398	A330	U270Q	G219	G142	A74
G993	G926	C855	C792	G658	U614	C546	A467	G399	A331	C270R	G220	C144	G75
C994	G927	C856	C793	G659	A616	C547	C468	G400	A332	G270S	A221	G76	C77
C995	G928	C857	A793	G660	G617	A548	C469	G401	G333	G270T	A222	G77	
A896	G929	U857	C796	G661	U618	A549	A470	C404	C334	C270U	A223	C148	G81
A896	U930	U858	C797	G662	G619	A550	A471	U405	C335	G270V	A224	A149	G82
G997	G931	G859	C798	G663	U620	G556	A472	G406	C336	G270W	G225	G152	G83
C998	G932	U860	G799	G664	G621	U557	G473	G407	C337	G270X	A226	C153	G84
U999	A933	A861	G799	G665	G622	G558	G474	G408	G227	G270Y	A227	G154	A84
A1000	G938	G862	A800	U667	A621	G559	A478	G409	U339	G271B	A228	C155	G85
A1001	G939	A863	G801	G668	G623	U562	A479	U410	A340	U271C	A229	U161	G88
G1002	G940	G864	A802	G669	G624	C563	A480	G411	G341	G271	U230	U162	G89
G1003	G941	C865	U803	A670	C624	C564	A481	G412	G342	G272	U231	U163	U90
C1004	G942	A866	A804	C671	A627	C565	A482	A415	C343	U273E	G232	U164	A91
C1005	G943	G870	G805	C672	G628	C566	A483	C416	G344	C273F	A233	U165	G92
C1006	G944	A871	U807	G673	A629	U567	A484	C417	G345	G274	C237	G171	G93
A1010	G945	A872	G808	G674	G630	U568	C485	G	G346	C275	C238	G172	
G1011	G946	C876	G809	A675	A631	U569	C486	G418	U350	A276	U239	G173	G98
U1012	G947	U877	U810	A676	A632	G570	C487	G419	G351	C277	G239	C174	U99
C1013	G948	U878	U811	G677	A633	C534	A491	G420	G352	C278	A241	G175	G101
U1014	G949	A878	U812	G678	C634	A571	A492	U421	G353	C279	G242	G176	G102
G950	G950	G879	U813	G679	C635	A572	C493	A422	G354		U243	G177	
C951	G951	G880	U814	G680	G636	G573	G494	A423	G355	A282	U244	G178	C105
G952	C951	G881	C815	G681	A637	C574	G495	G424	G356	C286	G245	G179	C106
U953	G953	G882	C816	G682	G638	A575	A501	G425	G357	C287	G246	G180	C107
A953	G954	G883	U817	G683	U639	U576	A502	G426	G358	C288	G247	G181	U108
C954	G955	C884	G818	G684	C641	A578	A503	U427	A359	G289	G248	G182	G109
U1023	U1023	C885	G819	G685	C642	G579	A504	A428	G360	C290	C249	C184	G110
G1024	G1024	C886	A821	C686	A643	C580	A505	U431	G361	C291	G250	U185	A111
G1025	A959	A887	U822	C687	A644	C581	A506	G432	G362		A251	G186	U112
U1026	A960	C888	G823	U688	C645	G582	A507	C433	G363	G295	G252	G187	G113
A1027	C961	C889	A824	G689	A646	C583	A508	G434	G363A	G296	G253	G188	U114
G1028	G962	A890	C825	C691	G647	C584	C509	G440	G363B	G298	G254	G189	C115
A1029	U963	G992	U826	C692	G648	G585	U511	U441	G363C	A299	A255	A190	C116
G1030	C964	C893	U827	C693	G649	A586	G512	G442	G363D	A300	A256	G192	G117
C965	C965	U895	A829	U694	C650	C587	C516	G443	U363E	G305	A257	C192	A118
G966	C966	A896	G830	G695	A654	C588	C517	C444	G364	U306	G258	U193	A119
C967	G967	C897	G831	C697	A654B	C589	G518	G445	G370	G307	G259	A195	U120
U1033	U1033	C898	G832	C698	G654C	C590	U519	A447	A371	G308	G260	A196	G121
G1034	G1034	A899	U833	C699	G654D	A590	G520	U448	G372	G309	G261	A197	G122
C1035	C1035	A900	C834	G700	G654E	G593	U524	A449	C376	A310	A265	C198	G123
G1036	G1036	A901	A835	G701	G654F	G594	U525	G450	G377	A311	G266	A199	G124
U1037	U1037	C899	G836	G702	G654G	G595	U526	C451	U380	G312	U267	A199	G125
C1038	C1038	A902	G837	G703	G654H	G596	A526	G452	G313	U269	G268	U200	G126
G1039	G1039	C900	C838	G704	G654I	G600	C527	G453	G314	C201	A127	C201	A127
C1040	C1040	U901	G839	G705	A654J	C601	A528	C454	A314	U202	C128	U202	C128
G1041	G1041	G906	U839	A706	G654K	G602	A529	C455	G315	C270C	C129	C129	C129
C1042	C1042	U907	C940	A707	G654L	A603	G530	C456	G316	G270D	A204	A204	C130
A1045	A1045	U908	A841	U709	G654M	G604	C531	C457	C319	U270E	G270F	A207	G131
A1046	A1046	C909	G842	G710	G654N	G605	A532	A458	G385	A270F	C270G	A207	G132
G1047	G1047	A910	G843	G711	G654O	G606	G533	G459	G386	C270G	C270G	C208	C133

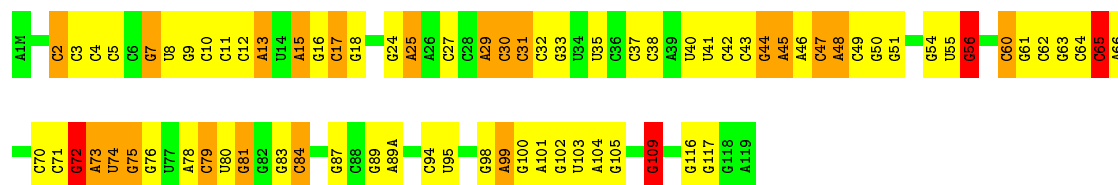
G1844	G1858	A1786	G1695	G1633	G1506	C1437	G1374	G1311	G1245	G1176	A1111	A1050
G1945	A1859	A1787	G1696	A1634	A1507	G1440	C1375	U1312	A1246	A1177	G1112	G1051
C1947	G1860	G1790	G1697	G1635	A1508	G1441	C1376	U1313	G1247	C1178	U1113	
		A1791	A1698	G1636	C1509	G1442	G1377	G1314	G1248	C1179	G1114	A1054
G1950	U1864	A1792	G1699	A1637	A1510	G1443	A1378	U1315	U1249	G1180	G1115	G1055
U1951	C1870	G1793	G1700	G1638	A1511	G1444	A1379	U1316	G1250	G1181	G1116	G1056
A1952			G1705	G1639	G1512	G1444A	G1380	A1317	G1251	A1182	G1117	A1057
			U1706	G1640	C1513	A1444A	G1381	C1318	G1252	G1183	G1118	U1058
U1955	G1878	U1794	U1706	A1641	U1514	A1445	G1382	C1319	G1253	G1184		U1059
U1956	C1879	U1796		G1642	C1515	G1446	C1383	G1319	A1254	U1060		U1061
C1957		U1716	U1716	G1643	U1516	G1447	A1384	A1321	G1255	G1186	G1122	G1062
C1958	G1882	G1717	G1717	G1644	G1517	G1448	G1385	U1322	G1256	G1187	G1124	G1063
G1959	A1884	U1727	U1727	G1645	C1518	A1449	C1386	U1323	G1257	A1188	G1125	G1064
				G1646	G1519	G1449A	C1387	G1324	C1258	A1189	A1126	
				G1647	U1520		G1388	G1325	G1259	G1190	A1127	U1065
				G1648	U1521		G1389	U1326	G1260	G1191	A1128	U1066
				G1649	G1522		U1390	C1327	G1261	G1192	A1129	A1067
				G1650			U1391	G1328	A1262	G1193	U1130	G1068
				G1651	G1525		U1392	U1329	U1263	A1194	G1131	A1069
				G1652	G1526		A1393	C1330	G1264	G1195	A1132	A1070
				G1653	G1527		U1394	A1331	A1265		U1133	G1071
				G1654	G1528		A1395	C1332	G1266	U1198	G	G1072
				G1655	A1529		U1396	C1333	U1267	U1199	C1135	A1073
				G1656	A1530		U1397	G1334	A1268	G1200	G1136	G1074
				G1657	C1531		G1461	U1398	A1269	C1201	G1137	C1075
				G1658	G1532		C1463	U1399	C1270	C1202	G1138	G1076
				G1659	C1533		G1464	G1400	G1271	G1203	G1139	A1077
				G1660	G1534		A1470	A1401	A1272	A1204	C1140	A1078
				G1661	U1535		G1471	C1402	G1281	U1205	G1141	G1079
				G1662	C1536		G1472	C1345			C1145	A1085
				G1663	G1537		G1473	G1346			G1149	A1086
				G1664	C1538		G1474	G1347	A1284	G1215	G1150	G1087
				G1665	G1539		A1475	G1348		G1216	G1151	A1088
				G1666	U1540		A1476	A1349			G1154	G1089
				G1667	G1541		G1477	U1352	U1288	G1219	G1155	U1090
				G1668	G1542		G1478	G1355	C1289	C1221	A1156	G1091
				G1669	A1543		G1479	G1356	C1290	C1222	A1157	C1092
				G1670	C1544		U1480	U1357	C1291	G1223	G1158	G1093
				G1671	A1545		U1481	G1358		G1224	C1159	U1094
				G1672	A1545A		U1482	G1359		A1095	U1159	A1096
				G1673	C1546		U1483	A1423	C1295	G1225	G1160	U1097
				G1674	C1547		U1484	G1424	G1296	G1226	C1161	A1098
				G1675	C1548		U1485	G1425	C1297	A1227	G1162	G1099
				G1676	C1549		U1486	G1426	C1298	G1228	G1163	A1099
				G1677	C1550		U1487	U1489	G1299	G1229	G1164	G1099
				G1678	A1554		G1488		U1300	G1229A	G1164	C1100
				G1679	G1555		U1489	C1363	A1301	C1230	U1165	U1101
				G1680	C1556		G1490	G1364	A1302	G1231	C1166	C1102
				G1681	G1557		U1491	A1365	G1296	G1232	C1167	A1103
				G1682	C1558		U1492	A1366	C1297	G1233	G1168	C1104
				G1683	A1559		U1493	A1367	C1298	G1234	G1169	U1105
				G1684	G1560		U1494	G1368	G1299	G1235	G1170	G1106
				G1685	G1561		U1495	G1369	U1300	U1240	G1171	G1107
				G1686	A1562		U1496	C1432	A1301	A1241	G1172	U1108
				G1687	G1563		U1497	C1433	A1302	G1242	G1173	C1109
				G1688	C1564		U1498	U1502	A1303	G1307	A1174	
				G1689	A1565		U1499	C1505	G1308	G1310	U1175	G1110
				G1690	G1566		U1500					
				G1691	A1567		U1501					
				G1692	A1568		U1502					
				G1693	A1569		U1503					
				G1694	A1570		U1504					
				G1695	A1571		U1505					
				G1696	A1572		U1506					
				G1697	A1573		U1507					
				G1698	A1574		U1508					
				G1699	A1575		U1509					
				G1700	A1576		U1510					
				G1701	A1577		U1511					
				G1702	A1578		U1512					
				G1703	A1579		U1513					
				G1704	A1580		U1514					
				G1705	A1581		U1515					
				G1706	A1582		U1516					
				G1707	A1583		U1517					
				G1708	A1584		U1518					
				G1709	A1585		U1519					
				G1710	A1586		U1520					
				G1711	A1587		U1521					
				G1712	A1588		U1522					
				G1713	A1589		U1523					
				G1714	A1590		U1524					
				G1715	A1591		U1525					
				G1716	A1592		U1526					
				G1717	A1593		U1527					
				G1718	A1594		U1528					
				G1719	A1595		U1529					
				G1720	A1596		U1530					
				G1721	A1597		U1531					
				G1722	A1598		U1532					
				G1723	A1599		U1533					
				G1724	A1600		U1534					
				G1725	A1601		U1535					
				G1726	A1602		U1536					
				G1727	A1603		U1537					
				G1728	A1604		U1538					
				G1729	A1605		U1539					
				G1730	A1606		U1540					
				G1731	A1607		U1541					
				G1732	A1608		U1542					
				G1733	A1609		U1543					
				G1734	A1610		U1544					
				G1735	A1611		U1545					
				G1736	A1612		U1546					
				G1737	A1613		U1547					
				G1738	A1614		U1548					
				G1739	A1615		U1549					
				G1740	A1616		U1550					
				G1741	A1617		U1551					
				G1742	A1618		U1552					
				G1743	A1619		U1553					
				G1744	A1620		U1554					
				G1745	A1621		U1555					
				G1746	A1622		U1556					
				G1747	A1623		U1557					
				G1748	A1624		U1558					
				G1749	A1625		U1559					
				G1750	A1626		U1560					
				G1751	A1627		U1561					
				G1752	A1628		U1562					
				G1753	A1629		U1563					
				G1754	A1630		U1564					
				G1755	A1631		U1565					
				G1756	A1632		U1566					
				G1757	A1633		U1567					
				G1758	A1634		U1568					
				G1759	A1635		U1569					
				G1760	A1636		U1570					
				G1761	A1637		U1571					
				G1762	A1638		U1572					
				G1763	A1639		U1573					
				G1764	A1640		U1574					
				G1765	A1641		U1575					
				G1766	A1642		U1576					
				G1767	A1643		U1577					
				G1768	A1644		U1578					
				G1769	A1645		U1579					
				G1770	A1646		U1580					
				G1771	A1647		U1581					
				G1772	A1648		U1582					
				G1773	A1649		U1583					
				G1774	A1650		U1584					
				G1775	A1651		U1585					
				G1776	A1652		U1586					
				G1777	A1653		U1587					



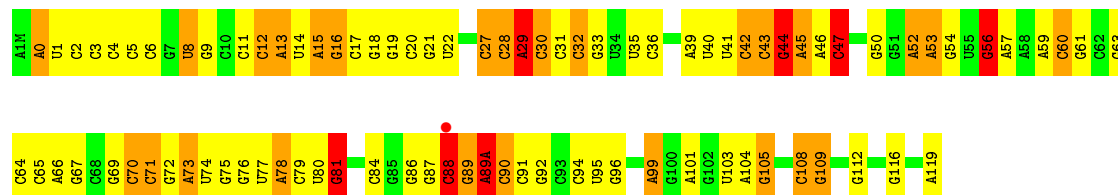
A941	G942	U943	G944	A945	G946	C949	G950	C951	G952	A953	G956	A957	U958	A959	A960	C961	G962	U963	G964	C965	G966	C967	G968	U969	C970	U971	G972	A973	G974	C974A	G977	A980	A981	C982	A983	A984	C985	C986	G987	A988	G989	A990	C991	C992	G993	A996	G997	C998	U999	G999	A1000	A1001	G1002	C1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
U877	G878	G879	G880	G881	G882	G883	A884	C885	C886	A887	C888	C889	A890	G892	C893	C894	U895	A896	C897	C898	G899	A900	C901	G902	C903	C904	U905	G906	U907	C908	A909	A910	U911	C912	U913	C914	G915	G916	A917	A918	G919	C920	G921	U922	C923	C924	C925	A926	G928	G929	G932	A933	G934	C935	G938																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U811	C812	U813	C814	C817	G818	A819	A820	A821	U822	G823	A824	C825	U826	U827	U828	A829	G830	G831	G832	U833	C834	A835	C836	C837	C838	C939	U940	C941	G942	C943	G944	A945	A946	C947	G948	G949	G952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
A746	U747	G748	C749	A750	A751	A752	C753	U757	C758	A761	U762	G763	A764	G765	G766	U767	G768	G769	G770	G771	C772	U773	C774	A775	G776	G777	U778	G779	C780	A781	A782	A783	A784	G785	C786	U787	A788	G789	C790	C791	G792	A793	U794	C795	C796	C797	A800	G801	A802	U803	A804	G805	C806	U807	C808	U809	A810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U421	G422	G423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	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

C1947	G1945	G1949	G1950	U1951	A1952	U1955	C1958	C1961	C1962	U1963	C1964	C1965	A1966	C1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	A1978	C1979	G1980	U1915	G1987	G1988	G1989	C1990	G1991	G1992	U1993	C1994	U1995	C1996	C1999	G2000	A2001	G2002	A2005	G2010	A2014	A2015	U2016	U2017	G2018	A2019	U2022	G2023	G2024																																																																																																																																																																																																																																																																																																																																																																																																															
G1883	A1884	A1885	C1886	G1887	G1888	A1889	A1890	G1891	C1892	C1893	C1894	C1895	G1896	A1897	U1898	A1899	A1900	A1901	G1902	G1903	A1904	C1905	G1906	G1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	U1926	A1927	A1928	G1929	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	U1940	G1941	G1942	U1943	U1944	G1945	U1946																																																																																																																																																																																																																																																																																																																																																																																																		
U1798	G1799	C1800	G1801	A1802	A1803	C1804	U1805	C1806	A1807	C1808	U1809	A1810	G1811	G1812	G1813	A1814	A1815	G1816	G1817	U1818	A1819	A1820	A1821	G1822	G1823	G1824	A1825	A1826	C1827	G1828	G1829	A1830	U1831	U1832	U1833	U1834	G1835	C1836	C1837	C1838	G1839	A1840	A1841	A1842	A1843	A1844	A1845	A1846	A1847	A1848	G1849	G1850	G1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	G1873	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																																																																																																																																																																																																																																																																																																													
G1712	U1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	G1771	G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	G1900	G1901	G1902	G1903	G1904	G1905	G1906	G1907	G1908	G1909	G1910	G1911	G1912	G1913	G1914	G1915	G1916	G1917	G1918	G1919	G1920	G1921	G1922	G1923	G1924	G1925	G1926	G1927	G1928	G1929	G1930	G1931	G1932	G1933	G1934	G1935	G1936	G1937	G1938	G1939	G1940	G1941	G1942	G1943	G1944	G1945	G1946																																																																																																																																																																																																																										
A1571	A1572	G1573	G1574	G1575	G1576	G1577	G1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	G1590	G1591	G1592	G1593	G1594	G1595	A1596	A1597	A1598	A1599	A1600	G1601	A1602	A1603	C1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	C1612	C1613	A1614	C1615	A1616	C1617	A1618	G1619	G1620	U1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	C1631	G1632	G1633	A1634	G1635	C1636	A1637	C1638	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																																																																										
U1497	C1498	C1499	G1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946
U1422	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																																																																																																																																																																																																																																																																																																																																																																																																																																		

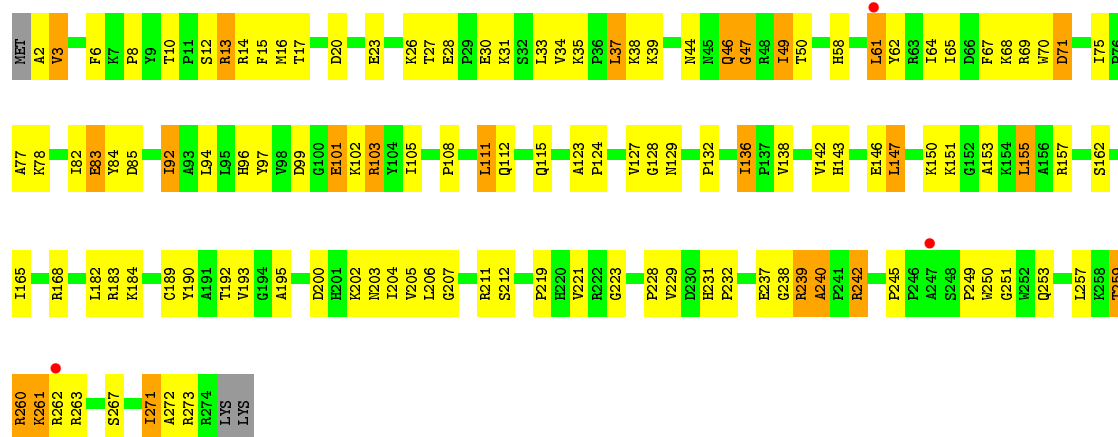




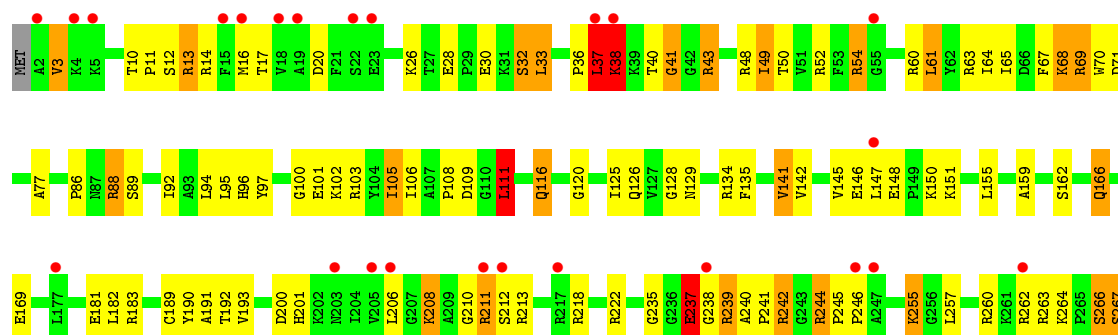
• Molecule 27: 5S ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

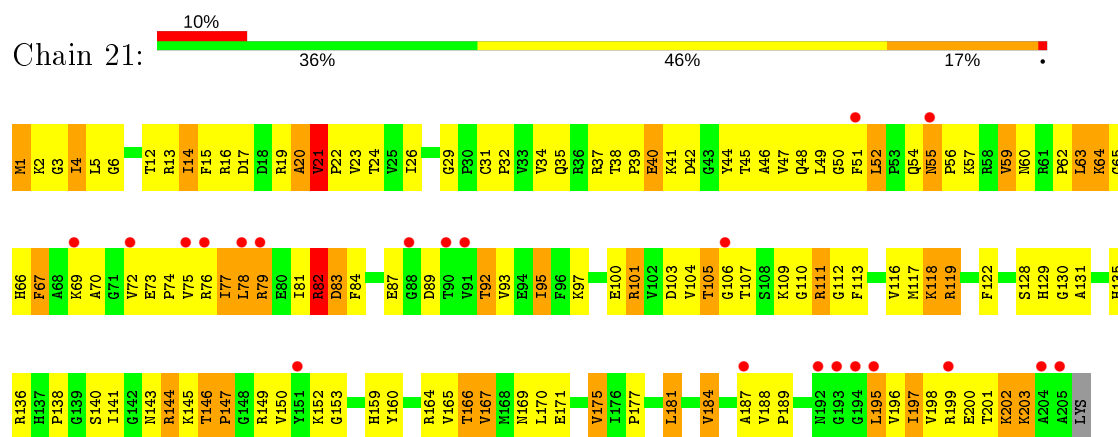


• Molecule 28: 50S ribosomal protein L2

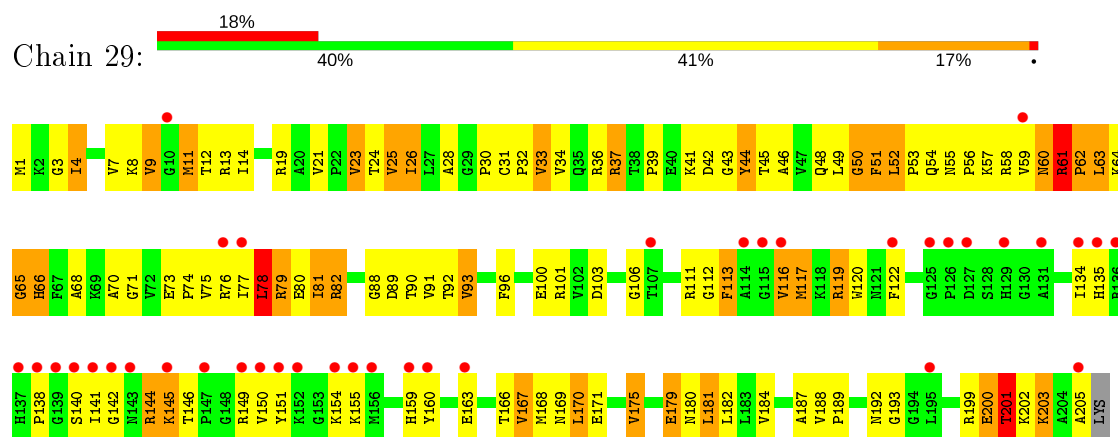




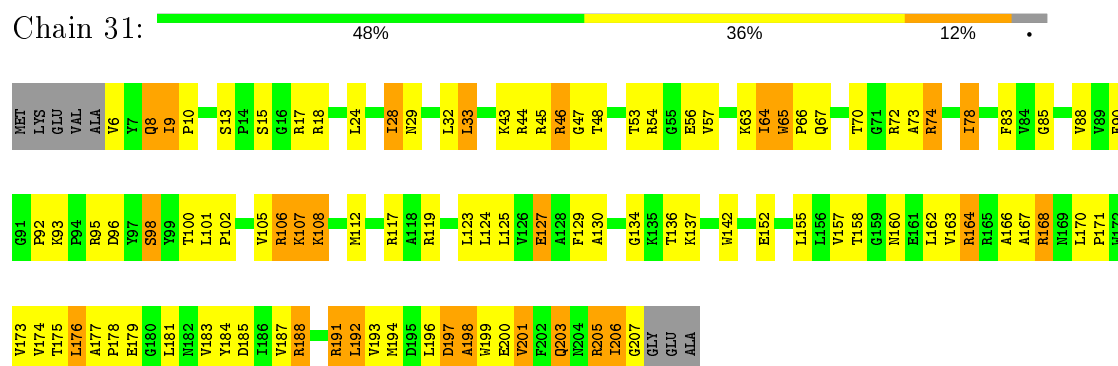
- Molecule 29: 50S ribosomal protein L3



- Molecule 29: 50S ribosomal protein L3

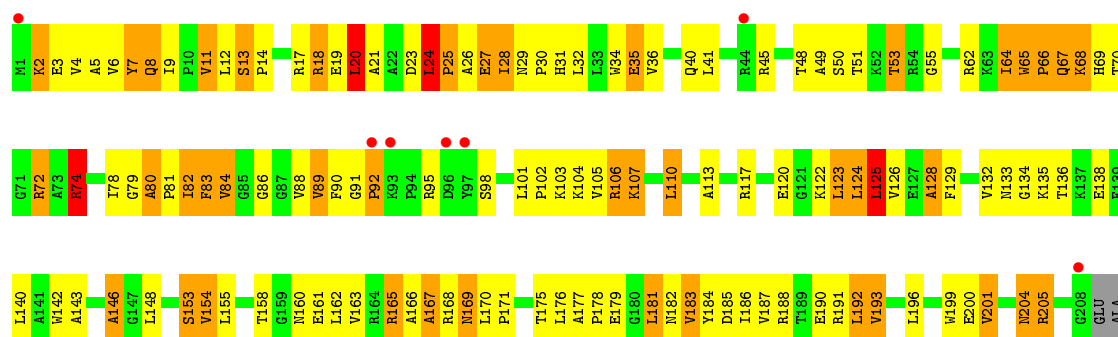


- Molecule 30: 50S ribosomal protein L4

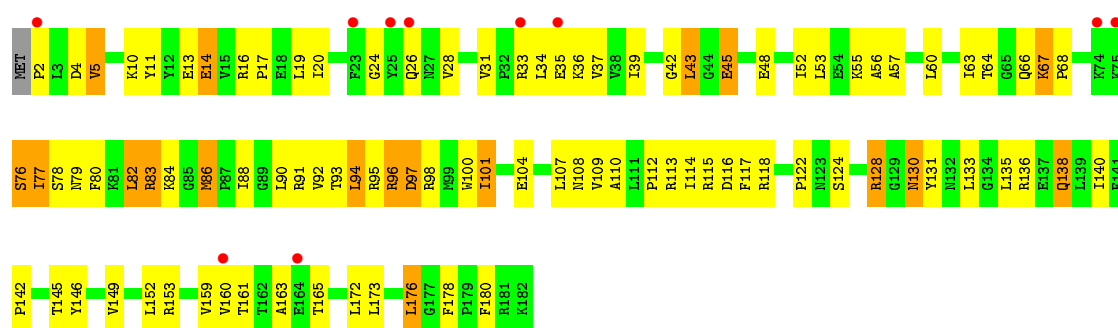


- Molecule 30: 50S ribosomal protein L4

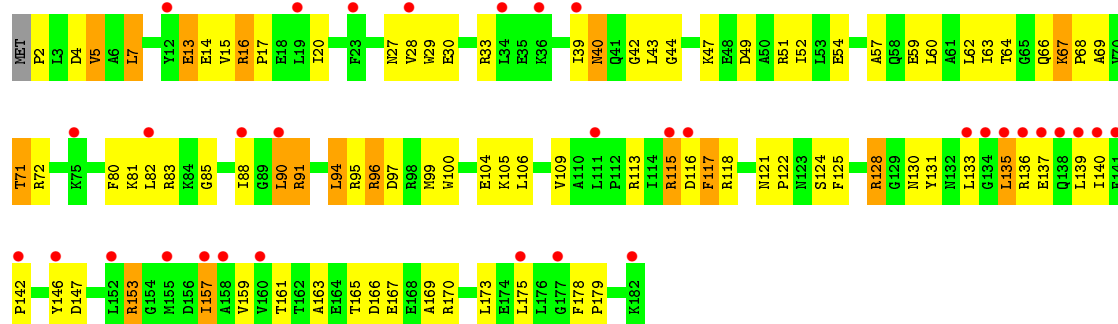




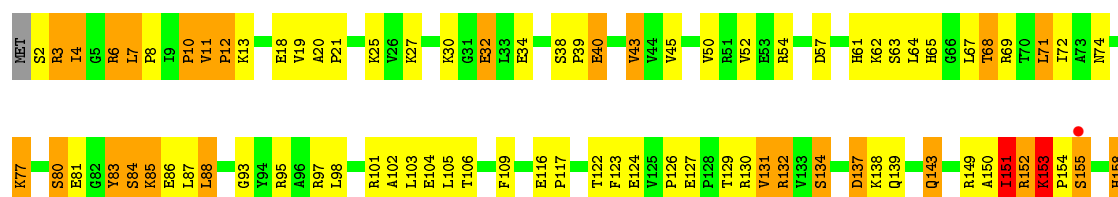
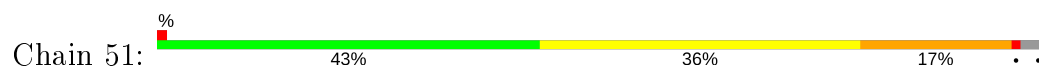
• Molecule 31: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L5

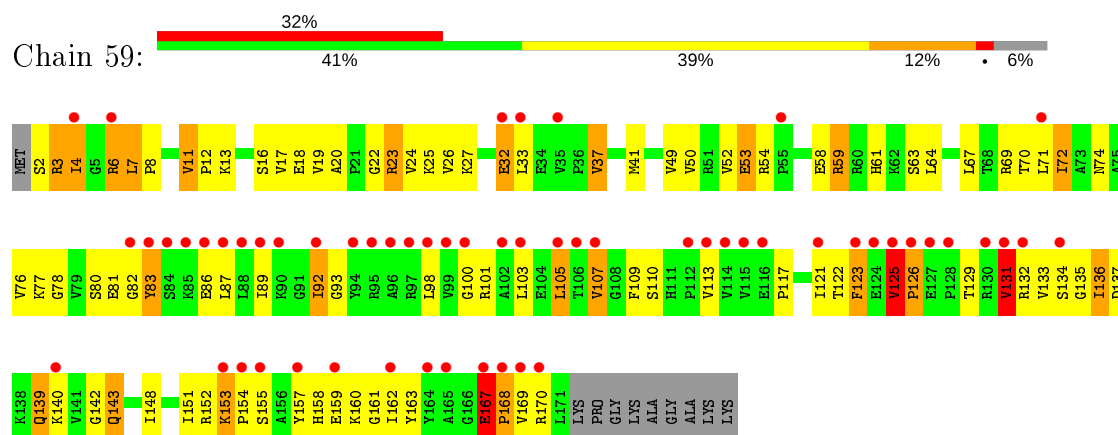


• Molecule 32: 50S ribosomal protein L6

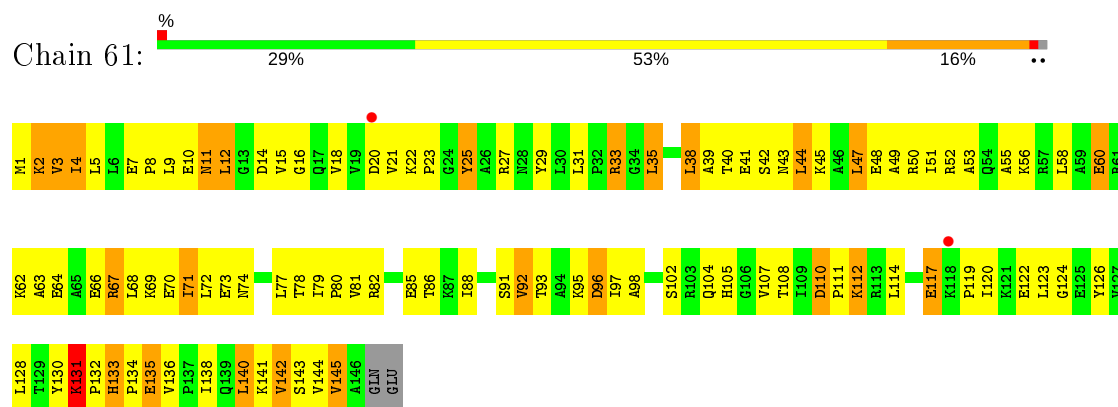




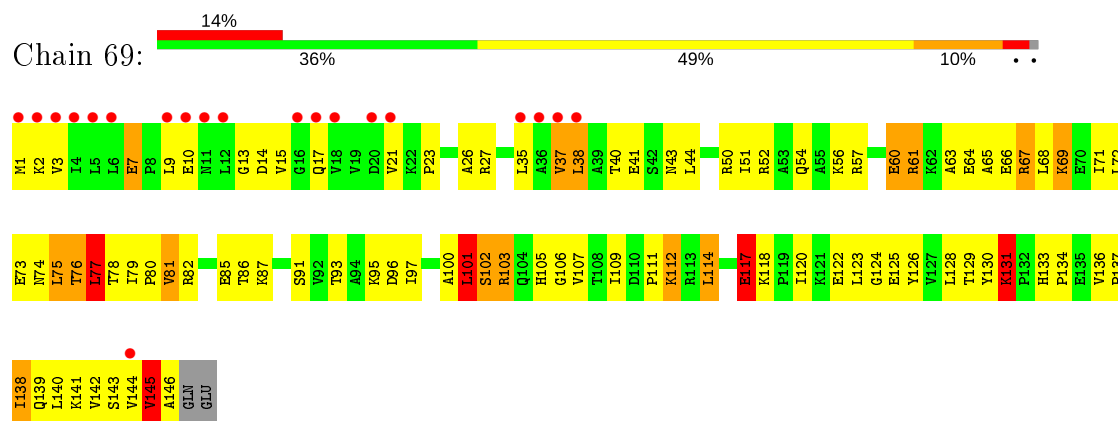
• Molecule 32: 50S ribosomal protein L6



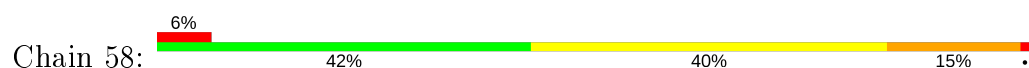
• Molecule 33: 50S ribosomal protein L9

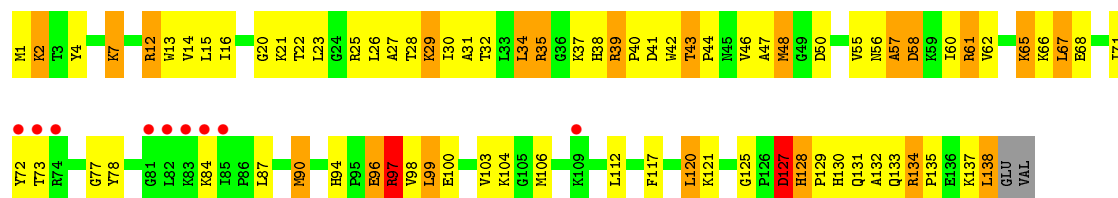


• Molecule 33: 50S ribosomal protein L9

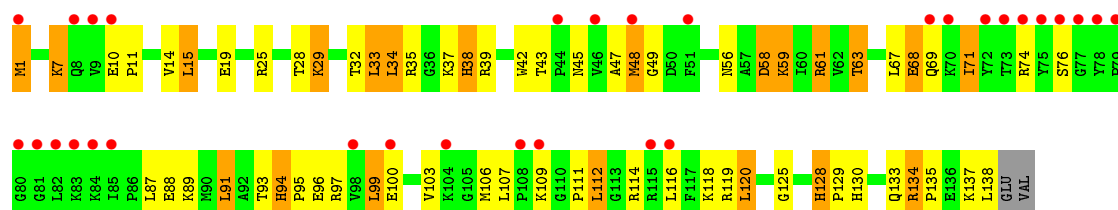


• Molecule 34: 50S ribosomal protein L13

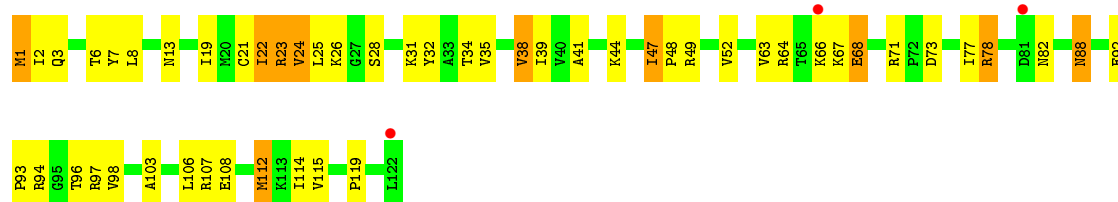




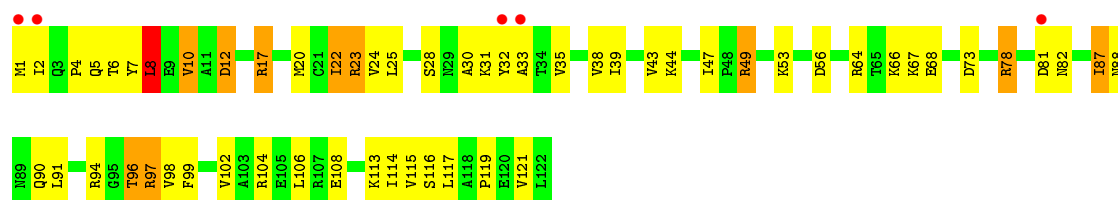
• Molecule 34: 50S ribosomal protein L13



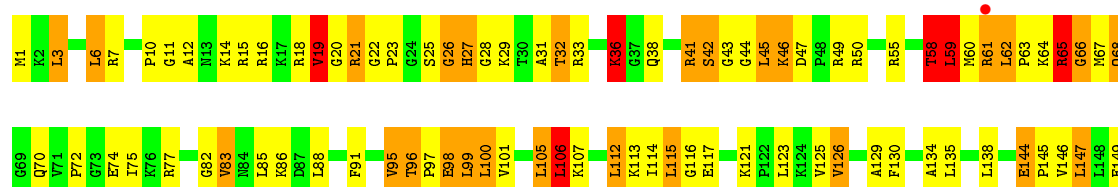
• Molecule 35: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L14

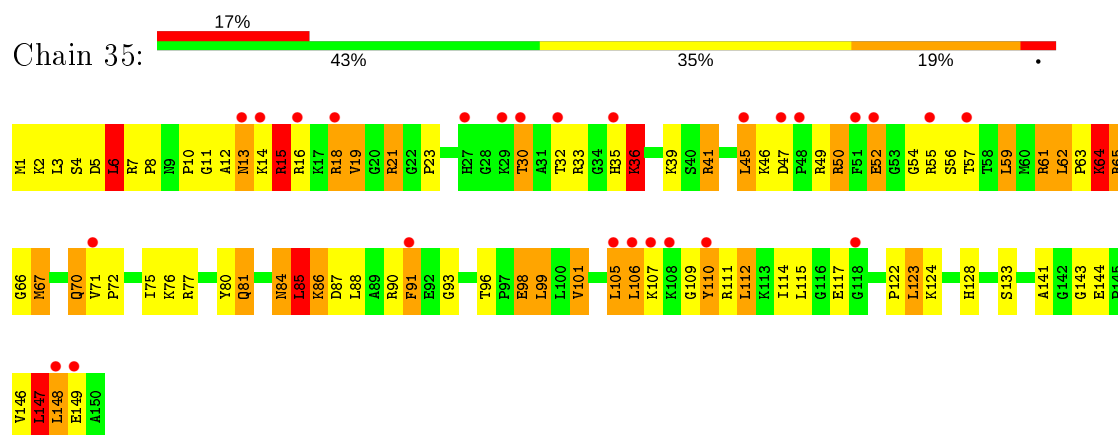


• Molecule 36: 50S ribosomal protein L15

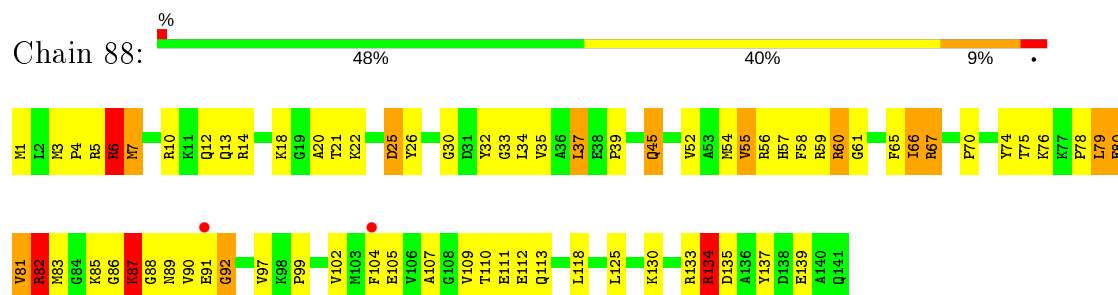


A150

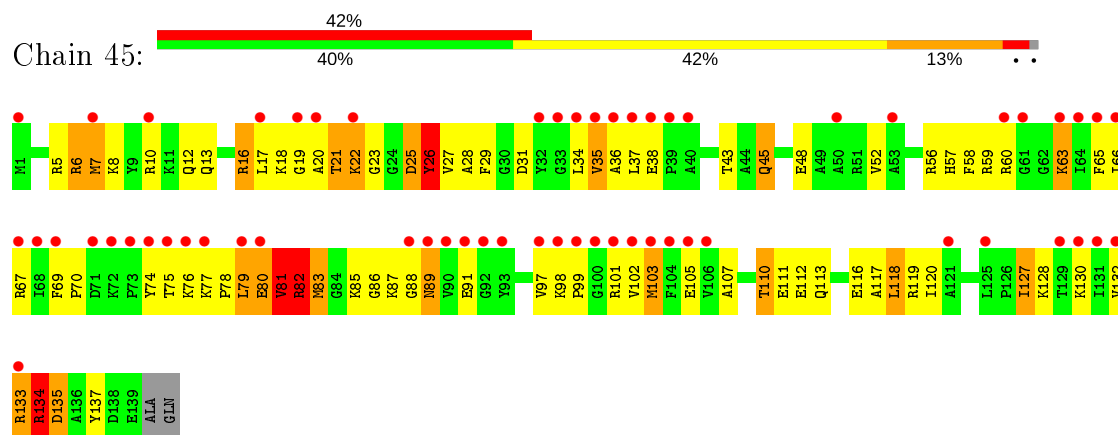
- Molecule 36: 50S ribosomal protein L15



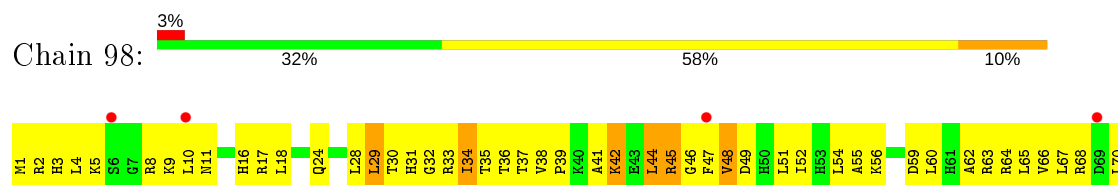
- Molecule 37: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L16

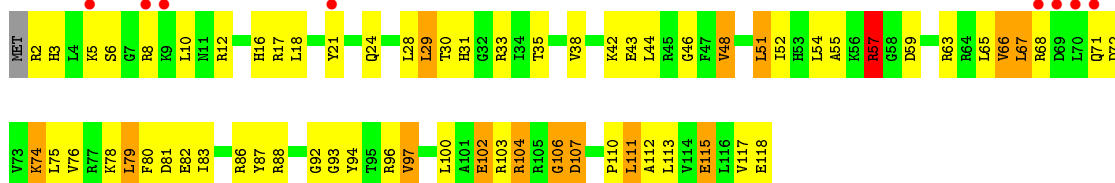
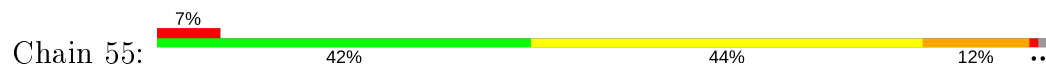


- Molecule 38: 50S ribosomal protein L17

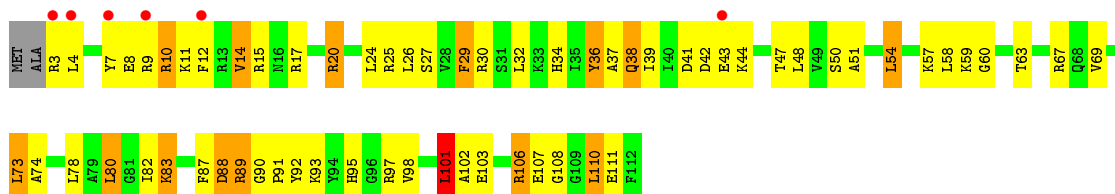




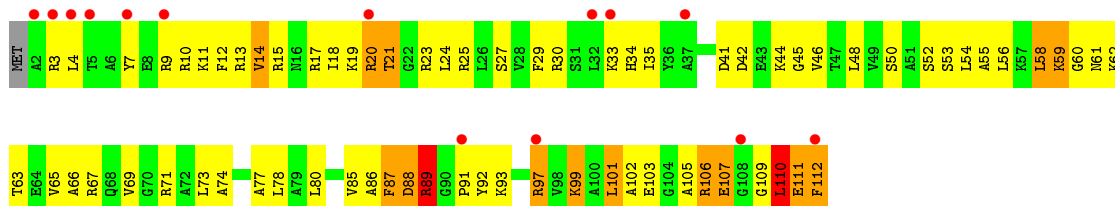
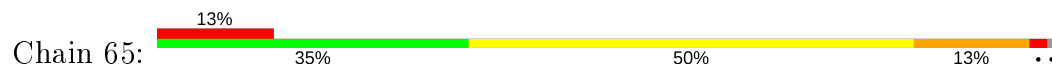
- Molecule 38: 50S ribosomal protein L17



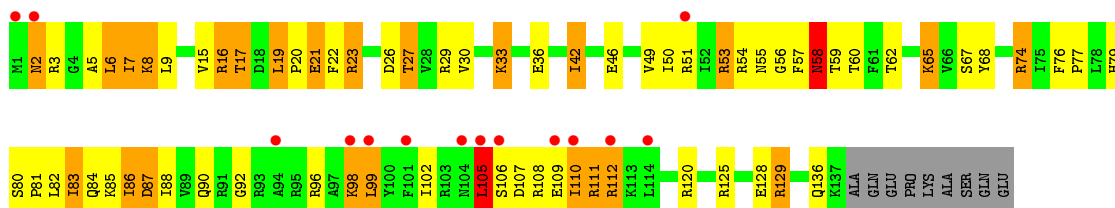
- Molecule 39: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L18

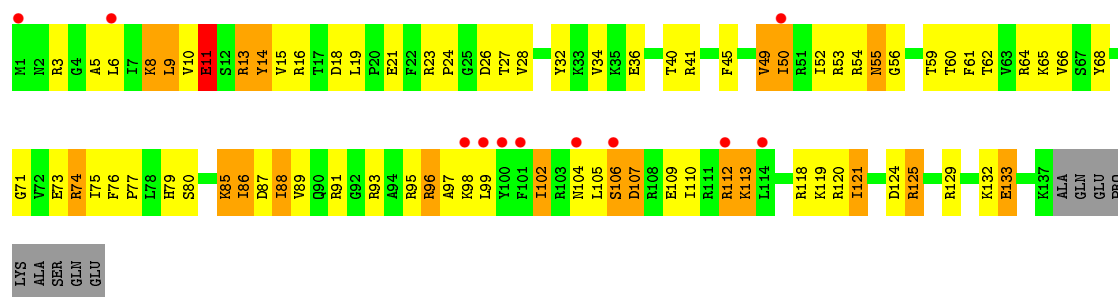


- Molecule 40: 50S ribosomal protein L19

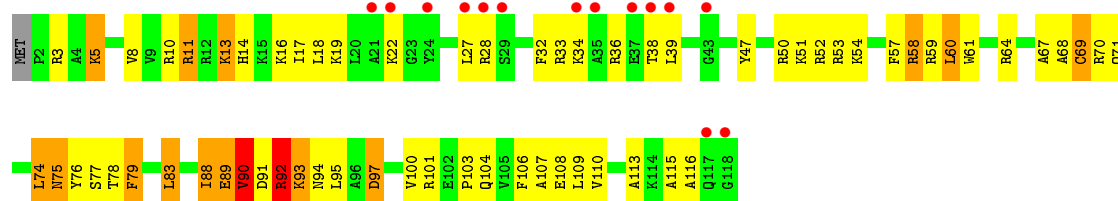
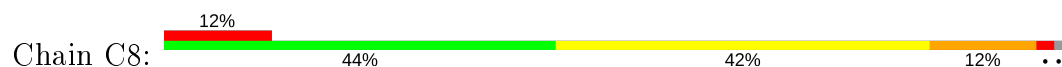


- Molecule 40: 50S ribosomal protein L19

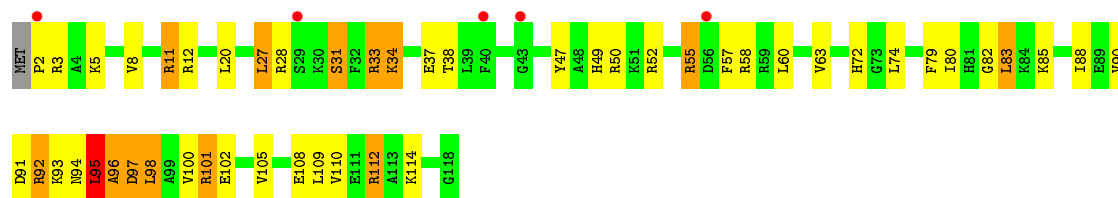




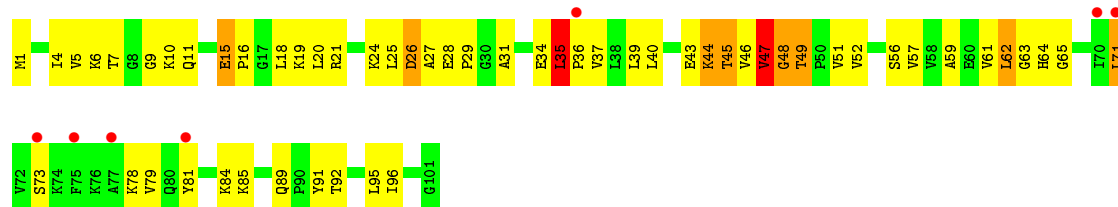
- Molecule 41: 50S ribosomal protein L20



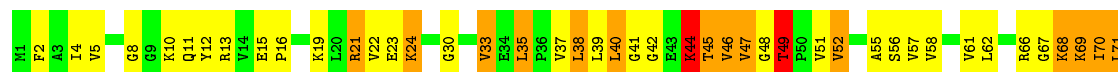
- Molecule 41: 50S ribosomal protein L20

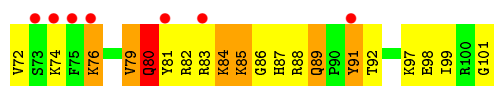


- Molecule 42: 50S ribosomal protein L21

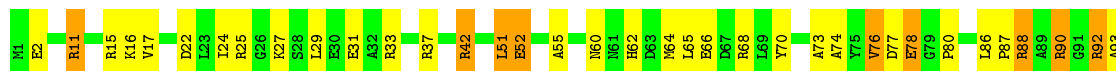


- Molecule 42: 50S ribosomal protein L21

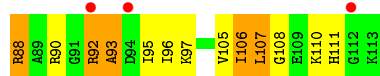
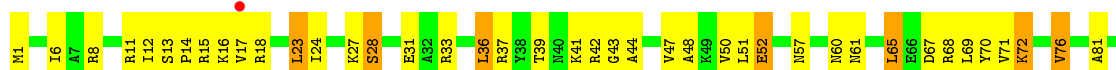




- Molecule 43: 50S ribosomal protein L22



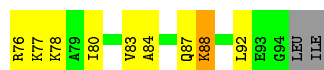
- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

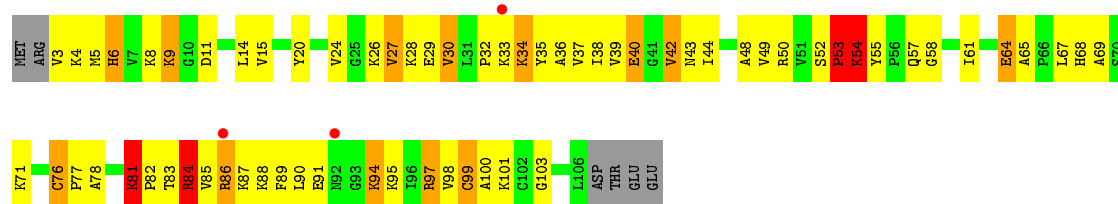


- Molecule 44: 50S ribosomal protein L23

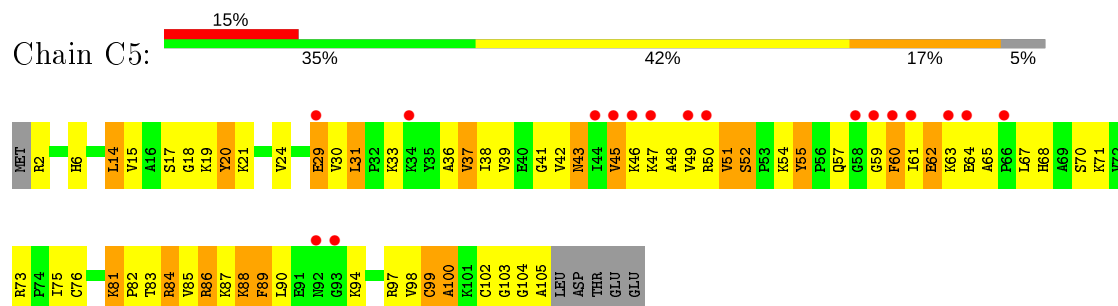


- Molecule 45: 50S ribosomal protein L24

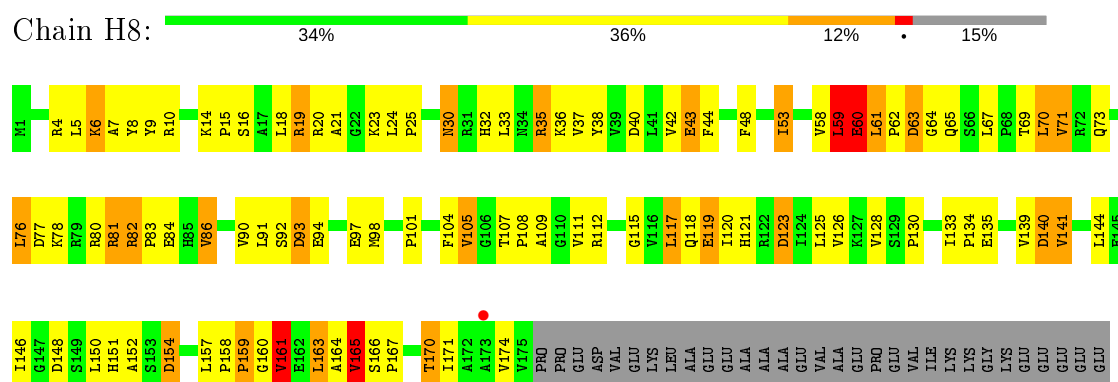




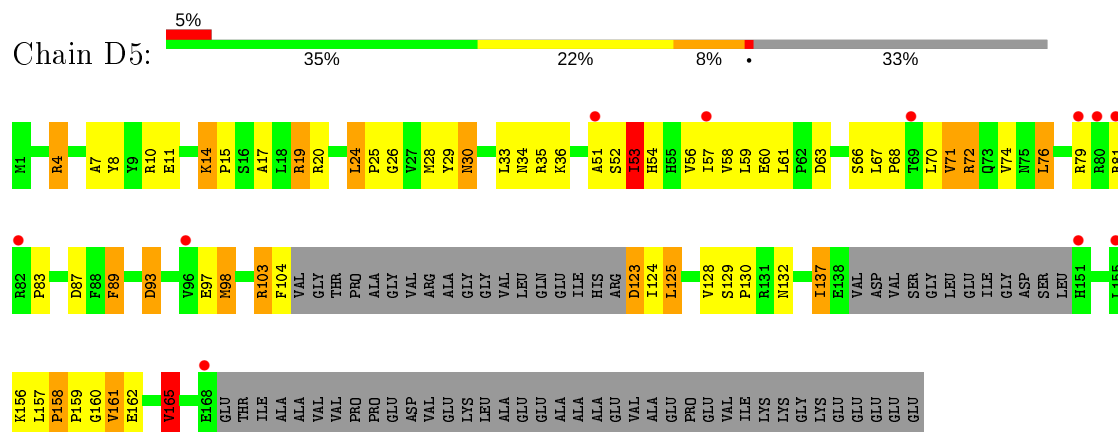
• Molecule 45: 50S ribosomal protein L24



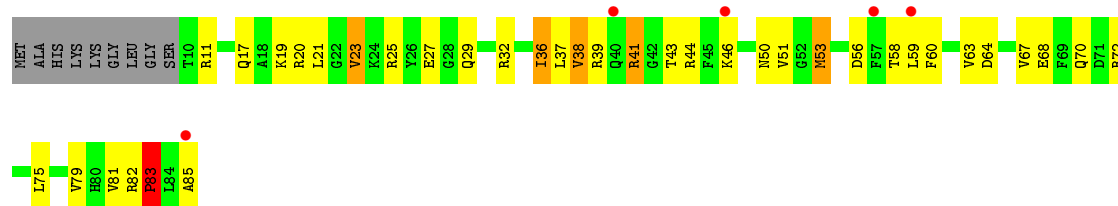
• Molecule 46: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L25



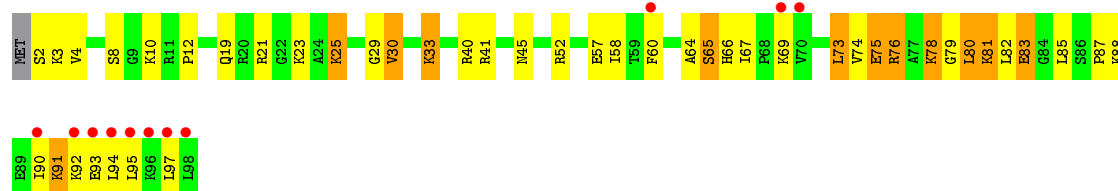
• Molecule 47: 50S ribosomal protein L27



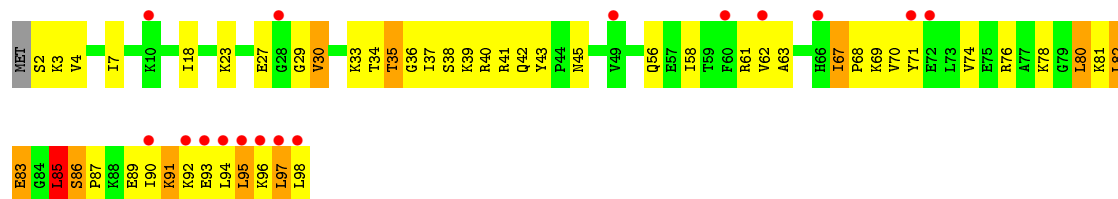
• Molecule 47: 50S ribosomal protein L27



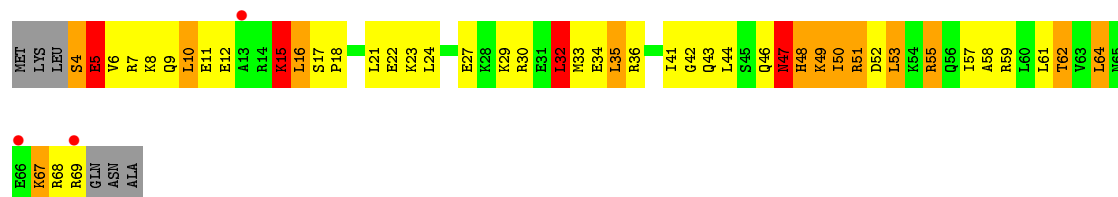
• Molecule 48: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29



- Chain N8: 



- Molecule 52: 50S ribosomal protein L32



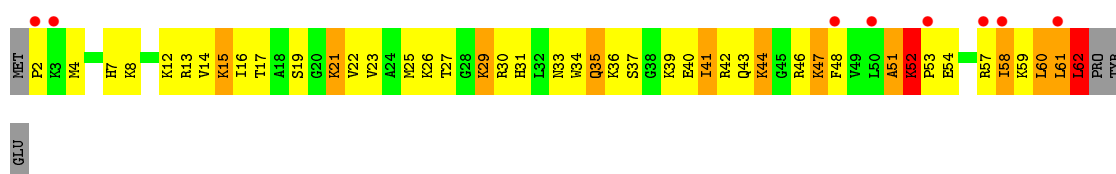
- Molecule 53: 50S ribosomal protein L34



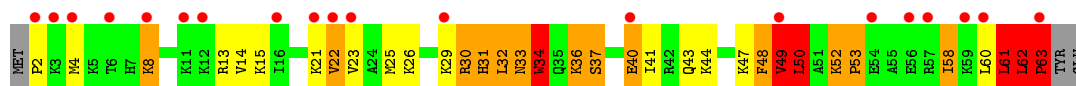
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: tRNA-Tyr



A67	A68	U69	C70	C71	C74	C75	C76	C77	C78	A79	C80	C81	A82	A85
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 450.90Å 622.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.45 – 3.05 225.45 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (225.45-3.05) 92.8 (225.45-3.05)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.249 0.196 , 0.248	Depositor DCC
R_{free} test set	1999 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.3	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	0.87	EDS
Total number of atoms	299607	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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, PAR, MIA, MG, ZN, 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	0.75	4/36215 (0.0%)	1.42	401/56524 (0.7%)
1	1G	0.66	1/36187 (0.0%)	1.30	253/56481 (0.4%)
2	12	0.38	0/1959	0.66	0/2642
2	1E	0.42	0/1959	0.70	1/2642 (0.0%)
3	22	0.42	0/1636	0.65	0/2205
3	2E	0.52	0/1629	0.72	0/2195
4	32	0.50	0/1732	0.76	2/2318 (0.1%)
4	3E	0.60	1/1732 (0.1%)	0.76	1/2318 (0.0%)
5	42	0.47	0/1171	0.70	0/1576
5	4E	0.54	0/1171	0.72	1/1576 (0.1%)
6	52	0.52	0/855	0.68	2/1154 (0.2%)
6	5E	0.54	0/855	0.70	0/1154
7	62	0.45	0/1275	0.64	0/1709
7	6E	0.45	0/1261	0.60	0/1689
8	72	0.44	0/1127	0.65	0/1517
8	7E	0.51	0/1135	0.74	1/1527 (0.1%)
9	82	0.40	0/988	0.66	0/1324
9	8E	0.44	0/1028	0.67	0/1379
10	1A	0.37	0/814	0.62	0/1095
10	1I	0.45	0/814	0.66	0/1095
11	2A	0.47	0/888	0.67	1/1198 (0.1%)
11	2I	0.51	0/879	0.74	1/1187 (0.1%)
12	3A	0.58	0/991	0.80	0/1327
12	3I	0.73	0/972	0.91	0/1301
13	4A	0.38	0/943	0.65	1/1265 (0.1%)
13	4I	0.49	0/938	0.71	0/1258
14	5A	0.44	0/484	0.74	0/643
14	5I	0.69	2/489 (0.4%)	0.86	1/650 (0.2%)
15	6A	0.47	0/744	0.65	0/992
15	6I	0.54	0/744	0.73	0/992
16	7A	0.53	0/721	0.71	0/970
16	7I	0.51	0/721	0.75	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.50	0/847	0.65	0/1131
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.50	0/586	0.72	1/779 (0.1%)
18	9I	0.49	0/595	0.79	1/790 (0.1%)
19	AA	0.44	0/638	0.72	1/860 (0.1%)
19	AI	0.53	0/680	0.81	0/915
20	BA	0.48	0/764	0.78	1/1007 (0.1%)
20	BI	0.41	0/764	0.68	0/1007
21	1B	0.52	0/221	0.66	0/288
21	1F	0.49	0/221	0.70	0/288
22	1K	0.49	0/1899	1.15	11/2952 (0.4%)
23	2K	0.81	0/1747	1.41	18/2723 (0.7%)
23	2L	0.69	0/1747	1.26	9/2723 (0.3%)
24	1L	0.47	1/1996 (0.1%)	1.08	5/3108 (0.2%)
24	3K	0.41	0/1996	1.01	1/3108 (0.0%)
25	4K	0.78	0/319	1.31	3/495 (0.6%)
25	4L	0.78	0/294	1.50	5/456 (1.1%)
26	14	0.89	62/70167 (0.1%)	1.58	1423/109541 (1.3%)
26	1H	1.03	114/70233 (0.2%)	1.76	2174/109643 (2.0%)
27	16	0.83	1/2928 (0.0%)	1.57	49/4568 (1.1%)
27	1J	0.70	0/2928	1.37	27/4568 (0.6%)
28	11	0.77	2/2170 (0.1%)	0.93	1/2926 (0.0%)
28	19	0.73	0/2170	0.94	6/2926 (0.2%)
29	21	0.70	0/1601	0.96	1/2160 (0.0%)
29	29	0.66	0/1601	0.98	3/2160 (0.1%)
30	31	0.72	0/1620	0.90	2/2194 (0.1%)
30	39	0.61	1/1662 (0.1%)	0.89	4/2249 (0.2%)
31	41	0.52	0/1498	0.75	1/2016 (0.0%)
31	49	0.42	0/1498	0.70	0/2016
32	51	0.65	0/1346	0.93	1/1821 (0.1%)
32	59	0.40	0/1332	0.74	3/1802 (0.2%)
33	61	0.52	0/1151	0.82	2/1558 (0.1%)
33	69	0.51	0/1151	0.77	3/1558 (0.2%)
34	15	0.49	0/1131	0.76	2/1525 (0.1%)
34	58	0.60	0/1131	0.83	0/1525
35	25	0.62	0/942	0.76	1/1269 (0.1%)
35	68	0.66	0/942	0.76	0/1269
36	35	0.67	0/1161	1.12	7/1544 (0.5%)
36	78	0.71	0/1161	1.13	7/1544 (0.5%)
37	45	0.70	2/1128 (0.2%)	0.98	3/1508 (0.2%)
37	88	0.82	1/1142 (0.1%)	1.11	4/1527 (0.3%)
38	55	0.65	0/973	0.84	1/1302 (0.1%)
38	98	0.57	0/981	0.79	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	65	0.54	0/891	0.90	2/1187 (0.2%)
39	A8	0.62	0/886	0.89	2/1180 (0.2%)
40	75	0.58	0/1155	0.76	0/1542
40	B8	0.62	0/1155	0.83	1/1542 (0.1%)
41	85	0.59	0/981	0.78	1/1306 (0.1%)
41	C8	0.71	1/981 (0.1%)	0.89	2/1306 (0.2%)
42	95	0.66	0/789	0.88	1/1057 (0.1%)
42	D8	0.60	0/789	0.82	2/1057 (0.2%)
43	A5	0.72	0/910	0.86	1/1220 (0.1%)
43	E8	0.65	0/910	0.84	0/1220
44	B5	0.80	1/739 (0.1%)	0.88	0/993
44	F8	0.73	0/744	0.83	0/1000
45	C5	0.61	0/807	0.89	1/1076 (0.1%)
45	G8	0.65	0/804	0.94	3/1073 (0.3%)
46	D5	0.43	0/1165	0.72	0/1574
46	H8	0.50	0/1427	0.80	1/1935 (0.1%)
47	E5	0.63	0/620	0.85	0/827
47	I8	0.71	0/614	0.89	0/819
48	F5	0.64	0/769	0.96	2/1022 (0.2%)
48	J8	0.70	0/769	0.86	0/1022
49	G5	0.60	0/560	0.81	0/741
49	K8	0.78	1/560 (0.2%)	0.98	2/741 (0.3%)
50	H5	0.48	0/473	0.69	0/635
50	L8	0.61	0/473	0.78	1/635 (0.2%)
51	I5	0.52	0/527	0.84	0/709
51	M8	0.50	0/545	0.87	0/733
52	J5	0.59	0/472	0.84	0/639
52	N8	0.65	0/472	0.86	1/639 (0.2%)
53	L5	0.70	0/399	0.88	0/526
53	P8	0.88	1/404 (0.2%)	0.97	0/533
54	M5	0.88	0/502	1.22	6/661 (0.9%)
54	Q8	0.85	0/494	1.10	1/649 (0.2%)
55	3L	0.39	0/1970	1.00	4/3065 (0.1%)
All	All	0.80	196/322722 (0.1%)	1.40	4482/483529 (0.9%)

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
1	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	1
2	1E	0	3
4	32	0	2
4	3E	0	1
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	2
14	5A	0	2
19	AA	0	1
19	AI	0	1
20	BA	0	2
26	14	1	0
28	11	0	1
28	19	0	4
29	21	0	5
29	29	0	4
30	39	0	6
31	41	0	1
31	49	0	2
32	51	0	3
32	59	0	1
33	61	0	4
33	69	0	2
34	58	0	1
36	35	0	4
36	78	0	7
37	45	0	8
37	88	0	2
38	55	0	1
38	98	0	1
39	A8	0	1
40	75	0	2
40	B8	0	2
41	85	0	4
41	C8	0	4
42	95	0	1
42	D8	0	2
43	A5	0	1
44	B5	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
45	C5	0	2
45	G8	0	3
46	D5	0	1
46	H8	0	3
47	E5	0	1
47	I8	0	1
48	F5	0	1
48	J8	0	2
49	G5	0	3
49	K8	0	3
51	I5	0	2
51	M8	0	1
52	N8	0	1
54	M5	0	5
54	Q8	0	3
All	All	2	128

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	783	A	N3-C4	-11.75	1.27	1.34
26	1H	2430	A	N9-C4	-11.09	1.31	1.37
26	14	783	A	N9-C4	-10.86	1.31	1.37
26	1H	71	A	N9-C4	-10.78	1.31	1.37
26	1H	676	A	N9-C4	-10.74	1.31	1.37

The worst 5 of 4482 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-20.97	113.42	126.00
26	14	1899	G	N3-C4-N9	-17.93	115.24	126.00
26	1H	1899	G	N3-C2-N2	-17.01	107.99	119.90
26	1H	2430	A	O5'-P-OP2	-17.00	90.30	110.70
26	1H	676	A	C2-N3-C4	-16.89	102.15	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	13	792	A	C1'
26	14	945	A	C1'

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
4	3E	29	PRO	Peptide
12	3I	47	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32352	0	16325	789	1
1	1G	32327	0	16316	749	3
2	12	1924	0	1975	103	0
2	1E	1924	0	1975	102	0
3	22	1612	0	1677	70	0
3	2E	1605	0	1668	56	0
4	32	1702	0	1763	78	0
4	3E	1702	0	1761	94	0
5	42	1155	0	1213	55	0
5	4E	1155	0	1213	49	0
6	52	842	0	857	32	0
6	5E	842	0	857	37	0
7	62	1256	0	1296	49	0
7	6E	1243	0	1284	50	0
8	72	1107	0	1165	53	0
8	7E	1115	0	1177	59	0
9	82	971	0	1001	55	0
9	8E	1009	0	1037	68	0
10	1A	801	0	849	52	0
10	1I	801	0	849	46	0
11	2A	873	0	894	47	0
11	2I	864	0	881	41	0
12	3A	975	0	1062	40	0
12	3I	956	0	1046	41	0
13	4A	933	0	992	53	0
13	4I	928	0	987	42	0
14	5A	475	0	511	25	0
14	5I	480	0	513	36	0
15	6A	733	0	771	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	733	0	771	27	0
16	7A	705	0	725	37	0
16	7I	705	0	725	49	0
17	8A	834	0	904	39	0
17	8I	834	0	904	54	0
18	9A	581	0	649	33	0
18	9I	590	0	662	29	0
19	AA	624	0	636	31	0
19	AI	665	0	686	39	0
20	BA	762	0	861	30	0
20	BI	762	0	861	52	0
21	1B	217	0	234	13	0
21	1F	217	0	234	12	0
22	1K	1824	0	945	57	0
23	2K	1645	0	841	30	0
23	2L	1645	0	841	33	0
24	1L	1807	0	920	32	0
24	3K	1807	0	920	47	0
25	4K	283	0	143	9	0
25	4L	261	0	132	6	0
26	14	62647	0	31582	1375	1
26	1H	62707	0	31612	1450	1
27	16	2617	0	1328	55	0
27	1J	2617	0	1328	80	0
28	11	2120	0	2197	92	0
28	19	2120	0	2197	89	0
29	21	1568	0	1634	111	0
29	29	1568	0	1634	113	0
30	31	1585	0	1632	87	0
30	39	1627	0	1680	110	0
31	41	1473	0	1535	72	0
31	49	1473	0	1535	63	0
32	51	1321	0	1388	82	0
32	59	1307	0	1382	64	1
33	61	1136	0	1223	65	1
33	69	1136	0	1223	50	0
34	15	1104	0	1180	57	0
34	58	1104	0	1180	81	0
35	25	932	0	996	42	0
35	68	932	0	996	40	0
36	35	1144	0	1228	92	0
36	78	1144	0	1228	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1107	0	1166	74	0
37	88	1121	0	1179	57	0
38	55	959	0	1021	47	0
38	98	967	0	1033	64	0
39	65	881	0	943	62	0
39	A8	876	0	938	47	0
40	75	1141	0	1202	71	0
40	B8	1141	0	1202	64	0
41	85	963	0	1022	44	0
41	C8	963	0	1022	66	0
42	95	778	0	852	69	0
42	D8	778	0	852	40	0
43	A5	899	0	964	27	0
43	E8	899	0	964	32	0
44	B5	725	0	778	36	0
44	F8	730	0	780	31	0
45	C5	794	0	884	54	0
45	G8	791	0	882	54	0
46	D5	1139	0	1163	53	0
46	H8	1397	0	1430	79	0
47	E5	612	0	633	31	0
47	I8	606	0	628	24	0
48	F5	762	0	848	36	0
48	J8	762	0	848	34	0
49	G5	558	0	610	30	0
49	K8	558	0	610	37	0
50	H5	468	0	518	13	0
50	L8	468	0	518	20	0
51	I5	515	0	514	54	0
51	M8	533	0	526	37	0
52	J5	458	0	480	21	0
52	N8	458	0	480	25	0
53	L5	391	0	432	9	0
53	P8	396	0	434	14	0
54	M5	495	0	567	62	0
54	Q8	488	0	560	55	0
55	3L	1814	0	932	51	0
56	11	2	0	0	0	0
56	13	146	0	0	0	0
56	14	391	0	0	0	0
56	16	12	0	0	0	0
56	1G	86	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	481	0	0	0	0
56	1J	6	0	0	0	0
56	1K	1	0	0	0	0
56	2I	2	0	0	0	0
56	25	1	0	0	0	0
56	29	3	0	0	0	0
56	2K	7	0	0	0	0
56	2L	4	0	0	0	0
56	3I	1	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	4I	1	0	0	0	0
56	45	1	0	0	0	0
56	5E	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	1	0	0	0	0
56	C5	1	0	0	0	0
56	I8	1	0	0	0	0
56	L5	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	13	42	0	45	2	0
57	1G	42	0	45	0	0
58	32	1	0	0	0	0
58	3E	1	0	0	0	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
59	11	10	0	0	1	0
59	13	141	0	0	25	0
59	14	474	0	0	139	0
59	16	11	0	0	2	0
59	19	9	0	0	4	0
59	1G	87	0	0	19	0
59	1H	633	0	0	156	0
59	1I	1	0	0	0	0
59	1J	6	0	0	0	0
59	1K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	5	0	0	3	0
59	29	3	0	0	1	0
59	2K	6	0	0	0	0
59	31	5	0	0	0	0
59	39	5	0	0	0	0
59	3E	1	0	0	0	0
59	3I	2	0	0	0	0
59	4K	3	0	0	0	0
59	55	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	6A	1	0	0	0	0
59	75	1	0	0	0	0
59	78	4	0	0	2	0
59	85	1	0	0	1	0
59	A5	1	0	0	0	0
59	BA	1	0	0	0	0
59	F8	1	0	0	0	0
59	G8	2	0	0	0	0
59	J8	1	0	0	0	0
59	L8	2	0	0	1	0
59	M5	2	0	0	0	0
All	All	299607	0	199932	8541	4

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

The worst 5 of 8541 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)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
4:32:26:CYS:HB3	4:32:31:CYS:SG	1.85	1.17
26:14:2701:C:H3'	26:14:2702:U:H5''	1.31	1.12
26:14:2711:A:OP2	59:14:3464:HOH:O	1.70	1.09
26:1H:229:A:H4'	26:1H:230:U:H5'	1.33	1.08

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:85:U:O2'	32:59:100:GLY:O[3_555]	1.97	0.23
1:1G:86:U:N3	26:14:275:G:OP2[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.19	0.01
33:61:91:SER:OG	1:1G:368:U:OP1[4_555]	2.19	0.01

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%)	195 (83%)	35 (15%)	5 (2%)	7	26
2	1E	235/256 (92%)	200 (85%)	34 (14%)	1 (0%)	34	64
3	22	204/239 (85%)	184 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	180 (89%)	22 (11%)	1 (0%)	29	60
4	32	206/209 (99%)	181 (88%)	24 (12%)	1 (0%)	29	60
4	3E	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	4E	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	22	52
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
7	6E	148/156 (95%)	140 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	10	35
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22	52
9	82	118/128 (92%)	105 (89%)	12 (10%)	1 (1%)	19	50
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	115/129 (89%)	104 (90%)	8 (7%)	3 (3%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	114/129 (88%)	101 (89%)	12 (10%)	1 (1%)	17	47
12	3A	123/132 (93%)	101 (82%)	19 (15%)	3 (2%)	6	23
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	50
13	4A	115/126 (91%)	95 (83%)	18 (16%)	2 (2%)	9	32
13	4I	114/126 (90%)	96 (84%)	16 (14%)	2 (2%)	8	30
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	8	30
14	5I	57/61 (93%)	46 (81%)	9 (16%)	2 (4%)	3	17
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	8A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
18	9A	69/88 (78%)	66 (96%)	3 (4%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	11	36
19	AA	76/93 (82%)	62 (82%)	11 (14%)	3 (4%)	3	15
19	AI	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	5	22
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	15	45
20	BI	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	15	45
21	1B	23/27 (85%)	21 (91%)	1 (4%)	1 (4%)	2	13
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276 (98%)	249 (92%)	18 (7%)	4 (2%)	10	35
28	19	271/276 (98%)	253 (93%)	13 (5%)	5 (2%)	8	30
29	21	203/206 (98%)	161 (79%)	33 (16%)	9 (4%)	2	12
29	29	203/206 (98%)	158 (78%)	36 (18%)	9 (4%)	2	12
30	31	200/210 (95%)	178 (89%)	21 (10%)	1 (0%)	29	60
30	39	206/210 (98%)	161 (78%)	38 (18%)	7 (3%)	3	17
31	41	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	9	32
31	49	179/182 (98%)	158 (88%)	20 (11%)	1 (1%)	25	55
32	51	171/180 (95%)	137 (80%)	21 (12%)	13 (8%)	1	4
32	59	168/180 (93%)	128 (76%)	31 (18%)	9 (5%)	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	61	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	7	26
33	69	144/148 (97%)	113 (78%)	27 (19%)	4 (3%)	5	21
34	15	136/140 (97%)	121 (89%)	14 (10%)	1 (1%)	22	52
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	4	20
35	25	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	50
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	35	148/150 (99%)	113 (76%)	32 (22%)	3 (2%)	7	27
36	78	148/150 (99%)	110 (74%)	30 (20%)	8 (5%)	2	9
37	45	137/141 (97%)	110 (80%)	25 (18%)	2 (2%)	10	35
37	88	139/141 (99%)	107 (77%)	26 (19%)	6 (4%)	2	13
38	55	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	9	32
38	98	116/118 (98%)	106 (91%)	9 (8%)	1 (1%)	17	47
39	65	109/112 (97%)	85 (78%)	22 (20%)	2 (2%)	8	30
39	A8	108/112 (96%)	89 (82%)	18 (17%)	1 (1%)	17	47
40	75	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
40	B8	135/146 (92%)	123 (91%)	12 (9%)	0	100	100
41	85	115/118 (98%)	98 (85%)	17 (15%)	0	100	100
41	C8	115/118 (98%)	107 (93%)	4 (4%)	4 (4%)	3	17
42	95	99/101 (98%)	77 (78%)	18 (18%)	4 (4%)	3	14
42	D8	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	19
43	A5	111/113 (98%)	101 (91%)	7 (6%)	3 (3%)	5	21
43	E8	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
44	B5	90/96 (94%)	76 (84%)	12 (13%)	2 (2%)	6	25
44	F8	91/96 (95%)	83 (91%)	6 (7%)	2 (2%)	6	25
45	C5	102/110 (93%)	76 (74%)	24 (24%)	2 (2%)	7	27
45	G8	102/110 (93%)	83 (81%)	13 (13%)	6 (6%)	1	8
46	D5	132/206 (64%)	104 (79%)	24 (18%)	4 (3%)	4	19
46	H8	173/206 (84%)	133 (77%)	33 (19%)	7 (4%)	3	14
47	E5	75/85 (88%)	68 (91%)	5 (7%)	2 (3%)	5	21
47	I8	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	5	21
48	F5	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	14	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	26
49	G5	64/72 (89%)	60 (94%)	2 (3%)	2 (3%)	4	19
49	K8	64/72 (89%)	59 (92%)	2 (3%)	3 (5%)	2	12
50	H5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	I5	61/71 (86%)	36 (59%)	21 (34%)	4 (7%)	1	6
51	M8	64/71 (90%)	36 (56%)	25 (39%)	3 (5%)	2	12
52	J5	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	30
52	N8	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
53	L5	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
53	P8	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	M5	60/65 (92%)	46 (77%)	11 (18%)	3 (5%)	2	11
54	Q8	59/65 (91%)	52 (88%)	3 (5%)	4 (7%)	1	6
All	All	11183/11946 (94%)	9677 (86%)	1306 (12%)	200 (2%)	8	30

5 of 200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	21	83	ASP
32	51	172	LYS
32	51	173	PRO
36	78	19	VAL

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%)	161 (78%)	44 (22%)	1	3
2	1E	205/220 (93%)	159 (78%)	46 (22%)	1	3
3	22	160/188 (85%)	121 (76%)	39 (24%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2E	159/188 (85%)	119 (75%)	40 (25%)	0	1
4	32	180/181 (99%)	139 (77%)	41 (23%)	1	3
4	3E	180/181 (99%)	138 (77%)	42 (23%)	1	2
5	42	116/123 (94%)	89 (77%)	27 (23%)	1	2
5	4E	116/123 (94%)	94 (81%)	22 (19%)	1	5
6	52	90/90 (100%)	71 (79%)	19 (21%)	1	4
6	5E	90/90 (100%)	71 (79%)	19 (21%)	1	4
7	62	126/127 (99%)	101 (80%)	25 (20%)	1	5
7	6E	126/127 (99%)	106 (84%)	20 (16%)	2	9
8	72	118/119 (99%)	96 (81%)	22 (19%)	1	6
8	7E	119/119 (100%)	92 (77%)	27 (23%)	1	3
9	82	95/99 (96%)	76 (80%)	19 (20%)	1	4
9	8E	98/99 (99%)	74 (76%)	24 (24%)	0	2
10	1A	89/92 (97%)	68 (76%)	21 (24%)	1	2
10	1I	89/92 (97%)	70 (79%)	19 (21%)	1	4
11	2A	89/99 (90%)	69 (78%)	20 (22%)	1	3
11	2I	88/99 (89%)	70 (80%)	18 (20%)	1	4
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	3
12	3I	103/109 (94%)	85 (82%)	18 (18%)	2	7
13	4A	94/101 (93%)	70 (74%)	24 (26%)	0	1
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	2
14	5A	48/50 (96%)	34 (71%)	14 (29%)	0	0
14	5I	48/50 (96%)	35 (73%)	13 (27%)	0	1
15	6A	79/80 (99%)	68 (86%)	11 (14%)	3	13
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	7
16	7A	72/74 (97%)	58 (81%)	14 (19%)	1	5
16	7I	72/74 (97%)	60 (83%)	12 (17%)	2	8
17	8A	95/97 (98%)	80 (84%)	15 (16%)	2	9
17	8I	95/97 (98%)	78 (82%)	17 (18%)	2	6
18	9A	62/77 (80%)	46 (74%)	16 (26%)	0	1
18	9I	63/77 (82%)	53 (84%)	10 (16%)	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AA	67/80 (84%)	50 (75%)	17 (25%)	0	1
19	AI	72/80 (90%)	56 (78%)	16 (22%)	1	3
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	2
20	BI	76/82 (93%)	54 (71%)	22 (29%)	0	1
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	25
21	1F	20/22 (91%)	18 (90%)	2 (10%)	7	25
28	11	214/218 (98%)	172 (80%)	42 (20%)	1	5
28	19	214/218 (98%)	170 (79%)	44 (21%)	1	4
29	21	165/166 (99%)	121 (73%)	44 (27%)	0	1
29	29	165/166 (99%)	124 (75%)	41 (25%)	0	2
30	31	161/166 (97%)	125 (78%)	36 (22%)	1	3
30	39	165/166 (99%)	121 (73%)	44 (27%)	0	1
31	41	155/156 (99%)	124 (80%)	31 (20%)	1	4
31	49	155/156 (99%)	123 (79%)	32 (21%)	1	4
32	51	142/148 (96%)	108 (76%)	34 (24%)	0	2
32	59	142/148 (96%)	107 (75%)	35 (25%)	0	2
33	61	122/124 (98%)	90 (74%)	32 (26%)	0	1
33	69	122/124 (98%)	86 (70%)	36 (30%)	0	0
34	15	117/119 (98%)	90 (77%)	27 (23%)	1	2
34	58	117/119 (98%)	91 (78%)	26 (22%)	1	3
35	25	100/100 (100%)	77 (77%)	23 (23%)	1	2
35	68	100/100 (100%)	82 (82%)	18 (18%)	1	6
36	35	116/116 (100%)	76 (66%)	40 (34%)	0	0
36	78	116/116 (100%)	81 (70%)	35 (30%)	0	0
37	45	110/111 (99%)	81 (74%)	29 (26%)	0	1
37	88	111/111 (100%)	85 (77%)	26 (23%)	1	2
38	55	100/101 (99%)	72 (72%)	28 (28%)	0	1
38	98	101/101 (100%)	76 (75%)	25 (25%)	0	2
39	65	87/88 (99%)	61 (70%)	26 (30%)	0	0
39	A8	87/88 (99%)	62 (71%)	25 (29%)	0	1
40	75	120/127 (94%)	86 (72%)	34 (28%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
40	B8	120/127 (94%)	89 (74%)	31 (26%)	0	1	
41	85	93/94 (99%)	69 (74%)	24 (26%)	0	1	
41	C8	93/94 (99%)	75 (81%)	18 (19%)	1	5	
42	95	82/82 (100%)	55 (67%)	27 (33%)	0	0	
42	D8	82/82 (100%)	63 (77%)	19 (23%)	1	2	
43	A5	92/92 (100%)	69 (75%)	23 (25%)	0	1	
43	E8	92/92 (100%)	72 (78%)	20 (22%)	1	3	
44	B5	74/78 (95%)	59 (80%)	15 (20%)	1	4	
44	F8	74/78 (95%)	62 (84%)	12 (16%)	2	9	
45	C5	85/91 (93%)	59 (69%)	26 (31%)	0	0	
45	G8	85/91 (93%)	60 (71%)	25 (29%)	0	0	
46	D5	127/179 (71%)	102 (80%)	25 (20%)	1	5	
46	H8	154/179 (86%)	118 (77%)	36 (23%)	1	2	
47	E5	62/67 (92%)	50 (81%)	12 (19%)	1	5	
47	I8	61/67 (91%)	50 (82%)	11 (18%)	1	6	
48	F5	82/83 (99%)	57 (70%)	25 (30%)	0	0	
48	J8	82/83 (99%)	67 (82%)	15 (18%)	1	6	
49	G5	62/67 (92%)	42 (68%)	20 (32%)	0	0	
49	K8	62/67 (92%)	41 (66%)	21 (34%)	0	0	
50	H5	51/52 (98%)	37 (72%)	14 (28%)	0	1	
50	L8	51/52 (98%)	38 (74%)	13 (26%)	0	1	
51	I5	57/63 (90%)	44 (77%)	13 (23%)	1	3	
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1	
52	J5	51/52 (98%)	45 (88%)	6 (12%)	5	18	
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	2	
53	L5	38/42 (90%)	31 (82%)	7 (18%)	1	6	
53	P8	38/42 (90%)	30 (79%)	8 (21%)	1	4	
54	M5	52/55 (94%)	36 (69%)	16 (31%)	0	0	
54	Q8	51/55 (93%)	38 (74%)	13 (26%)	0	1	
All	All	9444/9894 (96%)	7253 (77%)	2191 (23%)	1	2	

5 of 2191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	K8	24	LEU
6	52	25	ILE
44	B5	78	LYS
51	M8	15	ILE
3	22	3	ASN

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

Mol	Chain	Res	Type
37	88	13	GLN
46	H8	30	ASN
28	19	96	HIS
35	68	88	ASN
29	29	60	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1504/1522 (98%)	381 (25%)	35 (2%)
1	1G	1503/1522 (98%)	361 (24%)	37 (2%)
22	1K	82/85 (96%)	37 (45%)	8 (9%)
23	2K	76/77 (98%)	21 (27%)	3 (3%)
23	2L	76/77 (98%)	17 (22%)	1 (1%)
24	1L	84/85 (98%)	35 (41%)	8 (9%)
24	3K	84/85 (98%)	27 (32%)	4 (4%)
25	4K	11/30 (36%)	3 (27%)	1 (9%)
25	4L	12/30 (40%)	6 (50%)	3 (25%)
26	14	2908/2918 (99%)	759 (26%)	56 (1%)
26	1H	2911/2918 (99%)	725 (24%)	60 (2%)
27	16	121/122 (99%)	20 (16%)	0
27	1J	121/122 (99%)	33 (27%)	3 (2%)
55	3L	83/85 (97%)	34 (40%)	4 (4%)
All	All	9576/9678 (98%)	2459 (25%)	223 (2%)

5 of 2459 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	13	U

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2172	U
1	1G	429	U
26	14	2335	A
26	1H	2428	G
1	1G	89	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	OMC	2K	33	23	15,22,23	2.23	5 (33%)	17,31,34	1.18	1 (5%)
22	PSU	1K	40	22	17,21,22	0.95	2 (11%)	20,30,33	3.25	6 (30%)
23	OMC	2L	33	23	15,22,23	2.32	4 (26%)	17,31,34	1.93	3 (17%)
23	5MU	2K	55	23	15,22,23	2.14	3 (20%)	16,32,35	1.79	2 (12%)
23	PSU	2K	56	23	17,21,22	1.10	1 (5%)	20,30,33	3.11	5 (25%)
23	4SU	2K	8	23	14,21,22	3.38	2 (14%)	15,30,33	1.06	2 (13%)
55	MIA	3L	38	55	24,31,32	2.44	3 (12%)	26,44,47	2.60	10 (38%)
22	5MU	1K	63	22	15,22,23	2.09	3 (20%)	16,32,35	1.87	2 (12%)
23	PSU	2L	56	23	17,21,22	0.97	1 (5%)	20,30,33	3.19	6 (30%)
24	PSU	3K	40	24	17,21,22	1.00	1 (5%)	20,30,33	3.20	6 (30%)
55	PSU	3L	40	55	17,21,22	1.17	1 (5%)	20,30,33	3.52	6 (30%)
23	5MU	2L	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.90	2 (12%)
22	QUO	1K	35	25,22	28,35,36	5.57	9 (32%)	32,52,55	4.98	11 (34%)
22	MIA	1K	38	22	24,31,32	2.33	4 (16%)	26,44,47	3.09	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	4SU	2L	8	23	14,21,22	3.27	2 (14%)	15,30,33	0.86	1 (6%)
22	PSU	1K	64	22	17,21,22	1.02	1 (5%)	20,30,33	3.48	7 (35%)
24	PSU	1L	40	24	17,21,22	1.06	1 (5%)	20,30,33	3.17	6 (30%)

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
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
22	PSU	1K	40	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	2/7/27/28	0/2/2/2
23	5MU	2K	55	23	-	3/5/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
55	MIA	3L	38	55	-	4/11/33/34	0/3/3/3
22	5MU	1K	63	22	-	3/5/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
24	PSU	3K	40	24	-	0/7/25/26	0/2/2/2
55	PSU	3L	40	55	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
22	QUO	1K	35	25,22	-	4/6/43/44	0/4/4/4
22	MIA	1K	38	22	-	3/11/33/34	0/3/3/3
23	4SU	2L	8	23	-	0/5/25/26	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
24	PSU	1L	40	24	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	35	QUO	C4-N3	21.97	1.70	1.35
22	1K	35	QUO	C8-N9	-10.26	1.22	1.38
23	2K	8	4SU	C5-C4	10.24	1.50	1.38
22	1K	35	QUO	C7-C5	10.04	1.57	1.41
22	1K	35	QUO	C6-N1	-9.88	1.15	1.33

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	35	QUO	C6-C5-C4	20.45	126.56	115.01
22	1K	35	QUO	C8-N9-C1'	-13.50	113.53	125.48
55	3L	40	PSU	N1-C2-N3	-12.32	118.64	128.43
24	1L	40	PSU	N1-C2-N3	-11.17	119.55	128.43
22	1K	40	PSU	N1-C2-N3	-11.17	119.55	128.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2L	33	OMC	C2'-C1'-N1-C6
23	2L	33	OMC	O4'-C1'-N1-C6
23	2K	55	5MU	O4'-C1'-N1-C6
23	2K	55	5MU	O4'-C4'-C5'-O5'
55	3L	38	MIA	N1-C2-S10-C11

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	40	PSU	2	0
23	2L	33	OMC	6	0
23	2K	55	5MU	3	0
23	2K	56	PSU	1	0
23	2K	8	4SU	1	0
23	2L	56	PSU	1	0
22	1K	35	QUO	5	0
22	1K	38	MIA	6	0
23	2L	8	4SU	1	0
22	1K	64	PSU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1166 ligands modelled in this entry, 1164 are monoatomic - leaving 2 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PAR	13	1745	-	45,45,45	0.83	2 (4%)	64,67,67	2.07	18 (28%)
57	PAR	1G	1686	-	45,45,45	0.72	1 (2%)	64,67,67	1.85	12 (18%)

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
57	PAR	13	1745	-	-	6/18/94/94	0/4/4/4
57	PAR	1G	1686	-	-	5/18/94/94	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1686	PAR	C24-N24	-2.32	1.43	1.47
57	13	1745	PAR	C21-N21	-2.19	1.44	1.47
57	13	1745	PAR	C24-N24	-2.19	1.44	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1G	1686	PAR	C13-O52-C52	-6.63	101.57	117.96
57	13	1745	PAR	C11-O51-C51	5.23	123.95	113.69
57	13	1745	PAR	C14-O54-C54	5.04	123.58	113.69
57	1G	1686	PAR	C11-O51-C51	4.98	123.46	113.69
57	1G	1686	PAR	C14-O54-C54	4.89	123.29	113.69

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1G	1686	PAR	O51-C51-C61-O61
57	1G	1686	PAR	C33-C43-C53-O53
57	1G	1686	PAR	C41-C51-C61-O61
57	1G	1686	PAR	O51-C11-O11-C42

Continued on next page...

Continued from previous page...

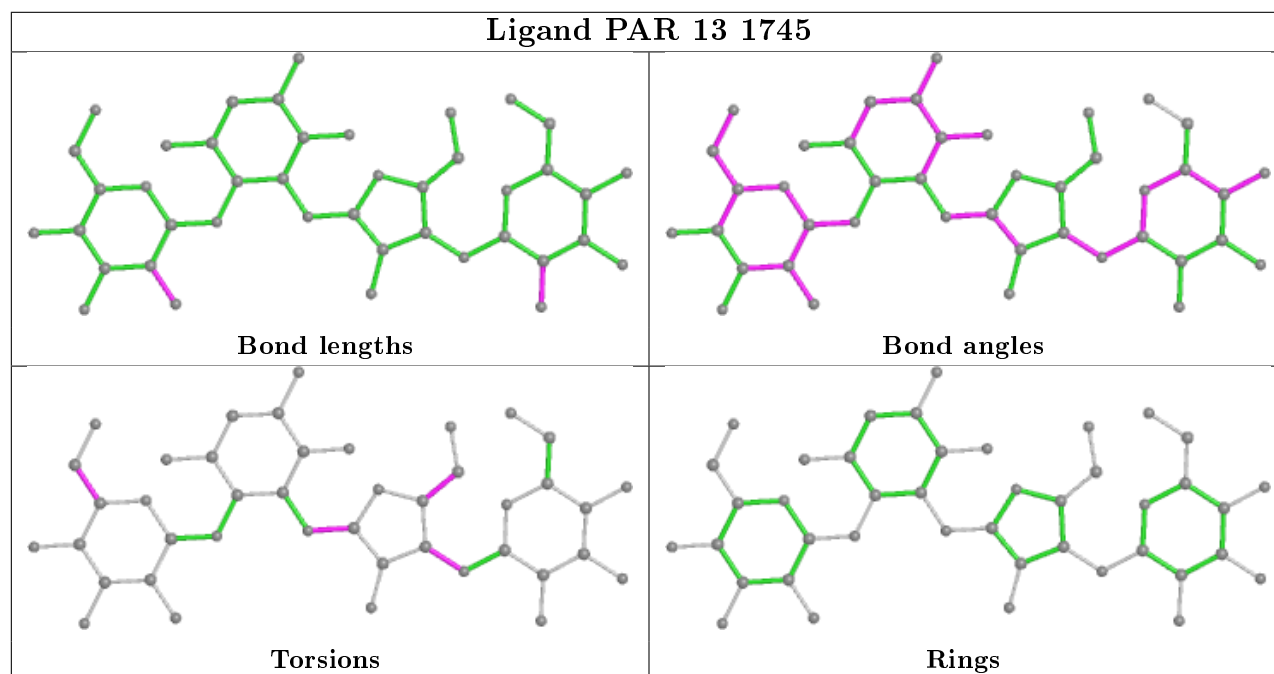
Mol	Chain	Res	Type	Atoms
57	13	1745	PAR	O43-C43-C53-O53

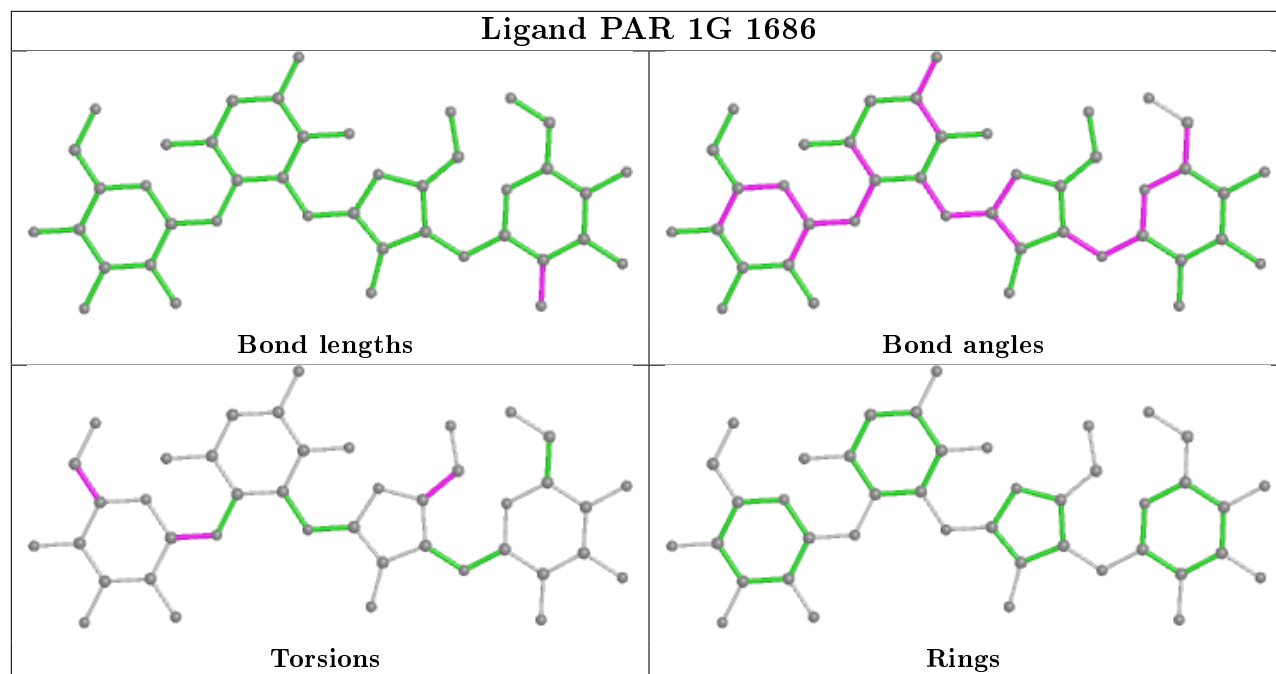
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	13	1745	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1505/1522 (98%)	0.12	30 (1%) 65 41	53, 96, 178, 280	0
1	1G	1504/1522 (98%)	0.10	34 (2%) 60 36	67, 108, 172, 272	0
2	12	237/256 (92%)	0.03	7 (2%) 50 25	122, 156, 179, 190	0
2	1E	237/256 (92%)	-0.04	5 (2%) 63 39	101, 137, 165, 175	0
3	22	206/239 (86%)	-0.00	8 (3%) 39 19	114, 132, 162, 173	0
3	2E	205/239 (85%)	0.16	10 (4%) 29 13	81, 103, 132, 138	0
4	32	208/209 (99%)	0.28	5 (2%) 59 34	88, 109, 130, 142	0
4	3E	208/209 (99%)	0.67	21 (10%) 7 2	77, 98, 122, 131	0
5	42	151/162 (93%)	0.53	15 (9%) 7 2	99, 115, 136, 155	0
5	4E	151/162 (93%)	0.42	13 (8%) 10 4	72, 91, 112, 150	0
6	52	101/101 (100%)	-0.39	0 100 100	78, 94, 114, 144	0
6	5E	101/101 (100%)	-0.12	2 (1%) 65 41	75, 94, 115, 132	0
7	62	155/156 (99%)	0.49	20 (12%) 3 1	105, 120, 143, 157	0
7	6E	152/156 (97%)	0.27	11 (7%) 15 5	96, 114, 137, 148	0
8	72	137/138 (99%)	1.22	37 (27%) 0 0	98, 119, 131, 137	0
8	7E	138/138 (100%)	1.00	28 (20%) 1 0	81, 100, 114, 126	0
9	82	122/128 (95%)	2.19	61 (50%) 0 0	102, 149, 166, 170	0
9	8E	127/128 (99%)	1.39	42 (33%) 0 0	81, 135, 158, 168	0
10	1A	99/105 (94%)	0.93	24 (24%) 0 0	111, 148, 164, 171	0
10	1I	99/105 (94%)	1.34	29 (29%) 0 0	73, 128, 159, 161	0
11	2A	117/129 (90%)	0.72	13 (11%) 5 2	81, 103, 120, 147	0
11	2I	116/129 (89%)	0.27	7 (6%) 21 9	72, 98, 120, 150	0
12	3A	125/132 (94%)	0.71	19 (15%) 2 1	78, 96, 129, 157	0
12	3I	122/132 (92%)	0.32	7 (5%) 23 10	61, 71, 97, 126	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	0.93	25 (21%) 0 0	102, 137, 157, 170	0
13	4I	116/126 (92%)	0.09	5 (4%) 35 16	78, 117, 136, 144	0
14	5A	58/61 (95%)	2.78	34 (58%) 0 0	116, 131, 146, 154	0
14	5I	59/61 (96%)	1.26	11 (18%) 1 0	82, 92, 108, 118	0
15	6A	88/89 (98%)	0.15	1 (1%) 80 60	80, 105, 121, 127	0
15	6I	88/89 (98%)	0.31	3 (3%) 45 22	67, 93, 110, 123	0
16	7A	84/88 (95%)	1.63	28 (33%) 0 0	85, 98, 124, 154	0
16	7I	84/88 (95%)	1.88	41 (48%) 0 0	90, 104, 132, 160	0
17	8A	100/105 (95%)	0.50	12 (12%) 4 1	91, 106, 124, 128	0
17	8I	100/105 (95%)	0.09	7 (7%) 16 6	81, 99, 111, 121	0
18	9A	71/88 (80%)	-0.33	0 100 100	84, 107, 134, 164	0
18	9I	72/88 (81%)	-0.02	0 100 100	80, 98, 126, 161	0
19	AA	78/93 (83%)	0.35	5 (6%) 19 7	124, 142, 171, 180	0
19	AI	83/93 (89%)	0.22	6 (7%) 15 5	90, 116, 137, 145	0
20	BA	99/106 (93%)	0.99	23 (23%) 0 0	83, 105, 133, 143	0
20	BI	99/106 (93%)	1.75	47 (47%) 0 0	101, 115, 146, 151	0
21	1B	25/27 (92%)	3.83	21 (84%) 0 0	110, 126, 143, 163	0
21	1F	25/27 (92%)	2.86	16 (64%) 0 0	90, 102, 117, 142	0
22	1K	80/85 (94%)	0.11	5 (6%) 20 8	81, 190, 249, 257	0
23	2K	73/77 (94%)	-0.05	2 (2%) 54 28	68, 96, 122, 140	0
23	2L	73/77 (94%)	-0.29	1 (1%) 75 53	76, 105, 138, 160	0
24	1L	84/85 (98%)	1.36	23 (27%) 0 0	107, 214, 302, 318	0
24	3K	84/85 (98%)	-0.18	2 (2%) 59 34	68, 209, 252, 259	0
25	4K	12/30 (40%)	1.37	3 (25%) 0 0	64, 94, 132, 145	0
25	4L	12/30 (40%)	1.32	4 (33%) 0 0	85, 117, 155, 188	0
26	14	2909/2918 (99%)	0.11	39 (1%) 77 56	48, 80, 223, 333	0
26	1H	2912/2918 (99%)	0.14	22 (0%) 86 70	38, 71, 217, 270	0
27	16	122/122 (100%)	-0.20	0 100 100	65, 91, 113, 185	0
27	1J	122/122 (100%)	-0.32	1 (0%) 86 70	73, 107, 128, 182	0
28	11	273/276 (98%)	0.34	3 (1%) 80 60	39, 62, 80, 92	0
28	19	273/276 (98%)	0.75	24 (8%) 10 3	42, 70, 88, 102	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	21	205/206 (99%)	0.80	21 (10%) 6 2	48, 85, 125, 137	0
29	29	205/206 (99%)	0.84	38 (18%) 1 0	56, 87, 129, 148	0
30	31	202/210 (96%)	0.02	0 100 100	38, 74, 110, 127	0
30	39	208/210 (99%)	0.20	7 (3%) 45 22	54, 95, 146, 178	0
31	41	181/182 (99%)	0.27	10 (5%) 25 10	79, 102, 133, 149	0
31	49	181/182 (99%)	1.02	33 (18%) 1 0	104, 125, 154, 169	0
32	51	173/180 (96%)	-0.03	2 (1%) 79 58	79, 102, 115, 151	0
32	59	170/180 (94%)	1.82	58 (34%) 0 0	134, 183, 210, 241	0
33	61	146/148 (98%)	-0.07	2 (1%) 75 53	74, 122, 140, 145	0
33	69	146/148 (98%)	0.47	20 (13%) 3 1	77, 118, 142, 146	0
34	15	138/140 (98%)	1.04	31 (22%) 0 0	75, 100, 129, 137	0
34	58	138/140 (98%)	0.47	9 (6%) 18 7	61, 88, 126, 143	0
35	25	122/122 (100%)	0.43	5 (4%) 37 18	61, 84, 102, 110	0
35	68	122/122 (100%)	0.49	3 (2%) 57 32	55, 74, 92, 101	0
36	35	150/150 (100%)	0.85	26 (17%) 1 0	54, 96, 133, 159	0
36	78	150/150 (100%)	0.24	1 (0%) 87 72	45, 81, 111, 152	0
37	45	139/141 (98%)	1.85	59 (42%) 0 0	69, 98, 116, 136	0
37	88	141/141 (100%)	0.36	2 (1%) 75 53	52, 77, 101, 129	0
38	55	117/118 (99%)	0.63	8 (6%) 17 6	56, 75, 92, 108	0
38	98	118/118 (100%)	0.51	4 (3%) 45 22	56, 80, 101, 107	0
39	65	111/112 (99%)	0.71	14 (12%) 3 1	75, 102, 120, 132	0
39	A8	110/112 (98%)	0.28	6 (5%) 25 10	70, 86, 110, 125	0
40	75	137/146 (93%)	0.34	11 (8%) 12 4	75, 91, 148, 185	0
40	B8	137/146 (93%)	0.50	14 (10%) 6 2	70, 89, 136, 159	0
41	85	117/118 (99%)	0.41	5 (4%) 35 16	62, 88, 122, 143	0
41	C8	117/118 (99%)	0.84	14 (11%) 4 1	50, 76, 107, 141	0
42	95	101/101 (100%)	0.28	7 (6%) 16 6	61, 116, 131, 136	0
42	D8	101/101 (100%)	0.29	7 (6%) 16 6	53, 100, 124, 139	0
43	A5	113/113 (100%)	0.40	4 (3%) 44 22	56, 71, 100, 159	0
43	E8	113/113 (100%)	0.16	0 100 100	52, 72, 105, 140	0
44	B5	92/96 (95%)	0.12	2 (2%) 62 38	64, 79, 106, 119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	F8	93/96 (96%)	-0.05	0 100 100	51, 67, 93, 102	0
45	C5	104/110 (94%)	0.99	17 (16%) 1 0	89, 119, 158, 166	0
45	G8	104/110 (94%)	0.45	3 (2%) 51 26	69, 96, 140, 148	0
46	D5	138/206 (66%)	0.40	11 (7%) 12 4	103, 134, 178, 186	0
46	H8	175/206 (84%)	-0.21	1 (0%) 89 76	84, 119, 190, 195	0
47	E5	77/85 (90%)	1.24	15 (19%) 1 0	64, 81, 99, 131	0
47	I8	76/85 (89%)	0.68	5 (6%) 18 7	52, 69, 85, 113	0
48	F5	97/98 (98%)	1.41	16 (16%) 1 0	57, 77, 122, 143	0
48	J8	97/98 (98%)	0.88	11 (11%) 5 1	48, 72, 124, 150	0
49	G5	66/72 (91%)	0.15	1 (1%) 73 51	74, 96, 114, 135	0
49	K8	66/72 (91%)	0.36	3 (4%) 33 15	59, 77, 90, 124	0
50	H5	59/60 (98%)	0.51	1 (1%) 70 46	74, 94, 132, 157	0
50	L8	59/60 (98%)	0.40	0 100 100	56, 78, 114, 137	0
51	I5	63/71 (88%)	2.20	28 (44%) 0 0	138, 171, 190, 192	0
51	M8	66/71 (92%)	0.50	6 (9%) 9 3	105, 154, 174, 184	0
52	J5	59/60 (98%)	0.50	3 (5%) 28 12	56, 80, 147, 187	0
52	N8	59/60 (98%)	0.66	6 (10%) 6 2	51, 86, 152, 158	0
53	L5	45/49 (91%)	0.45	1 (2%) 62 38	47, 56, 69, 84	0
53	P8	46/49 (93%)	0.10	0 100 100	40, 48, 66, 81	0
54	M5	62/65 (95%)	1.56	20 (32%) 0 0	65, 77, 93, 107	0
54	Q8	61/65 (93%)	1.01	8 (13%) 3 1	56, 66, 80, 98	0
55	3L	83/85 (97%)	0.32	9 (10%) 5 2	72, 217, 260, 269	0
All	All	20954/21624 (96%)	0.37	1450 (6%) 16 6	38, 95, 175, 333	0

The worst 5 of 1450 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	99	VAL	15.8
48	F5	98	LEU	14.8
48	F5	97	LEU	11.8
32	59	96	ALA	11.0
11	2A	11	LYS	10.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
23	OMC	2L	33	21/22	0.91	0.22	86,95,99,102	0
23	PSU	2L	56	20/21	0.91	0.10	101,108,114,119	0
23	4SU	2L	8	20/21	0.91	0.14	99,106,113,117	0
22	5MU	1K	63	21/22	0.92	0.16	106,124,138,141	0
22	PSU	1K	64	20/21	0.92	0.14	106,129,138,140	0
24	PSU	1L	40	20/21	0.92	0.26	99,116,121,124	0
55	PSU	3L	40	20/21	0.93	0.24	110,117,123,123	0
55	MIA	3L	38	29/30	0.93	0.26	102,116,135,141	0
22	QUO	1K	35	32/33	0.94	0.37	67,86,101,111	0
23	4SU	2K	8	20/21	0.94	0.16	83,89,99,107	0
22	PSU	1K	40	20/21	0.95	0.15	78,96,104,105	0
24	PSU	3K	40	20/21	0.95	0.12	106,113,117,119	0
23	5MU	2K	55	21/22	0.95	0.14	88,99,104,112	0
22	MIA	1K	38	29/30	0.95	0.29	67,84,98,112	0
23	PSU	2K	56	20/21	0.95	0.12	93,98,101,113	0
23	5MU	2L	55	21/22	0.95	0.11	101,110,116,118	0
23	OMC	2K	33	21/22	0.98	0.26	70,74,82,85	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
58	ZN	G8	201	1/1	0.23	0.14	178,178,178,178	0
56	MG	25	201	1/1	0.43	0.38	107,107,107,107	0
56	MG	14	3261	1/1	0.44	0.38	93,93,93,93	0
56	MG	1G	1641	1/1	0.49	0.26	73,73,73,73	0
56	MG	14	3182	1/1	0.49	0.24	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3223	1/1	0.51	0.58	102,102,102,102	0
56	MG	14	3289	1/1	0.53	0.28	79,79,79,79	0
56	MG	2L	102	1/1	0.54	0.22	79,79,79,79	0
56	MG	14	3254	1/1	0.54	0.27	102,102,102,102	0
58	ZN	C5	202	1/1	0.57	0.14	192,192,192,192	0
56	MG	1G	1684	1/1	0.58	0.12	122,122,122,122	0
56	MG	13	1685	1/1	0.59	0.22	91,91,91,91	0
56	MG	13	1647	1/1	0.59	0.21	77,77,77,77	0
56	MG	13	1743	1/1	0.61	0.36	102,102,102,102	0
56	MG	13	1617	1/1	0.62	0.26	86,86,86,86	0
56	MG	1H	3416	1/1	0.62	0.12	77,77,77,77	0
56	MG	14	3148	1/1	0.62	0.22	82,82,82,82	0
56	MG	14	3118	1/1	0.63	0.42	86,86,86,86	0
56	MG	1H	3239	1/1	0.63	0.22	72,72,72,72	0
56	MG	1G	1646	1/1	0.63	0.23	79,79,79,79	0
56	MG	1H	3275	1/1	0.64	0.44	75,75,75,75	0
56	MG	1H	3300	1/1	0.64	0.31	77,77,77,77	0
56	MG	1H	3185	1/1	0.64	0.19	71,71,71,71	0
56	MG	14	3151	1/1	0.64	0.23	72,72,72,72	0
56	MG	1H	3274	1/1	0.65	0.47	80,80,80,80	0
56	MG	13	1715	1/1	0.65	0.14	83,83,83,83	0
56	MG	14	3144	1/1	0.65	0.39	79,79,79,79	0
56	MG	14	3199	1/1	0.66	0.20	69,69,69,69	0
56	MG	14	3265	1/1	0.66	0.34	121,121,121,121	0
56	MG	14	3180	1/1	0.66	0.18	71,71,71,71	0
56	MG	14	3249	1/1	0.66	0.19	77,77,77,77	0
56	MG	1H	3451	1/1	0.66	0.13	46,46,46,46	0
56	MG	1H	3467	1/1	0.67	0.09	75,75,75,75	0
56	MG	1H	3178	1/1	0.67	0.27	63,63,63,63	0
56	MG	14	3293	1/1	0.67	0.48	88,88,88,88	0
56	MG	1H	3319	1/1	0.68	0.56	92,92,92,92	0
56	MG	13	1623	1/1	0.68	0.44	94,94,94,94	0
56	MG	13	1688	1/1	0.68	0.26	77,77,77,77	0
56	MG	1H	3295	1/1	0.69	0.17	76,76,76,76	0
56	MG	14	3139	1/1	0.69	0.20	81,81,81,81	0
56	MG	1H	3326	1/1	0.69	0.55	96,96,96,96	0
56	MG	1H	3030	1/1	0.69	0.34	81,81,81,81	0
56	MG	1H	3273	1/1	0.70	0.41	87,87,87,87	0
56	MG	13	1673	1/1	0.70	0.23	73,73,73,73	0
56	MG	14	3260	1/1	0.70	0.27	85,85,85,85	0
56	MG	1H	3098	1/1	0.70	0.20	87,87,87,87	0
56	MG	1H	3248	1/1	0.70	0.32	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3330	1/1	0.71	0.21	67,67,67,67	0
56	MG	1H	3144	1/1	0.71	0.27	66,66,66,66	0
56	MG	1H	3228	1/1	0.71	0.42	74,74,74,74	0
56	MG	14	3132	1/1	0.71	0.30	86,86,86,86	0
56	MG	1H	3201	1/1	0.71	0.20	59,59,59,59	0
56	MG	14	3377	1/1	0.71	0.12	96,96,96,96	0
56	MG	1G	1667	1/1	0.71	0.25	80,80,80,80	0
56	MG	1H	3282	1/1	0.71	0.40	83,83,83,83	0
56	MG	14	3282	1/1	0.72	0.32	86,86,86,86	0
56	MG	16	203	1/1	0.72	0.17	68,68,68,68	0
56	MG	1H	3207	1/1	0.72	0.21	73,73,73,73	0
56	MG	2K	102	1/1	0.72	0.23	83,83,83,83	0
56	MG	1H	3339	1/1	0.72	0.30	88,88,88,88	0
56	MG	1H	3459	1/1	0.72	0.08	77,77,77,77	0
56	MG	14	3167	1/1	0.73	0.14	59,59,59,59	0
56	MG	1H	3171	1/1	0.73	0.14	79,79,79,79	0
56	MG	14	3264	1/1	0.73	0.28	67,67,67,67	0
56	MG	14	3286	1/1	0.73	0.23	78,78,78,78	0
56	MG	1H	3349	1/1	0.73	0.35	85,85,85,85	0
56	MG	14	3169	1/1	0.73	0.14	77,77,77,77	0
56	MG	1H	3299	1/1	0.74	0.38	82,82,82,82	0
56	MG	1G	1620	1/1	0.74	0.34	78,78,78,78	0
56	MG	14	3094	1/1	0.74	0.18	69,69,69,69	0
56	MG	14	3158	1/1	0.74	0.41	67,67,67,67	0
56	MG	13	1741	1/1	0.74	0.09	110,110,110,110	0
56	MG	14	3226	1/1	0.74	0.18	82,82,82,82	0
56	MG	13	1658	1/1	0.74	0.24	70,70,70,70	0
56	MG	1H	3076	1/1	0.74	0.41	75,75,75,75	0
56	MG	1H	3217	1/1	0.74	0.46	93,93,93,93	0
56	MG	1H	3243	1/1	0.74	0.23	69,69,69,69	0
56	MG	1H	3386	1/1	0.75	0.12	53,53,53,53	0
56	MG	13	1720	1/1	0.75	0.11	62,62,62,62	0
56	MG	31	301	1/1	0.75	0.10	56,56,56,56	0
56	MG	14	3149	1/1	0.75	0.33	84,84,84,84	0
56	MG	14	3290	1/1	0.75	0.22	82,82,82,82	0
56	MG	1H	3205	1/1	0.76	0.36	62,62,62,62	0
56	MG	14	3217	1/1	0.76	0.28	68,68,68,68	0
56	MG	14	3250	1/1	0.76	0.22	74,74,74,74	0
56	MG	1H	3314	1/1	0.76	0.37	90,90,90,90	0
56	MG	13	1687	1/1	0.76	0.21	70,70,70,70	0
56	MG	1H	3311	1/1	0.76	0.27	78,78,78,78	0
56	MG	1H	3163	1/1	0.76	0.34	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1616	1/1	0.76	0.37	93,93,93,93	0
56	MG	1H	3293	1/1	0.76	0.46	90,90,90,90	0
56	MG	1H	3366	1/1	0.76	0.40	74,74,74,74	0
56	MG	1H	3264	1/1	0.77	0.22	58,58,58,58	0
56	MG	1H	3305	1/1	0.77	0.29	75,75,75,75	0
56	MG	39	301	1/1	0.77	0.23	71,71,71,71	0
56	MG	1H	3453	1/1	0.77	0.12	76,76,76,76	0
56	MG	14	3298	1/1	0.77	0.40	103,103,103,103	0
56	MG	1H	3222	1/1	0.77	0.36	80,80,80,80	0
56	MG	14	3305	1/1	0.77	0.17	79,79,79,79	0
56	MG	14	3275	1/1	0.77	0.27	60,60,60,60	0
56	MG	1H	3101	1/1	0.77	0.43	62,62,62,62	0
56	MG	14	3284	1/1	0.77	0.11	88,88,88,88	0
56	MG	14	3190	1/1	0.77	0.26	85,85,85,85	0
56	MG	13	1697	1/1	0.77	0.15	82,82,82,82	0
56	MG	1H	3328	1/1	0.77	0.47	91,91,91,91	0
56	MG	1H	3298	1/1	0.77	0.29	79,79,79,79	0
56	MG	1H	3332	1/1	0.78	0.47	88,88,88,88	0
56	MG	1H	3250	1/1	0.78	0.16	68,68,68,68	0
56	MG	14	3077	1/1	0.78	0.30	68,68,68,68	0
56	MG	14	3267	1/1	0.78	0.22	81,81,81,81	0
56	MG	13	1692	1/1	0.78	0.17	79,79,79,79	0
56	MG	13	1707	1/1	0.78	0.25	96,96,96,96	0
56	MG	13	1696	1/1	0.78	0.26	116,116,116,116	0
56	MG	1G	1665	1/1	0.78	0.13	94,94,94,94	0
56	MG	1H	3322	1/1	0.79	0.36	80,80,80,80	0
56	MG	1H	3461	1/1	0.79	0.09	108,108,108,108	0
56	MG	1H	3211	1/1	0.79	0.43	64,64,64,64	0
56	MG	14	3218	1/1	0.79	0.19	77,77,77,77	0
56	MG	14	3365	1/1	0.79	0.07	85,85,85,85	0
56	MG	1H	3341	1/1	0.79	0.33	67,67,67,67	0
56	MG	1H	3477	1/1	0.79	0.06	106,106,106,106	0
56	MG	1H	3368	1/1	0.79	0.27	74,74,74,74	0
56	MG	14	3302	1/1	0.79	0.15	72,72,72,72	0
56	MG	1H	3431	1/1	0.79	0.21	99,99,99,99	0
56	MG	14	3283	1/1	0.79	0.12	102,102,102,102	0
56	MG	1G	1648	1/1	0.79	0.43	121,121,121,121	0
56	MG	1H	3233	1/1	0.79	0.21	53,53,53,53	0
56	MG	1H	3393	1/1	0.79	0.10	65,65,65,65	0
56	MG	13	1649	1/1	0.79	0.21	85,85,85,85	0
56	MG	14	3153	1/1	0.80	0.17	94,94,94,94	0
56	MG	1H	3203	1/1	0.80	0.40	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3117	1/1	0.80	0.34	76,76,76,76	0
56	MG	1H	3358	1/1	0.80	0.25	80,80,80,80	0
56	MG	14	3280	1/1	0.80	0.43	87,87,87,87	0
56	MG	1H	3421	1/1	0.80	0.07	57,57,57,57	0
56	MG	1H	3342	1/1	0.80	0.30	98,98,98,98	0
56	MG	1H	3323	1/1	0.80	0.50	82,82,82,82	0
56	MG	14	3170	1/1	0.80	0.31	79,79,79,79	0
56	MG	13	1663	1/1	0.80	0.12	88,88,88,88	0
56	MG	1H	3238	1/1	0.80	0.21	54,54,54,54	0
56	MG	14	3287	1/1	0.80	0.20	79,79,79,79	0
56	MG	1H	3409	1/1	0.80	0.20	53,53,53,53	0
56	MG	14	3096	1/1	0.80	0.19	78,78,78,78	0
56	MG	1H	3462	1/1	0.80	0.06	92,92,92,92	0
56	MG	1G	1622	1/1	0.80	0.16	72,72,72,72	0
56	MG	1H	3068	1/1	0.80	0.29	67,67,67,67	0
56	MG	1H	3313	1/1	0.81	0.21	65,65,65,65	0
56	MG	13	1670	1/1	0.81	0.13	78,78,78,78	0
56	MG	1H	3240	1/1	0.81	0.18	73,73,73,73	0
56	MG	14	3216	1/1	0.81	0.17	83,83,83,83	0
56	MG	13	1710	1/1	0.81	0.12	128,128,128,128	0
56	MG	13	1662	1/1	0.81	0.30	73,73,73,73	0
56	MG	3E	301	1/1	0.81	0.11	112,112,112,112	0
56	MG	14	3091	1/1	0.81	0.22	84,84,84,84	0
56	MG	14	3122	1/1	0.81	0.14	68,68,68,68	0
56	MG	13	1708	1/1	0.81	0.22	85,85,85,85	0
56	MG	1G	1650	1/1	0.81	0.40	87,87,87,87	0
56	MG	C5	201	1/1	0.81	0.28	104,104,104,104	0
56	MG	13	1637	1/1	0.81	0.24	61,61,61,61	0
56	MG	1H	3146	1/1	0.81	0.24	75,75,75,75	0
56	MG	1G	1675	1/1	0.81	0.08	110,110,110,110	0
56	MG	14	3135	1/1	0.81	0.10	78,78,78,78	0
56	MG	14	3020	1/1	0.81	0.15	68,68,68,68	0
56	MG	14	3369	1/1	0.81	0.12	97,97,97,97	0
56	MG	14	3137	1/1	0.81	0.34	69,69,69,69	0
56	MG	14	3133	1/1	0.81	0.19	86,86,86,86	0
56	MG	1H	3139	1/1	0.81	0.17	66,66,66,66	0
56	MG	14	3127	1/1	0.81	0.17	64,64,64,64	0
56	MG	P8	101	1/1	0.81	0.29	68,68,68,68	0
56	MG	14	3342	1/1	0.81	0.13	74,74,74,74	0
56	MG	13	1701	1/1	0.81	0.12	80,80,80,80	0
56	MG	1G	1623	1/1	0.81	0.22	73,73,73,73	0
56	MG	14	3171	1/1	0.81	0.24	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3272	1/1	0.82	0.35	82,82,82,82	0
56	MG	1H	3281	1/1	0.82	0.37	74,74,74,74	0
56	MG	1H	3170	1/1	0.82	0.22	61,61,61,61	0
56	MG	1H	3290	1/1	0.82	0.41	84,84,84,84	0
56	MG	1H	3067	1/1	0.82	0.25	49,49,49,49	0
56	MG	14	3332	1/1	0.82	0.17	73,73,73,73	0
56	MG	13	1679	1/1	0.82	0.28	77,77,77,77	0
56	MG	1H	3288	1/1	0.82	0.13	54,54,54,54	0
56	MG	14	3378	1/1	0.82	0.10	79,79,79,79	0
56	MG	13	1703	1/1	0.82	0.20	89,89,89,89	0
56	MG	14	3033	1/1	0.82	0.17	64,64,64,64	0
56	MG	1H	3321	1/1	0.82	0.42	86,86,86,86	0
56	MG	14	3303	1/1	0.82	0.15	101,101,101,101	0
56	MG	1H	3259	1/1	0.83	0.20	81,81,81,81	0
56	MG	14	3189	1/1	0.83	0.16	60,60,60,60	0
56	MG	14	3121	1/1	0.83	0.17	58,58,58,58	0
56	MG	1H	3338	1/1	0.83	0.23	60,60,60,60	0
56	MG	16	207	1/1	0.83	0.28	71,71,71,71	0
56	MG	14	3161	1/1	0.83	0.24	86,86,86,86	0
56	MG	14	3214	1/1	0.83	0.17	65,65,65,65	0
56	MG	1H	3249	1/1	0.83	0.26	85,85,85,85	0
56	MG	1G	1652	1/1	0.83	0.30	74,74,74,74	0
56	MG	1H	3172	1/1	0.83	0.40	84,84,84,84	0
56	MG	1H	3202	1/1	0.83	0.17	66,66,66,66	0
56	MG	1G	1670	1/1	0.83	0.20	77,77,77,77	0
56	MG	1H	3168	1/1	0.83	0.44	79,79,79,79	0
56	MG	1H	3138	1/1	0.83	0.35	66,66,66,66	0
56	MG	1H	3053	1/1	0.83	0.36	72,72,72,72	0
56	MG	1H	3129	1/1	0.83	0.20	68,68,68,68	0
56	MG	1G	1656	1/1	0.83	0.28	72,72,72,72	0
56	MG	13	1704	1/1	0.83	0.20	80,80,80,80	0
56	MG	1G	1642	1/1	0.83	0.34	81,81,81,81	0
56	MG	1H	3331	1/1	0.83	0.23	76,76,76,76	0
56	MG	1H	3334	1/1	0.84	0.23	60,60,60,60	0
56	MG	1H	3057	1/1	0.84	0.36	57,57,57,57	0
56	MG	1H	3280	1/1	0.84	0.20	59,59,59,59	0
56	MG	16	205	1/1	0.84	0.30	77,77,77,77	0
56	MG	1G	1654	1/1	0.84	0.42	101,101,101,101	0
56	MG	14	3195	1/1	0.84	0.25	65,65,65,65	0
56	MG	1H	3197	1/1	0.84	0.29	66,66,66,66	0
56	MG	14	3159	1/1	0.84	0.22	73,73,73,73	0
56	MG	14	3142	1/1	0.84	0.21	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3221	1/1	0.84	0.24	80,80,80,80	0
56	MG	1H	3271	1/1	0.84	0.30	65,65,65,65	0
56	MG	14	3104	1/1	0.84	0.28	84,84,84,84	0
56	MG	1H	3125	1/1	0.84	0.20	49,49,49,49	0
56	MG	1H	3359	1/1	0.84	0.53	84,84,84,84	0
56	MG	1G	1659	1/1	0.84	0.20	93,93,93,93	0
56	MG	1H	3209	1/1	0.84	0.31	77,77,77,77	0
56	MG	14	3173	1/1	0.84	0.16	62,62,62,62	0
56	MG	1G	1636	1/1	0.84	0.16	84,84,84,84	0
56	MG	1G	1664	1/1	0.84	0.42	102,102,102,102	0
56	MG	14	3285	1/1	0.85	0.40	74,74,74,74	0
56	MG	14	3145	1/1	0.85	0.16	81,81,81,81	0
56	MG	2L	103	1/1	0.85	0.23	89,89,89,89	0
56	MG	14	3220	1/1	0.85	0.22	82,82,82,82	0
56	MG	1H	3153	1/1	0.85	0.33	64,64,64,64	0
56	MG	1G	1609	1/1	0.85	0.35	81,81,81,81	0
56	MG	1H	3435	1/1	0.85	0.05	90,90,90,90	0
56	MG	14	3136	1/1	0.85	0.28	73,73,73,73	0
56	MG	14	3268	1/1	0.85	0.19	57,57,57,57	0
56	MG	1H	3177	1/1	0.85	0.30	55,55,55,55	0
56	MG	1H	3312	1/1	0.85	0.47	78,78,78,78	0
56	MG	1H	3316	1/1	0.85	0.15	74,74,74,74	0
56	MG	1H	3128	1/1	0.85	0.28	57,57,57,57	0
56	MG	13	1728	1/1	0.85	0.11	85,85,85,85	0
56	MG	14	3115	1/1	0.85	0.36	88,88,88,88	0
56	MG	14	3154	1/1	0.85	0.12	82,82,82,82	0
56	MG	1H	3117	1/1	0.85	0.31	80,80,80,80	0
56	MG	14	3069	1/1	0.85	0.27	78,78,78,78	0
56	MG	1H	3077	1/1	0.85	0.23	73,73,73,73	0
56	MG	14	3223	1/1	0.85	0.24	62,62,62,62	0
56	MG	1H	3194	1/1	0.86	0.24	62,62,62,62	0
56	MG	13	1686	1/1	0.86	0.18	69,69,69,69	0
56	MG	13	1643	1/1	0.86	0.35	80,80,80,80	0
56	MG	1G	1668	1/1	0.86	0.26	82,82,82,82	0
56	MG	14	3130	1/1	0.86	0.26	71,71,71,71	0
56	MG	14	3389	1/1	0.86	0.18	97,97,97,97	0
56	MG	1G	1643	1/1	0.86	0.37	88,88,88,88	0
56	MG	14	3110	1/1	0.86	0.19	64,64,64,64	0
56	MG	14	3129	1/1	0.86	0.24	63,63,63,63	0
56	MG	3I	201	1/1	0.86	0.07	58,58,58,58	0
56	MG	14	3258	1/1	0.86	0.14	73,73,73,73	0
56	MG	1H	3276	1/1	0.86	0.34	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1628	1/1	0.86	0.13	48,48,48,48	0
56	MG	13	1733	1/1	0.86	0.06	73,73,73,73	0
56	MG	1H	3263	1/1	0.86	0.32	76,76,76,76	0
56	MG	1H	3199	1/1	0.86	0.31	57,57,57,57	0
56	MG	16	208	1/1	0.86	0.33	66,66,66,66	0
56	MG	1H	3269	1/1	0.86	0.36	62,62,62,62	0
56	MG	13	1644	1/1	0.86	0.34	76,76,76,76	0
56	MG	14	3292	1/1	0.86	0.24	82,82,82,82	0
56	MG	85	201	1/1	0.86	0.22	69,69,69,69	0
56	MG	14	3372	1/1	0.86	0.22	84,84,84,84	0
56	MG	1H	3156	1/1	0.86	0.11	54,54,54,54	0
56	MG	14	3042	1/1	0.86	0.16	72,72,72,72	0
56	MG	13	1730	1/1	0.86	0.11	86,86,86,86	0
56	MG	13	1716	1/1	0.86	0.14	92,92,92,92	0
56	MG	13	1711	1/1	0.86	0.21	79,79,79,79	0
56	MG	1H	3438	1/1	0.86	0.12	54,54,54,54	0
56	MG	13	1698	1/1	0.87	0.15	74,74,74,74	0
56	MG	1H	3213	1/1	0.87	0.32	77,77,77,77	0
56	MG	1H	3475	1/1	0.87	0.10	79,79,79,79	0
56	MG	1H	3150	1/1	0.87	0.20	59,59,59,59	0
56	MG	1G	1669	1/1	0.87	0.20	88,88,88,88	0
56	MG	11	302	1/1	0.87	0.19	42,42,42,42	0
56	MG	14	3276	1/1	0.87	0.15	76,76,76,76	0
56	MG	13	1668	1/1	0.87	0.22	76,76,76,76	0
56	MG	1H	3029	1/1	0.87	0.29	73,73,73,73	0
56	MG	1H	3078	1/1	0.87	0.14	63,63,63,63	0
56	MG	1H	3464	1/1	0.87	0.08	92,92,92,92	0
56	MG	1H	3301	1/1	0.87	0.28	79,79,79,79	0
56	MG	1H	3106	1/1	0.87	0.17	58,58,58,58	0
56	MG	1H	3463	1/1	0.87	0.18	101,101,101,101	0
56	MG	1H	3152	1/1	0.87	0.21	75,75,75,75	0
56	MG	13	1633	1/1	0.87	0.38	77,77,77,77	0
56	MG	14	3271	1/1	0.87	0.14	87,87,87,87	0
56	MG	14	3089	1/1	0.87	0.38	79,79,79,79	0
56	MG	13	1602	1/1	0.87	0.14	66,66,66,66	0
56	MG	1H	3122	1/1	0.87	0.24	49,49,49,49	0
56	MG	14	3274	1/1	0.87	0.26	82,82,82,82	0
56	MG	1H	3173	1/1	0.87	0.32	52,52,52,52	0
56	MG	1H	3401	1/1	0.87	0.07	64,64,64,64	0
56	MG	1H	3096	1/1	0.87	0.23	54,54,54,54	0
56	MG	16	202	1/1	0.87	0.38	59,59,59,59	0
56	MG	14	3207	1/1	0.87	0.59	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3116	1/1	0.87	0.25	56,56,56,56	0
56	MG	14	3345	1/1	0.87	0.15	81,81,81,81	0
56	MG	1H	3468	1/1	0.87	0.14	71,71,71,71	0
56	MG	1H	3458	1/1	0.87	0.15	84,84,84,84	0
56	MG	1H	3272	1/1	0.87	0.31	69,69,69,69	0
56	MG	1G	1677	1/1	0.87	0.19	104,104,104,104	0
56	MG	13	1684	1/1	0.87	0.30	62,62,62,62	0
56	MG	14	3208	1/1	0.87	0.15	68,68,68,68	0
56	MG	14	3241	1/1	0.88	0.26	91,91,91,91	0
56	MG	14	3034	1/1	0.88	0.10	86,86,86,86	0
56	MG	14	3175	1/1	0.88	0.15	56,56,56,56	0
56	MG	14	3095	1/1	0.88	0.20	56,56,56,56	0
56	MG	1H	3353	1/1	0.88	0.24	73,73,73,73	0
56	MG	1H	3384	1/1	0.88	0.07	57,57,57,57	0
56	MG	1H	3148	1/1	0.88	0.29	82,82,82,82	0
56	MG	14	3381	1/1	0.88	0.09	62,62,62,62	0
56	MG	1H	3444	1/1	0.88	0.13	59,59,59,59	0
56	MG	16	201	1/1	0.88	0.24	78,78,78,78	0
56	MG	14	3172	1/1	0.88	0.35	69,69,69,69	0
56	MG	1J	203	1/1	0.88	0.29	81,81,81,81	0
56	MG	14	3256	1/1	0.88	0.30	66,66,66,66	0
56	MG	1H	3443	1/1	0.88	0.06	58,58,58,58	0
56	MG	13	1653	1/1	0.88	0.09	75,75,75,75	0
56	MG	1G	1608	1/1	0.88	0.25	88,88,88,88	0
56	MG	14	3102	1/1	0.88	0.15	49,49,49,49	0
56	MG	14	3300	1/1	0.88	0.27	109,109,109,109	0
56	MG	14	3125	1/1	0.88	0.19	53,53,53,53	0
56	MG	1H	3174	1/1	0.88	0.27	63,63,63,63	0
56	MG	14	3367	1/1	0.88	0.13	70,70,70,70	0
56	MG	16	204	1/1	0.88	0.19	86,86,86,86	0
56	MG	1H	3261	1/1	0.88	0.15	61,61,61,61	0
56	MG	1H	3344	1/1	0.88	0.52	87,87,87,87	0
56	MG	14	3155	1/1	0.88	0.24	75,75,75,75	0
56	MG	41	201	1/1	0.88	0.37	82,82,82,82	0
56	MG	13	1717	1/1	0.88	0.23	74,74,74,74	0
56	MG	13	1660	1/1	0.88	0.13	91,91,91,91	0
56	MG	1G	1685	1/1	0.88	0.08	111,111,111,111	0
56	MG	1H	3042	1/1	0.88	0.30	74,74,74,74	0
56	MG	1H	3189	1/1	0.88	0.34	63,63,63,63	0
56	MG	1H	3110	1/1	0.88	0.37	57,57,57,57	0
56	MG	13	1641	1/1	0.88	0.16	59,59,59,59	0
56	MG	1H	3227	1/1	0.88	0.49	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1705	1/1	0.88	0.36	94,94,94,94	0
56	MG	1H	3255	1/1	0.88	0.26	76,76,76,76	0
56	MG	1H	3186	1/1	0.88	0.20	83,83,83,83	0
56	MG	1H	3159	1/1	0.89	0.12	71,71,71,71	0
56	MG	1H	3192	1/1	0.89	0.19	72,72,72,72	0
56	MG	1H	3406	1/1	0.89	0.10	45,45,45,45	0
56	MG	1H	3109	1/1	0.89	0.15	60,60,60,60	0
56	MG	14	3119	1/1	0.89	0.22	69,69,69,69	0
56	MG	13	1693	1/1	0.89	0.15	65,65,65,65	0
56	MG	1H	3154	1/1	0.89	0.34	74,74,74,74	0
56	MG	13	1666	1/1	0.89	0.12	58,58,58,58	0
56	MG	14	3341	1/1	0.89	0.11	48,48,48,48	0
56	MG	1H	3113	1/1	0.89	0.13	41,41,41,41	0
56	MG	13	1747	1/1	0.89	0.21	64,64,64,64	0
56	MG	13	1642	1/1	0.89	0.29	72,72,72,72	0
56	MG	14	3379	1/1	0.89	0.12	72,72,72,72	0
56	MG	1H	3394	1/1	0.89	0.10	57,57,57,57	0
56	MG	1H	3446	1/1	0.89	0.15	78,78,78,78	0
56	MG	2L	104	1/1	0.89	0.14	65,65,65,65	0
56	MG	14	3263	1/1	0.89	0.32	71,71,71,71	0
56	MG	1H	3167	1/1	0.89	0.15	67,67,67,67	0
56	MG	13	1719	1/1	0.89	0.24	89,89,89,89	0
56	MG	14	3177	1/1	0.89	0.19	72,72,72,72	0
56	MG	1H	3161	1/1	0.89	0.26	55,55,55,55	0
56	MG	14	3243	1/1	0.89	0.22	72,72,72,72	0
56	MG	1H	3137	1/1	0.89	0.20	49,49,49,49	0
56	MG	1H	3234	1/1	0.89	0.22	75,75,75,75	0
56	MG	1J	202	1/1	0.89	0.34	73,73,73,73	0
56	MG	1H	3091	1/1	0.89	0.21	55,55,55,55	0
56	MG	1H	3058	1/1	0.89	0.17	61,61,61,61	0
56	MG	1H	3224	1/1	0.89	0.22	61,61,61,61	0
56	MG	1H	3054	1/1	0.89	0.33	59,59,59,59	0
56	MG	13	1609	1/1	0.89	0.35	86,86,86,86	0
56	MG	14	3306	1/1	0.89	0.15	69,69,69,69	0
56	MG	1H	3364	1/1	0.89	0.09	68,68,68,68	0
56	MG	1H	3470	1/1	0.89	0.12	106,106,106,106	0
56	MG	14	3388	1/1	0.89	0.06	88,88,88,88	0
56	MG	1H	3372	1/1	0.89	0.08	37,37,37,37	0
56	MG	1H	3454	1/1	0.89	0.12	98,98,98,98	0
56	MG	1H	3336	1/1	0.89	0.26	79,79,79,79	0
56	MG	14	3059	1/1	0.89	0.23	52,52,52,52	0
56	MG	1H	3210	1/1	0.89	0.43	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3257	1/1	0.89	0.42	85,85,85,85	0
56	MG	1G	1610	1/1	0.89	0.37	77,77,77,77	0
56	MG	1G	1633	1/1	0.89	0.25	76,76,76,76	0
56	MG	14	3138	1/1	0.89	0.33	79,79,79,79	0
56	MG	1H	3165	1/1	0.89	0.23	61,61,61,61	0
56	MG	13	1631	1/1	0.89	0.28	73,73,73,73	0
56	MG	1H	3325	1/1	0.90	0.39	96,96,96,96	0
56	MG	L8	101	1/1	0.90	0.24	70,70,70,70	0
56	MG	13	1634	1/1	0.90	0.25	74,74,74,74	0
56	MG	1H	3218	1/1	0.90	0.14	61,61,61,61	0
56	MG	1G	1663	1/1	0.90	0.20	75,75,75,75	0
56	MG	1G	1628	1/1	0.90	0.22	77,77,77,77	0
56	MG	14	3278	1/1	0.90	0.19	98,98,98,98	0
56	MG	1H	3050	1/1	0.90	0.28	36,36,36,36	0
56	MG	1H	3379	1/1	0.90	0.10	46,46,46,46	0
56	MG	14	3088	1/1	0.90	0.43	71,71,71,71	0
56	MG	13	1651	1/1	0.90	0.20	87,87,87,87	0
56	MG	1H	3241	1/1	0.90	0.26	65,65,65,65	0
56	MG	1H	3452	1/1	0.90	0.13	49,49,49,49	0
56	MG	13	1646	1/1	0.90	0.18	95,95,95,95	0
56	MG	13	1690	1/1	0.90	0.25	113,113,113,113	0
56	MG	13	1659	1/1	0.90	0.21	66,66,66,66	0
56	MG	1H	3118	1/1	0.90	0.26	52,52,52,52	0
56	MG	14	3213	1/1	0.90	0.27	85,85,85,85	0
56	MG	13	1694	1/1	0.90	0.20	82,82,82,82	0
56	MG	14	3299	1/1	0.90	0.32	70,70,70,70	0
56	MG	1H	3147	1/1	0.90	0.47	68,68,68,68	0
56	MG	14	3339	1/1	0.90	0.17	94,94,94,94	0
56	MG	13	1740	1/1	0.90	0.12	88,88,88,88	0
56	MG	1H	3343	1/1	0.90	0.43	75,75,75,75	0
56	MG	13	1700	1/1	0.90	0.26	71,71,71,71	0
56	MG	14	3018	1/1	0.90	0.13	68,68,68,68	0
56	MG	1H	3081	1/1	0.90	0.22	61,61,61,61	0
56	MG	1H	3142	1/1	0.90	0.14	39,39,39,39	0
56	MG	14	3247	1/1	0.90	0.11	67,67,67,67	0
56	MG	1H	3285	1/1	0.90	0.21	61,61,61,61	0
56	MG	14	3233	1/1	0.90	0.11	61,61,61,61	0
56	MG	14	3210	1/1	0.90	0.26	71,71,71,71	0
56	MG	14	3192	1/1	0.90	0.35	80,80,80,80	0
56	MG	14	3164	1/1	0.90	0.16	64,64,64,64	0
56	MG	2K	105	1/1	0.90	0.35	78,78,78,78	0
56	MG	14	3097	1/1	0.90	0.21	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1J	205	1/1	0.90	0.10	82,82,82,82	0
56	MG	1H	3425	1/1	0.90	0.07	67,67,67,67	0
56	MG	13	1665	1/1	0.90	0.24	67,67,67,67	0
56	MG	14	3228	1/1	0.90	0.46	98,98,98,98	0
56	MG	1H	3169	1/1	0.90	0.35	62,62,62,62	0
56	MG	1H	3426	1/1	0.90	0.13	59,59,59,59	0
56	MG	1H	3033	1/1	0.90	0.15	67,67,67,67	0
56	MG	13	1648	1/1	0.90	0.19	69,69,69,69	0
56	MG	1H	3158	1/1	0.90	0.15	70,70,70,70	0
56	MG	14	3291	1/1	0.90	0.26	55,55,55,55	0
56	MG	14	3288	1/1	0.90	0.16	74,74,74,74	0
56	MG	1G	1662	1/1	0.90	0.19	73,73,73,73	0
56	MG	13	1689	1/1	0.90	0.38	120,120,120,120	0
56	MG	1H	3245	1/1	0.90	0.12	58,58,58,58	0
56	MG	14	3323	1/1	0.90	0.06	55,55,55,55	0
56	MG	14	3387	1/1	0.90	0.09	97,97,97,97	0
56	MG	1G	1671	1/1	0.90	0.09	73,73,73,73	0
56	MG	16	206	1/1	0.90	0.40	60,60,60,60	0
56	MG	14	3259	1/1	0.90	0.23	82,82,82,82	0
56	MG	1G	1626	1/1	0.91	0.27	79,79,79,79	0
56	MG	1H	3034	1/1	0.91	0.12	51,51,51,51	0
56	MG	14	3340	1/1	0.91	0.10	59,59,59,59	0
56	MG	1H	3215	1/1	0.91	0.22	85,85,85,85	0
56	MG	14	3140	1/1	0.91	0.31	92,92,92,92	0
56	MG	1H	3140	1/1	0.91	0.45	63,63,63,63	0
56	MG	1H	3424	1/1	0.91	0.14	58,58,58,58	0
56	MG	1H	3469	1/1	0.91	0.10	90,90,90,90	0
56	MG	1H	3284	1/1	0.91	0.18	62,62,62,62	0
56	MG	14	3238	1/1	0.91	0.23	85,85,85,85	0
56	MG	1H	3103	1/1	0.91	0.16	30,30,30,30	0
56	MG	1H	3335	1/1	0.91	0.26	87,87,87,87	0
56	MG	1H	3145	1/1	0.91	0.25	49,49,49,49	0
56	MG	1H	3478	1/1	0.91	0.10	102,102,102,102	0
56	MG	14	3350	1/1	0.91	0.11	83,83,83,83	0
56	MG	1H	3226	1/1	0.91	0.27	69,69,69,69	0
56	MG	14	3160	1/1	0.91	0.12	73,73,73,73	0
56	MG	14	3113	1/1	0.91	0.13	42,42,42,42	0
56	MG	1H	3356	1/1	0.91	0.14	79,79,79,79	0
56	MG	1H	3231	1/1	0.91	0.14	31,31,31,31	0
56	MG	1G	1680	1/1	0.91	0.27	94,94,94,94	0
56	MG	14	3269	1/1	0.91	0.19	59,59,59,59	0
56	MG	14	3185	1/1	0.91	0.11	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1625	1/1	0.91	0.38	84,84,84,84	0
56	MG	14	3375	1/1	0.91	0.06	91,91,91,91	0
56	MG	1H	3308	1/1	0.91	0.22	65,65,65,65	0
56	MG	14	3270	1/1	0.91	0.11	56,56,56,56	0
56	MG	14	3184	1/1	0.91	0.15	53,53,53,53	0
56	MG	1H	3092	1/1	0.91	0.11	50,50,50,50	0
56	MG	1H	3450	1/1	0.91	0.05	67,67,67,67	0
56	MG	1H	3151	1/1	0.91	0.20	66,66,66,66	0
56	MG	1H	3254	1/1	0.91	0.19	77,77,77,77	0
56	MG	14	3353	1/1	0.91	0.23	83,83,83,83	0
56	MG	14	3296	1/1	0.91	0.15	74,74,74,74	0
56	MG	1H	3333	1/1	0.91	0.46	93,93,93,93	0
56	MG	1H	3045	1/1	0.91	0.35	66,66,66,66	0
56	MG	14	3273	1/1	0.91	0.09	73,73,73,73	0
56	MG	1H	3346	1/1	0.91	0.21	73,73,73,73	0
56	MG	14	3196	1/1	0.91	0.20	90,90,90,90	0
56	MG	1H	3246	1/1	0.91	0.26	79,79,79,79	0
56	MG	14	3359	1/1	0.91	0.09	87,87,87,87	0
56	MG	14	3348	1/1	0.91	0.09	54,54,54,54	0
56	MG	1H	3265	1/1	0.92	0.84	54,54,54,54	0
56	MG	1H	3198	1/1	0.92	0.43	82,82,82,82	0
56	MG	1H	3188	1/1	0.92	0.15	60,60,60,60	0
56	MG	1G	1683	1/1	0.92	0.10	104,104,104,104	0
56	MG	13	1610	1/1	0.92	0.29	72,72,72,72	0
56	MG	1H	3085	1/1	0.92	0.21	66,66,66,66	0
56	MG	13	1669	1/1	0.92	0.19	76,76,76,76	0
56	MG	14	3301	1/1	0.92	0.27	86,86,86,86	0
56	MG	1H	3016	1/1	0.92	0.22	45,45,45,45	0
56	MG	13	1677	1/1	0.92	0.17	71,71,71,71	0
56	MG	1H	3347	1/1	0.92	0.56	85,85,85,85	0
56	MG	1H	3237	1/1	0.92	0.15	57,57,57,57	0
56	MG	13	1699	1/1	0.92	0.20	75,75,75,75	0
56	MG	14	3234	1/1	0.92	0.21	68,68,68,68	0
56	MG	14	3076	1/1	0.92	0.29	54,54,54,54	0
56	MG	1H	3474	1/1	0.92	0.11	64,64,64,64	0
56	MG	14	3054	1/1	0.92	0.35	74,74,74,74	0
56	MG	14	3307	1/1	0.92	0.17	60,60,60,60	0
56	MG	1H	3028	1/1	0.92	0.27	67,67,67,67	0
56	MG	1G	1629	1/1	0.92	0.24	79,79,79,79	0
56	MG	1H	3089	1/1	0.92	0.26	45,45,45,45	0
56	MG	14	3257	1/1	0.92	0.18	79,79,79,79	0
56	MG	1H	3278	1/1	0.92	0.25	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1746	1/1	0.92	0.18	72,72,72,72	0
56	MG	1H	3337	1/1	0.92	0.18	94,94,94,94	0
56	MG	14	3029	1/1	0.92	0.12	80,80,80,80	0
56	MG	14	3067	1/1	0.92	0.18	48,48,48,48	0
56	MG	1H	3135	1/1	0.92	0.23	54,54,54,54	0
56	MG	1J	204	1/1	0.92	0.12	95,95,95,95	0
56	MG	16	212	1/1	0.92	0.14	73,73,73,73	0
56	MG	13	1736	1/1	0.92	0.07	73,73,73,73	0
56	MG	1G	1634	1/1	0.92	0.33	76,76,76,76	0
56	MG	1H	3155	1/1	0.92	0.15	74,74,74,74	0
56	MG	1H	3236	1/1	0.92	0.18	68,68,68,68	0
56	MG	1H	3088	1/1	0.92	0.33	73,73,73,73	0
56	MG	1G	1666	1/1	0.92	0.16	74,74,74,74	0
56	MG	14	3205	1/1	0.92	0.25	71,71,71,71	0
56	MG	1H	3279	1/1	0.92	0.16	73,73,73,73	0
56	MG	14	3168	1/1	0.92	0.24	71,71,71,71	0
56	MG	1H	3465	1/1	0.92	0.10	94,94,94,94	0
56	MG	14	3252	1/1	0.92	0.38	96,96,96,96	0
56	MG	1H	3270	1/1	0.92	0.30	94,94,94,94	0
56	MG	1H	3306	1/1	0.92	0.27	86,86,86,86	0
56	MG	14	3051	1/1	0.92	0.14	78,78,78,78	0
56	MG	13	1674	1/1	0.92	0.19	94,94,94,94	0
56	MG	14	3385	1/1	0.92	0.20	72,72,72,72	0
56	MG	78	201	1/1	0.92	0.18	59,59,59,59	0
56	MG	14	3314	1/1	0.92	0.12	55,55,55,55	0
56	MG	1H	3317	1/1	0.92	0.18	61,61,61,61	0
56	MG	1H	3354	1/1	0.92	0.29	89,89,89,89	0
56	MG	1H	3304	1/1	0.92	0.29	69,69,69,69	0
56	MG	14	3240	1/1	0.92	0.10	77,77,77,77	0
56	MG	13	1672	1/1	0.92	0.07	91,91,91,91	0
56	MG	13	1742	1/1	0.92	0.10	115,115,115,115	0
56	MG	1H	3105	1/1	0.92	0.15	56,56,56,56	0
56	MG	1H	3320	1/1	0.92	0.18	91,91,91,91	0
56	MG	14	3124	1/1	0.92	0.22	63,63,63,63	0
56	MG	1H	3112	1/1	0.92	0.24	66,66,66,66	0
56	MG	16	210	1/1	0.92	0.28	89,89,89,89	0
56	MG	1H	3183	1/1	0.92	0.38	66,66,66,66	0
56	MG	1H	3310	1/1	0.92	0.28	69,69,69,69	0
56	MG	1G	1644	1/1	0.92	0.18	70,70,70,70	0
56	MG	14	3373	1/1	0.92	0.11	69,69,69,69	0
56	MG	88	201	1/1	0.92	0.20	78,78,78,78	0
56	MG	1H	3289	1/1	0.92	0.32	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3437	1/1	0.92	0.11	59,59,59,59	0
56	MG	14	3156	1/1	0.92	0.18	60,60,60,60	0
56	MG	1H	3204	1/1	0.92	0.25	59,59,59,59	0
56	MG	1H	3070	1/1	0.92	0.16	46,46,46,46	0
56	MG	1H	3180	1/1	0.92	0.18	59,59,59,59	0
56	MG	14	3246	1/1	0.92	0.12	66,66,66,66	0
56	MG	1H	3318	1/1	0.92	0.15	56,56,56,56	0
56	MG	L5	101	1/1	0.92	0.21	73,73,73,73	0
56	MG	1H	3479	1/1	0.92	0.15	90,90,90,90	0
56	MG	1H	3134	1/1	0.92	0.12	61,61,61,61	0
56	MG	1H	3066	1/1	0.92	0.17	67,67,67,67	0
56	MG	14	3023	1/1	0.92	0.17	40,40,40,40	0
56	MG	14	3224	1/1	0.92	0.48	48,48,48,48	0
56	MG	1H	3083	1/1	0.92	0.12	69,69,69,69	0
56	MG	1H	3051	1/1	0.92	0.15	65,65,65,65	0
56	MG	14	3279	1/1	0.93	0.11	60,60,60,60	0
56	MG	14	3058	1/1	0.93	0.19	61,61,61,61	0
56	MG	14	3186	1/1	0.93	0.28	54,54,54,54	0
56	MG	1H	3307	1/1	0.93	0.21	80,80,80,80	0
56	MG	1G	1631	1/1	0.93	0.21	86,86,86,86	0
56	MG	1H	3390	1/1	0.93	0.10	66,66,66,66	0
56	MG	1G	1624	1/1	0.93	0.18	63,63,63,63	0
56	MG	14	3198	1/1	0.93	0.25	78,78,78,78	0
56	MG	35	201	1/1	0.93	0.20	60,60,60,60	0
56	MG	1H	3429	1/1	0.93	0.08	40,40,40,40	0
56	MG	14	3017	1/1	0.93	0.17	49,49,49,49	0
56	MG	1H	3086	1/1	0.93	0.29	66,66,66,66	0
56	MG	14	3352	1/1	0.93	0.08	84,84,84,84	0
56	MG	1H	3434	1/1	0.93	0.08	75,75,75,75	0
56	MG	1H	3131	1/1	0.93	0.28	67,67,67,67	0
56	MG	13	1721	1/1	0.93	0.14	90,90,90,90	0
56	MG	14	3166	1/1	0.93	0.21	70,70,70,70	0
56	MG	1G	1657	1/1	0.93	0.17	126,126,126,126	0
56	MG	14	3141	1/1	0.93	0.11	76,76,76,76	0
56	MG	1H	3039	1/1	0.93	0.19	47,47,47,47	0
56	MG	1H	3247	1/1	0.93	0.24	64,64,64,64	0
56	MG	1H	3037	1/1	0.93	0.21	62,62,62,62	0
56	MG	14	3229	1/1	0.93	0.14	65,65,65,65	0
56	MG	13	1722	1/1	0.93	0.11	76,76,76,76	0
56	MG	14	3197	1/1	0.93	0.28	89,89,89,89	0
56	MG	1H	3327	1/1	0.93	0.47	79,79,79,79	0
56	MG	13	1671	1/1	0.93	0.11	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3120	1/1	0.93	0.28	75,75,75,75	0
56	MG	14	3201	1/1	0.93	0.25	72,72,72,72	0
56	MG	14	3092	1/1	0.93	0.28	41,41,41,41	0
56	MG	1K	101	1/1	0.93	0.19	75,75,75,75	0
56	MG	14	3231	1/1	0.93	0.22	74,74,74,74	0
56	MG	1H	3348	1/1	0.93	0.53	80,80,80,80	0
56	MG	1H	3047	1/1	0.93	0.21	70,70,70,70	0
56	MG	1H	3097	1/1	0.93	0.15	67,67,67,67	0
56	MG	14	3176	1/1	0.93	0.35	81,81,81,81	0
56	MG	1H	3041	1/1	0.93	0.28	87,87,87,87	0
56	MG	13	1682	1/1	0.93	0.11	86,86,86,86	0
56	MG	1H	3216	1/1	0.93	0.24	67,67,67,67	0
56	MG	14	3026	1/1	0.93	0.13	65,65,65,65	0
56	MG	1H	3388	1/1	0.93	0.14	64,64,64,64	0
56	MG	14	3087	1/1	0.93	0.33	62,62,62,62	0
56	MG	1H	3212	1/1	0.93	0.15	63,63,63,63	0
56	MG	14	3363	1/1	0.93	0.07	74,74,74,74	0
56	MG	14	3011	1/1	0.93	0.18	43,43,43,43	0
56	MG	14	3131	1/1	0.93	0.17	70,70,70,70	0
56	MG	1H	3350	1/1	0.93	0.08	67,67,67,67	0
56	MG	13	1636	1/1	0.93	0.18	66,66,66,66	0
56	MG	14	3391	1/1	0.93	0.71	58,58,58,58	0
56	MG	1J	206	1/1	0.93	0.13	73,73,73,73	0
56	MG	14	3072	1/1	0.93	0.15	45,45,45,45	0
56	MG	14	3251	1/1	0.93	0.15	48,48,48,48	0
56	MG	1G	1681	1/1	0.93	0.18	110,110,110,110	0
56	MG	14	3266	1/1	0.93	0.21	68,68,68,68	0
56	MG	1H	3351	1/1	0.93	0.25	70,70,70,70	0
56	MG	1G	1647	1/1	0.93	0.16	102,102,102,102	0
56	MG	1H	3032	1/1	0.93	0.30	78,78,78,78	0
56	MG	13	1706	1/1	0.93	0.17	79,79,79,79	0
56	MG	21	302	1/1	0.93	0.32	66,66,66,66	0
56	MG	14	3147	1/1	0.93	0.18	78,78,78,78	0
56	MG	1H	3361	1/1	0.93	0.21	53,53,53,53	0
56	MG	13	1691	1/1	0.93	0.12	64,64,64,64	0
56	MG	1H	3157	1/1	0.93	0.37	72,72,72,72	0
56	MG	1G	1672	1/1	0.93	0.10	78,78,78,78	0
56	MG	1G	1627	1/1	0.93	0.18	57,57,57,57	0
56	MG	13	1713	1/1	0.93	0.16	70,70,70,70	0
56	MG	14	3297	1/1	0.93	0.08	74,74,74,74	0
56	MG	14	3193	1/1	0.93	0.14	59,59,59,59	0
56	MG	1H	3065	1/1	0.93	0.20	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1613	1/1	0.93	0.27	71,71,71,71	0
56	MG	14	3281	1/1	0.93	0.22	73,73,73,73	0
56	MG	1H	3422	1/1	0.93	0.09	54,54,54,54	0
56	MG	1H	3360	1/1	0.93	0.32	73,73,73,73	0
56	MG	13	1612	1/1	0.94	0.16	63,63,63,63	0
56	MG	1H	3471	1/1	0.94	0.09	68,68,68,68	0
56	MG	14	3354	1/1	0.94	0.10	71,71,71,71	0
56	MG	1H	3373	1/1	0.94	0.15	45,45,45,45	0
56	MG	14	3255	1/1	0.94	0.14	65,65,65,65	0
56	MG	13	1622	1/1	0.94	0.35	79,79,79,79	0
56	MG	1H	3179	1/1	0.94	0.25	55,55,55,55	0
56	MG	14	3015	1/1	0.94	0.18	71,71,71,71	0
56	MG	2K	106	1/1	0.94	0.06	84,84,84,84	0
56	MG	13	1655	1/1	0.94	0.13	73,73,73,73	0
56	MG	14	3383	1/1	0.94	0.10	86,86,86,86	0
56	MG	1H	3460	1/1	0.94	0.13	55,55,55,55	0
56	MG	1G	1658	1/1	0.94	0.17	79,79,79,79	0
56	MG	14	3376	1/1	0.94	0.13	87,87,87,87	0
56	MG	2K	101	1/1	0.94	0.34	79,79,79,79	0
56	MG	1H	3094	1/1	0.94	0.28	41,41,41,41	0
56	MG	14	3327	1/1	0.94	0.10	58,58,58,58	0
56	MG	14	3045	1/1	0.94	0.32	57,57,57,57	0
56	MG	14	3002	1/1	0.94	0.18	43,43,43,43	0
56	MG	1G	1619	1/1	0.94	0.19	84,84,84,84	0
56	MG	1H	3190	1/1	0.94	0.14	67,67,67,67	0
56	MG	1G	1674	1/1	0.94	0.11	70,70,70,70	0
56	MG	1H	3069	1/1	0.94	0.09	44,44,44,44	0
56	MG	14	3308	1/1	0.94	0.12	46,46,46,46	0
56	MG	14	3346	1/1	0.94	0.12	59,59,59,59	0
56	MG	14	3037	1/1	0.94	0.16	61,61,61,61	0
56	MG	1H	3055	1/1	0.94	0.11	61,61,61,61	0
56	MG	14	3174	1/1	0.94	0.18	66,66,66,66	0
56	MG	14	3349	1/1	0.94	0.20	63,63,63,63	0
56	MG	1H	3283	1/1	0.94	0.31	74,74,74,74	0
56	MG	14	3304	1/1	0.94	0.10	68,68,68,68	0
56	MG	1H	3220	1/1	0.94	0.11	50,50,50,50	0
56	MG	1H	3038	1/1	0.94	0.13	55,55,55,55	0
56	MG	14	3225	1/1	0.94	0.20	78,78,78,78	0
56	MG	1H	3181	1/1	0.94	0.14	54,54,54,54	0
56	MG	I8	101	1/1	0.94	0.39	53,53,53,53	0
56	MG	1H	3043	1/1	0.94	0.45	84,84,84,84	0
56	MG	1H	3095	1/1	0.94	0.41	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3215	1/1	0.94	0.12	50,50,50,50	0
56	MG	1H	3060	1/1	0.94	0.20	74,74,74,74	0
56	MG	1H	3377	1/1	0.94	0.07	44,44,44,44	0
56	MG	14	3157	1/1	0.94	0.12	88,88,88,88	0
56	MG	14	3237	1/1	0.94	0.13	54,54,54,54	0
56	MG	1H	3187	1/1	0.94	0.30	56,56,56,56	0
56	MG	13	1607	1/1	0.94	0.18	77,77,77,77	0
56	MG	21	301	1/1	0.94	0.15	53,53,53,53	0
56	MG	1G	1617	1/1	0.94	0.16	80,80,80,80	0
56	MG	1G	1621	1/1	0.94	0.15	81,81,81,81	0
56	MG	14	3107	1/1	0.94	0.24	40,40,40,40	0
56	MG	13	1729	1/1	0.94	0.06	97,97,97,97	0
56	MG	1H	3324	1/1	0.94	0.26	87,87,87,87	0
56	MG	1J	201	1/1	0.94	0.16	87,87,87,87	0
56	MG	1H	3244	1/1	0.94	0.17	39,39,39,39	0
56	MG	14	3315	1/1	0.94	0.13	68,68,68,68	0
56	MG	14	3022	1/1	0.94	0.14	72,72,72,72	0
56	MG	14	3338	1/1	0.94	0.13	53,53,53,53	0
56	MG	13	1709	1/1	0.94	0.22	89,89,89,89	0
56	MG	1G	1679	1/1	0.94	0.10	90,90,90,90	0
56	MG	1H	3420	1/1	0.94	0.16	48,48,48,48	0
56	MG	1H	3130	1/1	0.94	0.24	54,54,54,54	0
56	MG	14	3146	1/1	0.94	0.29	69,69,69,69	0
56	MG	1H	3141	1/1	0.94	0.38	60,60,60,60	0
56	MG	13	1611	1/1	0.94	0.30	70,70,70,70	0
56	MG	14	3008	1/1	0.94	0.21	54,54,54,54	0
56	MG	13	1681	1/1	0.94	0.23	81,81,81,81	0
56	MG	13	1632	1/1	0.94	0.18	63,63,63,63	0
56	MG	14	3239	1/1	0.94	0.16	76,76,76,76	0
56	MG	1H	3399	1/1	0.94	0.08	47,47,47,47	0
56	MG	1G	1632	1/1	0.94	0.20	70,70,70,70	0
56	MG	1H	3355	1/1	0.94	0.22	60,60,60,60	0
56	MG	1G	1673	1/1	0.94	0.06	74,74,74,74	0
56	MG	13	1657	1/1	0.94	0.27	69,69,69,69	0
56	MG	1H	3340	1/1	0.94	0.14	74,74,74,74	0
56	MG	1H	3315	1/1	0.94	0.28	66,66,66,66	0
56	MG	14	3028	1/1	0.94	0.18	73,73,73,73	0
56	MG	1H	3345	1/1	0.94	0.11	60,60,60,60	0
56	MG	1H	3062	1/1	0.94	0.36	65,65,65,65	0
56	MG	1H	3292	1/1	0.94	0.21	60,60,60,60	0
56	MG	1H	3397	1/1	0.94	0.11	66,66,66,66	0
56	MG	1H	3048	1/1	0.94	0.24	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3390	1/1	0.94	0.15	90,90,90,90	0
56	MG	1H	3229	1/1	0.94	0.33	95,95,95,95	0
56	MG	14	3310	1/1	0.94	0.09	50,50,50,50	0
56	MG	14	3380	1/1	0.94	0.10	93,93,93,93	0
56	MG	1H	3457	1/1	0.94	0.06	92,92,92,92	0
56	MG	14	3106	1/1	0.94	0.13	50,50,50,50	0
56	MG	1H	3329	1/1	0.94	0.39	73,73,73,73	0
56	MG	14	3322	1/1	0.94	0.10	77,77,77,77	0
56	MG	14	3209	1/1	0.94	0.16	74,74,74,74	0
56	MG	13	1714	1/1	0.94	0.34	99,99,99,99	0
56	MG	13	1718	1/1	0.94	0.20	90,90,90,90	0
56	MG	1H	3235	1/1	0.95	0.14	38,38,38,38	0
56	MG	14	3194	1/1	0.95	0.16	52,52,52,52	0
56	MG	14	3181	1/1	0.95	0.18	55,55,55,55	0
56	MG	14	3206	1/1	0.95	0.15	48,48,48,48	0
56	MG	1H	3251	1/1	0.95	0.10	61,61,61,61	0
56	MG	1H	3430	1/1	0.95	0.07	76,76,76,76	0
56	MG	1H	3143	1/1	0.95	0.13	49,49,49,49	0
56	MG	1H	3427	1/1	0.95	0.23	76,76,76,76	0
56	MG	14	3066	1/1	0.95	0.14	49,49,49,49	0
56	MG	14	3047	1/1	0.95	0.11	60,60,60,60	0
56	MG	14	3326	1/1	0.95	0.14	65,65,65,65	0
56	MG	1H	3256	1/1	0.95	0.20	57,57,57,57	0
56	MG	14	3057	1/1	0.95	0.16	68,68,68,68	0
56	MG	13	1645	1/1	0.95	0.10	79,79,79,79	0
56	MG	14	3253	1/1	0.95	0.30	74,74,74,74	0
56	MG	14	3384	1/1	0.95	0.09	62,62,62,62	0
56	MG	13	1737	1/1	0.95	0.07	62,62,62,62	0
56	MG	1G	1638	1/1	0.95	0.16	75,75,75,75	0
56	MG	1H	3031	1/1	0.95	0.17	71,71,71,71	0
56	MG	14	3356	1/1	0.95	0.09	72,72,72,72	0
56	MG	1H	3214	1/1	0.95	0.34	68,68,68,68	0
56	MG	1H	3191	1/1	0.95	0.18	75,75,75,75	0
56	MG	2K	104	1/1	0.95	0.29	98,98,98,98	0
56	MG	1H	3286	1/1	0.95	0.21	70,70,70,70	0
56	MG	14	3114	1/1	0.95	0.25	44,44,44,44	0
56	MG	1H	3396	1/1	0.95	0.18	57,57,57,57	0
56	MG	1G	1661	1/1	0.95	0.20	73,73,73,73	0
56	MG	1H	3063	1/1	0.95	0.44	65,65,65,65	0
56	MG	13	1678	1/1	0.95	0.21	74,74,74,74	0
56	MG	1H	3303	1/1	0.95	0.18	65,65,65,65	0
56	MG	1G	1635	1/1	0.95	0.34	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1726	1/1	0.95	0.13	77,77,77,77	0
56	MG	14	3162	1/1	0.95	0.38	56,56,56,56	0
56	MG	2K	103	1/1	0.95	0.18	81,81,81,81	0
56	MG	1G	1653	1/1	0.95	0.23	90,90,90,90	0
56	MG	1H	3044	1/1	0.95	0.16	51,51,51,51	0
56	MG	1H	3432	1/1	0.95	0.12	65,65,65,65	0
56	MG	1G	1611	1/1	0.95	0.13	72,72,72,72	0
56	MG	1H	3309	1/1	0.95	0.48	98,98,98,98	0
56	MG	1H	3253	1/1	0.95	0.15	78,78,78,78	0
56	MG	14	3219	1/1	0.95	0.14	56,56,56,56	0
56	MG	1G	1604	1/1	0.95	0.12	77,77,77,77	0
56	MG	1H	3004	1/1	0.95	0.41	47,47,47,47	0
56	MG	14	3074	1/1	0.95	0.17	66,66,66,66	0
56	MG	1H	3219	1/1	0.95	0.15	53,53,53,53	0
56	MG	1H	3162	1/1	0.95	0.25	68,68,68,68	0
56	MG	14	3024	1/1	0.95	0.15	74,74,74,74	0
56	MG	5E	201	1/1	0.95	0.18	70,70,70,70	0
56	MG	14	3007	1/1	0.95	0.13	48,48,48,48	0
56	MG	14	3204	1/1	0.95	0.19	51,51,51,51	0
56	MG	1H	3132	1/1	0.95	0.21	45,45,45,45	0
56	MG	14	3128	1/1	0.95	0.29	58,58,58,58	0
56	MG	13	1624	1/1	0.95	0.28	48,48,48,48	0
56	MG	14	3382	1/1	0.95	0.08	69,69,69,69	0
56	MG	1H	3383	1/1	0.95	0.18	52,52,52,52	0
56	MG	1H	3382	1/1	0.95	0.09	45,45,45,45	0
56	MG	1G	1660	1/1	0.95	0.10	74,74,74,74	0
56	MG	14	3244	1/1	0.95	0.15	65,65,65,65	0
56	MG	1H	3195	1/1	0.95	0.27	65,65,65,65	0
56	MG	1H	3262	1/1	0.95	0.39	56,56,56,56	0
56	MG	14	3134	1/1	0.95	0.17	64,64,64,64	0
56	MG	13	1635	1/1	0.95	0.12	59,59,59,59	0
56	MG	13	1723	1/1	0.95	0.08	86,86,86,86	0
56	MG	14	3103	1/1	0.95	0.21	67,67,67,67	0
56	MG	1H	3369	1/1	0.95	0.12	45,45,45,45	0
56	MG	1H	3073	1/1	0.95	0.27	63,63,63,63	0
56	MG	14	3235	1/1	0.95	0.26	72,72,72,72	0
56	MG	14	3035	1/1	0.95	0.14	54,54,54,54	0
56	MG	14	3044	1/1	0.95	0.08	53,53,53,53	0
56	MG	1H	3120	1/1	0.95	0.13	60,60,60,60	0
56	MG	1H	3064	1/1	0.95	0.26	56,56,56,56	0
56	MG	14	3056	1/1	0.95	0.18	51,51,51,51	0
56	MG	1H	3375	1/1	0.95	0.09	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3352	1/1	0.95	0.13	61,61,61,61	0
56	MG	14	3366	1/1	0.95	0.13	66,66,66,66	0
56	MG	1H	3378	1/1	0.95	0.14	55,55,55,55	0
56	MG	14	3075	1/1	0.95	0.15	53,53,53,53	0
56	MG	1H	3370	1/1	0.95	0.12	54,54,54,54	0
56	MG	1G	1606	1/1	0.95	0.25	79,79,79,79	0
56	MG	1H	3439	1/1	0.95	0.10	69,69,69,69	0
56	MG	14	3337	1/1	0.95	0.06	55,55,55,55	0
56	MG	1H	3196	1/1	0.95	0.08	68,68,68,68	0
56	MG	1H	3119	1/1	0.95	0.29	52,52,52,52	0
56	MG	14	3294	1/1	0.95	0.24	74,74,74,74	0
56	MG	1H	3121	1/1	0.95	0.18	64,64,64,64	0
56	MG	13	1661	1/1	0.95	0.29	54,54,54,54	0
56	MG	1H	3436	1/1	0.95	0.10	60,60,60,60	0
56	MG	14	3343	1/1	0.95	0.14	46,46,46,46	0
56	MG	16	209	1/1	0.95	0.20	56,56,56,56	0
56	MG	1H	3082	1/1	0.95	0.27	70,70,70,70	0
56	MG	1H	3294	1/1	0.95	0.19	47,47,47,47	0
56	MG	14	3245	1/1	0.96	0.21	70,70,70,70	0
56	MG	1H	3208	1/1	0.96	0.26	78,78,78,78	0
56	MG	14	3165	1/1	0.96	0.16	58,58,58,58	0
56	MG	14	3277	1/1	0.96	0.17	66,66,66,66	0
56	MG	1H	3287	1/1	0.96	0.14	50,50,50,50	0
56	MG	1H	3040	1/1	0.96	0.14	49,49,49,49	0
56	MG	1H	3018	1/1	0.96	0.17	52,52,52,52	0
56	MG	1H	3398	1/1	0.96	0.11	55,55,55,55	0
56	MG	14	3031	1/1	0.96	0.27	60,60,60,60	0
56	MG	1H	3449	1/1	0.96	0.06	72,72,72,72	0
56	MG	14	3100	1/1	0.96	0.17	63,63,63,63	0
56	MG	14	3386	1/1	0.96	0.22	60,60,60,60	0
56	MG	14	3358	1/1	0.96	0.22	77,77,77,77	0
56	MG	14	3082	1/1	0.96	0.16	67,67,67,67	0
56	MG	14	3200	1/1	0.96	0.13	66,66,66,66	0
56	MG	14	3295	1/1	0.96	0.23	64,64,64,64	0
56	MG	14	3371	1/1	0.96	0.13	56,56,56,56	0
56	MG	1H	3182	1/1	0.96	0.20	87,87,87,87	0
56	MG	14	3109	1/1	0.96	0.09	78,78,78,78	0
56	MG	14	3362	1/1	0.96	0.08	69,69,69,69	0
56	MG	1G	1651	1/1	0.96	0.17	84,84,84,84	0
56	MG	1H	3027	1/1	0.96	0.22	32,32,32,32	0
56	MG	1H	3405	1/1	0.96	0.20	61,61,61,61	0
56	MG	14	3048	1/1	0.96	0.15	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3330	1/1	0.96	0.06	48,48,48,48	0
56	MG	1H	3466	1/1	0.96	0.06	56,56,56,56	0
56	MG	1H	3176	1/1	0.96	0.16	60,60,60,60	0
56	MG	1H	3008	1/1	0.96	0.33	42,42,42,42	0
56	MG	13	1734	1/1	0.96	0.07	86,86,86,86	0
56	MG	13	1619	1/1	0.96	0.26	64,64,64,64	0
56	MG	1H	3260	1/1	0.96	0.11	72,72,72,72	0
56	MG	1H	3074	1/1	0.96	0.28	70,70,70,70	0
56	MG	14	3081	1/1	0.96	0.25	52,52,52,52	0
56	MG	14	3334	1/1	0.96	0.08	79,79,79,79	0
56	MG	1H	3116	1/1	0.96	0.37	62,62,62,62	0
56	MG	1H	3363	1/1	0.96	0.23	68,68,68,68	0
56	MG	1H	3391	1/1	0.96	0.09	71,71,71,71	0
56	MG	1H	3164	1/1	0.96	0.18	52,52,52,52	0
56	MG	14	3043	1/1	0.96	0.15	67,67,67,67	0
56	MG	14	3211	1/1	0.96	0.15	67,67,67,67	0
56	MG	13	1712	1/1	0.96	0.16	77,77,77,77	0
56	MG	13	1739	1/1	0.96	0.21	73,73,73,73	0
56	MG	1H	3011	1/1	0.96	0.20	48,48,48,48	0
56	MG	1G	1603	1/1	0.96	0.12	76,76,76,76	0
56	MG	1H	3075	1/1	0.96	0.39	70,70,70,70	0
56	MG	1H	3184	1/1	0.96	0.19	45,45,45,45	0
56	MG	14	3179	1/1	0.96	0.28	64,64,64,64	0
56	MG	14	3317	1/1	0.96	0.10	41,41,41,41	0
56	MG	14	3108	1/1	0.96	0.21	76,76,76,76	0
56	MG	1H	3123	1/1	0.96	0.23	52,52,52,52	0
56	MG	1H	3166	1/1	0.96	0.26	72,72,72,72	0
56	MG	1G	1614	1/1	0.96	0.27	72,72,72,72	0
56	MG	1H	3297	1/1	0.96	0.33	71,71,71,71	0
56	MG	1H	3258	1/1	0.96	0.22	63,63,63,63	0
56	MG	14	3004	1/1	0.96	0.17	46,46,46,46	0
56	MG	1H	3046	1/1	0.96	0.34	67,67,67,67	0
56	MG	13	1695	1/1	0.96	0.21	79,79,79,79	0
56	MG	13	1603	1/1	0.96	0.15	58,58,58,58	0
56	MG	13	1725	1/1	0.96	0.08	62,62,62,62	0
56	MG	1H	3005	1/1	0.96	0.23	53,53,53,53	0
56	MG	1H	3013	1/1	0.96	0.20	31,31,31,31	0
56	MG	1H	3433	1/1	0.96	0.09	83,83,83,83	0
56	MG	14	3309	1/1	0.96	0.11	58,58,58,58	0
56	MG	14	3325	1/1	0.96	0.12	63,63,63,63	0
56	MG	14	3068	1/1	0.96	0.19	69,69,69,69	0
56	MG	1H	3392	1/1	0.96	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3268	1/1	0.96	0.23	46,46,46,46	0
56	MG	14	3328	1/1	0.96	0.10	62,62,62,62	0
56	MG	14	3212	1/1	0.96	0.12	65,65,65,65	0
56	MG	1H	3193	1/1	0.96	0.29	69,69,69,69	0
56	MG	13	1744	1/1	0.96	0.07	95,95,95,95	0
56	MG	1G	1637	1/1	0.96	0.41	81,81,81,81	0
56	MG	1H	3481	1/1	0.96	0.12	77,77,77,77	0
56	MG	1G	1612	1/1	0.96	0.18	63,63,63,63	0
56	MG	14	3039	1/1	0.96	0.17	38,38,38,38	0
56	MG	14	3016	1/1	0.96	0.12	54,54,54,54	0
56	MG	1H	3296	1/1	0.96	0.25	90,90,90,90	0
56	MG	29	302	1/1	0.96	0.29	65,65,65,65	0
56	MG	14	3055	1/1	0.96	0.15	64,64,64,64	0
56	MG	1H	3015	1/1	0.96	0.22	59,59,59,59	0
56	MG	13	1639	1/1	0.96	0.12	56,56,56,56	0
56	MG	1H	3133	1/1	0.96	0.17	60,60,60,60	0
56	MG	14	3321	1/1	0.96	0.08	62,62,62,62	0
56	MG	13	1732	1/1	0.96	0.12	62,62,62,62	0
56	MG	14	3203	1/1	0.96	0.19	55,55,55,55	0
56	MG	1G	1645	1/1	0.96	0.12	73,73,73,73	0
56	MG	1H	3381	1/1	0.96	0.11	40,40,40,40	0
56	MG	1G	1687	1/1	0.96	0.10	81,81,81,81	0
56	MG	14	3036	1/1	0.96	0.16	42,42,42,42	0
56	MG	1H	3127	1/1	0.96	0.19	52,52,52,52	0
56	MG	14	3232	1/1	0.96	0.29	62,62,62,62	0
56	MG	14	3013	1/1	0.96	0.18	54,54,54,54	0
56	MG	14	3188	1/1	0.96	0.17	56,56,56,56	0
56	MG	1H	3456	1/1	0.96	0.12	92,92,92,92	0
56	MG	1H	3441	1/1	0.96	0.10	86,86,86,86	0
56	MG	1G	1682	1/1	0.96	0.08	74,74,74,74	0
56	MG	1H	3376	1/1	0.96	0.08	36,36,36,36	0
56	MG	14	3336	1/1	0.96	0.09	52,52,52,52	0
56	MG	14	3248	1/1	0.96	0.16	76,76,76,76	0
56	MG	1G	1655	1/1	0.96	0.39	79,79,79,79	0
56	MG	13	1683	1/1	0.96	0.14	69,69,69,69	0
56	MG	1G	1616	1/1	0.96	0.15	86,86,86,86	0
56	MG	13	1614	1/1	0.96	0.19	79,79,79,79	0
56	MG	1H	3012	1/1	0.96	0.34	45,45,45,45	0
56	MG	13	1650	1/1	0.96	0.16	68,68,68,68	0
56	MG	1H	3059	1/1	0.96	0.13	68,68,68,68	0
56	MG	14	3312	1/1	0.96	0.07	67,67,67,67	0
56	MG	14	3112	1/1	0.96	0.11	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3003	1/1	0.96	0.26	35,35,35,35	0
56	MG	1H	3052	1/1	0.97	0.22	46,46,46,46	0
56	MG	1H	3025	1/1	0.97	0.23	53,53,53,53	0
56	MG	1H	3277	1/1	0.97	0.27	70,70,70,70	0
56	MG	14	3027	1/1	0.97	0.13	70,70,70,70	0
56	MG	1G	1613	1/1	0.97	0.08	87,87,87,87	0
56	MG	14	3242	1/1	0.97	0.17	74,74,74,74	0
56	MG	45	201	1/1	0.97	0.11	50,50,50,50	0
56	MG	1H	3102	1/1	0.97	0.14	60,60,60,60	0
56	MG	14	3080	1/1	0.97	0.07	69,69,69,69	0
56	MG	1H	3021	1/1	0.97	0.22	45,45,45,45	0
56	MG	14	3222	1/1	0.97	0.18	83,83,83,83	0
56	MG	13	1620	1/1	0.97	0.21	51,51,51,51	0
56	MG	13	1667	1/1	0.97	0.19	92,92,92,92	0
56	MG	13	1638	1/1	0.97	0.19	53,53,53,53	0
56	MG	1H	3365	1/1	0.97	0.17	64,64,64,64	0
56	MG	14	3098	1/1	0.97	0.22	54,54,54,54	0
56	MG	2L	101	1/1	0.97	0.15	76,76,76,76	0
56	MG	1H	3024	1/1	0.97	0.32	46,46,46,46	0
56	MG	14	3202	1/1	0.97	0.38	55,55,55,55	0
56	MG	14	3006	1/1	0.97	0.16	48,48,48,48	0
56	MG	1H	3357	1/1	0.97	0.29	62,62,62,62	0
56	MG	14	3152	1/1	0.97	0.11	67,67,67,67	0
56	MG	1G	1615	1/1	0.97	0.17	87,87,87,87	0
56	MG	1H	3019	1/1	0.97	0.22	38,38,38,38	0
56	MG	1H	3476	1/1	0.97	0.07	79,79,79,79	0
56	MG	1G	1605	1/1	0.97	0.13	74,74,74,74	0
56	MG	1H	3206	1/1	0.97	0.23	63,63,63,63	0
56	MG	14	3012	1/1	0.97	0.26	77,77,77,77	0
56	MG	1H	3385	1/1	0.97	0.10	54,54,54,54	0
56	MG	1H	3252	1/1	0.97	0.12	49,49,49,49	0
56	MG	1H	3404	1/1	0.97	0.08	45,45,45,45	0
56	MG	1H	3473	1/1	0.97	0.17	73,73,73,73	0
56	MG	1G	1639	1/1	0.97	0.10	85,85,85,85	0
56	MG	14	3101	1/1	0.97	0.26	84,84,84,84	0
56	MG	14	3357	1/1	0.97	0.15	62,62,62,62	0
56	MG	1H	3232	1/1	0.97	0.13	43,43,43,43	0
56	MG	1H	3006	1/1	0.97	0.16	49,49,49,49	0
56	MG	13	1731	1/1	0.97	0.10	94,94,94,94	0
56	MG	14	3083	1/1	0.97	0.15	60,60,60,60	0
56	MG	1H	3414	1/1	0.97	0.13	53,53,53,53	0
56	MG	1H	3200	1/1	0.97	0.19	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3448	1/1	0.97	0.06	88,88,88,88	0
56	MG	14	3032	1/1	0.97	0.17	65,65,65,65	0
56	MG	1H	3225	1/1	0.97	0.32	57,57,57,57	0
58	ZN	3E	302	1/1	0.97	0.35	89,89,89,89	0
56	MG	13	1654	1/1	0.97	0.23	75,75,75,75	0
56	MG	1H	3367	1/1	0.97	0.30	66,66,66,66	0
57	PAR	13	1745	42/42	0.97	0.22	57,66,72,75	0
56	MG	14	3183	1/1	0.97	0.26	46,46,46,46	0
56	MG	14	3331	1/1	0.97	0.12	70,70,70,70	0
56	MG	13	1626	1/1	0.97	0.29	68,68,68,68	0
56	MG	1H	3400	1/1	0.97	0.13	47,47,47,47	0
56	MG	14	3191	1/1	0.97	0.20	57,57,57,57	0
56	MG	1H	3080	1/1	0.97	0.29	53,53,53,53	0
56	MG	1H	3302	1/1	0.97	0.12	59,59,59,59	0
56	MG	1H	3160	1/1	0.97	0.14	56,56,56,56	0
56	MG	14	3324	1/1	0.97	0.10	52,52,52,52	0
56	MG	14	3364	1/1	0.97	0.08	75,75,75,75	0
56	MG	14	3335	1/1	0.97	0.06	55,55,55,55	0
56	MG	13	1664	1/1	0.97	0.21	59,59,59,59	0
56	MG	1G	1649	1/1	0.97	0.14	72,72,72,72	0
56	MG	14	3316	1/1	0.97	0.10	49,49,49,49	0
56	MG	1G	1676	1/1	0.97	0.07	75,75,75,75	0
58	ZN	5A	101	1/1	0.97	0.14	121,121,121,121	0
56	MG	14	3221	1/1	0.97	0.29	58,58,58,58	0
56	MG	13	1627	1/1	0.97	0.21	62,62,62,62	0
56	MG	14	3361	1/1	0.97	0.07	60,60,60,60	0
56	MG	14	3014	1/1	0.97	0.22	58,58,58,58	0
56	MG	13	1656	1/1	0.97	0.26	91,91,91,91	0
56	MG	1H	3036	1/1	0.97	0.33	57,57,57,57	0
56	MG	1H	3411	1/1	0.97	0.08	53,53,53,53	0
56	MG	1H	3100	1/1	0.97	0.17	43,43,43,43	0
56	MG	14	3041	1/1	0.97	0.21	39,39,39,39	0
56	MG	14	3060	1/1	0.97	0.15	48,48,48,48	0
56	MG	14	3313	1/1	0.97	0.06	50,50,50,50	0
56	MG	14	3374	1/1	0.97	0.17	76,76,76,76	0
56	MG	13	1735	1/1	0.97	0.06	71,71,71,71	0
56	MG	1H	3415	1/1	0.97	0.17	68,68,68,68	0
57	PAR	1G	1686	42/42	0.97	0.25	69,76,87,91	0
56	MG	1H	3371	1/1	0.97	0.16	46,46,46,46	0
56	MG	14	3123	1/1	0.97	0.13	60,60,60,60	0
56	MG	14	3070	1/1	0.97	0.21	39,39,39,39	0
56	MG	1H	3149	1/1	0.97	0.34	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3073	1/1	0.97	0.16	80,80,80,80	0
56	MG	1H	3071	1/1	0.97	0.16	53,53,53,53	0
56	MG	14	3085	1/1	0.97	0.13	50,50,50,50	0
56	MG	14	3329	1/1	0.97	0.12	45,45,45,45	0
56	MG	14	3052	1/1	0.97	0.24	62,62,62,62	0
56	MG	13	1680	1/1	0.97	0.28	69,69,69,69	0
56	MG	1G	1640	1/1	0.97	0.19	80,80,80,80	0
56	MG	1H	3440	1/1	0.97	0.12	61,61,61,61	0
56	MG	14	3079	1/1	0.97	0.15	57,57,57,57	0
56	MG	1H	3447	1/1	0.97	0.11	76,76,76,76	0
56	MG	14	3093	1/1	0.97	0.26	48,48,48,48	0
56	MG	14	3001	1/1	0.97	0.23	53,53,53,53	0
56	MG	13	1606	1/1	0.97	0.20	63,63,63,63	0
56	MG	14	3126	1/1	0.97	0.31	66,66,66,66	0
56	MG	1H	3014	1/1	0.97	0.27	43,43,43,43	0
56	MG	14	3163	1/1	0.97	0.20	80,80,80,80	0
56	MG	13	1738	1/1	0.97	0.09	72,72,72,72	0
56	MG	14	3090	1/1	0.97	0.20	52,52,52,52	0
56	MG	14	3065	1/1	0.97	0.28	46,46,46,46	0
56	MG	13	1676	1/1	0.97	0.16	62,62,62,62	0
56	MG	14	3178	1/1	0.97	0.21	80,80,80,80	0
56	MG	1H	3023	1/1	0.97	0.22	51,51,51,51	0
56	MG	1H	3001	1/1	0.97	0.18	49,49,49,49	0
56	MG	13	1702	1/1	0.97	0.26	62,62,62,62	0
56	MG	13	1724	1/1	0.97	0.18	78,78,78,78	0
56	MG	1H	3026	1/1	0.97	0.23	53,53,53,53	0
56	MG	1H	3417	1/1	0.98	0.15	61,61,61,61	0
56	MG	14	3019	1/1	0.98	0.12	74,74,74,74	0
56	MG	1H	3115	1/1	0.98	0.34	51,51,51,51	0
56	MG	1H	3022	1/1	0.98	0.27	53,53,53,53	0
56	MG	2K	107	1/1	0.98	0.20	59,59,59,59	0
56	MG	1H	3291	1/1	0.98	0.25	40,40,40,40	0
56	MG	14	3009	1/1	0.98	0.18	51,51,51,51	0
56	MG	1H	3428	1/1	0.98	0.15	47,47,47,47	0
56	MG	1H	3009	1/1	0.98	0.27	43,43,43,43	0
56	MG	14	3143	1/1	0.98	0.21	67,67,67,67	0
56	MG	13	1640	1/1	0.98	0.10	75,75,75,75	0
56	MG	14	3040	1/1	0.98	0.21	43,43,43,43	0
56	MG	1H	3442	1/1	0.98	0.11	42,42,42,42	0
56	MG	14	3064	1/1	0.98	0.15	71,71,71,71	0
56	MG	1H	3090	1/1	0.98	0.21	44,44,44,44	0
56	MG	14	3320	1/1	0.98	0.23	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3049	1/1	0.98	0.28	60,60,60,60	0
56	MG	14	3021	1/1	0.98	0.19	55,55,55,55	0
58	ZN	32	301	1/1	0.98	0.36	96,96,96,96	0
56	MG	1G	1607	1/1	0.98	0.16	81,81,81,81	0
56	MG	1H	3242	1/1	0.98	0.29	58,58,58,58	0
56	MG	13	1604	1/1	0.98	0.10	68,68,68,68	0
56	MG	14	3084	1/1	0.98	0.18	43,43,43,43	0
56	MG	1H	3126	1/1	0.98	0.34	60,60,60,60	0
56	MG	13	1621	1/1	0.98	0.27	74,74,74,74	0
56	MG	1H	3402	1/1	0.98	0.10	48,48,48,48	0
56	MG	1H	3104	1/1	0.98	0.16	41,41,41,41	0
56	MG	14	3227	1/1	0.98	0.13	88,88,88,88	0
56	MG	1H	3079	1/1	0.98	0.26	45,45,45,45	0
56	MG	13	1630	1/1	0.98	0.18	43,43,43,43	0
56	MG	13	1727	1/1	0.98	0.06	76,76,76,76	0
56	MG	1G	1601	1/1	0.98	0.20	65,65,65,65	0
56	MG	14	3150	1/1	0.98	0.18	51,51,51,51	0
56	MG	14	3105	1/1	0.98	0.19	47,47,47,47	0
56	MG	14	3368	1/1	0.98	0.10	53,53,53,53	0
56	MG	14	3262	1/1	0.98	0.13	66,66,66,66	0
56	MG	1H	3387	1/1	0.98	0.08	54,54,54,54	0
56	MG	13	1675	1/1	0.98	0.10	73,73,73,73	0
56	MG	13	1615	1/1	0.98	0.28	92,92,92,92	0
56	MG	14	3086	1/1	0.98	0.06	65,65,65,65	0
56	MG	14	3370	1/1	0.98	0.10	68,68,68,68	0
56	MG	1H	3395	1/1	0.98	0.09	45,45,45,45	0
56	MG	1H	3412	1/1	0.98	0.15	32,32,32,32	0
56	MG	1H	3407	1/1	0.98	0.07	57,57,57,57	0
56	MG	14	3311	1/1	0.98	0.12	51,51,51,51	0
56	MG	1G	1678	1/1	0.98	0.16	98,98,98,98	0
56	MG	1H	3099	1/1	0.98	0.33	53,53,53,53	0
56	MG	16	211	1/1	0.98	0.13	85,85,85,85	0
56	MG	14	3333	1/1	0.98	0.12	58,58,58,58	0
56	MG	14	3010	1/1	0.98	0.22	58,58,58,58	0
56	MG	14	3236	1/1	0.98	0.23	75,75,75,75	0
56	MG	14	3025	1/1	0.98	0.22	84,84,84,84	0
56	MG	14	3319	1/1	0.98	0.08	62,62,62,62	0
56	MG	1H	3002	1/1	0.98	0.18	40,40,40,40	0
56	MG	13	1629	1/1	0.98	0.18	46,46,46,46	0
56	MG	14	3355	1/1	0.98	0.09	47,47,47,47	0
56	MG	14	3344	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3380	1/1	0.98	0.12	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3360	1/1	0.98	0.13	63,63,63,63	0
56	MG	1H	3007	1/1	0.98	0.32	46,46,46,46	0
56	MG	14	3038	1/1	0.98	0.15	34,34,34,34	0
56	MG	1G	1618	1/1	0.98	0.13	88,88,88,88	0
56	MG	1H	3418	1/1	0.98	0.06	42,42,42,42	0
56	MG	14	3111	1/1	0.98	0.22	55,55,55,55	0
56	MG	1H	3230	1/1	0.98	0.19	37,37,37,37	0
56	MG	1H	3267	1/1	0.98	0.24	60,60,60,60	0
56	MG	1H	3084	1/1	0.98	0.28	48,48,48,48	0
56	MG	1H	3408	1/1	0.98	0.11	47,47,47,47	0
56	MG	14	3187	1/1	0.98	0.21	53,53,53,53	0
56	MG	1H	3017	1/1	0.98	0.20	41,41,41,41	0
56	MG	1H	3389	1/1	0.98	0.14	68,68,68,68	0
56	MG	1H	3108	1/1	0.98	0.20	34,34,34,34	0
56	MG	1H	3413	1/1	0.98	0.17	44,44,44,44	0
56	MG	14	3078	1/1	0.98	0.29	50,50,50,50	0
56	MG	14	3003	1/1	0.98	0.09	54,54,54,54	0
56	MG	1H	3072	1/1	0.98	0.19	43,43,43,43	0
56	MG	1H	3362	1/1	0.98	0.23	69,69,69,69	0
56	MG	13	1625	1/1	0.98	0.34	45,45,45,45	0
56	MG	1H	3010	1/1	0.98	0.18	54,54,54,54	0
56	MG	1H	3175	1/1	0.98	0.29	67,67,67,67	0
56	MG	1G	1602	1/1	0.98	0.11	64,64,64,64	0
56	MG	1G	1630	1/1	0.98	0.24	75,75,75,75	0
56	MG	1H	3093	1/1	0.98	0.09	47,47,47,47	0
56	MG	1H	3410	1/1	0.98	0.11	46,46,46,46	0
58	ZN	5I	101	1/1	0.98	0.16	88,88,88,88	0
56	MG	13	1605	1/1	0.98	0.18	67,67,67,67	0
56	MG	1H	3056	1/1	0.98	0.33	70,70,70,70	0
56	MG	1H	3445	1/1	0.98	0.10	52,52,52,52	0
56	MG	1H	3114	1/1	0.98	0.23	48,48,48,48	0
56	MG	1H	3035	1/1	0.98	0.15	61,61,61,61	0
56	MG	1H	3480	1/1	0.99	0.20	56,56,56,56	0
56	MG	14	3347	1/1	0.99	0.07	56,56,56,56	0
56	MG	1H	3107	1/1	0.99	0.28	65,65,65,65	0
56	MG	1H	3472	1/1	0.99	0.14	56,56,56,56	0
56	MG	14	3050	1/1	0.99	0.20	63,63,63,63	0
56	MG	14	3230	1/1	0.99	0.30	73,73,73,73	0
56	MG	1H	3111	1/1	0.99	0.20	43,43,43,43	0
56	MG	29	301	1/1	0.99	0.18	44,44,44,44	0
56	MG	1H	3087	1/1	0.99	0.37	43,43,43,43	0
56	MG	13	1618	1/1	0.99	0.17	58,58,58,58	0

Continued on next page...

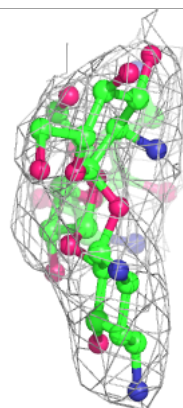
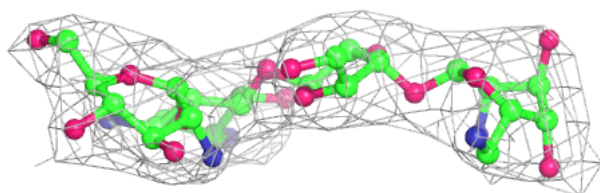
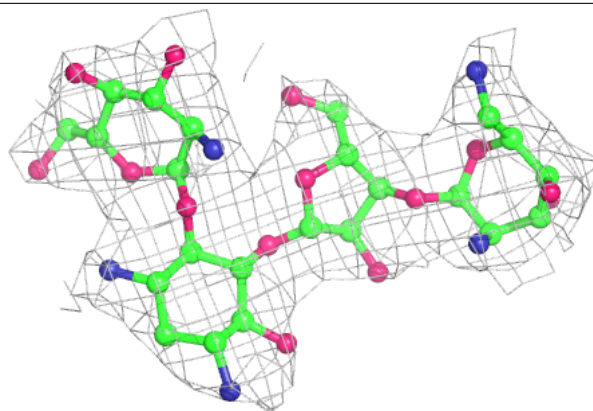
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3049	1/1	0.99	0.18	54,54,54,54	0
56	MG	14	3030	1/1	0.99	0.14	55,55,55,55	0
56	MG	14	3062	1/1	0.99	0.18	56,56,56,56	0
56	MG	14	3061	1/1	0.99	0.22	50,50,50,50	0
56	MG	1H	3020	1/1	0.99	0.20	47,47,47,47	0
56	MG	14	3046	1/1	0.99	0.09	53,53,53,53	0
56	MG	13	1601	1/1	0.99	0.23	46,46,46,46	0
56	MG	13	1652	1/1	0.99	0.20	80,80,80,80	0
56	MG	1H	3266	1/1	0.99	0.07	64,64,64,64	0
56	MG	14	3053	1/1	0.99	0.22	52,52,52,52	0
56	MG	1H	3403	1/1	0.99	0.16	43,43,43,43	0
56	MG	11	301	1/1	0.99	0.20	48,48,48,48	0
56	MG	1H	3136	1/1	0.99	0.27	41,41,41,41	0
56	MG	14	3005	1/1	0.99	0.21	53,53,53,53	0
56	MG	1H	3061	1/1	0.99	0.12	48,48,48,48	0
56	MG	13	1608	1/1	0.99	0.17	71,71,71,71	0
56	MG	14	3351	1/1	0.99	0.13	43,43,43,43	0
56	MG	1H	3124	1/1	0.99	0.19	52,52,52,52	0
56	MG	1H	3423	1/1	0.99	0.07	44,44,44,44	0
56	MG	1H	3419	1/1	0.99	0.10	37,37,37,37	0
56	MG	29	303	1/1	0.99	0.20	71,71,71,71	0
56	MG	14	3071	1/1	0.99	0.19	61,61,61,61	0
56	MG	14	3099	1/1	0.99	0.19	46,46,46,46	0
56	MG	14	3063	1/1	0.99	0.29	66,66,66,66	0
56	MG	1H	3455	1/1	0.99	0.08	57,57,57,57	0
56	MG	1H	3374	1/1	0.99	0.10	50,50,50,50	0
56	MG	14	3318	1/1	0.99	0.10	57,57,57,57	0

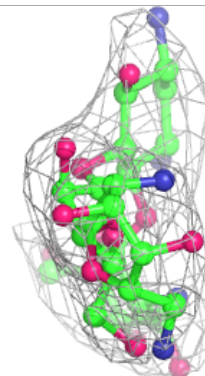
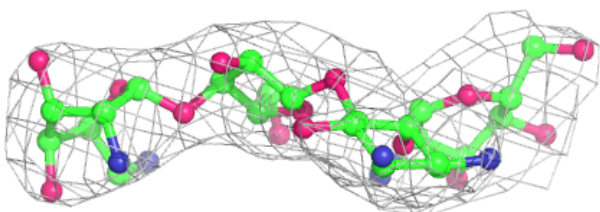
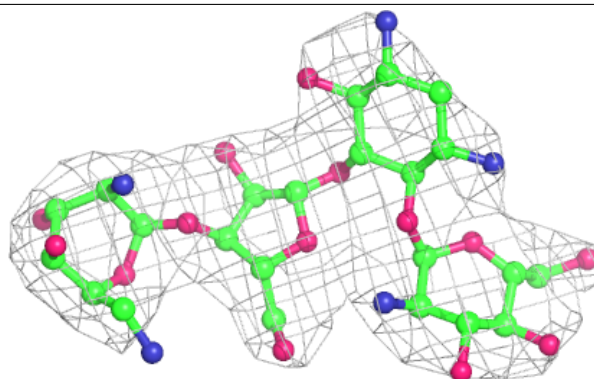
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR 13 1745:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PAR 1G 1686:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.