wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 01:02 am GMT

PDB ID	:	5IB7
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet, near-cognate tRNALys with U-G mismatch in the A-site and antibiotic paromomycin
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2016-02-22
Resolution	:	2.99 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

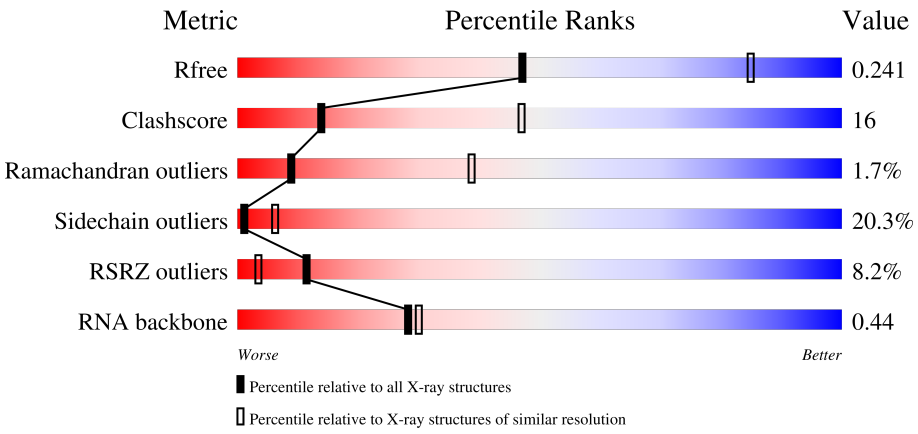
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 <=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	37% 45% 15% • •
1	1G	1522	% 39% 44% 14% • •
2	12	256	10% 34% 36% 9% • 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1E	256	5% 39% 38% 12% • 10%
3	22	239	21% 41% 34% 7% 18%
3	2E	239	9% 53% 26% 6% 14%
4	32	209	7% 49% 42% 8%
4	3E	209	6% 44% 44% 11% •
5	42	162	7% 51% 33% 8% 7%
5	4E	162	2% 51% 35% 6% 8%
6	52	101	66% 27% 7%
6	5E	101	7% 50% 44% 5% •
7	62	156	21% 38% 43% 8% 12%
7	6E	156	23% 55% 36% 8% •
8	72	138	11% 52% 41% 7% •
8	7E	138	21% 52% 38% 9% •
9	82	128	39% 39% 46% 9% 5%
9	8E	128	4% 44% 41% 13% •
10	1A	105	21% 35% 29% 10% • 24%
10	1I	105	27% 51% 33% 5% 10%
11	2A	129	21% 55% 22% 9% • 12%
11	2I	129	19% 50% 29% 7% 14%
12	3A	132	34% 48% 33% 11% • 8%
12	3I	132	11% 60% 26% 7% 8%
13	4A	126	21% 37% 39% 10% 13%
13	4I	126	3% 38% 44% 11% 7%
14	5A	61	67% 44% 44% 7% • •
14	5I	61	13% 49% 31% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6A	89	3% 61% 35%
15	6I	89	3% 55% 35% 8%
16	7A	88	2% 58% 34% 5%
16	7I	88	23% 40% 44% 10% 6%
17	8A	105	26% 63% 30% 6%
17	8I	105	17% 48% 42% 5% 6%
18	9A	88	5% 43% 28% 5% 24%
18	9I	88	2% 44% 27% 6% 23%
19	AA	93	14% 40% 27% 30%
19	AI	93	3% 46% 30% 12% 12%
20	BA	106	17% 48% 37% 8% 7%
20	BI	106	25% 42% 41% 8% 8%
21	1B	27	30% 48% 30% 19%
21	1F	27	44% 26% 15% 15%
22	1K	76	7% 26% 47% 18% 5%
23	2K	77	% 42% 40% 14%
23	2L	77	40% 44% 12%
24	1L	76	14% 32% 38% 14% 13%
24	3K	76	13% 17% 37% 36% 8%
24	3L	76	4% 21% 46% 26% 5%
25	4K	30	13% 23% 23% 17% 37%
25	4L	30	10% 10% 30% 20% 37%
26	14	2917	% 34% 41% 18%
26	1H	2917	32% 41% 21%
27	16	122	% 44% 35% 15% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	1J	122	29% 50% 17%
28	71	229	9% 28% 23% 6% 42%
29	11	276	2% 53% 36% 9%
29	19	276	3% 55% 33% 10%
30	21	206	5% 44% 35% 17%
30	29	206	19% 46% 40% 12%
31	31	210	4% 51% 36% 9%
31	39	210	7% 40% 43% 13%
32	41	182	12% 51% 40% 7%
32	49	182	26% 46% 43% 10%
33	51	180	2% 52% 26% 17%
33	59	180	51% 47% 31% 14% 6%
34	61	148	11% 52% 34% 11%
34	69	148	8% 49% 38% 10%
35	15	140	18% 52% 35% 11%
35	58	140	13% 54% 32% 11%
36	25	122	11% 48% 41% 11%
36	68	122	2% 61% 34%
37	35	150	14% 43% 41% 12%
37	78	150	7% 37% 41% 15% 5%
38	45	141	19% 43% 42% 13%
38	88	141	7% 51% 35% 13%
39	55	118	6% 51% 41% 8%
39	98	118	10% 47% 40% 13%
40	65	112	20% 40% 43% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	A8	112	16% 38% 47% 13%
41	75	146	5% 41% 38% 11% 9%
41	B8	146	3% 36% 39% 16% 8%
42	85	118	3% 56% 31% 11%
42	C8	118	3% 58% 29% 9%
43	95	101	22% 56% 36% 6%
43	D8	101	15% 49% 39% 10%
44	A5	113	4% 64% 27% 7%
44	E8	113	7% 58% 31% 8%
45	B5	96	16% 54% 35% 8%
45	F8	96	% 68% 23% 8%
46	C5	110	33% 42% 36% 14% 5%
46	G8	110	5% 46% 34% 13% 6%
47	D5	206	34% 34% 40% 11% 14%
47	H8	206	32% 43% 29% 8% 17%
48	E5	85	15% 47% 34% 7% 11%
48	I8	85	6% 49% 31% 11% 9%
49	F5	98	18% 52% 35% 9%
49	J8	98	9% 49% 37% 9%
50	G5	72	7% 43% 43% 7%
50	K8	72	% 35% 40% 15% 6%
51	H5	60	48% 57% 37%
51	L8	60	3% 52% 40% 5%
52	M8	71	23% 35% 32% 14% 15%
53	J5	60	12% 53% 37% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	N8	60	43% 28% 7% 20%
54	O8	54	74% 26% 43% 11% 17%
55	L5	49	4% 65% 27%
55	P8	49	2% 53% 39%
56	M5	65	28% 52% 32% 14%
56	Q8	65	43% 35% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1647	-	-	-	X
57	MG	13	1662	-	-	-	X
57	MG	13	1664	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1673	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	14	3064	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3109	-	-	-	X
57	MG	14	3115	-	-	-	X
57	MG	14	3118	-	-	-	X
57	MG	14	3127	-	-	-	X
57	MG	14	3128	-	-	-	X
57	MG	14	3132	-	-	-	X
57	MG	14	3138	-	-	-	X
57	MG	14	3161	-	-	-	X
57	MG	14	3166	-	-	-	X
57	MG	14	3173	-	-	-	X
57	MG	14	3185	-	-	-	X
57	MG	14	3197	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1609	-	-	-	X
57	MG	1G	1618	-	-	-	X
57	MG	1G	1634	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3004	-	-	-	X
57	MG	1H	3053	-	-	-	X
57	MG	1H	3065	-	-	-	X
57	MG	1H	3081	-	-	-	X
57	MG	1H	3111	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3135	-	-	-	X
57	MG	1H	3144	-	-	-	X
57	MG	1H	3145	-	-	-	X
57	MG	1H	3150	-	-	-	X
57	MG	1H	3153	-	-	-	X
57	MG	1H	3163	-	-	-	X
57	MG	1H	3168	-	-	-	X
57	MG	1H	3177	-	-	-	X
57	MG	1H	3180	-	-	-	X
57	MG	1H	3205	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3211	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3237	-	-	-	X
57	MG	E5	101	-	-	-	X
57	MG	P8	101	-	-	-	X
59	SF4	32	302	-	-	X	-

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 297444 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
			Total	C	N	O	P			
1	13	1499	32223	14342	5973	10409	1499	0	0	0
1	1G	1508	32414	14427	6005	10474	1508	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3E	207	1698	1064	338	289	7	0	0	0
4	32	208	1702	1066	339	290	7	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	6E	154	1242	770	250	216	6	0	0	0
7	62	138	1110	689	221	194	6	0	0	0

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1I	94	749	468	147	133	1	0	0	0
			Total	C	N	O				
10	1A	80	646	403	129	114		0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	3I	122	956	603	193	159	1	0	0	0
			Total	C	N	O	S			
12	3A	121	947	597	191	158	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

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

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	3K	70	1483	664	260	490	69	0	0	0
24	1L	66	1401	626	244	465	66	0	0	0
24	3L	72	1528	684	270	503	71	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	4K	19	420	188	89	124	19	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	4L	19	419	188	89	123	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	1H	2860	61609	27418	11525	19806	2860	0	0	0
26	14	2826	60877	27092	11393	19566	2826	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	21	203	1546	978	295	267	6	0	0	0
30	29	204	1563	988	299	270	6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	88	141	1117	712	211	187	7	0	0	0
38	45	138	1099	702	208	183	6	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	98	118	967	604	203	159	1	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	55	118	967	604	203	159	1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	A8	111	881	556	176	149	0	0	0
40	65	110	876	553	175	148	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	F8	95	750	488	135	126	1	0	0	0
45	B5	94	735	477	133	125		0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M8	60	475	300	84	86	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	N8	48	369	229	75	60	5	0	0	0
53	J5	56	434	272	87	70	5	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

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

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	P8	47	401	246	99	54	2	0	0	0
55	L5	47	401	246	99	54	2	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	Q8	64	516	331	102	81	2	0	0	0
56	M5	64	516	331	102	81	2	0	0	0

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

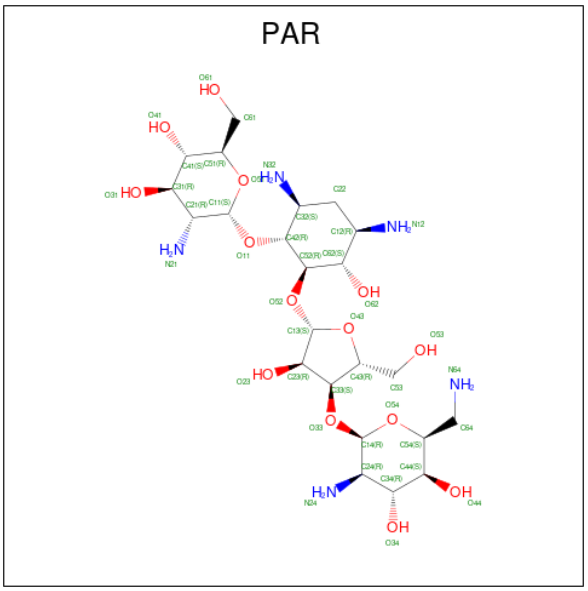
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	13	140	140	140	0	0
57	3I	1	1	1	0	0
57	4I	1	1	1	0	0
57	5I	1	1	1	0	0
57	2K	2	2	2	0	0
57	1H	525	525	525	0	0
57	16	11	11	11	0	0
57	21	3	3	3	0	0
57	31	2	2	2	0	0
57	41	1	1	1	0	0
57	78	1	1	1	0	0
57	88	3	3	3	0	0
57	I8	2	2	2	0	0
57	P8	1	1	1	0	0
57	Q8	1	1	1	0	0
57	1G	102	102	102	0	0
57	32	1	1	1	0	0
57	42	1	1	1	0	0

Continued on next page...

Continued from previous page...

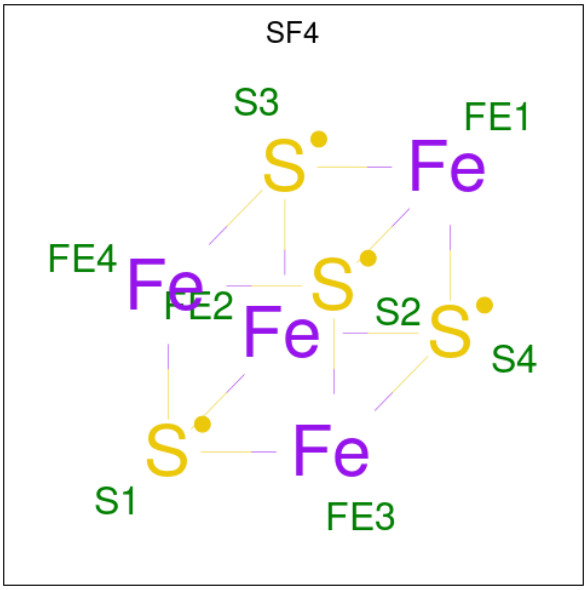
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	52	1	1	1	0	0
57	7A	1	1	1	0	0
57	2L	2	2	2	0	0
57	4L	1	1	1	0	0
57	14	435	435	435	0	0
57	1J	8	8	8	0	0
57	19	1	1	1	0	0
57	29	1	1	1	0	0
57	39	2	2	2	0	0
57	25	1	1	1	0	0
57	35	1	1	1	0	0
57	45	2	2	2	0	0
57	C5	1	1	1	0	0
57	E5	1	1	1	0	0
57	M5	1	1	1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

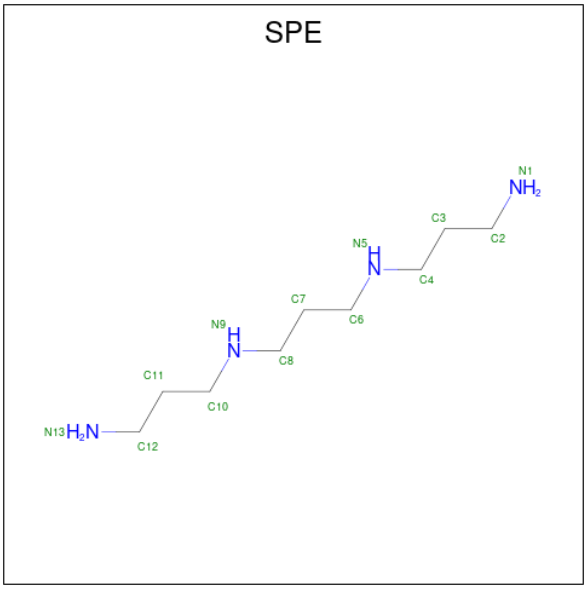


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	1	Total Zn 1 1	0	0
60	G8	1	Total Zn 1 1	0	0
60	5A	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0

- Molecule 61 is THERMINE (three-letter code: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	13	320	Total O 320 320	0	0
62	4E	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	8E	2	Total O 2 2	0	0
62	1I	2	Total O 2 2	0	0
62	3I	2	Total O 2 2	0	0
62	5I	2	Total O 2 2	0	0
62	6I	3	Total O 3 3	0	0
62	7I	1	Total O 1 1	0	0
62	BI	2	Total O 2 2	0	0
62	1F	1	Total O 1 1	0	0
62	1K	2	Total O 2 2	0	0
62	2K	8	Total O 8 8	0	0
62	4K	5	Total O 5 5	0	0
62	1H	1470	Total O 1470 1470	0	0
62	16	12	Total O 12 12	0	0
62	11	17	Total O 17 17	0	0
62	21	7	Total O 7 7	0	0
62	31	5	Total O 5 5	0	0
62	41	1	Total O 1 1	0	0
62	58	2	Total O 2 2	0	0
62	78	10	Total O 10 10	0	0
62	B8	1	Total O 1 1	0	0
62	C8	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	F8	2	Total O 2 2	0	0
62	G8	2	Total O 2 2	0	0
62	I8	6	Total O 6 6	0	0
62	J8	4	Total O 4 4	0	0
62	L8	3	Total O 3 3	0	0
62	P8	1	Total O 1 1	0	0
62	Q8	5	Total O 5 5	0	0
62	1G	317	Total O 317 317	0	0
62	32	1	Total O 1 1	0	0
62	52	4	Total O 4 4	0	0
62	1A	1	Total O 1 1	0	0
62	6A	2	Total O 2 2	0	0
62	7A	5	Total O 5 5	0	0
62	9A	2	Total O 2 2	0	0
62	BA	2	Total O 2 2	0	0
62	2L	6	Total O 6 6	0	0
62	4L	6	Total O 6 6	0	0
62	14	1144	Total O 1144 1144	0	0
62	1J	12	Total O 12 12	0	0
62	19	15	Total O 15 15	0	0
62	29	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

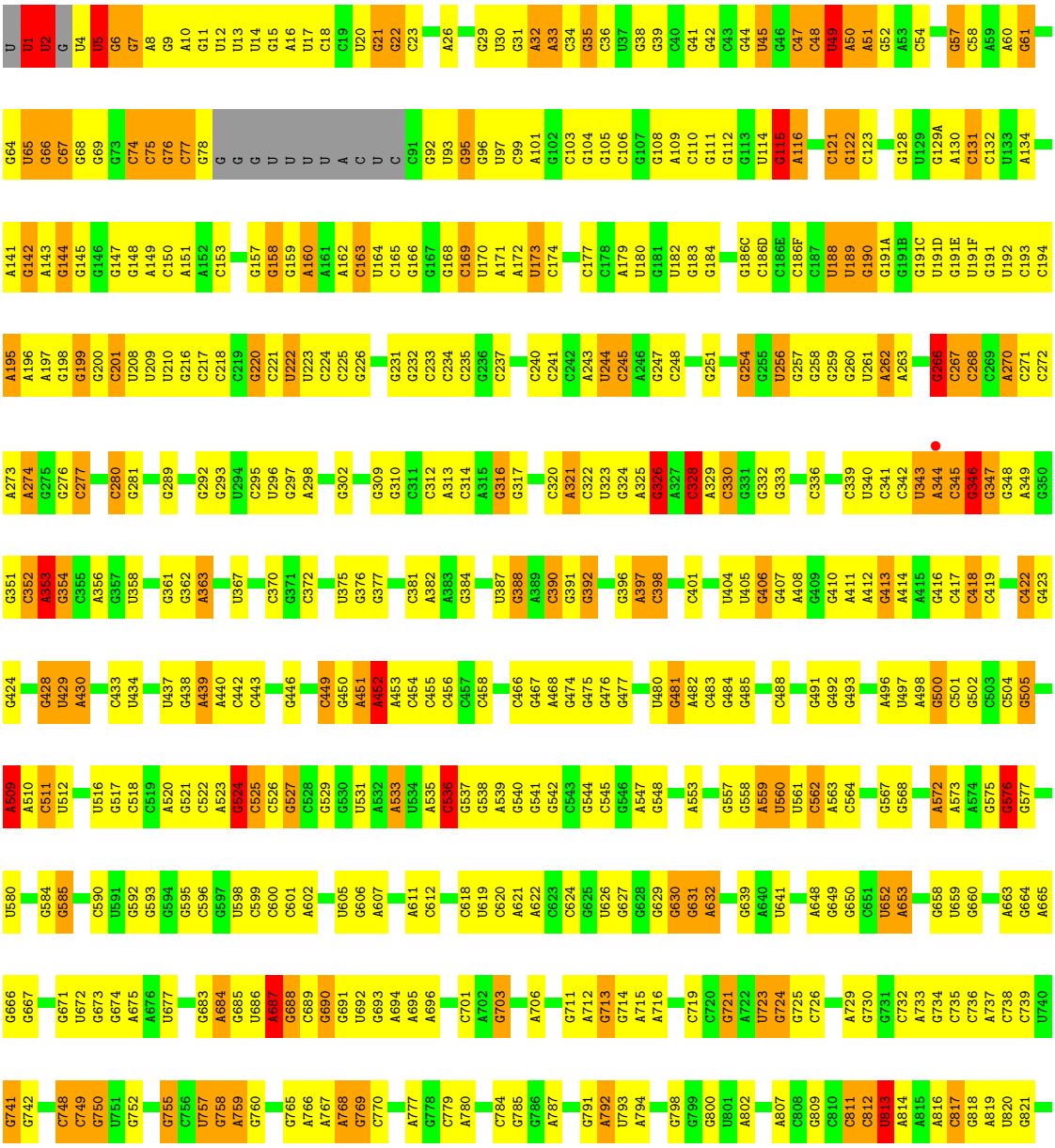
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	39	5	Total O 5 5	0	0
62	15	1	Total O 1 1	0	0
62	25	6	Total O 6 6	0	0
62	35	8	Total O 8 8	0	0
62	55	3	Total O 3 3	0	0
62	85	2	Total O 2 2	0	0
62	A5	1	Total O 1 1	0	0
62	B5	1	Total O 1 1	0	0
62	C5	3	Total O 3 3	0	0
62	F5	1	Total O 1 1	0	0
62	H5	2	Total O 2 2	0	0
62	M5	9	Total O 9 9	0	0

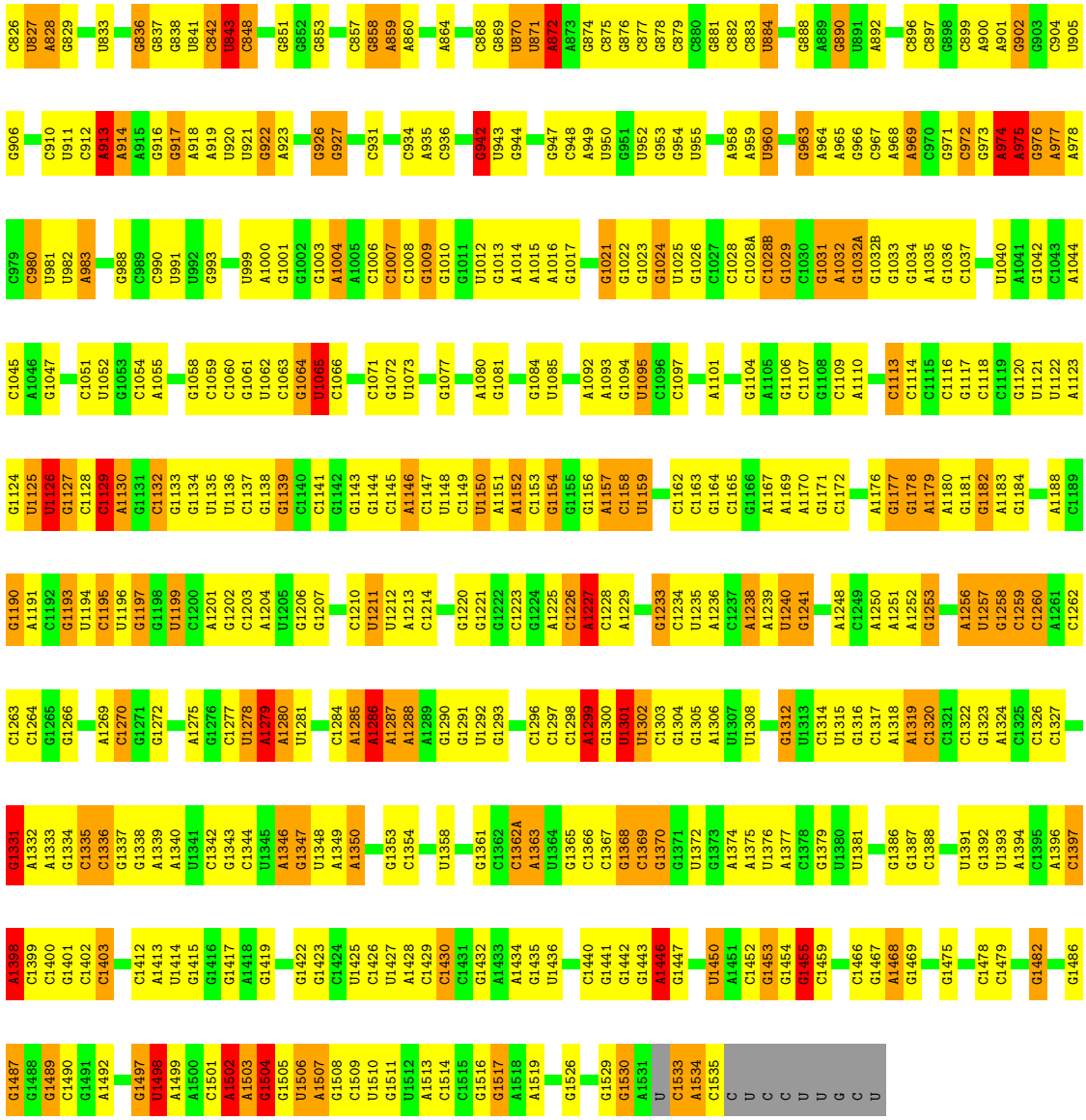
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

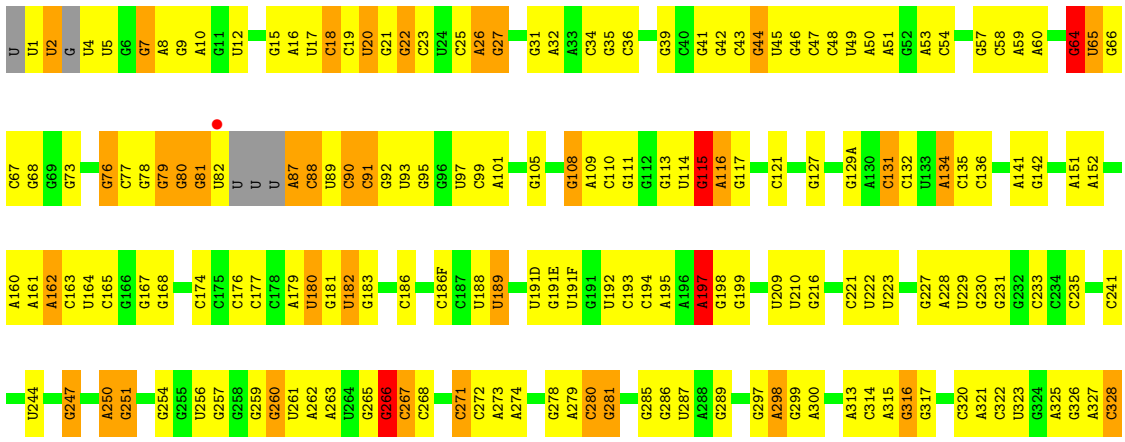
Chain 13:

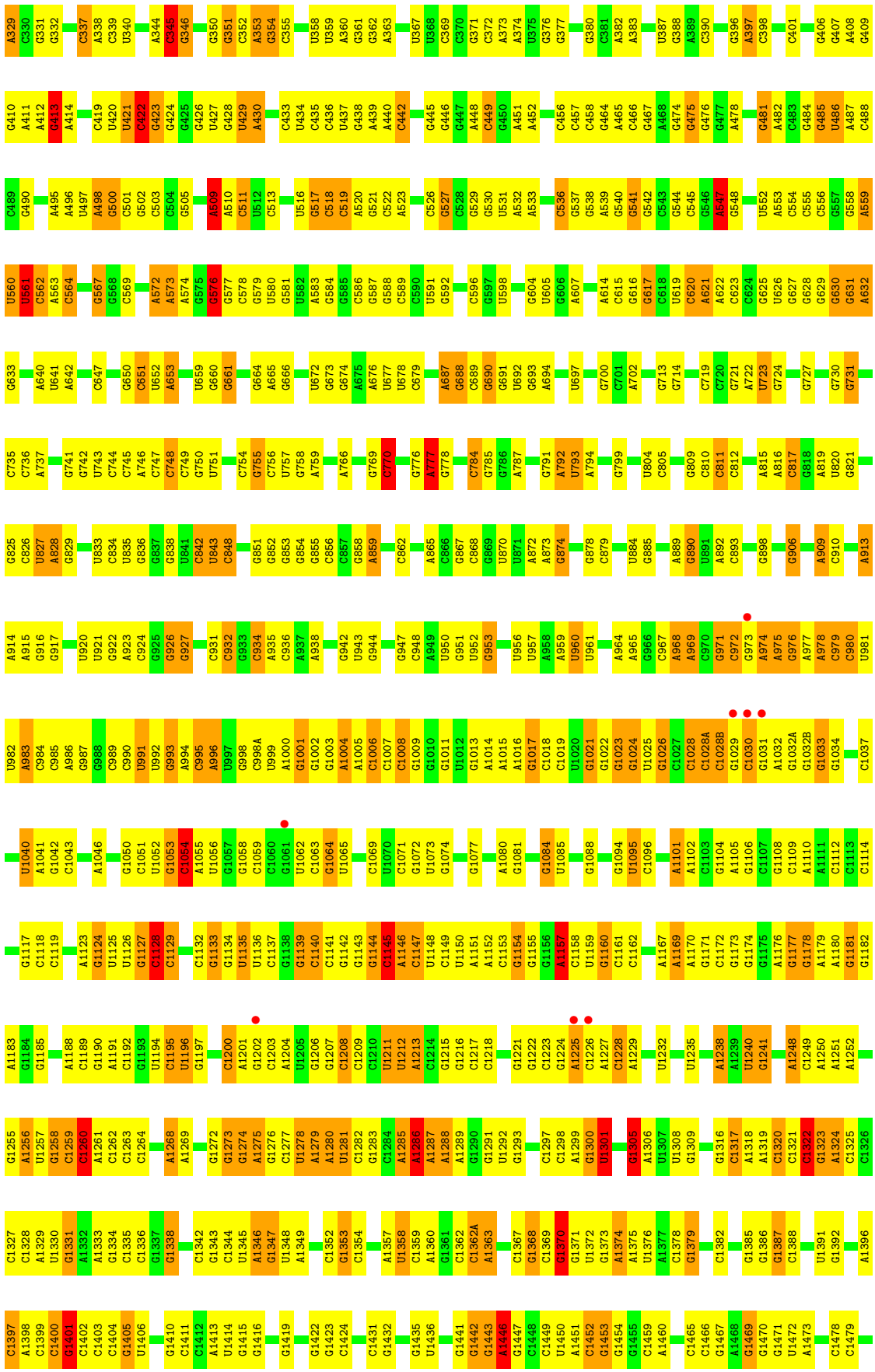




• Molecule 1: 16S ribosomal RNA

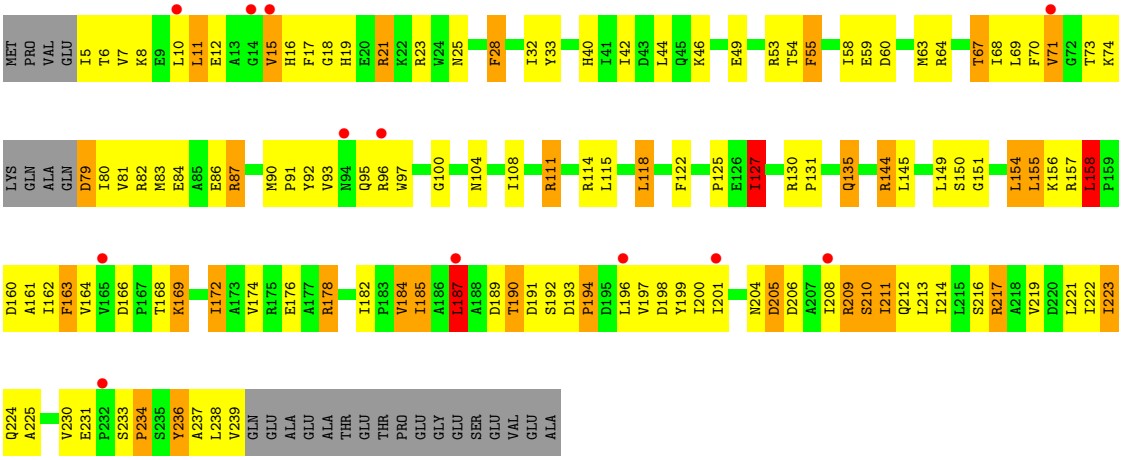
Chain 1G:




A329 C330 G331 G332 C337 A338 C339 U340 A344 C345 G346 G350 G351 C352 A353 G354 C355 U358 U359 A360 G361 G362 A363 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G377 G380 C381 A382 A383 U387 G388 A389 C390 G396 A397 C398 C401 G406 G407 A408 G409
G410 A411 A412 G413 A414 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 C433 U434 C435 C436 U437 G438 A439 A440 C442 G445 G446 G447 A448 C449 G450 A451 A452 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G476 G477 A478 G481 A482 C483 G484 G485 U486 A487 C488
C489 G490 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 U516 G517 C518 C519 A520 G521 C522 A523 C526 G527 C528 G529 G530 U531 A532 A533 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 U552 A553 C554 C555 C556 G557 G558 A559
U560 U561 C562 A563 C564 G567 G568 C569 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 C596 G597 U598 G604 U605 G606 A607 A614 C615 G616 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632
G633 A640 U641 A642 C647 G650 C651 U652 A653 U659 G660 G661 G664 A665 G666 U672 G673 G674 A675 A676 U677 U678 C679 A687 G688 C689 G690 G691 U692 G693 A694 U697 G700 C701 A702 G713 G714 C719 C720 G721 A722 U723 G724 G727 G730 G731
C735 C736 A737 G741 G742 U743 C744 C745 A746 C747 C748 C749 G750 U751 C754 G755 C756 U757 C758 A759 A766 G769 C770 G776 A777 G778 C784 G785 G786 A787 G791 A792 U793 A794 G799 U804 C805 G809 C810 C811 C812 A815 A816 C817 G818 A819 U820 G821
G825 C826 U827 A828 G829 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 G851 G852 G853 G854 G855 C856 C857 G858 A859 C862 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 G878 C879 U884 G885 A889 G890 U891 A892 C893 G898 G906 A909 C910 A913
A914 A915 G916 G917 U920 U921 G922 A923 C924 G925 G926 G927 C931 C932 G933 C934 A935 C936 A937 A938 G942 U943 G944 G947 C948 A949 U950 G951 U952 G953 U956 U957 A958 A959 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981
U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1034 C1037
U1040 A1041 G1042 C1043 A1046 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1069 U1070 C1071 G1072 U1073 G1074 G1077 A1080 G1081 G1084 U1085 G1088 G1094 U1095 C1096 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114
G1117 C1118 C1119 A1123 G1124 U1125 U1126 G1127 C1128 C1129 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1167 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182
A1183 G1184 G1185 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 U1232 U1235 A1238 A1239 U1240 G1241 A1248 C1249 A1250 A1251 A1252
G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 A1268 A1269 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 C1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 C1297 C1298 A1299 G1300 U1301 G1305 A1306 U1307 U1308 G1309 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326
C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 C1335 C1336 G1337 G1338 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 C1352 G1353 C1354 A1357 U1358 C1359 A1360 G1361 C1362 C1362A A1363 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 C1382 G1385 G1386 G1387 C1388 U1391 G1392 A1396
C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 G1410 C1411 C1412 A1413 U1414 G1415 G1416 G1419 G1422 G1423 C1424 C1431 G1432 G1435 U1436 G1441 G1442 G1443 A1446 G1447 C1448 C1449 U1450 A1451 C1452 G1453 G1454 G1455 C1459 A1460 C1465 C1466 G1467 A1468 G1469 G1470 G1471 U1472 A1473 C1478 C1479

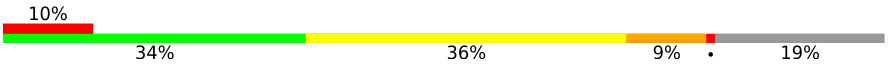
• Molecule 2: 30S ribosomal protein S2

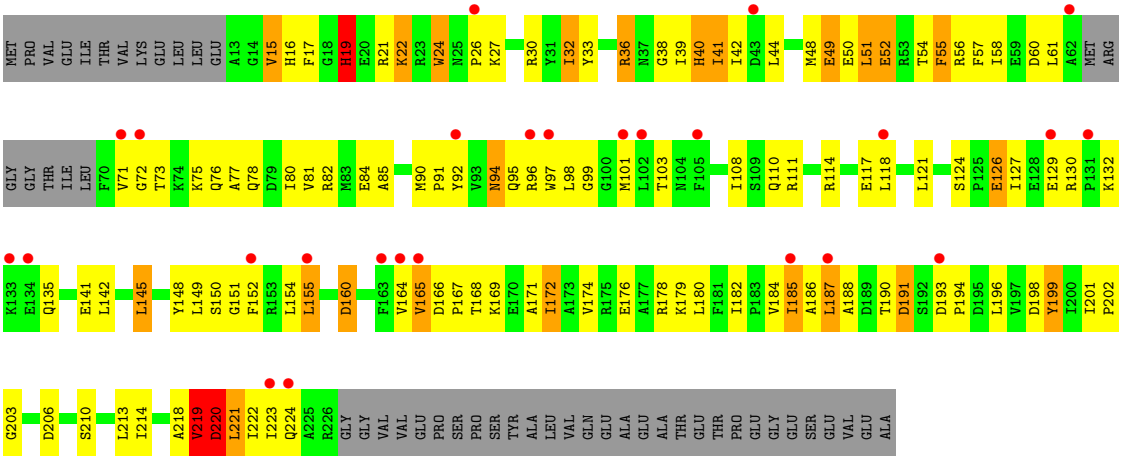
Chain 1E:



• Molecule 2: 30S ribosomal protein S2

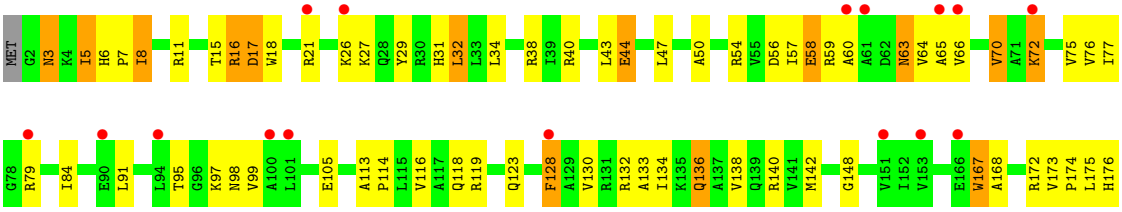
Chain 12:

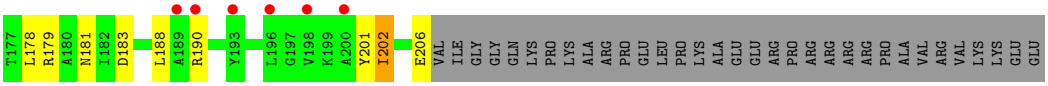




• Molecule 3: 30S ribosomal protein S3

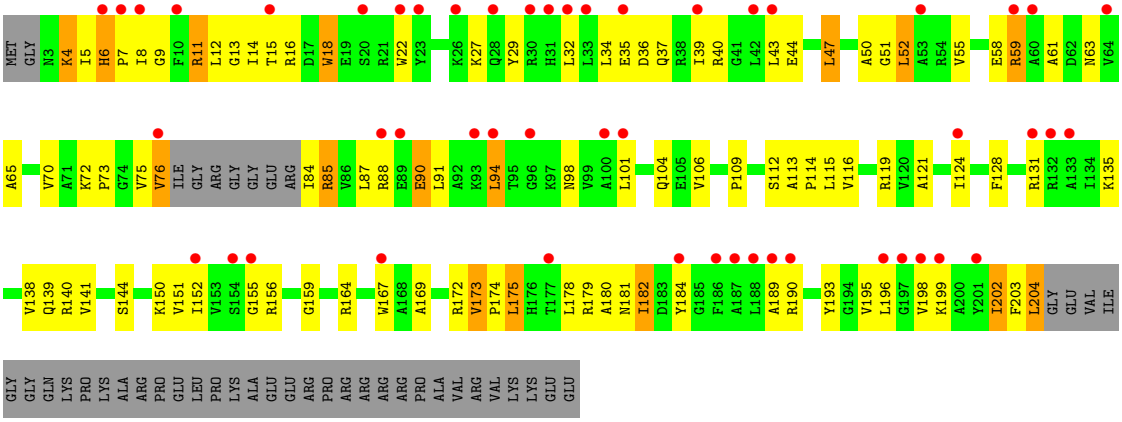
Chain 2E:





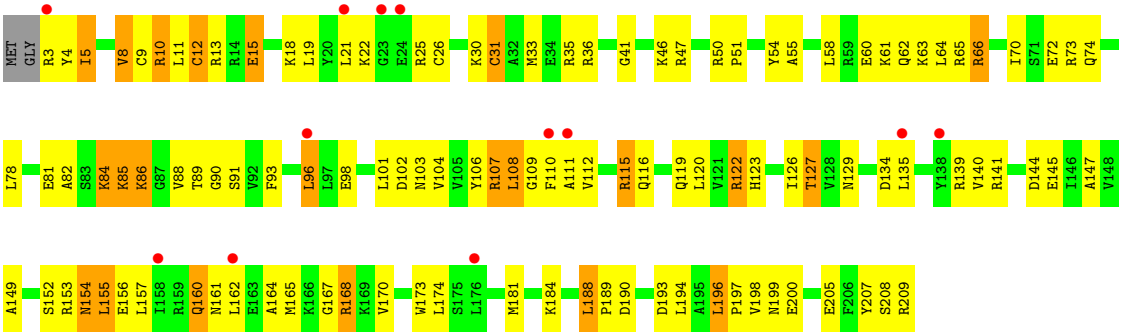
- Molecule 3: 30S ribosomal protein S3

Chain 22:



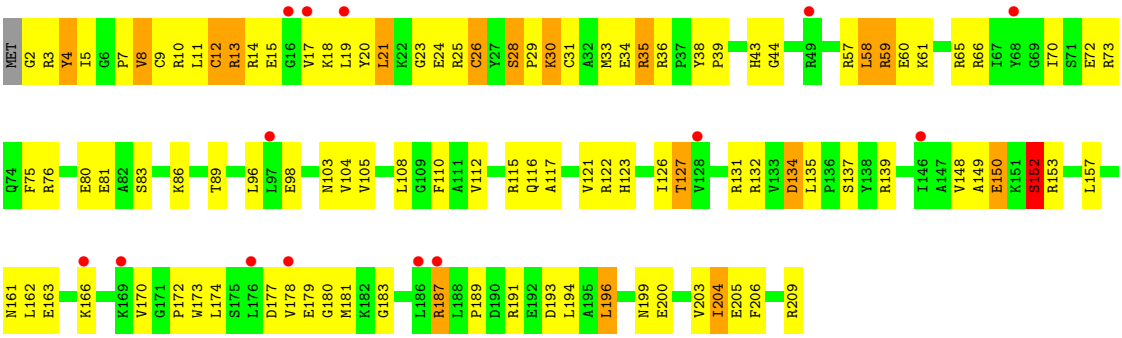
- Molecule 4: 30S ribosomal protein S4

Chain 3E:



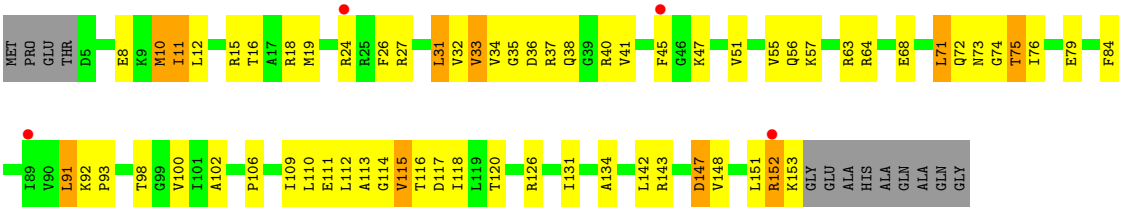
- Molecule 4: 30S ribosomal protein S4

Chain 32:



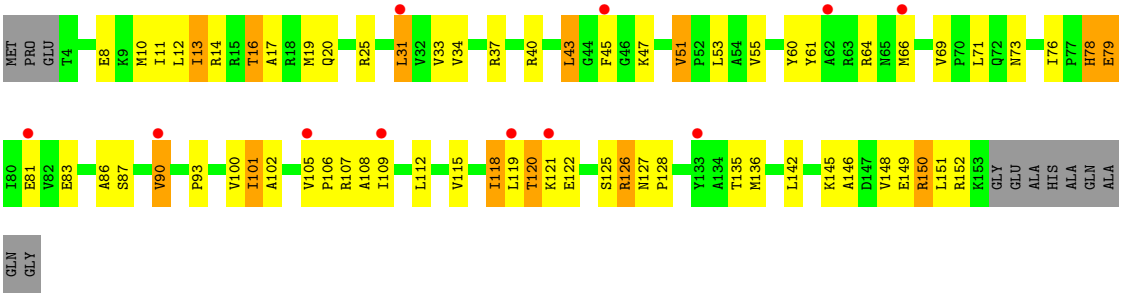
- Molecule 5: 30S ribosomal protein S5

Chain 4E:



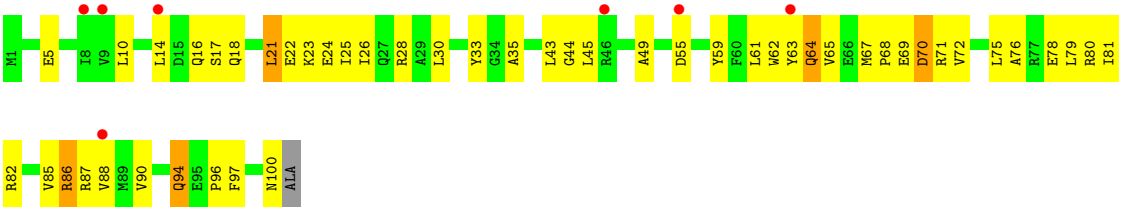
- Molecule 5: 30S ribosomal protein S5

Chain 42:



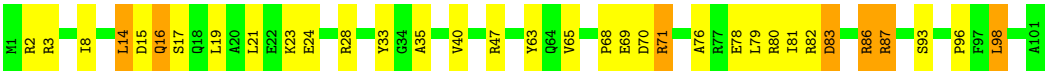
- Molecule 6: 30S ribosomal protein S6

Chain 5E:



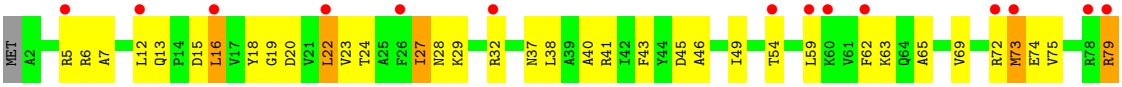
- Molecule 6: 30S ribosomal protein S6

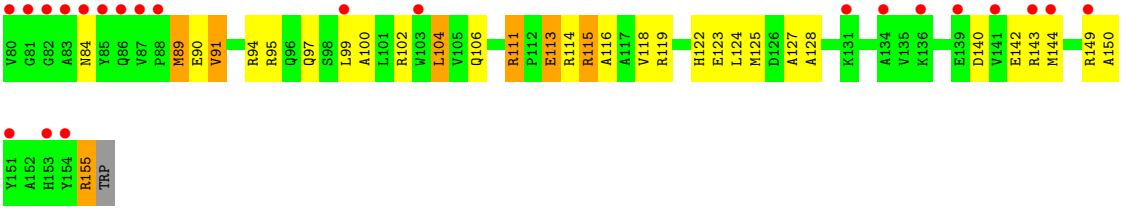
Chain 52:



- Molecule 7: 30S ribosomal protein S7

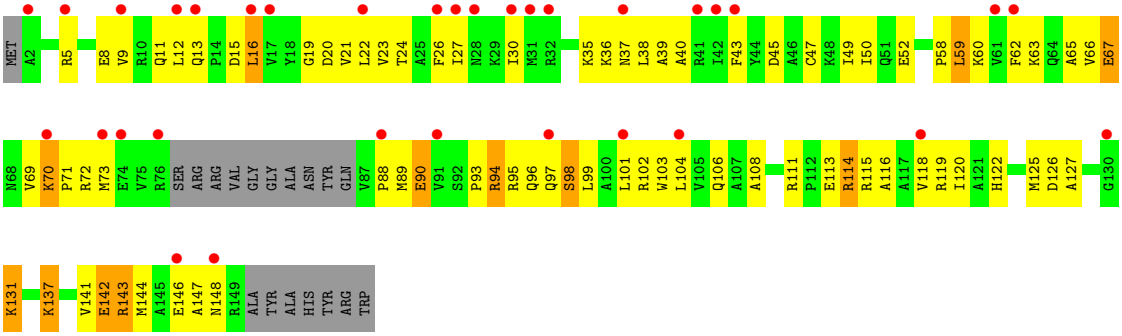
Chain 6E:





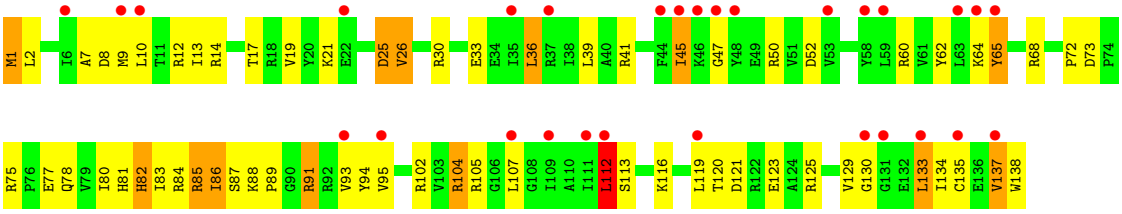
• Molecule 7: 30S ribosomal protein S7

Chain 62:



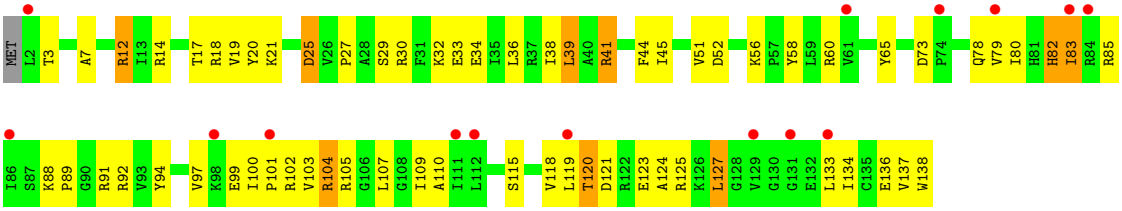
• Molecule 8: 30S ribosomal protein S8

Chain 7E:



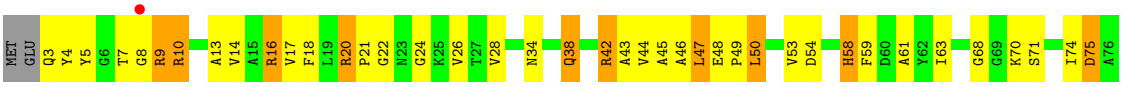
• Molecule 8: 30S ribosomal protein S8

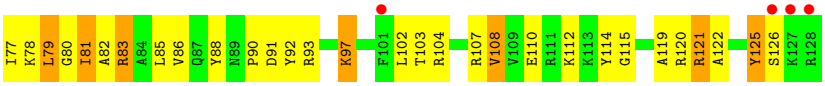
Chain 72:



• Molecule 9: 30S ribosomal protein S9

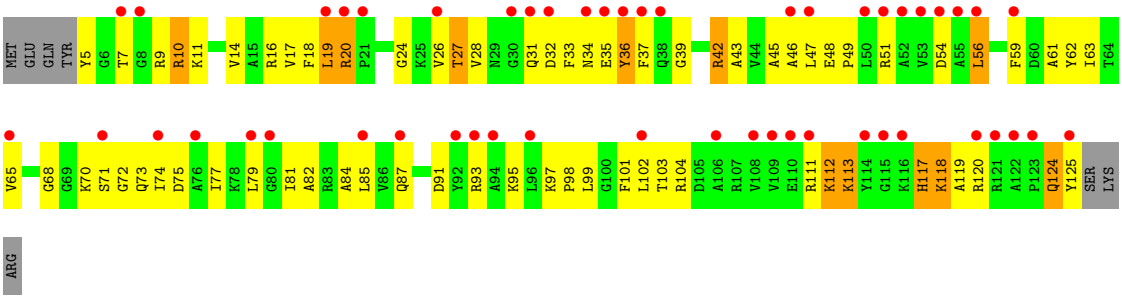
Chain 8E:





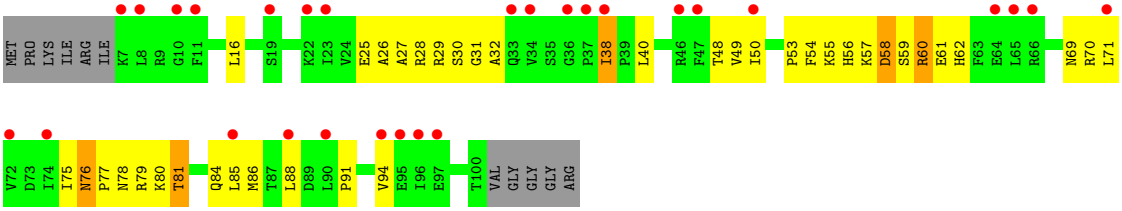
• Molecule 9: 30S ribosomal protein S9

Chain 82:



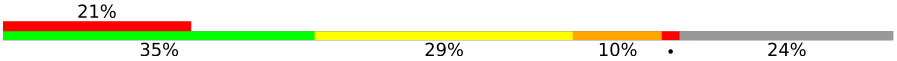
• Molecule 10: 30S ribosomal protein S10

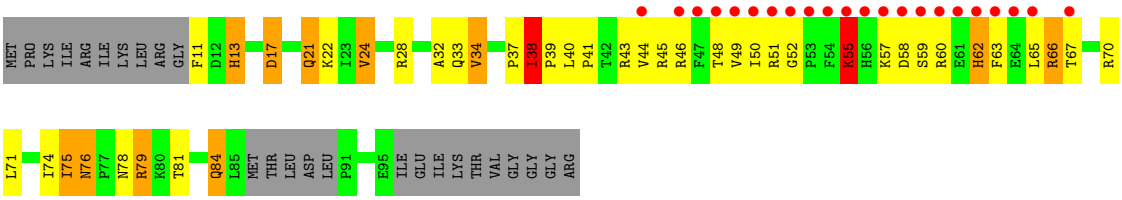
Chain 1I:



• Molecule 10: 30S ribosomal protein S10

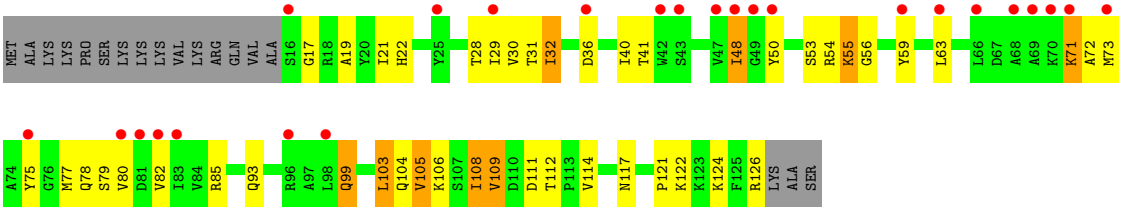
Chain 1A:





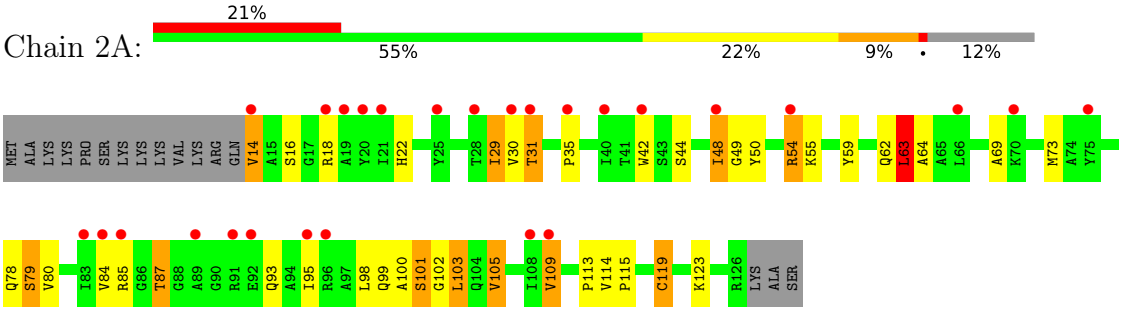
• Molecule 11: 30S ribosomal protein S11

Chain 2I:



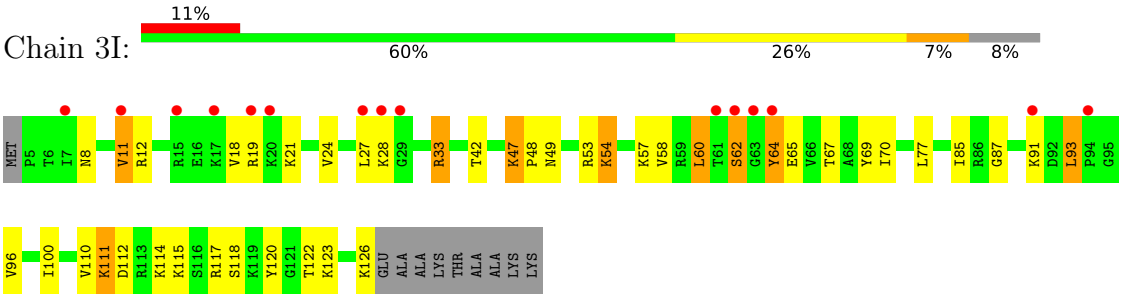
• Molecule 11: 30S ribosomal protein S11

Chain 2A:



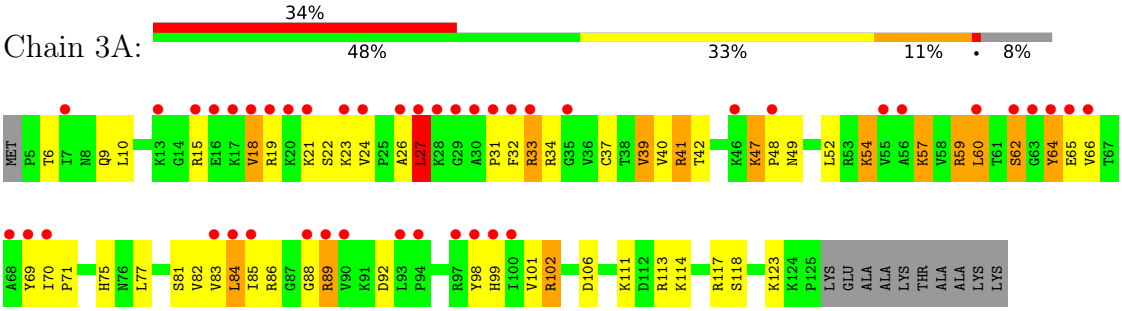
- Molecule 12: 30S ribosomal protein S12

Chain 3I:



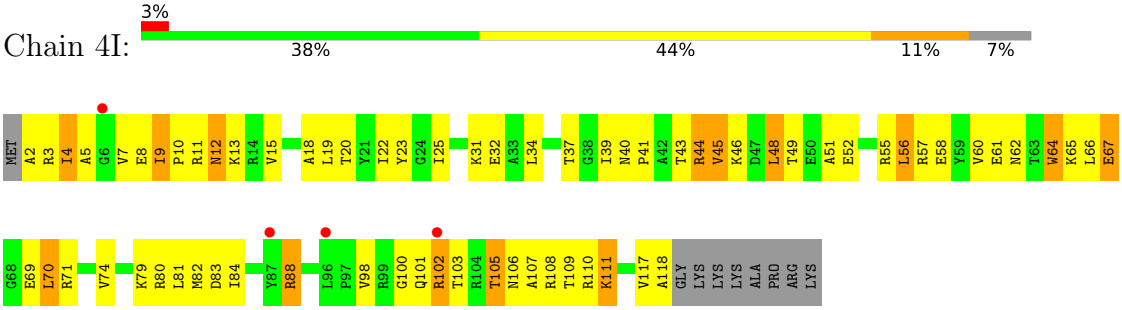
- Molecule 12: 30S ribosomal protein S12

Chain 3A:



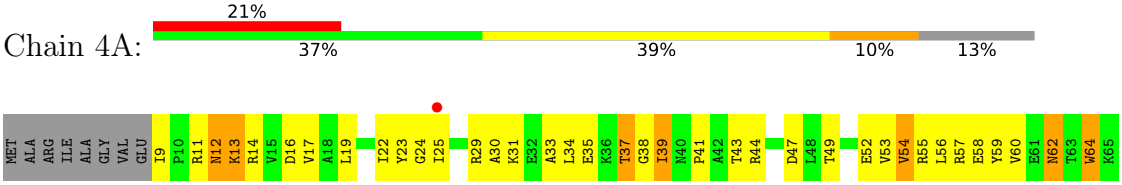
- Molecule 13: 30S ribosomal protein S13

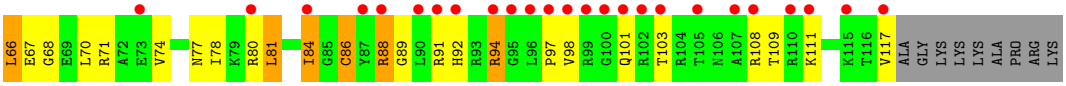
Chain 4I:



- Molecule 13: 30S ribosomal protein S13

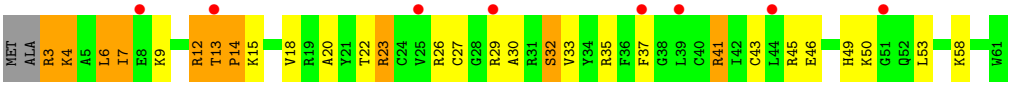
Chain 4A:





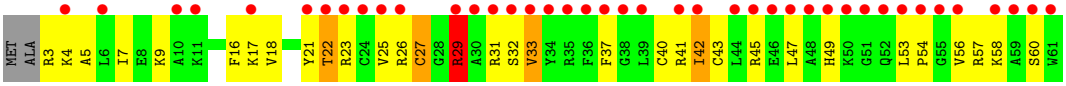
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



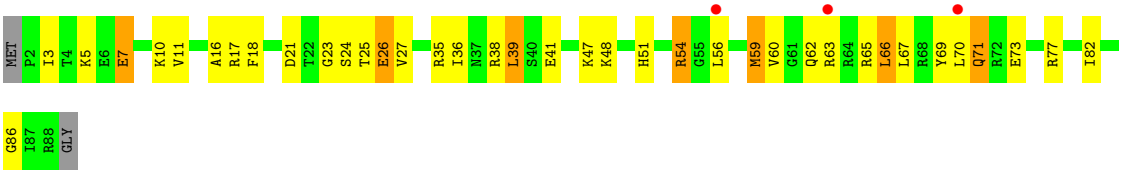
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



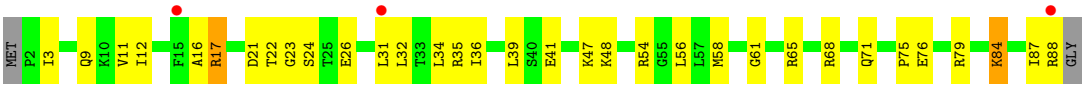
• Molecule 15: 30S ribosomal protein S15

Chain 6I:



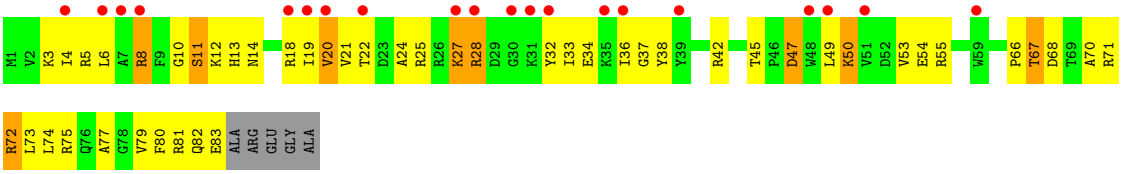
• Molecule 15: 30S ribosomal protein S15

Chain 6A:



• Molecule 16: 30S ribosomal protein S16

Chain 7I:

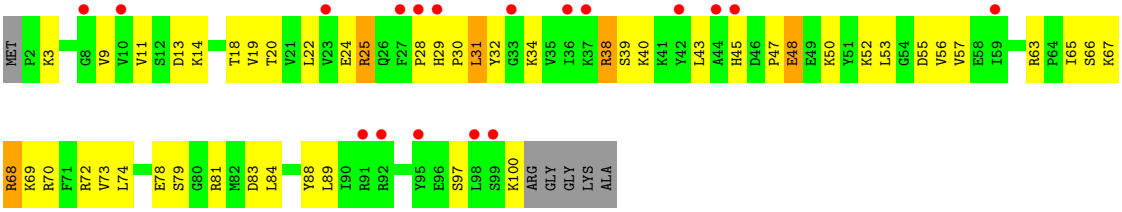


• Molecule 16: 30S ribosomal protein S16

Chain 7A:

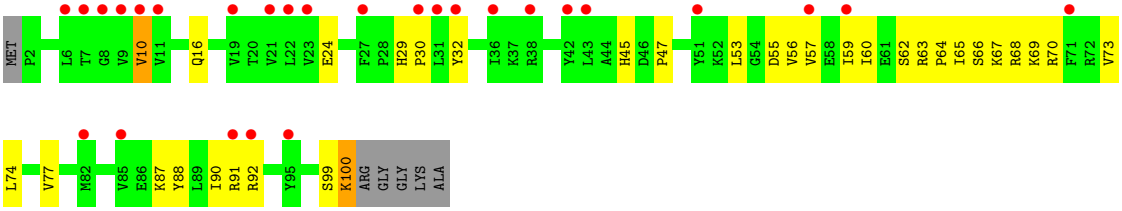
• Molecule 17: 30S ribosomal protein S17

Chain 8I:



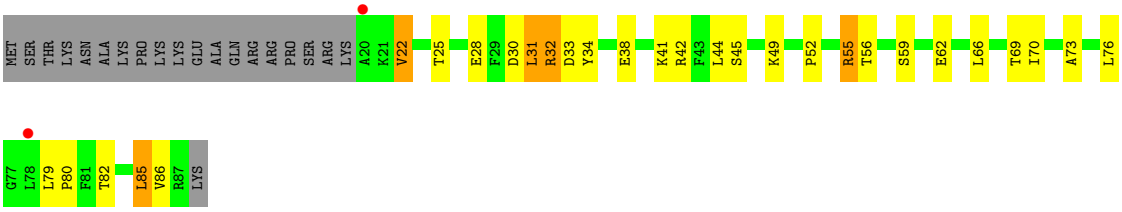
• Molecule 17: 30S ribosomal protein S17

Chain 8A:



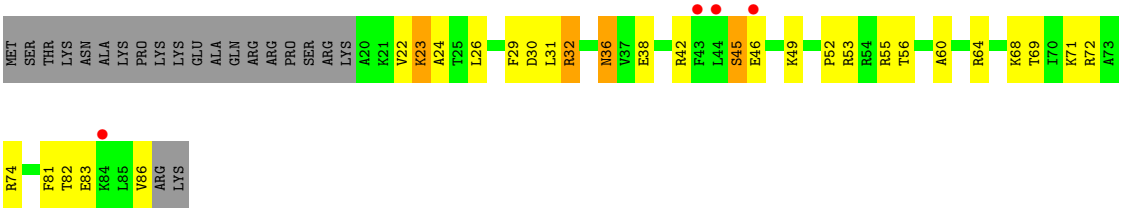
• Molecule 18: 30S ribosomal protein S18

Chain 9I:



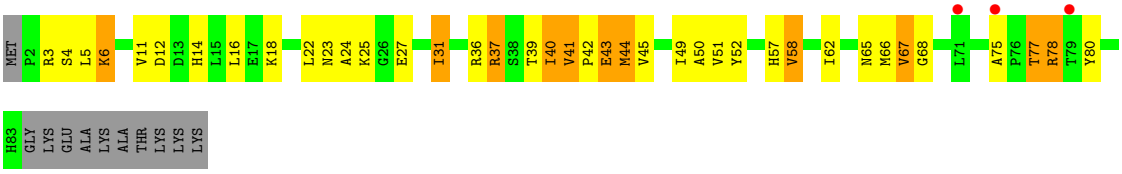
• Molecule 18: 30S ribosomal protein S18

Chain 9A:



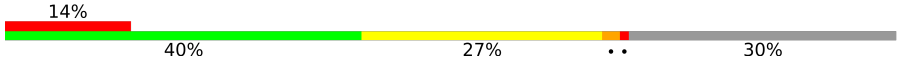
• Molecule 19: 30S ribosomal protein S19

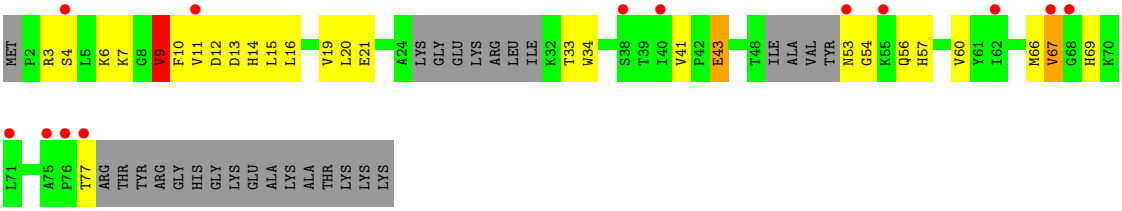
Chain AI:



• Molecule 19: 30S ribosomal protein S19

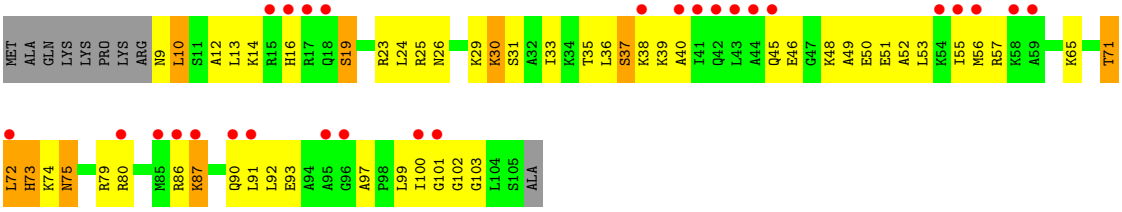
Chain AA:





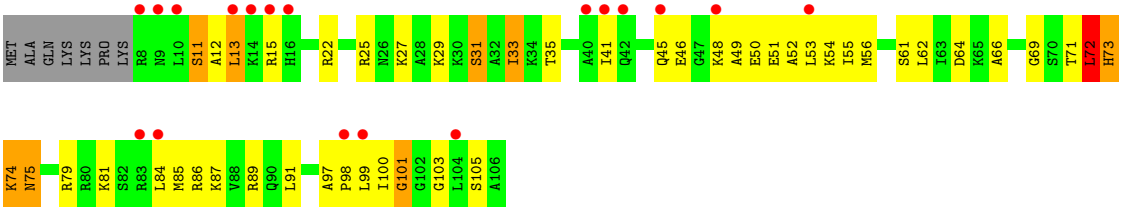
• Molecule 20: 30S ribosomal protein S20

Chain BI:



• Molecule 20: 30S ribosomal protein S20

Chain BA:

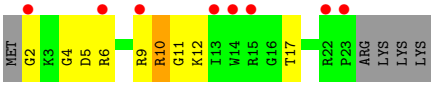


• Molecule 21: 30S ribosomal protein Thx

Chain 1F:

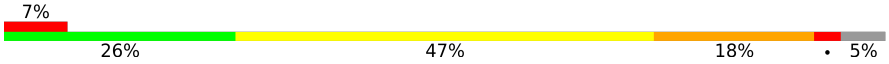
• Molecule 21: 30S ribosomal protein Thx

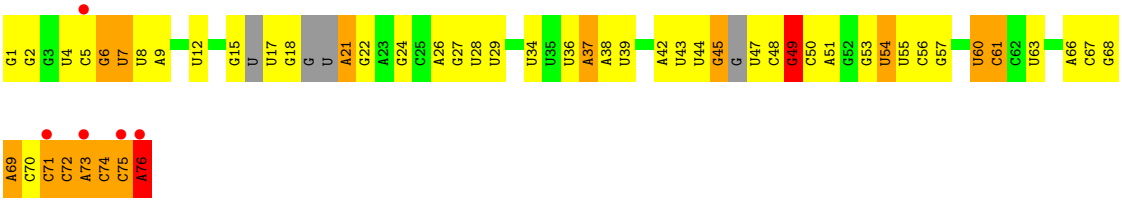
Chain 1B:



• Molecule 22: tRNALys

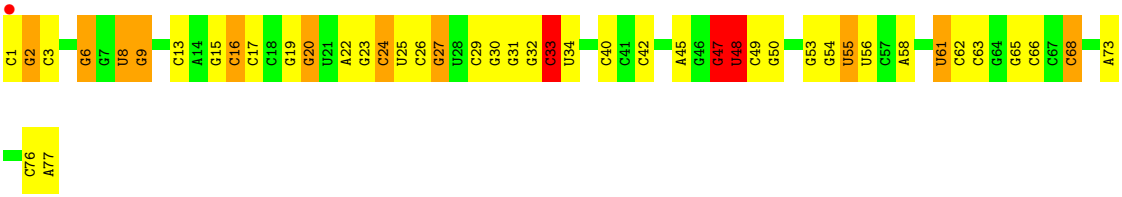
Chain 1K:





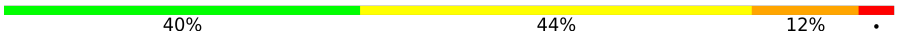
• Molecule 23: tRNAfMet

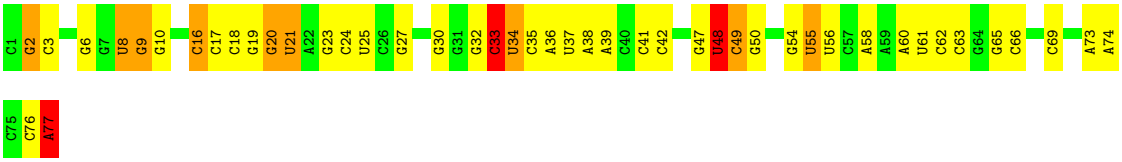
Chain 2K:



• Molecule 23: tRNAfMet

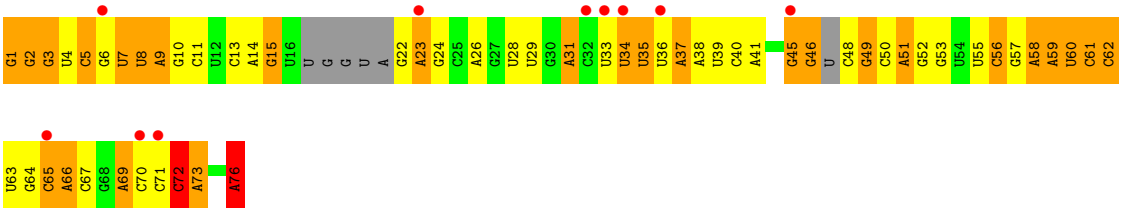
Chain 2L:





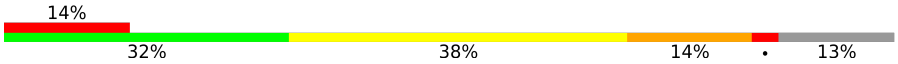
• Molecule 24: tRNALys

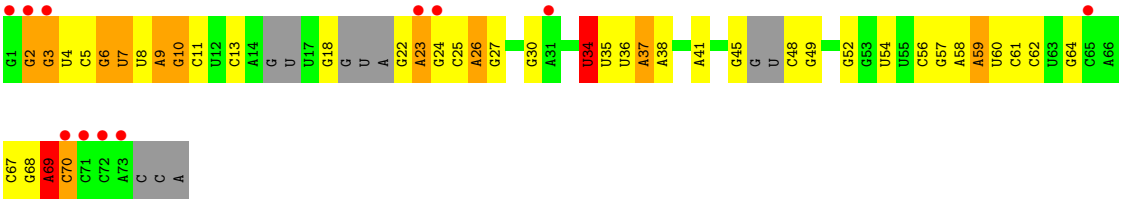
Chain 3K:



• Molecule 24: tRNALys

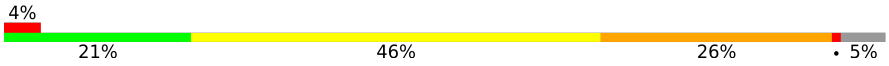
Chain 1L:

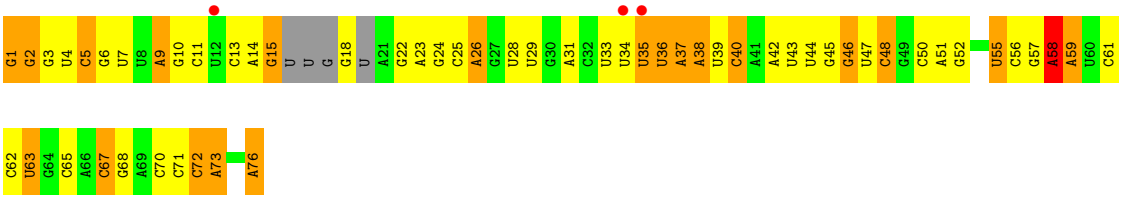




- Molecule 24: tRNALys

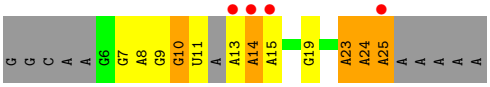
Chain 3L:





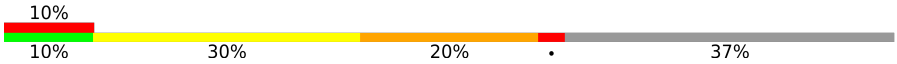
- Molecule 25: mRNA

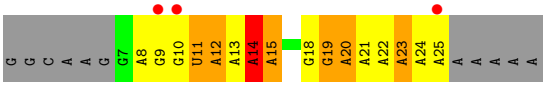
Chain 4K:



- Molecule 25: mRNA

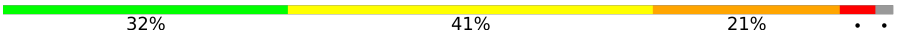
Chain 4L:

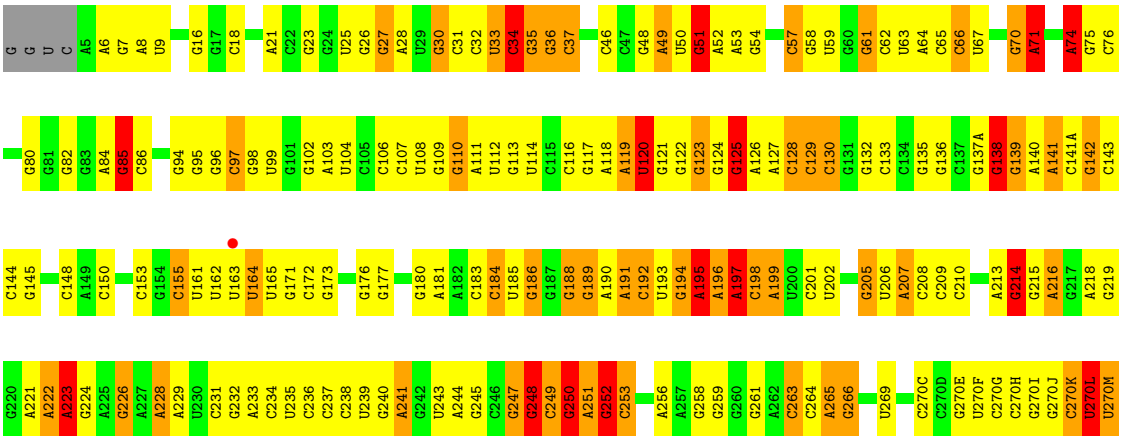


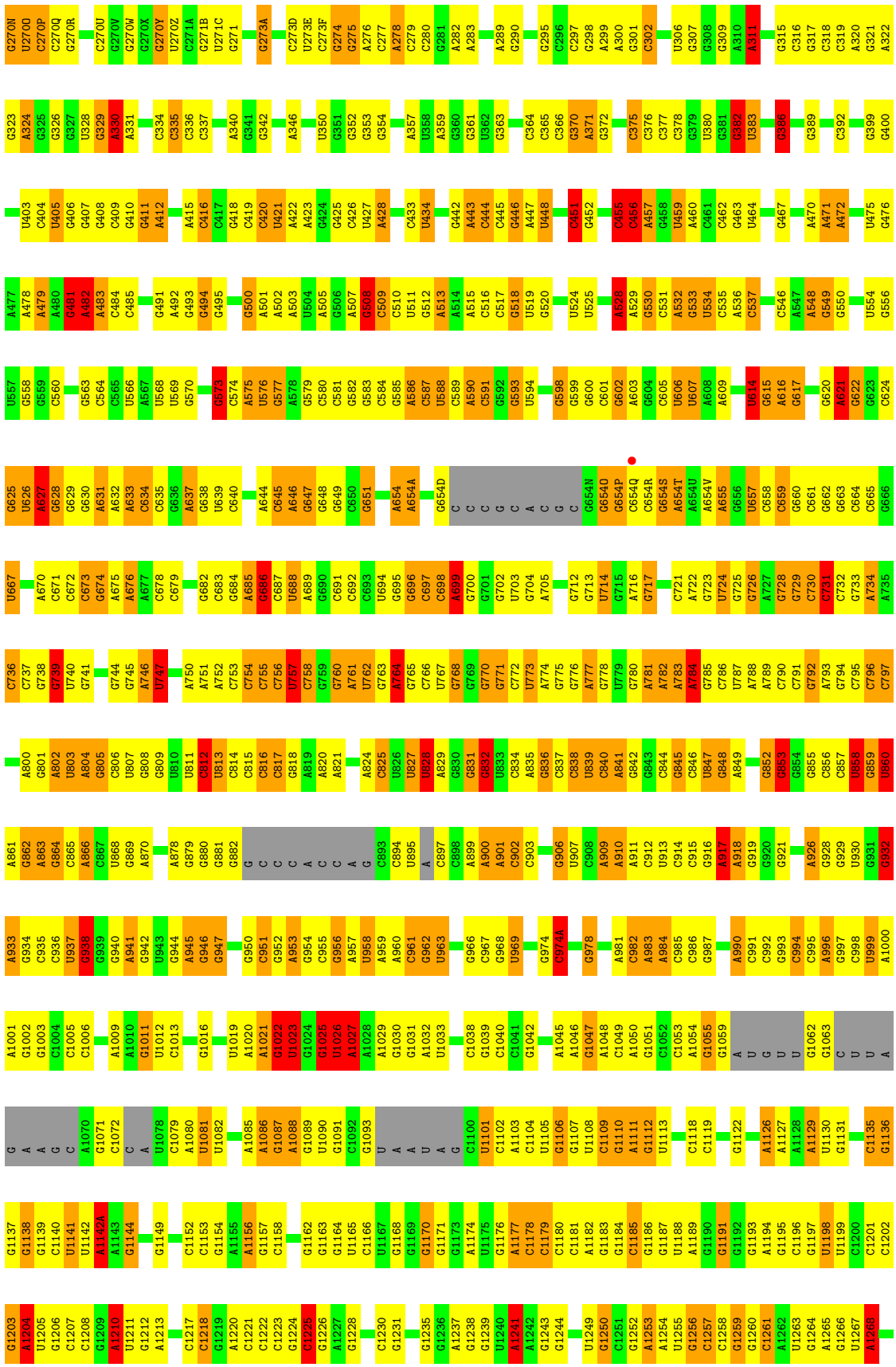


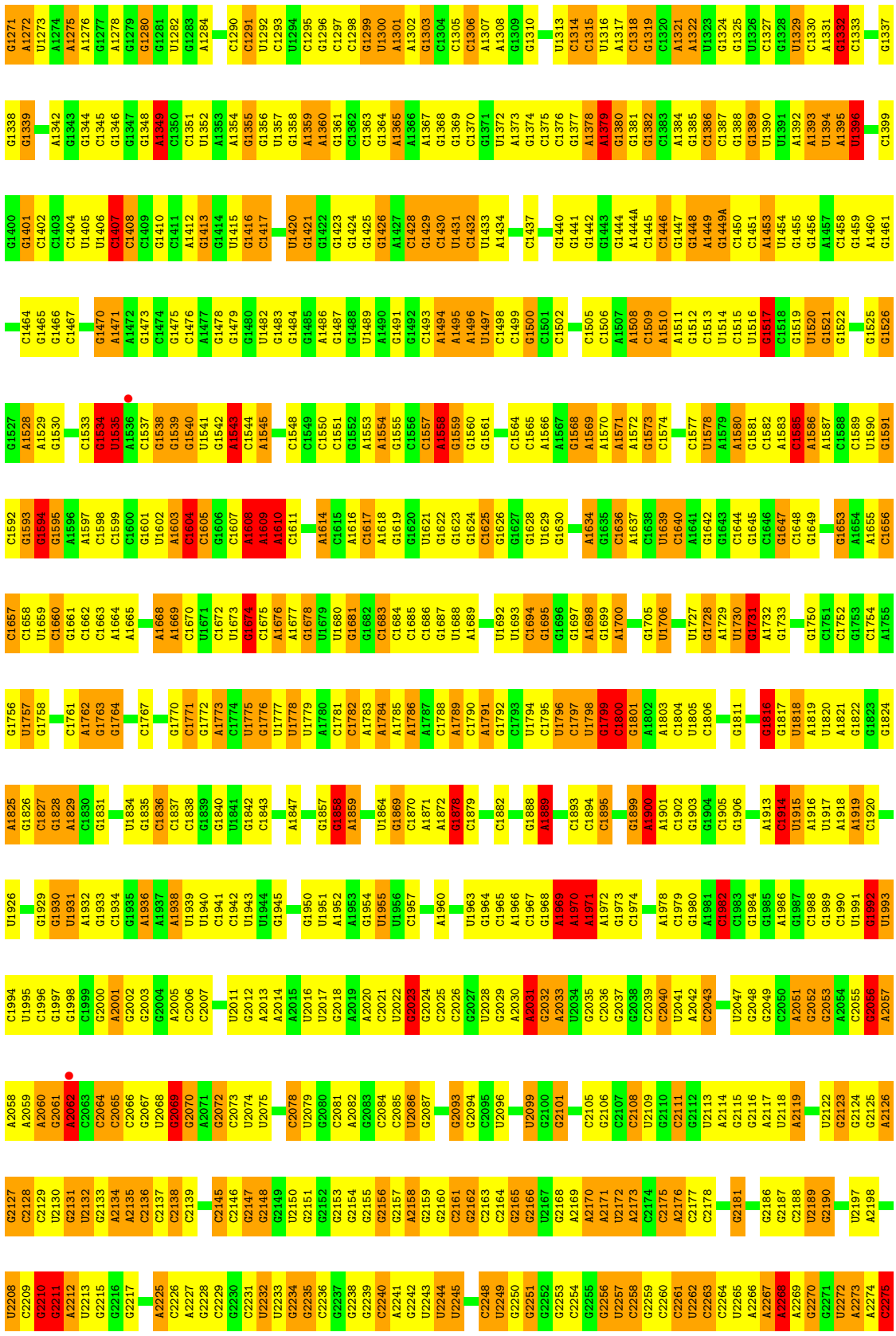
- Molecule 26: 23S ribosomal RNA

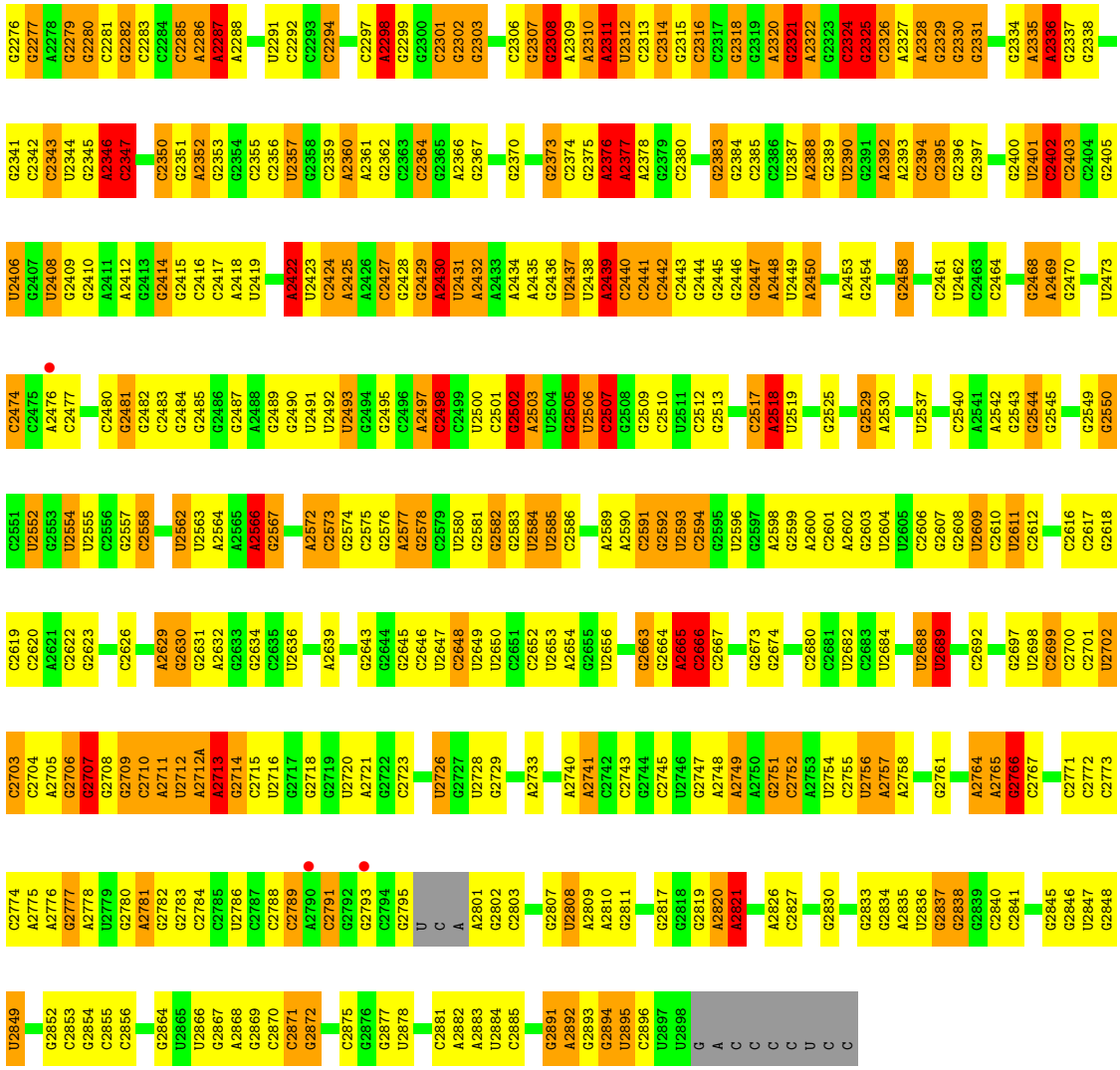
Chain 1H:





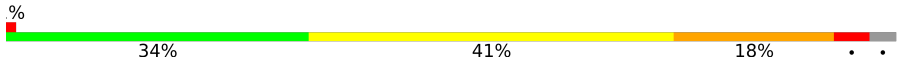

G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 C1217 C1218 G1219 A1220 C1221 C1222 C1223 G1224 C1225 G1226 A1227 G1228 C1230 G1231 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268
G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 G1149 C1152 C1153 G1154 A1155 A1156 C1157 C1158 G1162 G1163 G1164 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1180 C1181 A1182 G1183 C1184 C1185 G1186 G1187 U1188 G1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 C1202
G A A G C A1070 G1071 C1072 C A U1078 C1079 A1080 U1081 U1082 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U A A U A G C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1118 C1119 G1122 A1126 A1127 A1128 A1129 U1130 G1131 C1135 G1136
A1001 G1002 G1003 C1004 C1005 C1006 A1009 A1010 G1011 U1012 C1013 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 C1038 G1039 C1040 C1041 G1042 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1059 A U G U U C U U A
A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G950 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 G966 C967 G968 U969 G974 C974A G978 A981 C982 A983 A984 C985 C986 G987 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000
A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 A878 G879 G880 G881 G882 G C C C A C C A G C893 C894 U895 A C897 C898 A899 A900 A901 C902 C903 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 A926 G928 G929 U930 G931 G932
A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 G812 U813 C814 C815 C816 C817 G818 A819 A820 A821 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 G852 G853 G854 G855 C856 C857 U858 U860
C736 C737 G738 G739 U740 G741 G744 G745 A746 U747 A750 A751 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 G771 C772 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797
U667 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G682 C683 G684 A685 G686 C687 U688 A689 G690 C691 C692 C693 U694 G695 G696 C697 C698 A699 G700 G701 G702 U703 G704 A705 G712 G713 U714 G715 A716 G717 C721 A722 G723 U724 G725 G726 A727 G728 G729 C730 C731 C732 G733 A734 A735
U557 G558 G559 C560 G563 C564 C565 U566 A567 U568 U569 G570 G573 C574 A575 U576 G577 A578 G579 C580 C581 C582 G583 C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 U594 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 U614 G615 A616 G617 G620 A621 G622 G623 C624
G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 A644 C645 A646 G647 G648 G649 C650 G651 A654 A654A G654D C C C G C A C G C G654N G6540 G654P C654Q C654R G654S A654T A654U A654V A655 G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666
A477 A478 A479 A480 G481 A482 A483 C484 C485 G491 A492 G493 G494 G495 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 A515 C516 C517 G518 U519 G520 U524 U525 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 C546 A547 A548 G549 G550 U554 G556
G323 A324 G325 G326 G327 U328 G329 A330 A331 C334 C335 C336 C337 A340 G341 G342 A346 U350 G351 G352 G353 G354 A357 U358 A359 G360 G361 U362 G363 C364 C365 C366 G370 A371 G372 C375 C376 C377 C378 G379 U380 G381 G382 U383 G386 G389 C392 G399 G400
U403 C404 U405 G406 G407 G408 C409 G410 G411 A412 A415 C416 C417 G418 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 C433 U434 G442 A443 C444 C445 G446 A447 U448 C451 G452 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G467 A470 A471 A472 U475 G476
G270N U270O C270P C270Q G270R C270U G270V G270W G270X G270Y U270Z C271A G271B U271C G271 G273A C273D U273E C273F G274 G275 A276 C277 A278 C279 C280 G281 A282 A283 A289 G290 G295 C296 C297 G298 A299 A300 G301 C302 U306 G307 G308 G309 A310 A311 G315 C316 G317 C318 C319 A320 G321 A322

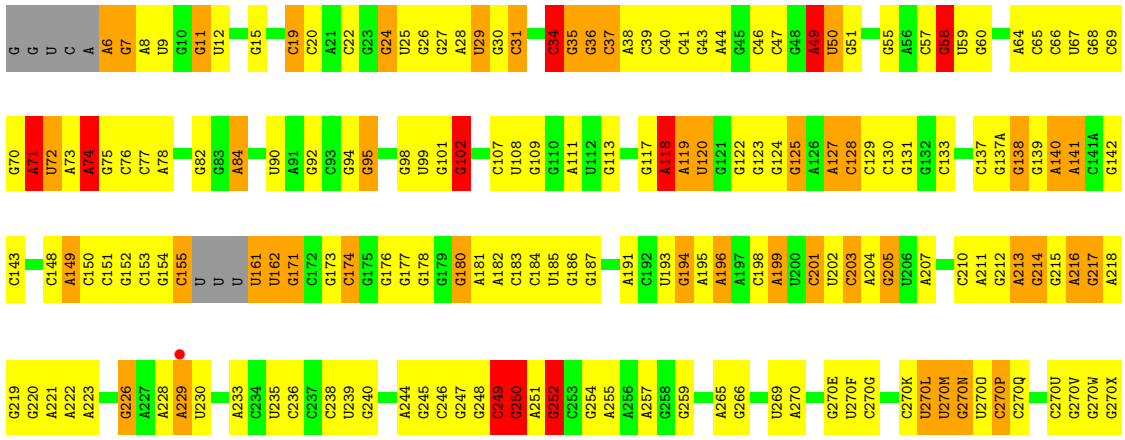


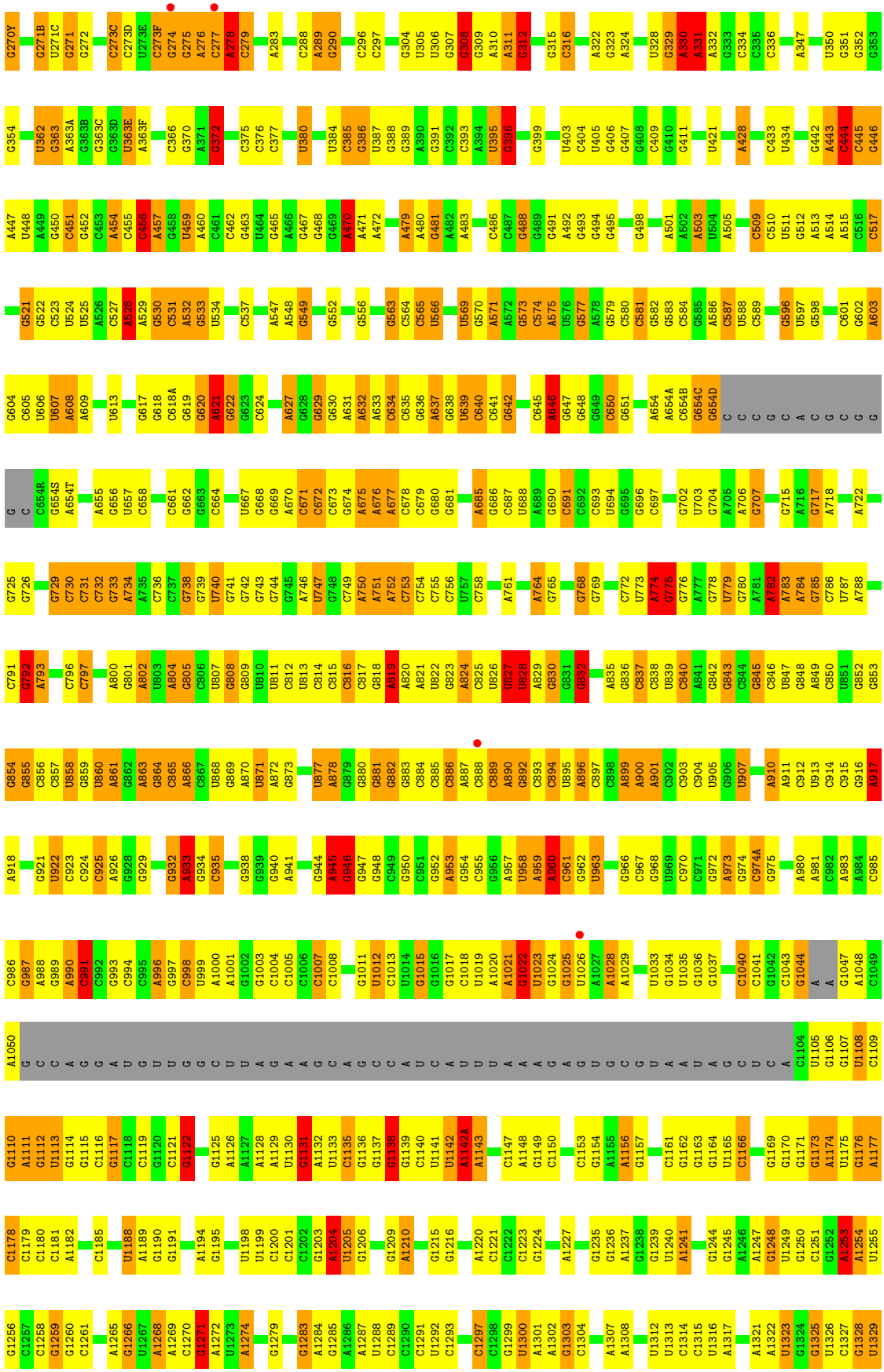


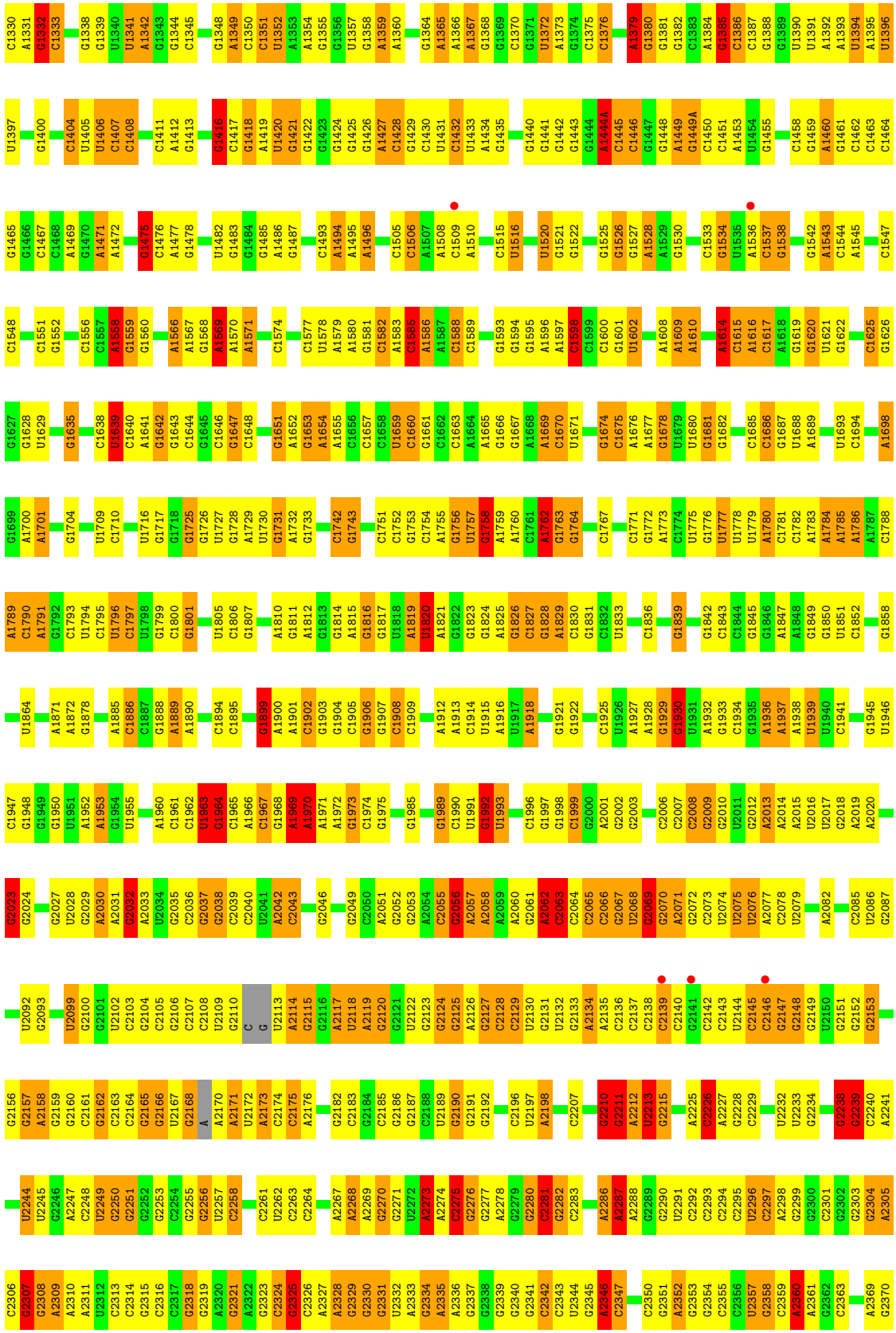
• Molecule 26: 23S ribosomal RNA

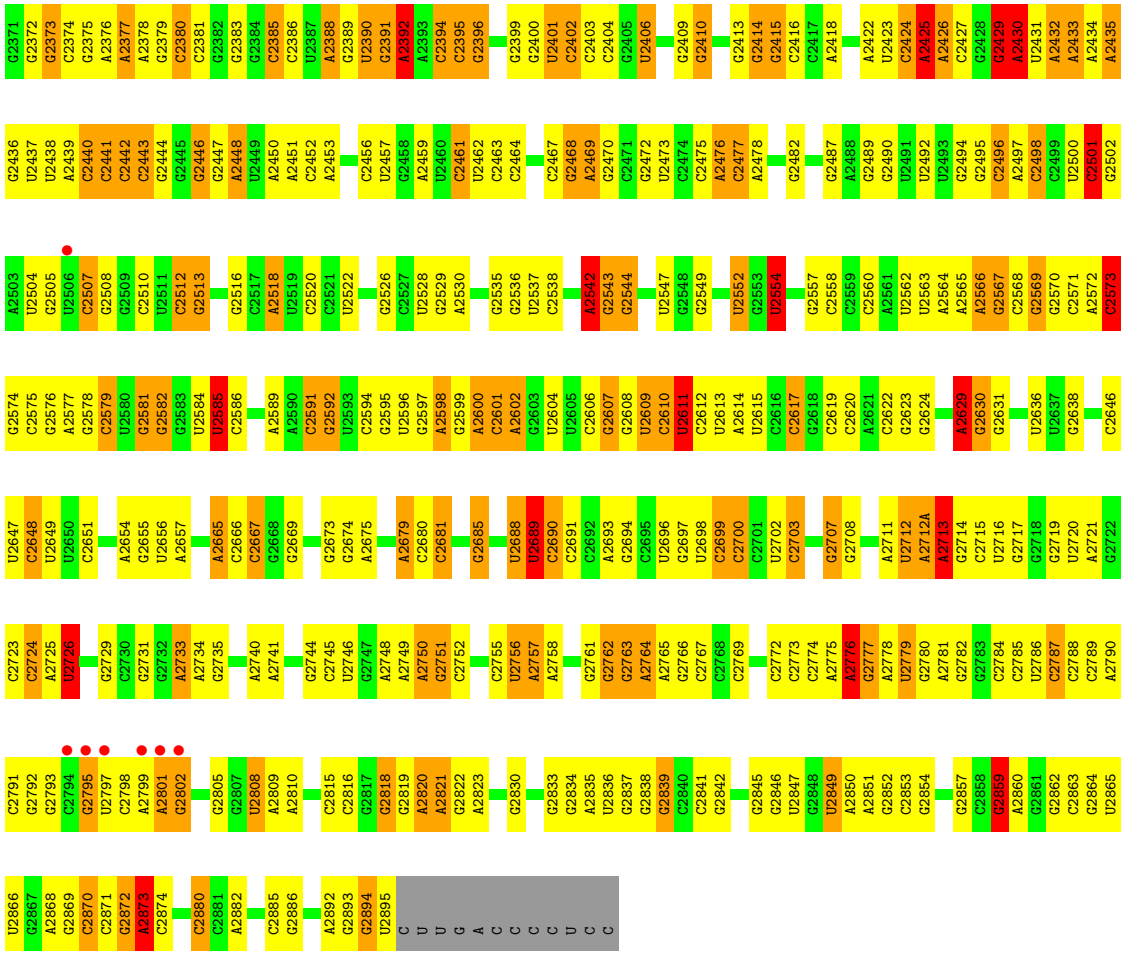
Chain 14:





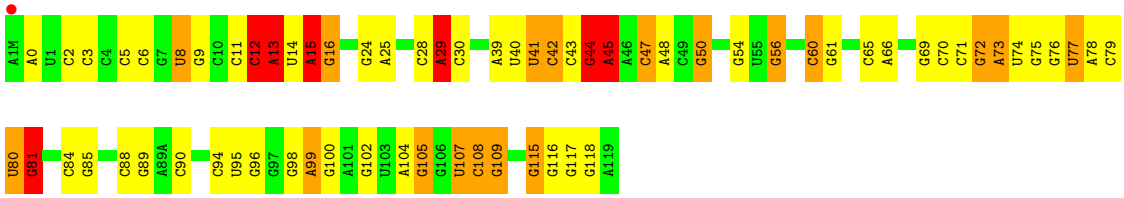

G270Y G271B U271C G271 G272 C273C C273D U273E C273F G274 G275 A276 C277 A278 C279 A283 C288 A289 G290 C296 C297 G304 U305 U306 G307 G308 G309 A310 A311 G312 G315 C316 A322 G323 A324 U328 G329 A330 A331 A332 G333 C334 C335 C336 A347 U350 G351 G352 G353
G354 U362 G363 A363A G363B G363C G363D U363E A363F C366 G370 A371 G372 C375 C376 C377 U380 U384 C385 G386 U387 G388 G389 A390 G391 C392 C393 A394 U395 G396 G399 U403 C404 U405 G406 G407 G408 C409 G410 G411 U421 A428 C433 U434 G442 A443 C444 C445 C446
A447 U448 A449 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 A479 A480 G481 A482 A483 C486 C487 G488 G489 G491 A492 G493 G494 G495 G498 A501 A502 A503 U504 A505 C509 C510 U511 G512 A513 A514 A515 C516 C517
G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C537 A547 A548 G549 G552 G556 G563 C564 C565 U566 U569 G570 A571 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 G596 U597 G598 C601 G602 A603
G604 C605 U606 U607 A608 A609 U613 G617 G618 C618A G619 G620 A621 G622 G623 C624 A627 G628 G629 G630 A631 A632 A633 C634 C635 C636 A637 G638 U639 C640 C641 G642 C645 A646 G647 G648 G649 C650 G651 A654 A654A C654B G654C G654D C C C C G G C A C G C G G
G C C654R G654S A654T A655 G656 U657 C658 C661 G662 G663 C664 U667 G668 G669 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G680 G681 A685 G686 C687 U688 A689 G690 C691 C692 C693 U694 G695 G696 C697 G702 U703 G704 A705 A706 G707 G715 A716 G717 A718 A722
G725 G726 G729 C730 C731 C732 G733 A734 A735 C736 C737 G738 G739 U740 G741 G742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 C755 C756 U757 C758 A761 A764 G765 G768 G769 C772 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788
C791 G792 A793 C796 C797 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 A835 G836 C837 C838 U839 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852 G853
G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 U871 A872 G873 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 A910 A911 C912 U913 C914 C915 G916 A917
A918 G921 U922 C923 C924 C925 A926 G928 G929 G932 A933 G934 G935 G938 G939 G940 A941 G944 A945 G946 G947 G948 C949 G950 C951 C952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 G966 C967 G968 U969 C970 C971 G972 A973 G974 C974A G975 A980 A981 C982 A983 A984 C985
C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 U1033 G1034 U1035 G1036 G1037 C1040 C1041 G1042 C1043 G1044 A A A1050 G C C A C C A G C A G U C A G U U A A U U G G C U U U A U U C A U U A A G C G U A A U A G C U C A C1104 U1105 G1106 G1107 U1108 C1109
G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 C1147 A1148 G1149 C1150 C1153 G1154 A1155 A1156 G1157 C1161 G1162 G1163 G1164 U1165 C1166 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177
C1178 C1179 C1180 C1181 A1182 C1185 U1188 A1189 G1190 G1191 A1194 G1195 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 G1209 A1210 G1215 G1216 A1220 C1221 C1222 C1223 G1224 A1227 G1235 G1236 A1237 G1238 G1239 U1240 A1241 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255
G1256 C1257 C1258 G1259 C1260 C1261 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1279 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1293 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1304 A1307 A1308 U1312 U1313 C1314 C1315 U1316 A1317 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329


C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 G2316 C2317 G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 G2337 G2338 G2339 G2340 G2341 C2342 U2344 G2345 A2346 C2347 C2350 G2351 A2352 G2353 G2354 C2355 C2356 U2357 G2358 C2359 A2360 A2361 G2362 C2363 A2369 G2370
U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253 C2254 G2255 G2256 U2257 C2258 C2261 U2262 C2263 C2264 A2267 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 C2282 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2300 C2301 G2302 G2303 G2304 A2305
G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A A2170 A2171 U2172 A2173 C2174 C2175 A2176 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 C2196 U2197 A2198 C2207 G2210 G2211 A2212 U2213 G2215 A2225 C2226 A2227 G2228 C2229 U2232 U2233 G2234 G2236 G2239 C2240 A2241
U2092 G2093 U2099 G2100 G2101 U2102 C2103 G2104 G2105 G2106 C2107 C2108 U2109 G2110 C G U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2150 G2151 G2152 G2153
G2023 G2024 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079 A2082 C2085 U2086 G2087
C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 G1985 G1989 C1990 U1991 G1992 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 G2003 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2013 A2014 A2015 U2016 U2017 G2018 A2019 A2020
U1864 A1871 A1872 G1878 A1885 C1886 C1887 G1888 A1889 A1890 C1894 C1895 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 A1912 A1913 C1914 U1915 A1916 U1917 A1918 G1921 G1922 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 G1945 U1946
A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 U1805 C1806 G1807 A1810 G1811 A1812 G1813 C1814 A1815 G1816 C1817 U1818 A1819 U1820 A1821 G1822 C1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 C1836 G1839 G1842 C1843 C1844 G1845 G1846 A1847 A1848 G1849 G1850 U1851 C1852 G1858
G1699 A1700 A1701 G1704 U1709 C1710 U1716 G1717 G1718 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1742 G1743 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1767 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788
G1627 G1628 U1629 G1635 C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1685 C1686 G1687 U1688 A1689 U1693 C1694 A1698
C1548 C1551 G1552 C1556 C1557 A1558 G1559 G1560 A1566 A1567 G1568 A1569 A1570 A1571 C1574 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1587 C1588 C1589 G1593 G1594 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 A1608 A1609 A1610 A1614 C1615 A1616 C1617 A1618 G1619 G1620 U1621 G1622 C1625 G1626
G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1475 C1476 A1477 G1478 U1482 G1483 G1484 G1485 A1486 G1487 C1493 A1494 A1495 A1496 C1505 C1506 A1507 A1508 C1509 A1510 C1515 U1516 U1520 G1521 G1522 G1525 G1526 G1527 A1528 A1529 G1530 C1533 G1534 U1535 A1536 C1537 G1538 G1542 A1543 C1544 A1545 C1547
U1397 G1400 C1404 U1405 U1406 C1407 C1408 C1411 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1440 G1441 G1442 G1443 G1444 A1444A C1445 C1446 G1447 G1448 A1449 G1449A C1450 C1451 A1453 U1454 G1455 C1458 G1459 A1460 G1461 C1462 C1463 C1464
C1330 A1331 G1332 C1333 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 G1348 A1349 C1350 C1351 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396



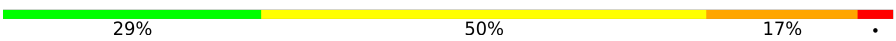
- Molecule 27: 5S ribosomal RNA

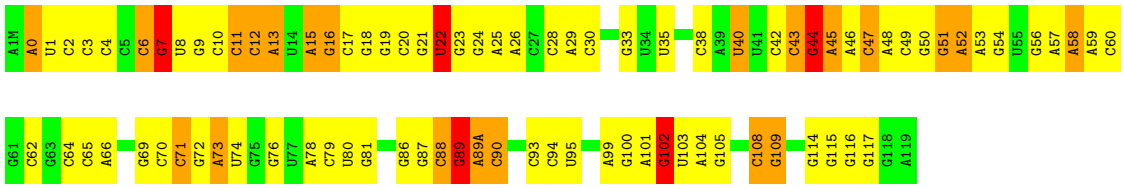
Chain 16:



- Molecule 27: 5S ribosomal RNA

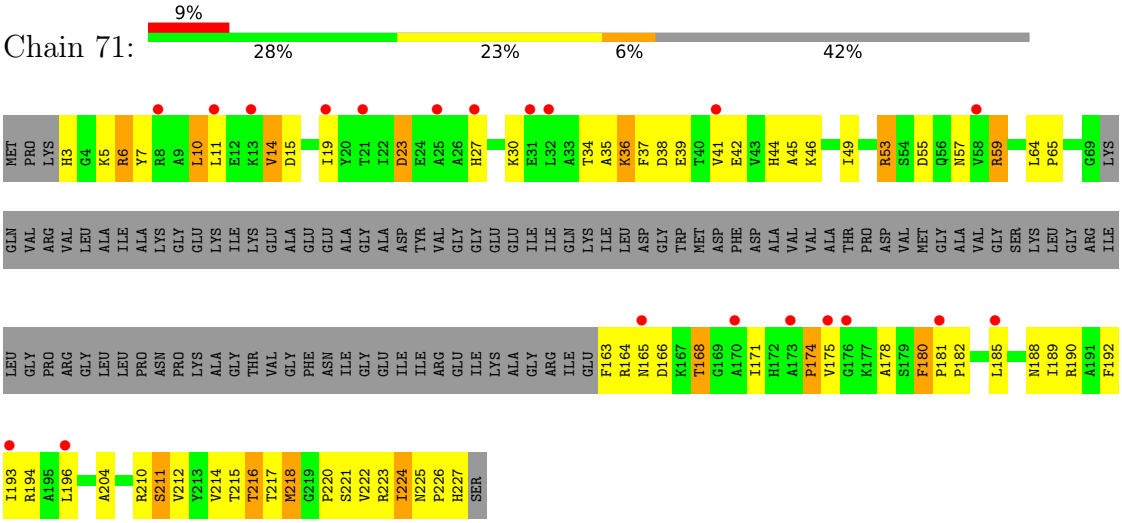
Chain 1J:





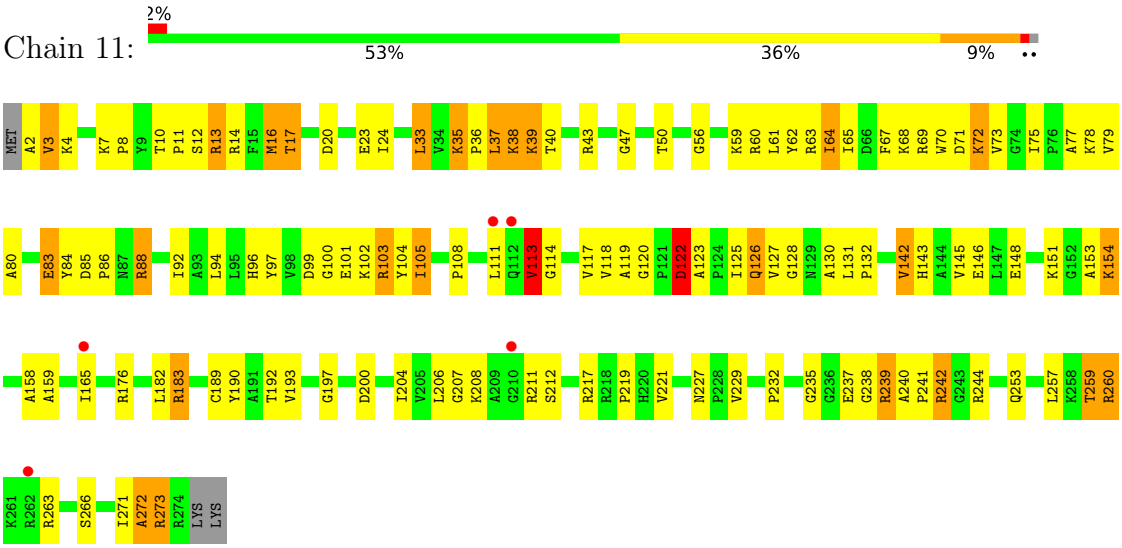
- Molecule 28: 50S ribosomal protein L1

Chain 71:



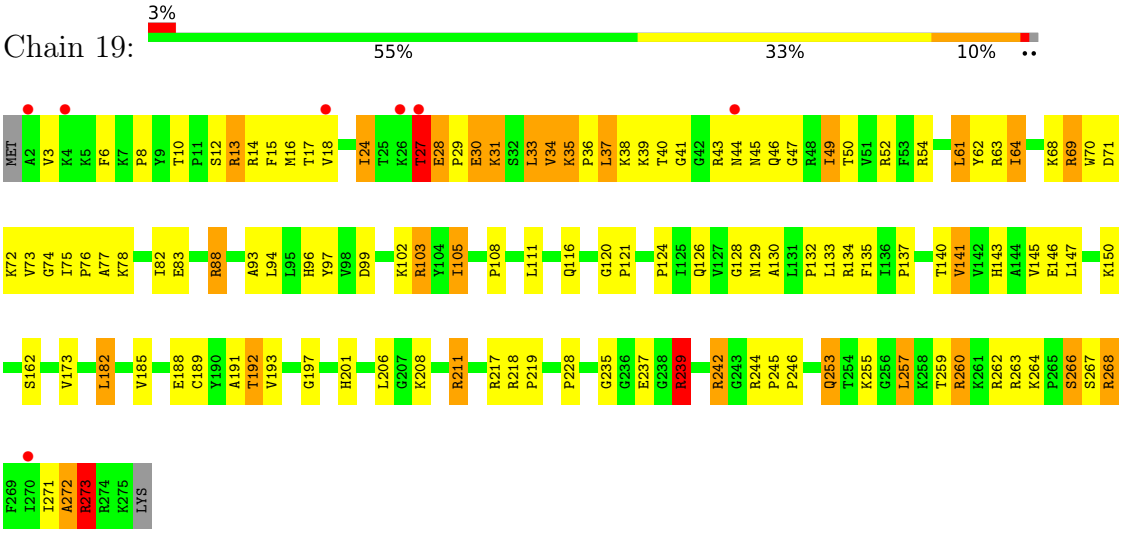
• Molecule 29: 50S ribosomal protein L2

Chain 11:



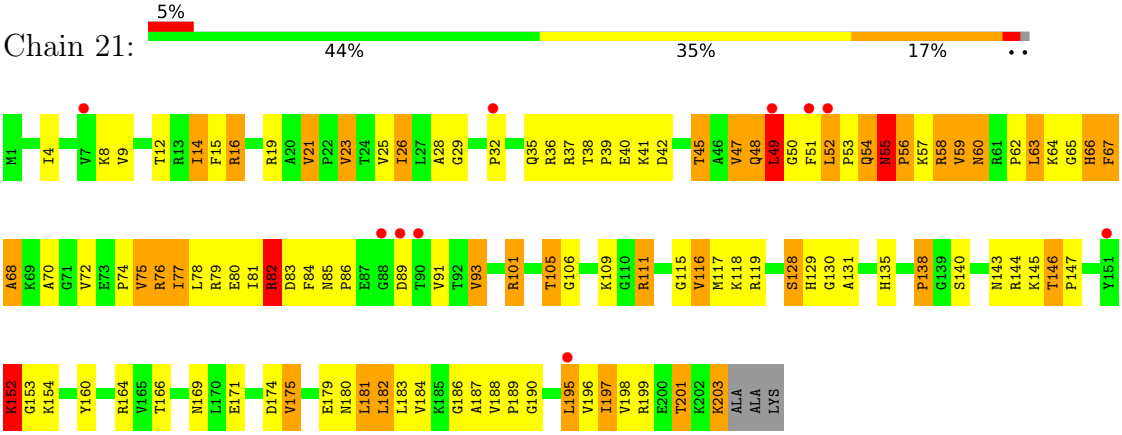
• Molecule 29: 50S ribosomal protein L2

Chain 19:



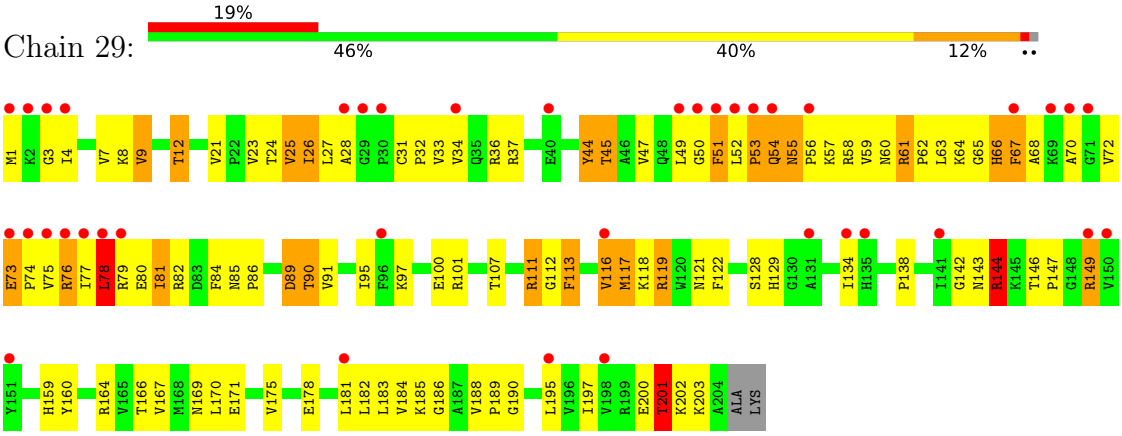
• Molecule 30: 50S ribosomal protein L3

Chain 21:



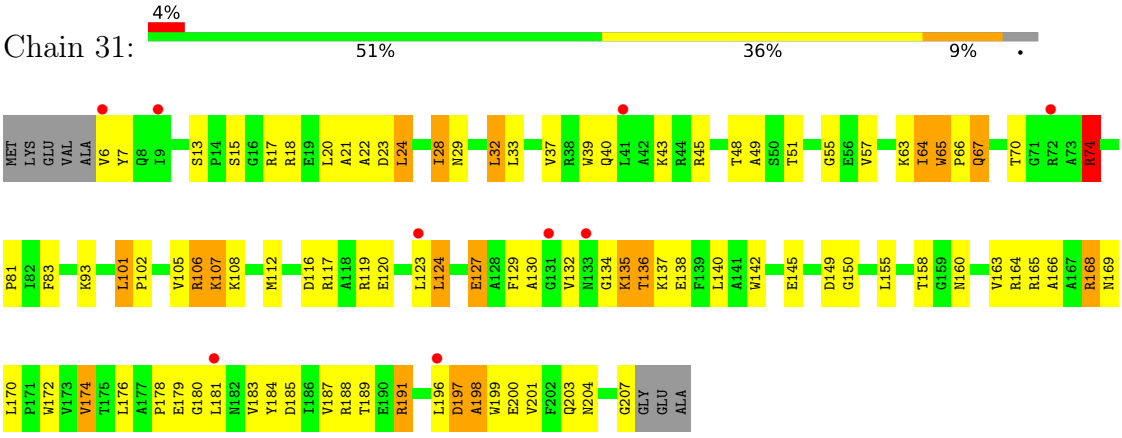
• Molecule 30: 50S ribosomal protein L3

Chain 29:



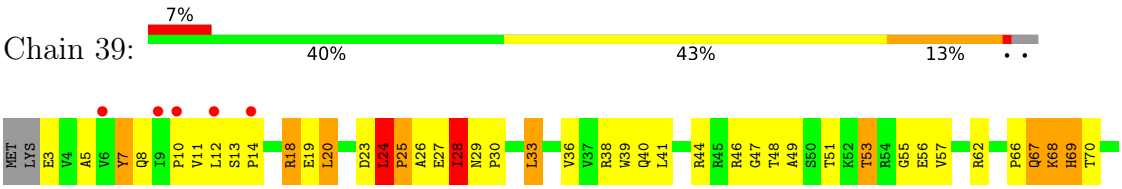
• Molecule 31: 50S ribosomal protein L4

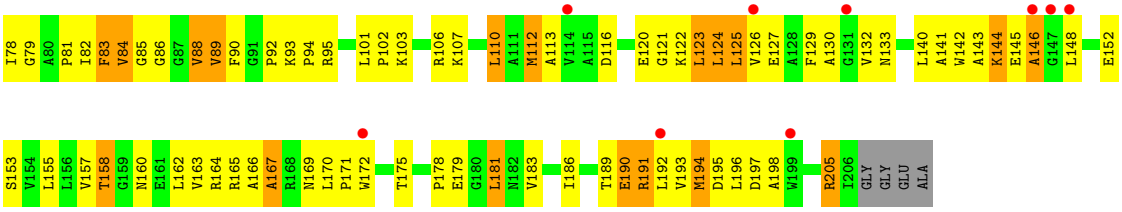
Chain 31:



• Molecule 31: 50S ribosomal protein L4

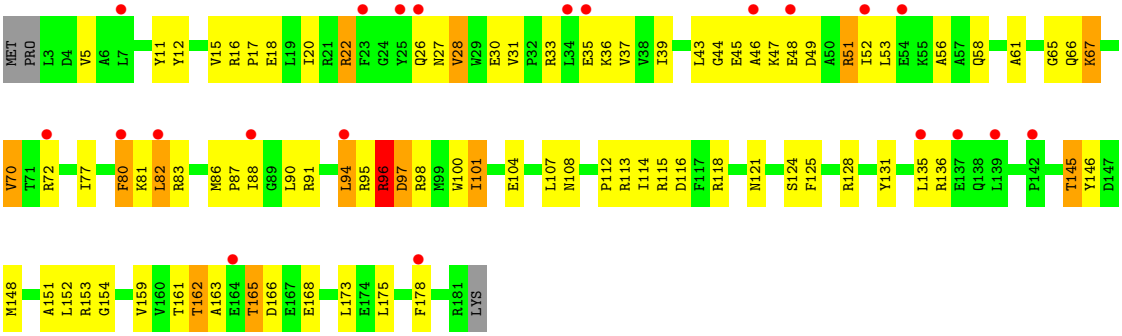
Chain 39:





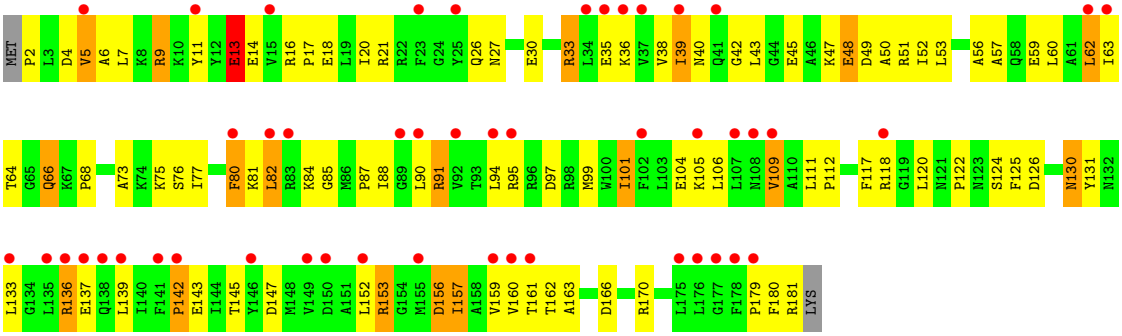
• Molecule 32: 50S ribosomal protein L5

Chain 41:



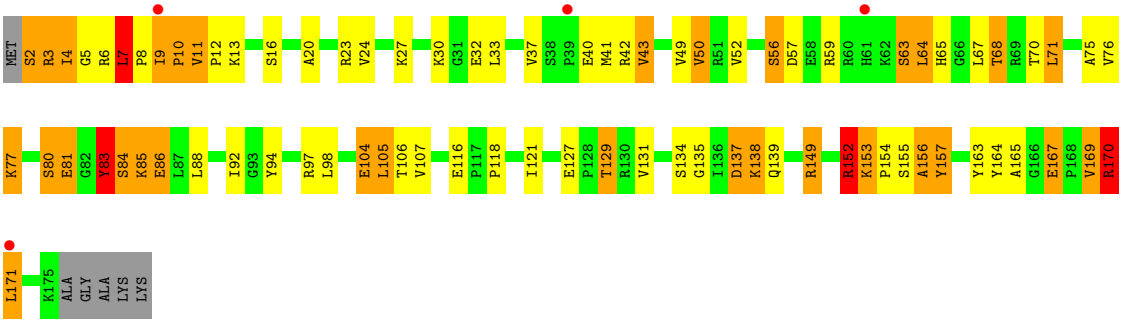
• Molecule 32: 50S ribosomal protein L5

Chain 49:



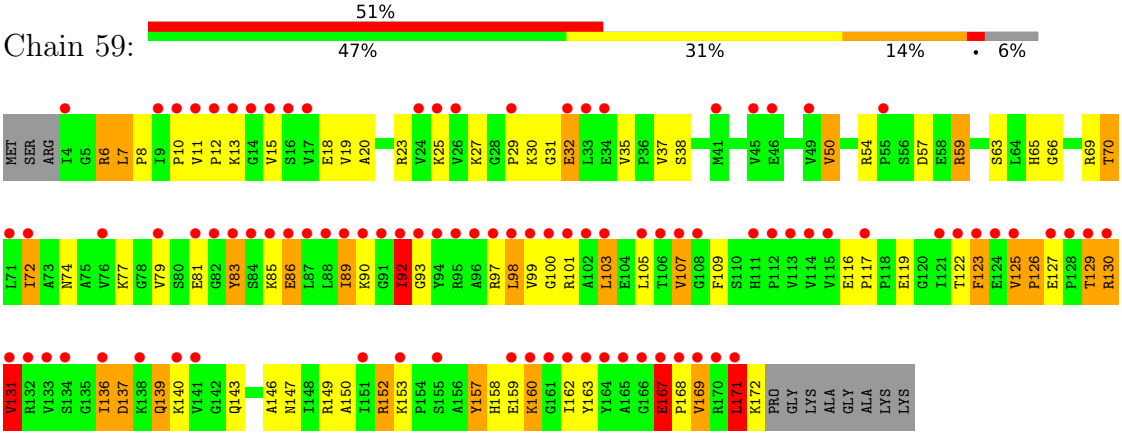
• Molecule 33: 50S ribosomal protein L6

Chain 51:



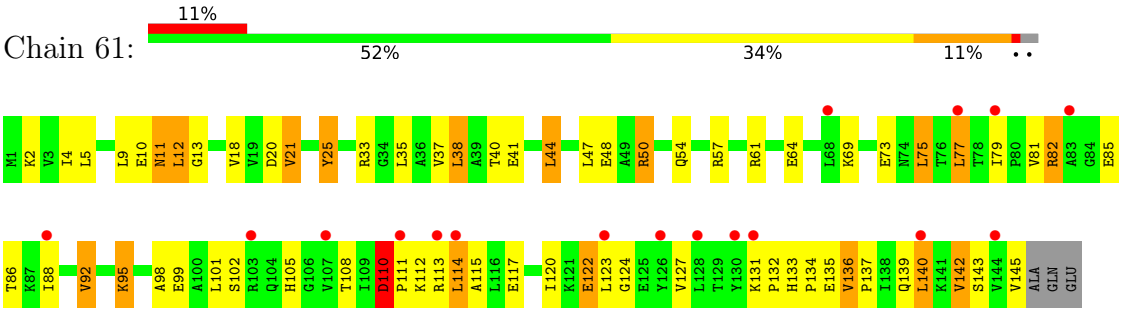
• Molecule 33: 50S ribosomal protein L6

Chain 59:



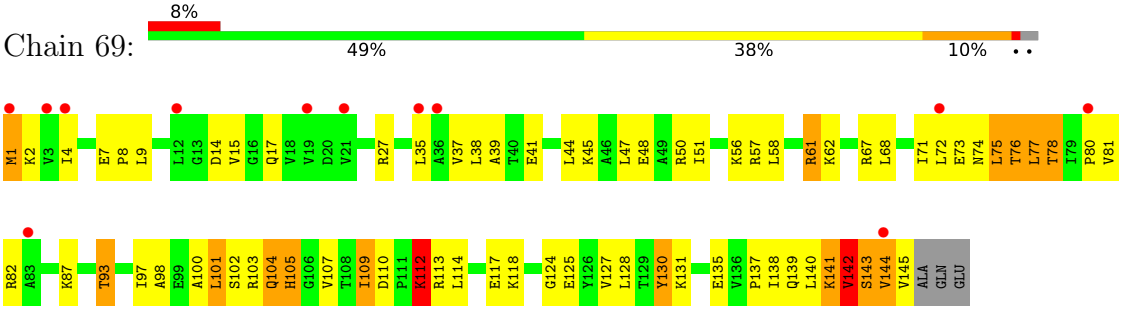
• Molecule 34: 50S ribosomal protein L9

Chain 61:



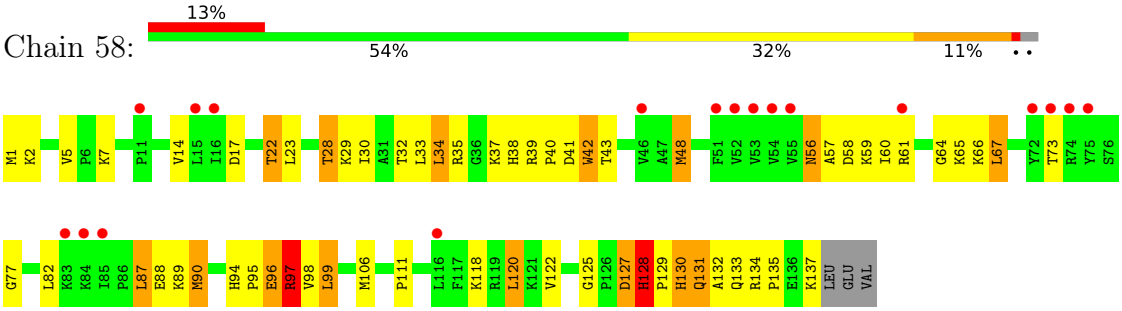
• Molecule 34: 50S ribosomal protein L9

Chain 69:



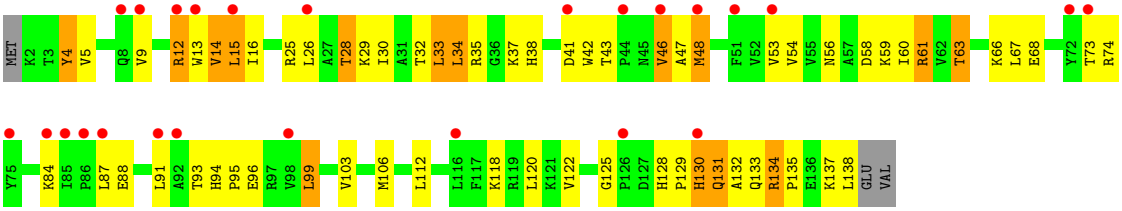
• Molecule 35: 50S ribosomal protein L13

Chain 58:



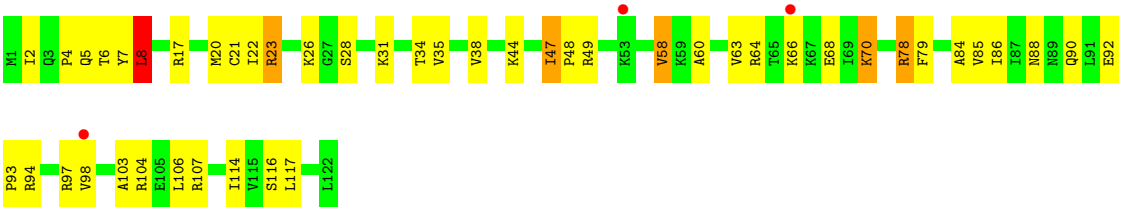
• Molecule 35: 50S ribosomal protein L13

Chain 15:



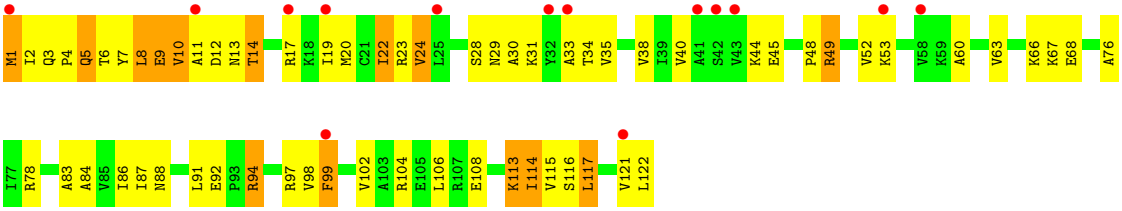
- Molecule 36: 50S ribosomal protein L14

Chain 68:



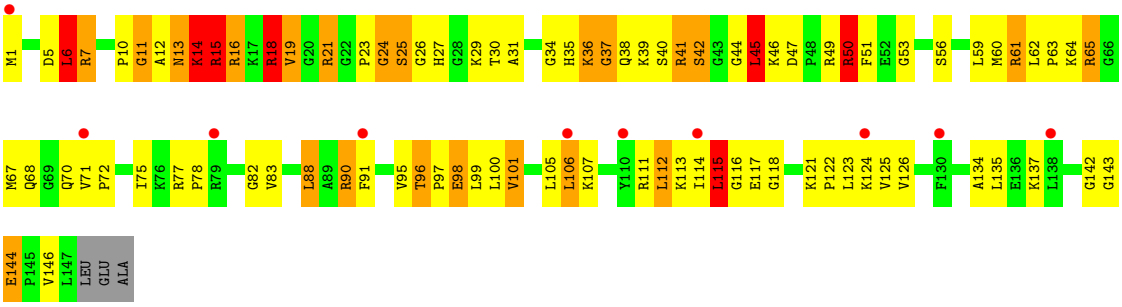
- Molecule 36: 50S ribosomal protein L14

Chain 25:



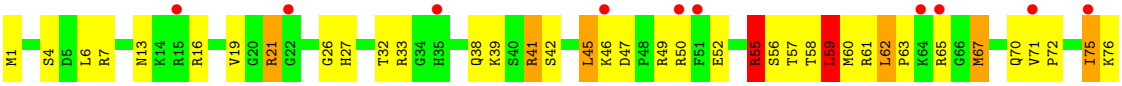
- Molecule 37: 50S ribosomal protein L15

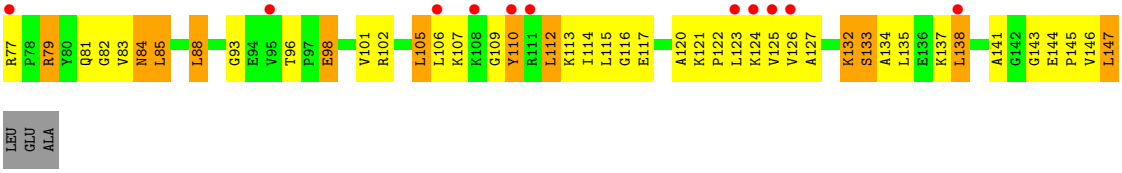
Chain 78:



- Molecule 37: 50S ribosomal protein L15

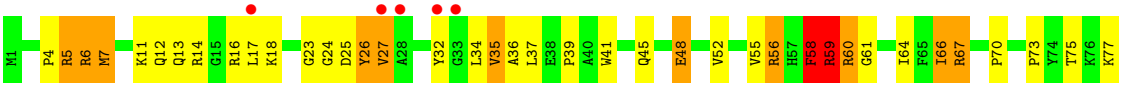
Chain 35:

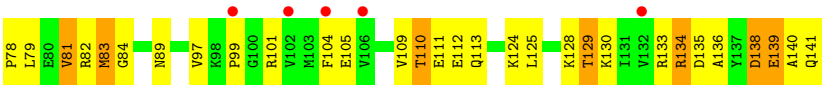




• Molecule 38: 50S ribosomal protein L16

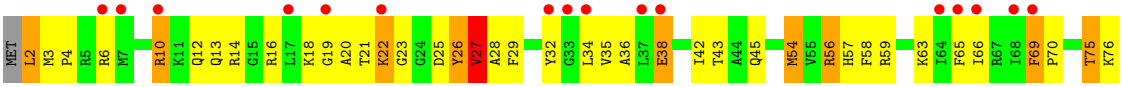
Chain 88:





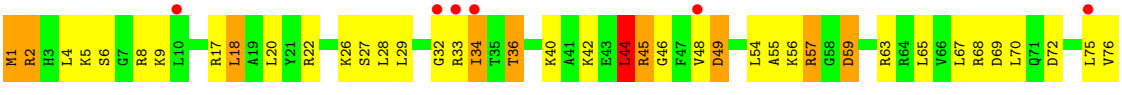
• Molecule 38: 50S ribosomal protein L16

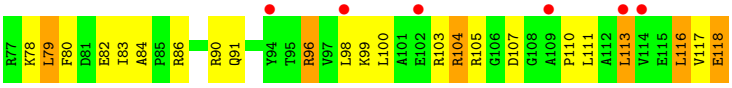
Chain 45:



• Molecule 39: 50S ribosomal protein L17

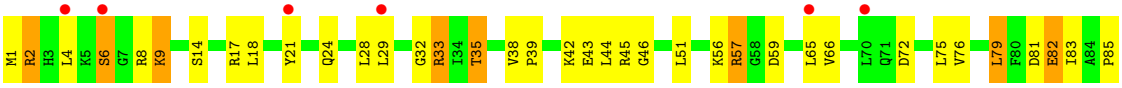
Chain 98:

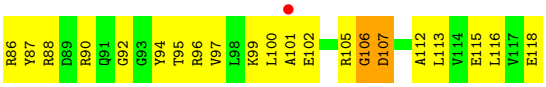




• Molecule 39: 50S ribosomal protein L17

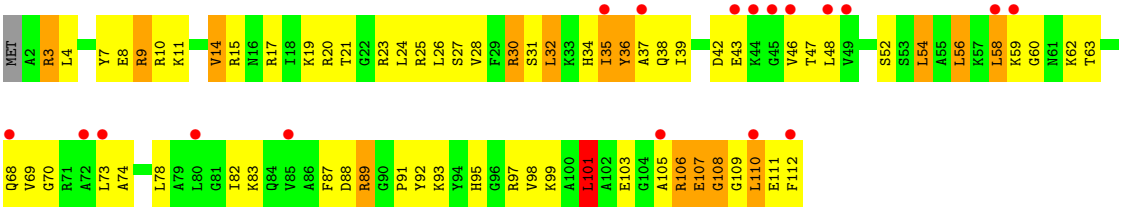
Chain 55:





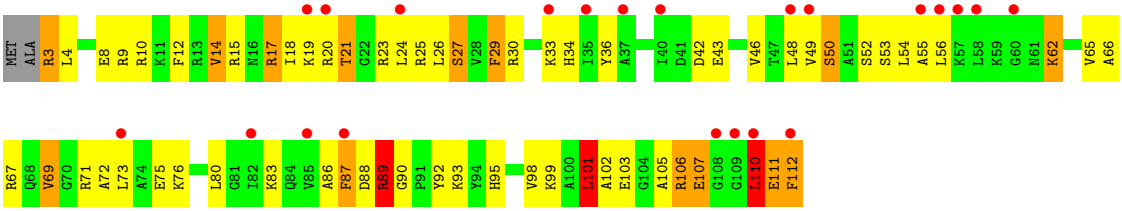
- Molecule 40: 50S ribosomal protein L18

Chain A8:



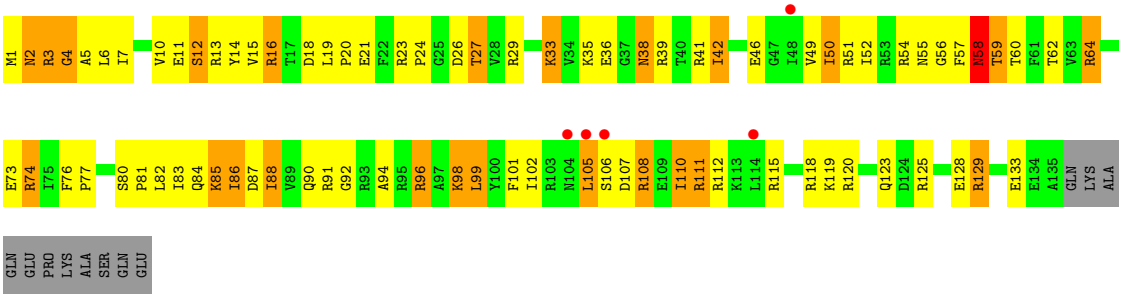
- Molecule 40: 50S ribosomal protein L18

Chain 65:



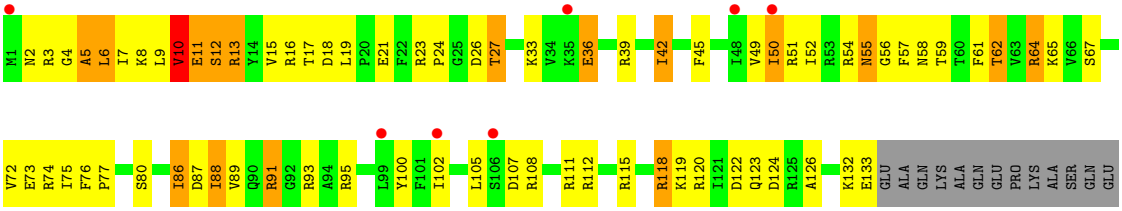
- Molecule 41: 50S ribosomal protein L19

Chain B8:



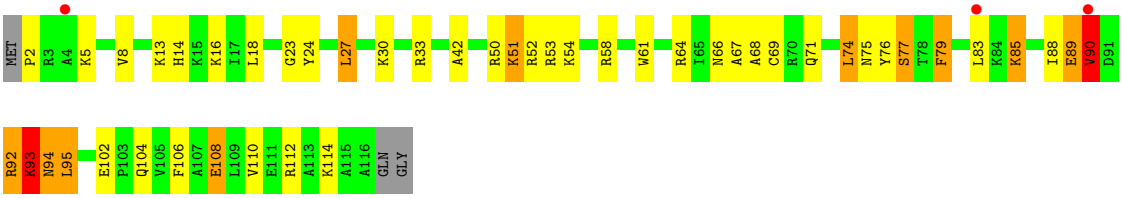
- Molecule 41: 50S ribosomal protein L19

Chain 75:



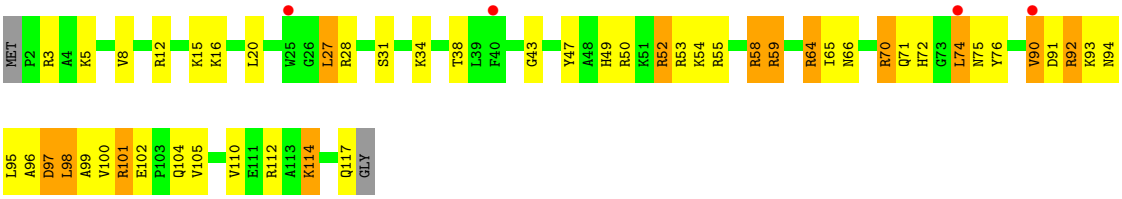
- Molecule 42: 50S ribosomal protein L20

Chain C8:



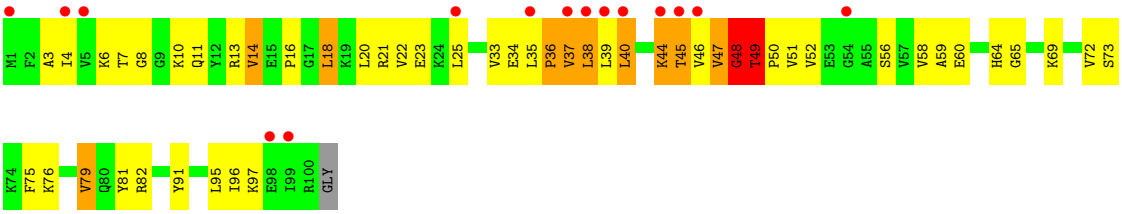
• Molecule 42: 50S ribosomal protein L20

Chain 85:



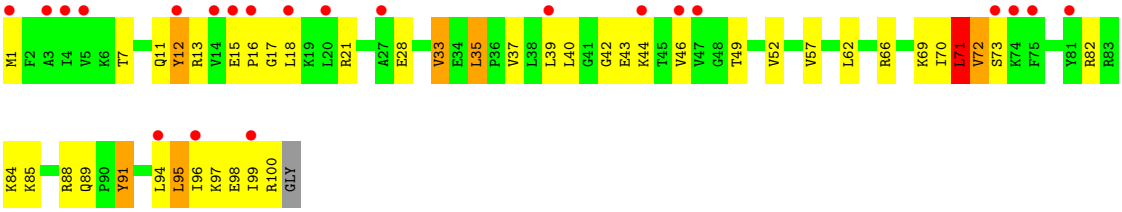
• Molecule 43: 50S ribosomal protein L21

Chain D8:



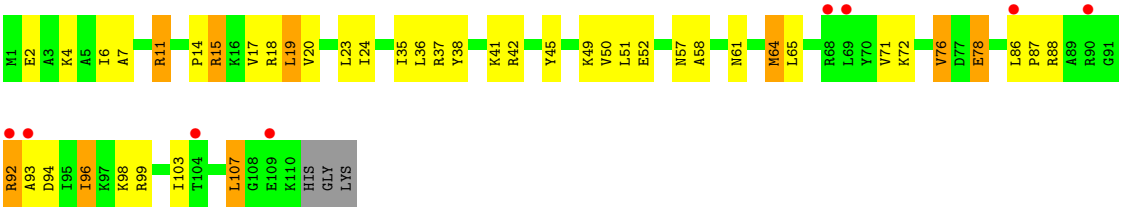
• Molecule 43: 50S ribosomal protein L21

Chain 95:



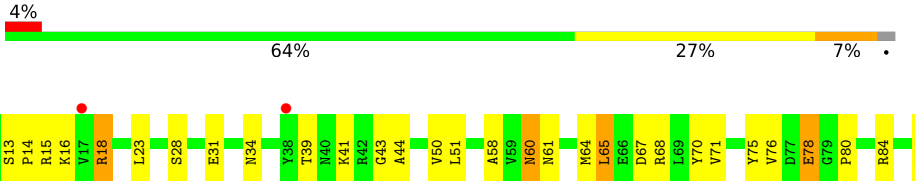
• Molecule 44: 50S ribosomal protein L22

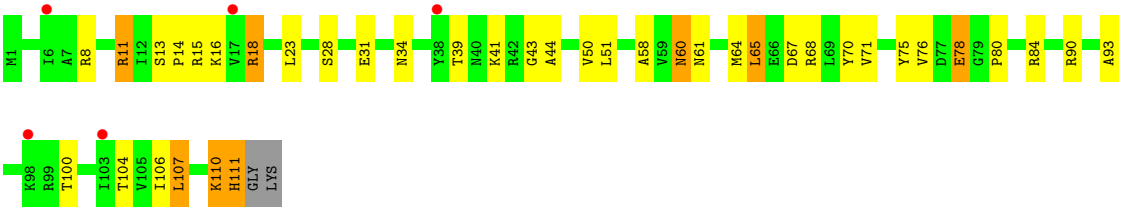
Chain E8:



• Molecule 44: 50S ribosomal protein L22

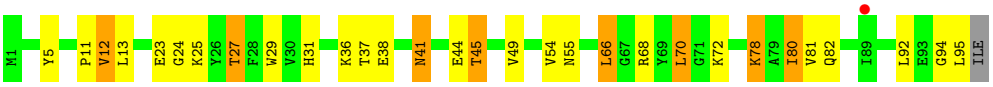
Chain A5:





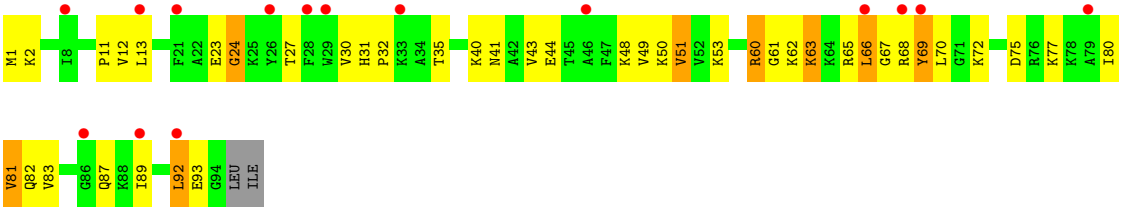
• Molecule 45: 50S ribosomal protein L23

Chain F8:



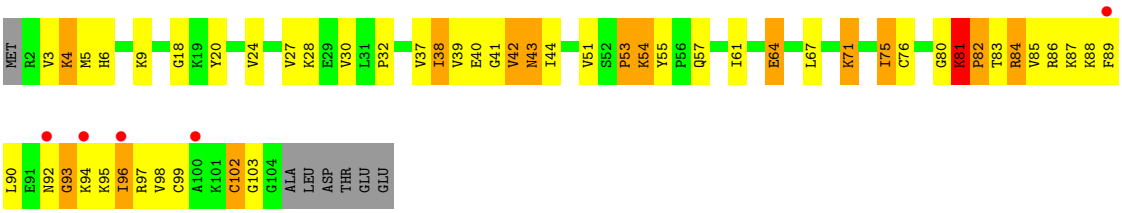
• Molecule 45: 50S ribosomal protein L23

Chain B5:



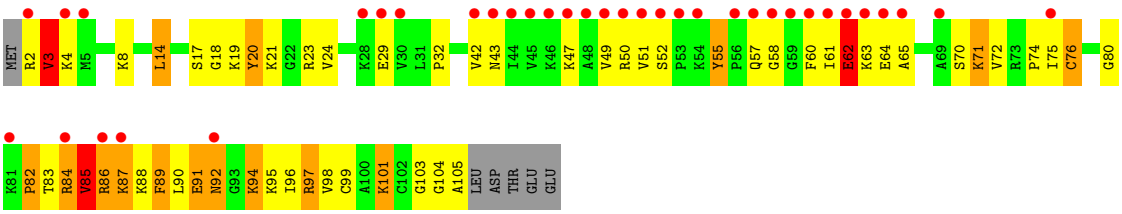
• Molecule 46: 50S ribosomal protein L24

Chain G8:



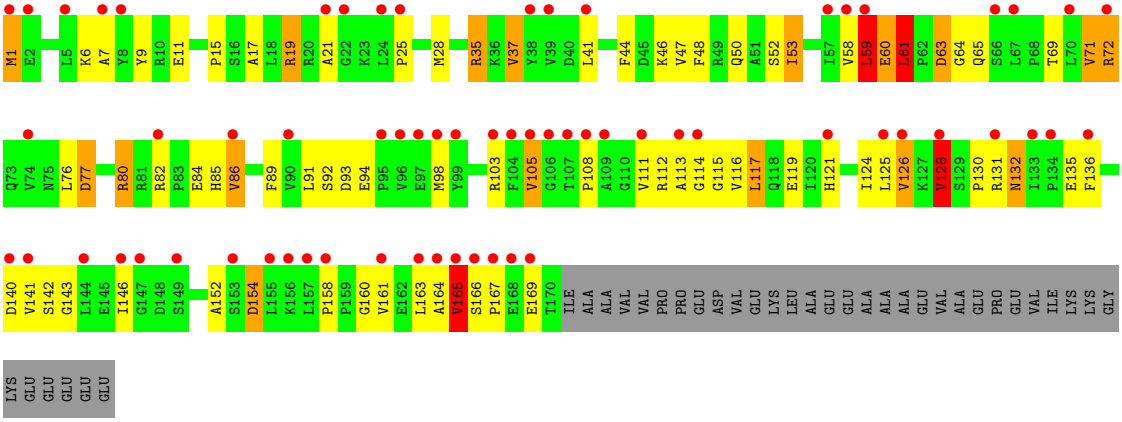
• Molecule 46: 50S ribosomal protein L24

Chain C5:



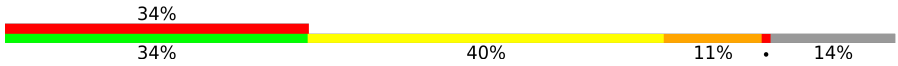
• Molecule 47: 50S ribosomal protein L25

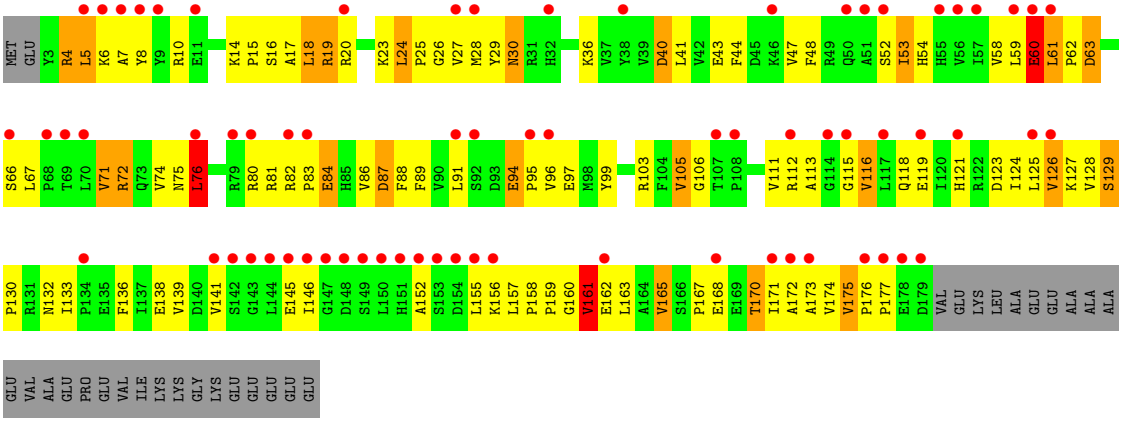
Chain H8:



• Molecule 47: 50S ribosomal protein L25

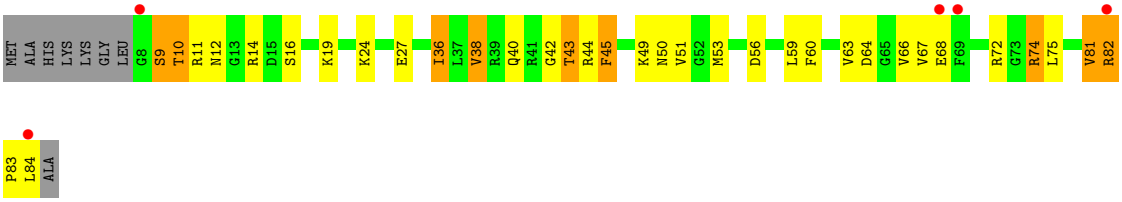
Chain D5:





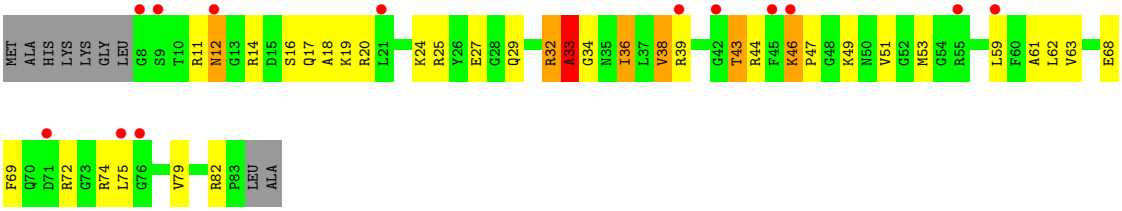
• Molecule 48: 50S ribosomal protein L27

Chain I8:



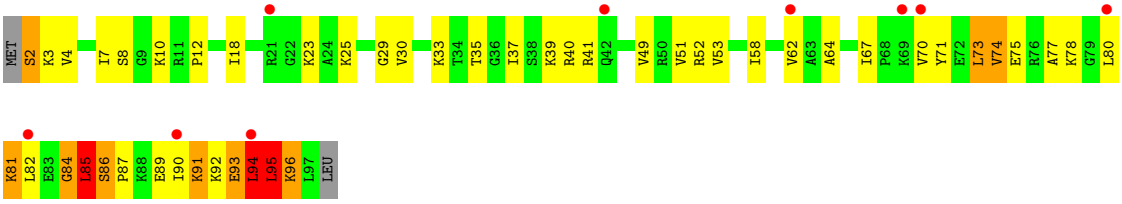
• Molecule 48: 50S ribosomal protein L27

Chain E5:



• Molecule 49: 50S ribosomal protein L28

Chain J8:

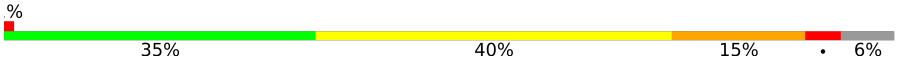


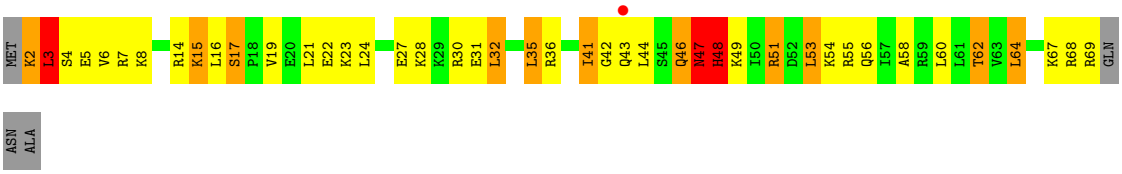
• Molecule 49: 50S ribosomal protein L28

Chain F5:

• Molecule 50: 50S ribosomal protein L29

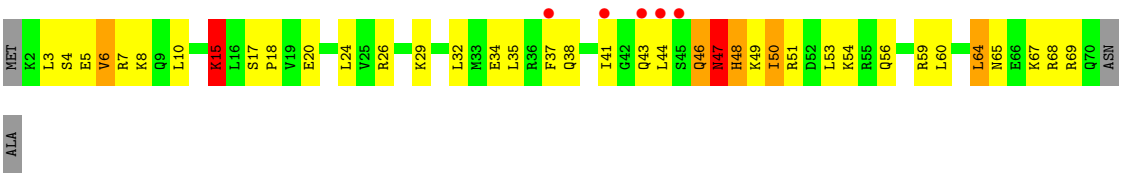
Chain K8:





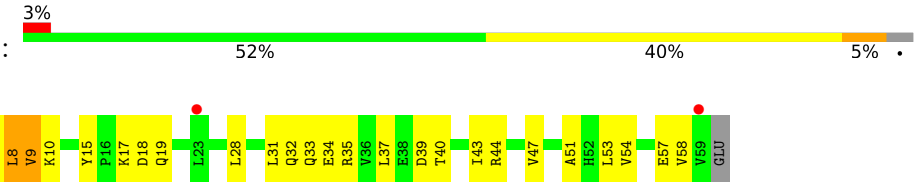
• Molecule 50: 50S ribosomal protein L29

Chain G5:



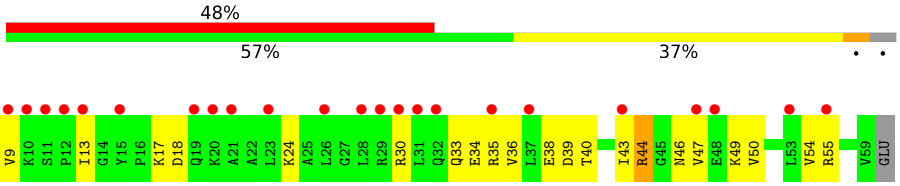
• Molecule 51: 50S ribosomal protein L30

Chain L8:



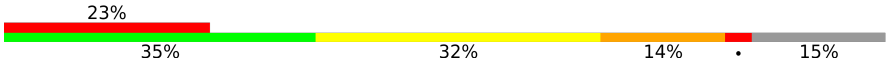
• Molecule 51: 50S ribosomal protein L30

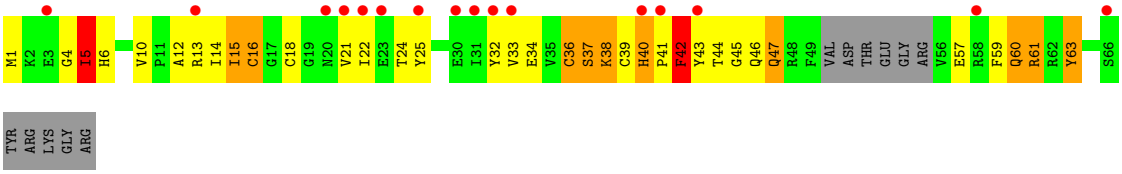
Chain H5:



• Molecule 52: 50S ribosomal protein L31

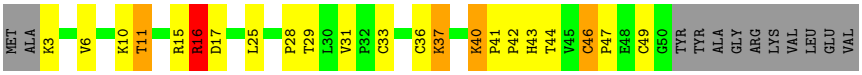
Chain M8:





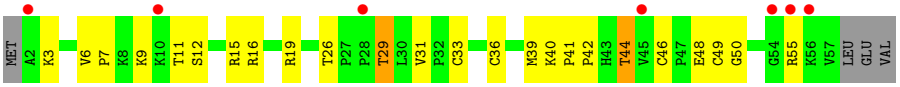
• Molecule 53: 50S ribosomal protein L32

Chain N8:



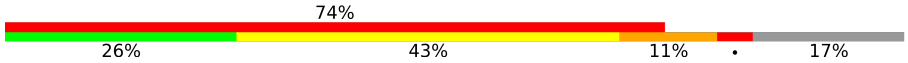
• Molecule 53: 50S ribosomal protein L32

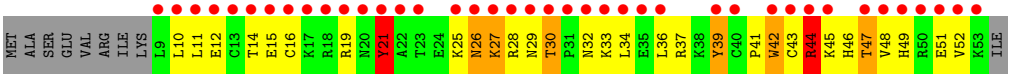
Chain J5:



• Molecule 54: 50S ribosomal protein L33

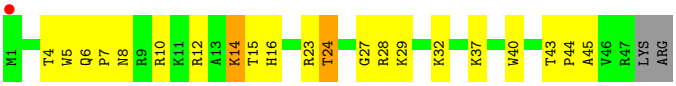
Chain O8:





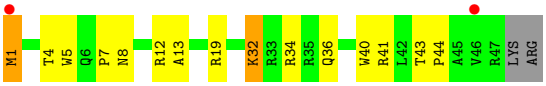
• Molecule 55: 50S ribosomal protein L34

Chain P8:



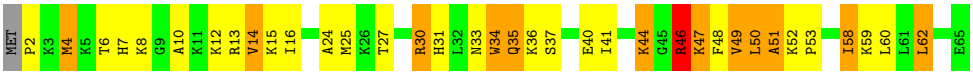
• Molecule 55: 50S ribosomal protein L34

Chain L5:



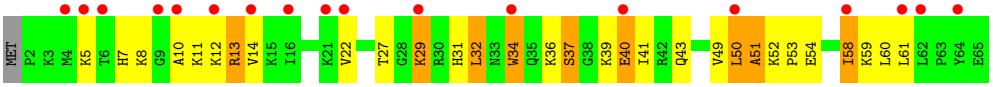
• Molecule 56: 50S ribosomal protein L35

Chain Q8:



• Molecule 56: 50S ribosomal protein L35

Chain M5:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.30Å 448.80Å 620.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 161.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (161.81-2.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.241 0.202 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.70	1/36068 (0.0%)	1.35	292/56287 (0.5%)
1	1G	0.61	0/36282	1.22	170/56623 (0.3%)
2	12	0.37	0/1727	0.61	1/2326 (0.0%)
2	1E	0.40	0/1908	0.63	2/2573 (0.1%)
3	22	0.43	1/1560 (0.1%)	0.56	0/2104
3	2E	0.47	1/1629 (0.1%)	0.62	1/2195 (0.0%)
4	32	0.45	1/1732 (0.1%)	0.64	0/2318
4	3E	0.48	1/1728 (0.1%)	0.62	1/2313 (0.0%)
5	42	0.38	0/1156	0.60	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.49	0/855	0.66	1/1154 (0.1%)
6	5E	0.46	0/850	0.61	0/1147
7	62	0.39	0/1122	0.61	0/1500
7	6E	0.39	0/1259	0.54	0/1686
8	72	0.37	0/1127	0.57	0/1517
8	7E	0.41	0/1135	0.64	1/1527 (0.1%)
9	82	0.36	0/971	0.62	0/1304
9	8E	0.39	0/1019	0.61	0/1367
10	1A	1.00	2/658 (0.3%)	0.56	0/885
10	1I	0.40	0/762	0.62	0/1027
11	2A	0.40	0/850	0.61	1/1150 (0.1%)
11	2I	0.47	0/838	0.65	0/1133
12	3A	0.44	0/963	0.66	1/1290 (0.1%)
12	3I	0.63	0/972	0.80	1/1301 (0.1%)
13	4A	0.35	0/889	0.59	0/1192
13	4I	0.50	0/943	0.67	0/1265
14	5A	0.34	0/495	0.65	0/657
14	5I	0.47	0/495	0.69	1/657 (0.2%)
15	6A	0.40	0/740	0.58	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.43	0/721	0.65	0/970
16	7I	0.43	0/716	0.68	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.51	0/836	0.65	0/1117
18	9A	0.46	0/549	0.67	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.67	0/700
19	AI	0.42	0/676	0.72	0/910
20	BA	0.35	0/764	0.67	1/1007 (0.1%)
20	BI	0.50	1/748 (0.1%)	0.63	0/986
21	1B	0.40	0/192	0.61	0/252
21	1F	0.42	0/203	0.71	0/266
22	1K	0.56	0/1589	1.11	6/2464 (0.2%)
23	2K	0.77	0/1721	1.42	16/2682 (0.6%)
23	2L	0.66	1/1721 (0.1%)	1.22	7/2682 (0.3%)
24	1L	0.39	0/1560	0.96	3/2418 (0.1%)
24	3K	0.52	0/1654	1.19	13/2570 (0.5%)
24	3L	0.52	0/1705	1.12	9/2650 (0.3%)
25	4K	0.74	0/473	1.15	0/735
25	4L	0.69	0/473	1.29	3/737 (0.4%)
26	14	0.84	45/68181 (0.1%)	1.54	1291/106432 (1.2%)
26	1H	1.01	117/68997 (0.2%)	1.75	2061/107696 (1.9%)
27	16	0.83	0/2928	1.57	59/4568 (1.3%)
27	1J	0.70	0/2928	1.37	32/4568 (0.7%)
28	71	0.29	0/1049	0.54	0/1417
29	11	0.66	1/2170 (0.0%)	0.90	4/2926 (0.1%)
29	19	0.64	1/2175 (0.0%)	0.85	2/2933 (0.1%)
30	21	0.57	0/1579	0.92	3/2131 (0.1%)
30	29	0.53	0/1596	0.80	3/2153 (0.1%)
31	31	0.63	1/1620 (0.1%)	0.90	3/2194 (0.1%)
31	39	0.51	0/1637	0.80	1/2218 (0.0%)
32	41	0.47	0/1481	0.68	0/1994
32	49	0.38	0/1483	0.63	1/1997 (0.1%)
33	51	0.53	0/1354	0.86	4/1833 (0.2%)
33	59	0.35	0/1320	0.69	3/1787 (0.2%)
34	61	0.41	0/1146	0.71	1/1551 (0.1%)
34	69	0.41	0/1146	0.70	1/1551 (0.1%)
35	15	0.41	0/1123	0.61	0/1515
35	58	0.52	0/1123	0.75	0/1514
36	25	0.48	0/942	0.71	1/1269 (0.1%)
36	68	0.55	0/942	0.76	2/1269 (0.2%)
37	35	0.53	0/1139	0.83	2/1514 (0.1%)
37	78	0.61	0/1139	1.04	8/1514 (0.5%)
38	45	0.61	2/1120 (0.2%)	0.81	0/1498
38	88	0.69	0/1138	0.92	1/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	55	0.51	0/981	0.83	0/1312
39	98	0.49	0/981	0.81	1/1312 (0.1%)
40	65	0.47	0/886	0.83	3/1180 (0.3%)
40	A8	0.59	0/891	0.83	2/1187 (0.2%)
41	75	0.51	0/1123	0.74	2/1500 (0.1%)
41	B8	0.58	0/1133	0.83	2/1514 (0.1%)
42	85	0.50	0/977	0.67	0/1301
42	C8	0.61	0/968	0.82	2/1289 (0.2%)
43	95	0.47	0/781	0.76	0/1048
43	D8	0.53	0/785	0.74	1/1052 (0.1%)
44	A5	0.55	0/897	0.77	1/1204 (0.1%)
44	E8	0.57	0/886	0.81	0/1189
45	B5	0.57	0/749	0.71	0/1007
45	F8	0.64	0/764	0.80	1/1025 (0.1%)
46	C5	0.52	0/807	0.81	1/1076 (0.1%)
46	G8	0.65	0/796	0.95	2/1062 (0.2%)
47	D5	0.54	1/1443 (0.1%)	0.64	1/1960 (0.1%)
47	H8	0.44	0/1395	0.73	1/1890 (0.1%)
48	E5	0.52	0/611	0.77	0/814
48	I8	0.76	1/619 (0.2%)	0.94	1/825 (0.1%)
49	F5	0.52	0/744	0.90	1/989 (0.1%)
49	J8	0.69	0/754	0.96	4/1003 (0.4%)
50	G5	0.53	0/578	0.73	0/766
50	K8	0.69	0/577	1.02	3/763 (0.4%)
51	H5	0.46	0/464	0.64	0/623
51	L8	0.50	0/464	0.73	0/623
52	M8	0.47	0/485	0.83	0/652
53	J5	0.58	0/448	0.76	0/606
53	N8	0.61	0/381	0.83	1/516 (0.2%)
54	O8	0.63	1/396 (0.3%)	0.90	1/529 (0.2%)
55	L5	0.57	0/409	0.78	0/540
55	P8	0.75	0/409	0.98	2/540 (0.4%)
56	M5	0.65	0/524	0.87	1/691 (0.1%)
56	Q8	0.69	0/524	1.02	3/691 (0.4%)
All	All	0.76	179/317928 (0.1%)	1.36	4051/476129 (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
2	12	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	2
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AA	0	2
19	AI	0	1
20	BA	0	2
29	11	0	5
29	19	0	3
30	21	0	8
30	29	0	5
31	39	0	7
32	41	0	1
32	49	0	2
33	51	0	5
33	59	0	1
34	61	0	3
34	69	0	4
35	58	0	1
37	35	0	2
37	78	0	6
38	45	0	2
38	88	0	4
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	2
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	2
43	D8	0	3
44	A5	0	1
45	B5	0	2
46	C5	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
46	G8	0	5
47	D5	0	3
47	H8	0	6
48	E5	0	2
48	I8	0	1
49	F5	0	1
49	J8	0	1
50	G5	0	2
50	K8	0	2
52	M8	0	3
54	O8	0	1
55	P8	0	1
56	M5	0	2
56	Q8	0	3
All	All	0	145

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1A	38	ILE	C-N	19.47	1.71	1.34
47	D5	94	GLU	C-N	14.46	1.61	1.34
10	1A	76	ASN	C-N	14.15	1.61	1.34
26	1H	774	A	N9-C4	-13.65	1.29	1.37
26	14	783	A	N9-C4	-12.02	1.30	1.37

The worst 5 of 4051 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-23.89	111.67	126.00
26	1H	945	A	C6-C5-N7	-20.89	117.67	132.30
26	1H	945	A	N1-C6-N6	20.76	131.05	118.60
26	1H	1899	G	N3-C4-C5	20.42	138.81	128.60
26	1H	2430	A	C2-N3-C4	-20.30	100.45	110.60

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	234	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	1E	236	TYR	Peptide
9	8E	4	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32223	0	16267	692	0
1	1G	32414	0	16360	752	0
2	12	1696	0	1730	89	0
2	1E	1874	0	1926	95	0
3	22	1537	0	1603	84	0
3	2E	1605	0	1668	54	0
4	32	1702	0	1765	93	0
4	3E	1698	0	1759	84	0
5	42	1141	0	1199	40	0
5	4E	1142	0	1204	40	0
6	52	842	0	857	19	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	53	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	62	0
9	8E	1000	0	1031	63	0
10	1A	646	0	662	45	0
10	1I	749	0	767	42	0
11	2A	835	0	847	25	0
11	2I	823	0	833	29	0
12	3A	947	0	1033	45	0
12	3I	956	0	1046	35	0
13	4A	879	0	935	46	0
13	4I	933	0	992	57	0
14	5A	486	0	525	35	0
14	5I	486	0	524	29	0
15	6A	729	0	768	26	0
15	6I	729	0	768	23	0
16	7A	705	0	725	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7I	700	0	720	45	0
17	8A	823	0	891	22	0
17	8I	823	0	891	34	0
18	9A	544	0	605	19	0
18	9I	549	0	607	21	0
19	AA	510	0	507	21	0
19	AI	661	0	683	43	0
20	BA	762	0	861	43	0
20	BI	746	0	843	44	0
21	1B	188	0	195	8	0
21	1F	199	0	208	9	0
22	1K	1542	0	790	25	0
23	2K	1646	0	845	18	0
23	2L	1646	0	845	25	0
24	1L	1401	0	713	22	0
24	3K	1483	0	756	50	0
24	3L	1528	0	778	42	0
25	4K	420	0	209	7	0
25	4L	419	0	208	17	0
26	14	60877	0	30690	1171	0
26	1H	61609	0	31058	1189	0
27	16	2617	0	1328	50	0
27	1J	2617	0	1328	76	0
28	71	1027	0	1043	57	0
29	11	2120	0	2197	100	0
29	19	2125	0	2199	105	0
30	21	1546	0	1602	86	0
30	29	1563	0	1629	93	0
31	31	1585	0	1632	70	0
31	39	1602	0	1649	88	0
32	41	1457	0	1514	68	0
32	49	1459	0	1507	65	0
33	51	1328	0	1396	64	0
33	59	1295	0	1366	58	0
34	61	1131	0	1218	36	0
34	69	1131	0	1218	49	0
35	15	1096	0	1168	47	0
35	58	1096	0	1169	48	0
36	25	932	0	996	46	0
36	68	932	0	996	41	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	45	1099	0	1154	73	0
38	88	1117	0	1168	58	0
39	55	967	0	1033	42	0
39	98	967	0	1033	45	0
40	65	876	0	938	63	0
40	A8	881	0	943	54	0
41	75	1109	0	1170	61	0
41	B8	1119	0	1177	72	0
42	85	959	0	1019	40	0
42	C8	950	0	1011	58	0
43	95	770	0	838	32	0
43	D8	774	0	849	40	0
44	A5	886	0	948	23	0
44	E8	876	0	941	30	0
45	B5	735	0	785	30	0
45	F8	750	0	814	19	0
46	C5	794	0	885	52	0
46	G8	783	0	869	49	0
47	D5	1411	0	1436	82	0
47	H8	1365	0	1391	57	0
48	E5	603	0	620	33	0
48	I8	611	0	631	34	0
49	F5	737	0	813	32	0
49	J8	747	0	817	42	0
50	G5	576	0	625	27	0
50	K8	575	0	634	42	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	475	0	465	34	0
53	J5	434	0	454	22	0
53	N8	369	0	388	21	0
54	O8	389	0	404	26	0
55	L5	401	0	436	10	0
55	P8	401	0	436	11	0
56	M5	516	0	582	25	0
56	Q8	516	0	582	37	0
57	13	140	0	0	0	0
57	14	435	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	102	0	0	0	0
57	1H	525	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1J	8	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	31	2	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	2	0	0	0	0
57	4I	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	2	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	43	0	0
58	1G	42	0	45	1	0
59	32	8	0	0	3	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	14	26	0	45	8	0
61	1G	13	0	24	0	0
62	11	17	0	0	4	0
62	13	320	0	0	12	0
62	14	1144	0	0	65	0
62	15	1	0	0	0	0
62	16	12	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	19	15	0	0	3	0
62	1A	1	0	0	0	0
62	1F	1	0	0	0	0
62	1G	317	0	0	21	0
62	1H	1470	0	0	90	0
62	1I	2	0	0	0	0
62	1J	12	0	0	1	0
62	1K	2	0	0	0	0
62	21	7	0	0	1	0
62	25	6	0	0	0	0
62	29	4	0	0	0	0
62	2K	8	0	0	1	0
62	2L	6	0	0	0	0
62	31	5	0	0	0	0
62	32	1	0	0	0	0
62	35	8	0	0	1	0
62	39	5	0	0	1	0
62	3I	2	0	0	0	0
62	41	1	0	0	0	0
62	4E	3	0	0	0	0
62	4K	5	0	0	0	0
62	4L	6	0	0	0	0
62	52	4	0	0	0	0
62	55	3	0	0	0	0
62	58	2	0	0	0	0
62	5I	2	0	0	0	0
62	6A	2	0	0	0	0
62	6I	3	0	0	0	0
62	78	10	0	0	0	0
62	7A	5	0	0	0	0
62	7I	1	0	0	0	0
62	85	2	0	0	0	0
62	8E	2	0	0	0	0
62	9A	2	0	0	0	0
62	A5	1	0	0	0	0
62	B5	1	0	0	0	0
62	B8	1	0	0	0	0
62	BA	2	0	0	0	0
62	BI	2	0	0	1	0
62	C5	3	0	0	0	0
62	C8	3	0	0	0	0
62	F5	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	F8	2	0	0	0	0
62	G8	2	0	0	0	0
62	H5	2	0	0	1	0
62	I8	6	0	0	1	0
62	J8	4	0	0	0	0
62	L8	3	0	0	1	0
62	M5	9	0	0	1	0
62	P8	1	0	0	0	0
62	Q8	5	0	0	2	0
All	All	297444	0	197360	7486	0

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 16.

The worst 5 of 7486 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.44
38:45:27:VAL:HB	38:45:28:ALA:HA	1.19	1.13
29:11:182:LEU:H	29:11:272:ALA:HB3	1.23	1.02
37:78:63:PRO:HB2	56:Q8:30:ARG:HH21	1.23	1.01
26:1H:1496:A:H8	26:1H:1577:C:HO2'	1.00	0.99

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	203/256 (79%)	173 (85%)	25 (12%)	5 (2%)	5 28
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12 45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	191/239 (80%)	171 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	32	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	29	68
4	3E	205/209 (98%)	192 (94%)	12 (6%)	1 (0%)	29	68
5	42	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	22	60
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22	60
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	42
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	60
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	19	57
9	8E	124/128 (97%)	108 (87%)	16 (13%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	85 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	8	37
11	2I	109/129 (84%)	94 (86%)	12 (11%)	3 (3%)	5	25
12	3A	119/132 (90%)	100 (84%)	15 (13%)	4 (3%)	3	20
12	3I	120/132 (91%)	107 (89%)	12 (10%)	1 (1%)	19	57
13	4A	107/126 (85%)	88 (82%)	18 (17%)	1 (1%)	17	55
13	4I	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	17	55
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	37
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	20
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	53
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9I	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	42
19	AA	59/93 (63%)	49 (83%)	8 (14%)	2 (3%)	3	20
19	AI	80/93 (86%)	68 (85%)	9 (11%)	3 (4%)	3	18
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	15	53
20	BI	95/106 (90%)	84 (88%)	10 (10%)	1 (1%)	14	50
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	128/229 (56%)	120 (94%)	8 (6%)	0	100	100
29	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	37
29	19	272/276 (99%)	246 (90%)	23 (8%)	3 (1%)	14	50
30	21	201/206 (98%)	158 (79%)	33 (16%)	10 (5%)	2	12
30	29	202/206 (98%)	149 (74%)	42 (21%)	11 (5%)	2	11
31	31	200/210 (95%)	181 (90%)	17 (8%)	2 (1%)	15	53
31	39	202/210 (96%)	162 (80%)	34 (17%)	6 (3%)	4	24
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	9	39
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	25	64
33	51	172/180 (96%)	141 (82%)	20 (12%)	11 (6%)	1	7
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	3	19
34	61	143/148 (97%)	122 (85%)	19 (13%)	2 (1%)	11	43
34	69	143/148 (97%)	111 (78%)	29 (20%)	3 (2%)	7	33
35	15	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
35	58	135/140 (96%)	114 (84%)	17 (13%)	4 (3%)	4	24
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	119 (82%)	26 (18%)	0	100	100
37	78	145/150 (97%)	114 (79%)	22 (15%)	9 (6%)	1	8
38	45	136/141 (96%)	115 (85%)	19 (14%)	2 (2%)	10	42
38	88	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	3	19
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	55
39	98	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	17	55
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	5	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	117 (89%)	12 (9%)	2 (2%)	10	42
41	B8	133/146 (91%)	118 (89%)	15 (11%)	0	100	100
42	85	114/118 (97%)	104 (91%)	9 (8%)	1 (1%)	17	55
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	26
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	4	23
43	D8	98/101 (97%)	88 (90%)	6 (6%)	4 (4%)	3	16
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	17	55
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	6	31
45	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	6
46	G8	101/110 (92%)	81 (80%)	16 (16%)	4 (4%)	3	17
47	D5	175/206 (85%)	136 (78%)	31 (18%)	8 (5%)	2	14
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	16
48	E5	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	5	26
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	45
49	F5	92/98 (94%)	79 (86%)	12 (13%)	1 (1%)	14	50
49	J8	94/98 (96%)	83 (88%)	9 (10%)	2 (2%)	7	33
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	4	24
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	14
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	40 (71%)	15 (27%)	1 (2%)	8	37
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	O8	43/54 (80%)	30 (70%)	12 (28%)	1 (2%)	6	30
55	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
56	M5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	9	40
56	Q8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11128/12158 (92%)	9762 (88%)	1180 (11%)	186 (2%)	9 39

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
30	21	83	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	12	179/220 (81%)	143 (80%)	36 (20%)	1 6
2	1E	200/220 (91%)	154 (77%)	46 (23%)	1 4
3	22	154/188 (82%)	128 (83%)	26 (17%)	2 11
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2 10
4	32	180/181 (99%)	151 (84%)	29 (16%)	2 12
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1 8
5	42	114/123 (93%)	87 (76%)	27 (24%)	1 3
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1 8
6	52	90/90 (100%)	74 (82%)	16 (18%)	2 9
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6 25
7	62	114/127 (90%)	88 (77%)	26 (23%)	1 4
7	6E	125/127 (98%)	105 (84%)	20 (16%)	2 12
8	72	118/119 (99%)	101 (86%)	17 (14%)	3 15
8	7E	119/119 (100%)	99 (83%)	20 (17%)	2 11
9	82	92/99 (93%)	73 (79%)	19 (21%)	1 6
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	2
10	1I	81/92 (88%)	73 (90%)	8 (10%)	8	30
11	2A	85/99 (86%)	67 (79%)	18 (21%)	1	5
11	2I	84/99 (85%)	70 (83%)	14 (17%)	2	11
12	3A	102/109 (94%)	79 (78%)	23 (22%)	1	4
12	3I	103/109 (94%)	91 (88%)	12 (12%)	5	22
13	4A	90/101 (89%)	68 (76%)	22 (24%)	0	3
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	29
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	7A	72/74 (97%)	61 (85%)	11 (15%)	2	13
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	19
17	8I	94/97 (97%)	82 (87%)	12 (13%)	4	19
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	8
18	9I	58/77 (75%)	49 (84%)	9 (16%)	2	13
19	AA	56/80 (70%)	47 (84%)	9 (16%)	2	12
19	AI	72/80 (90%)	61 (85%)	11 (15%)	2	13
20	BA	76/82 (93%)	66 (87%)	10 (13%)	4	18
20	BI	75/82 (92%)	61 (81%)	14 (19%)	1	8
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	71	108/181 (60%)	87 (81%)	21 (19%)	1	7
29	11	214/218 (98%)	173 (81%)	41 (19%)	1	8
29	19	214/218 (98%)	171 (80%)	43 (20%)	1	6
30	21	162/166 (98%)	118 (73%)	44 (27%)	0	2
30	29	165/166 (99%)	135 (82%)	30 (18%)	1	9
31	31	161/166 (97%)	128 (80%)	33 (20%)	1	6
31	39	163/166 (98%)	126 (77%)	37 (23%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	126 (82%)	27 (18%)	2	10
32	49	152/156 (97%)	125 (82%)	27 (18%)	2	9
33	51	143/148 (97%)	106 (74%)	37 (26%)	0	2
33	59	140/148 (95%)	106 (76%)	34 (24%)	0	3
34	61	122/124 (98%)	86 (70%)	36 (30%)	0	1
34	69	122/124 (98%)	89 (73%)	33 (27%)	0	2
35	15	116/119 (98%)	90 (78%)	26 (22%)	1	4
35	58	116/119 (98%)	87 (75%)	29 (25%)	0	3
36	25	100/100 (100%)	76 (76%)	24 (24%)	0	3
36	68	100/100 (100%)	90 (90%)	10 (10%)	7	29
37	35	114/116 (98%)	82 (72%)	32 (28%)	0	2
37	78	114/116 (98%)	78 (68%)	36 (32%)	0	1
38	45	109/111 (98%)	88 (81%)	21 (19%)	1	8
38	88	110/111 (99%)	90 (82%)	20 (18%)	1	9
39	55	101/101 (100%)	80 (79%)	21 (21%)	1	5
39	98	101/101 (100%)	72 (71%)	29 (29%)	0	2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	A8	87/88 (99%)	66 (76%)	21 (24%)	0	3
41	75	117/127 (92%)	95 (81%)	22 (19%)	1	8
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0	2
42	85	93/94 (99%)	73 (78%)	20 (22%)	1	5
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10
43	95	81/82 (99%)	68 (84%)	13 (16%)	2	12
43	D8	82/82 (100%)	63 (77%)	19 (23%)	1	4
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	8
44	E8	90/92 (98%)	73 (81%)	17 (19%)	1	8
45	B5	74/78 (95%)	56 (76%)	18 (24%)	0	3
45	F8	77/78 (99%)	64 (83%)	13 (17%)	2	11
46	C5	85/91 (93%)	63 (74%)	22 (26%)	0	2
46	G8	84/91 (92%)	66 (79%)	18 (21%)	1	5
47	D5	156/179 (87%)	124 (80%)	32 (20%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	H8	151/179 (84%)	124 (82%)	27 (18%)	2 9
48	E5	61/67 (91%)	55 (90%)	6 (10%)	8 30
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3 15
49	F5	79/83 (95%)	63 (80%)	16 (20%)	1 6
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3 14
50	G5	63/67 (94%)	46 (73%)	17 (27%)	0 2
50	K8	64/67 (96%)	43 (67%)	21 (33%)	0 1
51	H5	50/52 (96%)	38 (76%)	12 (24%)	0 3
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1 7
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0 2
53	J5	48/52 (92%)	41 (85%)	7 (15%)	3 15
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1 5
54	O8	44/52 (85%)	29 (66%)	15 (34%)	0 1
55	L5	38/42 (90%)	32 (84%)	6 (16%)	2 12
55	P8	38/42 (90%)	31 (82%)	7 (18%)	1 9
56	M5	54/55 (98%)	43 (80%)	11 (20%)	1 6
56	Q8	54/55 (98%)	44 (82%)	10 (18%)	1 8
All	All	9397/10064 (93%)	7493 (80%)	1904 (20%)	1 6

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	L8	58	VAL
45	B5	82	GLN
8	72	41	ARG
44	A5	107	LEU
55	L5	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
18	9A	36	ASN
29	19	227	ASN
51	H5	33	GLN
40	65	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	G5	47	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	331 (22%)	33 (2%)
1	1G	1506/1522 (98%)	352 (23%)	33 (2%)
22	1K	68/76 (89%)	27 (39%)	4 (5%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	15 (19%)	2 (2%)
24	1L	61/76 (80%)	24 (39%)	2 (3%)
24	3K	67/76 (88%)	37 (55%)	2 (2%)
24	3L	69/76 (90%)	30 (43%)	2 (2%)
25	4K	17/30 (56%)	9 (52%)	1 (5%)
25	4L	18/30 (60%)	12 (66%)	1 (5%)
26	14	2821/2917 (96%)	675 (23%)	42 (1%)
26	1H	2850/2917 (97%)	630 (22%)	52 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	32 (26%)	3 (2%)
All	All	9368/9640 (97%)	2219 (23%)	180 (1%)

5 of 2219 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G

5 of 180 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	992	U
26	14	503	A
1	1G	1145	C
23	2L	33	OMC
26	14	960	A

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

15 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	7MG	2K	47	23	22,26,27	2.88	7 (31%)	29,39,42	2.89	10 (34%)
23	PSU	2K	56	23	18,21,22	1.32	2 (11%)	22,30,33	1.79	3 (13%)
23	4SU	2L	8	23	18,21,22	1.95	4 (22%)	26,30,33	2.36	5 (19%)
23	PSU	2L	56	23	18,21,22	1.25	2 (11%)	22,30,33	1.45	2 (9%)
22	U8U	1K	34	25,22	19,24,25	2.61	7 (36%)	23,34,37	1.18	2 (8%)
22	T6A	1K	37	22	27,34,35	2.48	5 (18%)	29,49,52	2.41	7 (24%)
23	4SU	2K	8	23	18,21,22	1.66	3 (16%)	26,30,33	2.38	4 (15%)
23	5MU	2L	55	23	19,22,23	4.00	5 (26%)	28,32,35	3.11	8 (28%)
23	5MU	2K	55	23	19,22,23	3.89	5 (26%)	28,32,35	3.15	9 (32%)
23	7MG	2L	47	23	22,26,27	3.01	8 (36%)	29,39,42	2.86	10 (34%)
22	5MU	1K	54	22	19,22,23	3.94	5 (26%)	28,32,35	2.92	7 (25%)
23	OMC	2L	33	23	19,22,23	1.78	4 (21%)	26,31,34	1.26	2 (7%)
22	PSU	1K	39	22	18,21,22	1.02	1 (5%)	22,30,33	1.53	4 (18%)
22	PSU	1K	55	22	18,21,22	1.28	1 (5%)	22,30,33	1.56	4 (18%)
23	OMC	2K	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.03	2 (7%)

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	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	3/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	0/9/28/29	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	T6A	1K	37	22	-	6/19/41/42	0/3/3/3
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.89	1.59	1.38
22	1K	54	5MU	C2-N1	12.63	1.58	1.38
23	2K	55	5MU	C2-N1	12.52	1.58	1.38
23	2L	47	7MG	C5-N7	8.90	1.45	1.35
23	2K	47	7MG	C5-N7	8.03	1.44	1.35

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2L	55	5MU	C5-C4-N3	9.89	123.75	115.31
23	2K	55	5MU	C5-C4-N3	9.69	123.58	115.31
22	1K	54	5MU	C5-C4-N3	9.41	123.34	115.31
23	2L	8	4SU	C4-N3-C2	-8.13	119.44	127.34
23	2K	8	4SU	C4-N3-C2	-7.63	119.93	127.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2K	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1269 ligands modelled in this entry, 1262 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
61	SPE	14	3437	26	12,12,12	0.83	0	11,11,11	0.96	1 (9%)
58	PAR	13	1741	1	45,45,45	0.68	0	64,67,67	1.48	10 (15%)
59	SF4	32	302	4	0,12,12	-	-	-		
59	SF4	3E	301	4	0,12,12	-	-	-		
61	SPE	1G	1703	-	12,12,12	0.35	0	11,11,11	0.76	0
58	PAR	1G	1702	-	45,45,45	0.67	1 (2%)	64,67,67	1.39	9 (14%)
61	SPE	14	3436	-	12,12,12	0.43	0	11,11,11	0.65	0

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
61	SPE	14	3437	26	-	5/10/10/10	-
58	PAR	13	1741	1	-	5/18/94/94	0/4/4/4
59	SF4	32	302	4	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5
61	SPE	1G	1703	-	-	3/10/10/10	-
58	PAR	1G	1702	-	-	1/18/94/94	0/4/4/4
61	SPE	14	3436	-	-	5/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.22	1.43	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	13	1741	PAR	C32-C22-C12	3.69	118.76	111.18
58	13	1741	PAR	C11-O51-C51	3.65	120.85	113.69
58	1G	1702	PAR	C14-O33-C33	-3.57	109.14	117.96
58	13	1741	PAR	C22-C12-C62	3.28	115.00	110.04
58	1G	1702	PAR	C13-O52-C52	-3.28	109.84	117.96

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	13	1741	PAR	C44-C54-C64-N64
58	13	1741	PAR	O54-C54-C64-N64
61	1G	1703	SPE	C2-C3-C4-N5
61	14	3437	SPE	C6-C7-C8-N9
61	14	3437	SPE	N9-C10-C11-C12

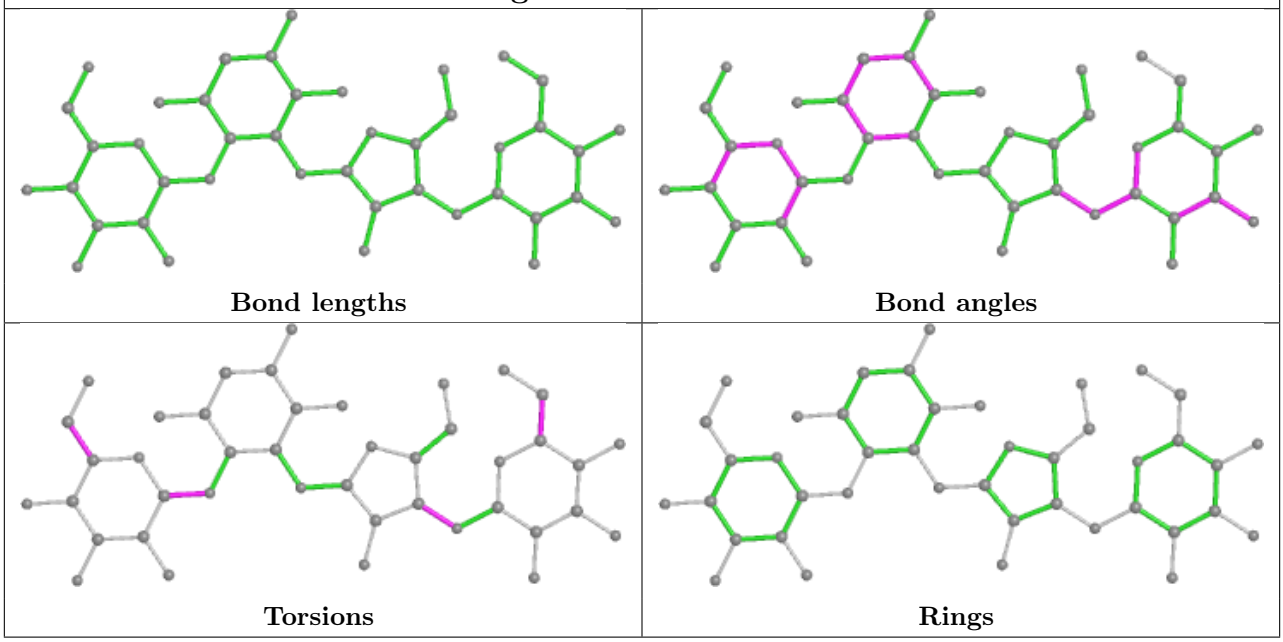
There are no ring outliers.

5 monomers are involved in 13 short contacts:

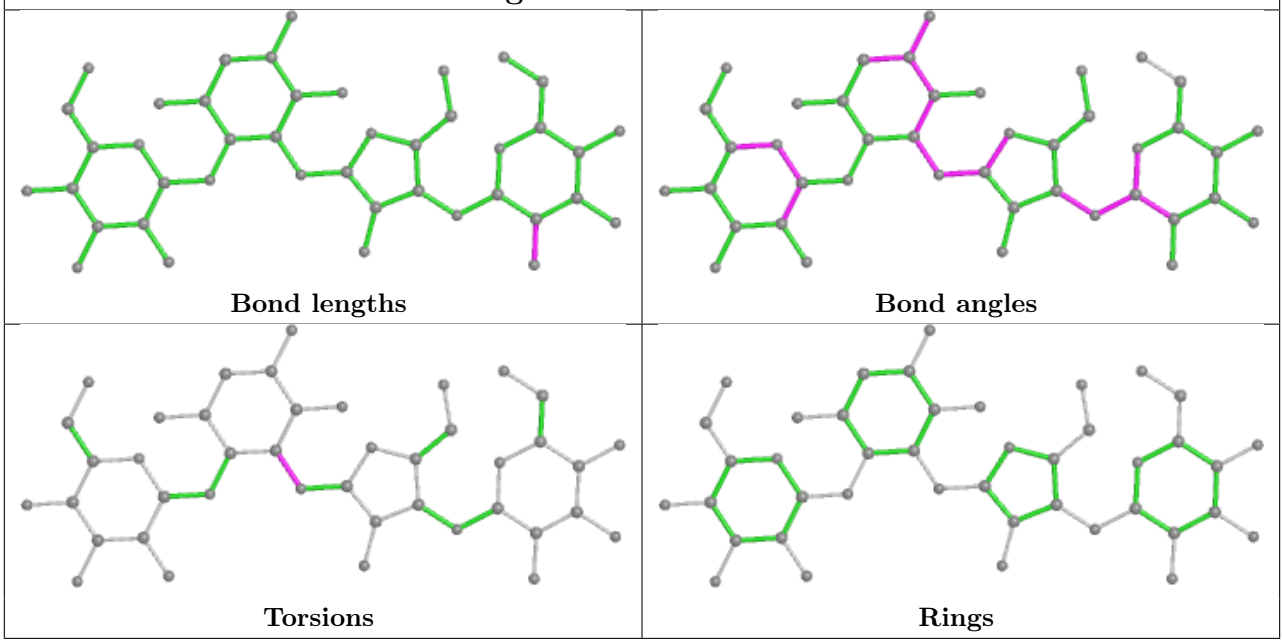
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	14	3437	SPE	6	0
59	32	302	SF4	3	0
59	3E	301	SF4	1	0
58	1G	1702	PAR	1	0
61	14	3436	SPE	2	0

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 then 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.

Ligand PAR 13 1741



Ligand PAR 1G 1702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	1A	2
26	1H	1
24	1L	1
47	D5	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13	1499/1522 (98%)	-0.23	1 (0%)	95	89	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.17	10 (0%)	87	69	71, 119, 192, 267	0
2	12	207/256 (80%)	0.75	26 (12%)	3	1	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.24	12 (5%)	27	10	112, 143, 169, 174	0
3	22	195/239 (81%)	1.21	50 (25%)	0	0	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.67	22 (10%)	6	2	88, 111, 143, 151	0
4	32	208/209 (99%)	0.66	14 (6%)	17	5	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.31	12 (5%)	23	7	84, 108, 132, 144	0
5	42	150/162 (92%)	0.49	11 (7%)	15	4	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.30	4 (2%)	54	26	82, 103, 121, 131	0
6	52	101/101 (100%)	0.02	0	100	100	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.52	7 (7%)	16	5	85, 105, 120, 132	0
7	62	138/156 (88%)	1.18	33 (23%)	0	0	116, 130, 141, 147	0
7	6E	154/156 (98%)	1.23	36 (23%)	0	0	102, 120, 150, 171	0
8	72	137/138 (99%)	0.73	15 (10%)	5	2	100, 131, 142, 149	0
8	7E	138/138 (100%)	1.07	29 (21%)	1	0	93, 110, 122, 134	0
9	82	121/128 (94%)	1.87	50 (41%)	0	0	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.24	5 (3%)	38	15	87, 138, 157, 163	0
10	1A	80/105 (76%)	1.02	22 (27%)	0	0	133, 156, 169, 174	0
10	1I	94/105 (89%)	1.42	28 (29%)	0	0	81, 131, 168, 173	0
11	2A	113/129 (87%)	1.33	27 (23%)	0	0	84, 109, 124, 135	0
11	2I	111/129 (86%)	1.14	25 (22%)	0	0	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.72	45 (37%)	0	0	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.72	15 (12%)	4	1	66, 76, 102, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	109/126 (86%)	0.85	26 (23%) 0 0	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.32	4 (3%) 45 19	88, 116, 131, 138	0
14	5A	59/61 (96%)	3.90	41 (69%) 0 0	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.83	8 (13%) 3 1	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.13	3 (3%) 45 19	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.35	3 (3%) 45 19	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.26	2 (2%) 59 30	92, 105, 129, 155	0
16	7I	83/88 (94%)	1.13	20 (24%) 0 0	96, 111, 137, 155	0
17	8A	99/105 (94%)	1.30	27 (27%) 0 0	97, 113, 130, 135	0
17	8I	99/105 (94%)	1.10	18 (18%) 1 0	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.35	4 (5%) 21 7	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.20	2 (2%) 51 23	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.17	13 (20%) 1 0	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.24	3 (3%) 41 17	96, 117, 138, 151	0
20	BA	99/106 (93%)	1.15	18 (18%) 1 0	90, 114, 140, 152	0
20	BI	97/106 (91%)	1.37	27 (27%) 0 0	106, 119, 145, 151	0
21	1B	22/27 (81%)	1.72	8 (36%) 0 0	127, 141, 145, 148	0
21	1F	23/27 (85%)	0.24	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	0.54	5 (7%) 14 4	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.03	1 (1%) 75 49	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.07	0 100 100	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.06	11 (16%) 1 0	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.91	10 (14%) 2 1	76, 229, 251, 253	0
24	3L	72/76 (94%)	0.16	3 (4%) 36 14	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.97	4 (21%) 1 0	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.35	3 (15%) 2 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.06	17 (0%) 89 72	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.10	7 (0%) 95 87	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.35	1 (0%) 86 65	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.45	0 100 100	85, 119, 145, 205	0
28	71	132/229 (57%)	0.80	20 (15%) 2 1	146, 210, 235, 243	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
29	11	273/276 (98%)	0.46	5 (1%)	68	40	41, 63, 79, 93	0
29	19	274/276 (99%)	0.59	7 (2%)	56	27	47, 73, 88, 107	0
30	21	203/206 (98%)	0.63	10 (4%)	29	11	48, 84, 120, 130	0
30	29	204/206 (99%)	1.03	39 (19%)	1	0	60, 95, 134, 149	0
31	31	202/210 (96%)	0.63	9 (4%)	33	12	46, 76, 112, 127	0
31	39	204/210 (97%)	0.56	14 (6%)	16	5	57, 101, 148, 177	0
32	41	179/182 (98%)	0.77	21 (11%)	4	1	79, 100, 134, 146	0
32	49	180/182 (98%)	1.22	48 (26%)	0	0	117, 138, 156, 174	0
33	51	174/180 (96%)	0.30	4 (2%)	60	31	77, 102, 119, 130	0
33	59	169/180 (93%)	2.48	92 (54%)	0	0	152, 196, 220, 233	0
34	61	145/148 (97%)	0.52	17 (11%)	4	1	76, 131, 149, 157	0
34	69	145/148 (97%)	0.46	12 (8%)	11	3	86, 122, 149, 156	0
35	15	137/140 (97%)	1.16	25 (18%)	1	0	81, 108, 135, 151	0
35	58	137/140 (97%)	0.86	18 (13%)	3	1	63, 85, 121, 138	0
36	25	122/122 (100%)	0.91	14 (11%)	4	1	69, 88, 105, 117	0
36	68	122/122 (100%)	0.39	3 (2%)	57	29	56, 72, 90, 99	0
37	35	147/150 (98%)	0.86	21 (14%)	2	1	58, 102, 135, 152	0
37	78	147/150 (98%)	0.57	10 (6%)	17	5	47, 80, 104, 115	0
38	45	138/141 (97%)	0.95	27 (19%)	1	0	76, 105, 124, 155	0
38	88	141/141 (100%)	0.71	10 (7%)	16	5	54, 75, 95, 123	0
39	55	118/118 (100%)	0.60	7 (5%)	22	7	65, 80, 97, 112	0
39	98	118/118 (100%)	0.81	12 (10%)	6	2	60, 78, 94, 106	0
40	65	110/112 (98%)	1.06	22 (20%)	1	0	89, 112, 132, 137	0
40	A8	111/112 (99%)	1.09	18 (16%)	1	0	72, 85, 105, 116	0
41	75	133/146 (91%)	0.40	7 (5%)	26	10	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.14	5 (3%)	41	17	67, 84, 128, 139	0
42	85	116/118 (98%)	0.54	4 (3%)	45	19	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.31	3 (2%)	56	27	53, 77, 102, 108	0
43	95	100/101 (99%)	1.08	22 (22%)	0	0	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.89	15 (15%)	2	1	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.79	5 (4%)	33	12	57, 75, 101, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	E8	110/113 (97%)	0.49	8 (7%) 15 4	53, 70, 94, 106	0
45	B5	94/96 (97%)	1.09	15 (15%) 1 1	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.21	1 (1%) 80 56	49, 66, 97, 110	0
46	C5	104/110 (94%)	2.12	36 (34%) 0 0	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.26	5 (4%) 29 11	73, 95, 122, 130	0
47	D5	177/206 (85%)	1.81	70 (39%) 0 0	108, 148, 226, 236	0
47	H8	170/206 (82%)	1.81	65 (38%) 0 0	80, 116, 202, 210	0
48	E5	76/85 (89%)	1.15	13 (17%) 1 0	66, 88, 102, 115	0
48	I8	77/85 (90%)	0.58	5 (6%) 18 5	54, 69, 91, 102	0
49	F5	94/98 (95%)	1.21	18 (19%) 1 0	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.85	9 (9%) 8 3	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.44	5 (7%) 15 4	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.12	1 (1%) 73 46	59, 79, 96, 120	0
51	H5	58/60 (96%)	2.04	29 (50%) 0 0	77, 99, 122, 135	0
51	L8	58/60 (96%)	0.54	2 (3%) 45 19	60, 77, 103, 110	0
52	M8	60/71 (84%)	1.54	16 (26%) 0 0	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.72	7 (12%) 3 1	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.36	0 100 100	46, 78, 119, 127	0
54	O8	45/54 (83%)	4.57	40 (88%) 0 0	117, 153, 171, 177	0
55	L5	47/49 (95%)	0.47	2 (4%) 35 13	47, 60, 87, 97	0
55	P8	47/49 (95%)	0.09	1 (2%) 63 34	42, 50, 72, 87	0
56	M5	64/65 (98%)	1.47	18 (28%) 0 0	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.36	0 100 100	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.42	1700 (8%) 11 3	40, 99, 184, 267	0

The worst 5 of 1700 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	C5	59	GLY	14.7
14	5A	38	GLY	12.9
33	59	96	ALA	12.6
46	C5	49	VAL	12.1
52	M8	40	HIS	11.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
22	PSU	1K	55	20/21	0.87	0.16	107,127,140,145	0
23	4SU	2L	8	20/21	0.88	0.16	107,118,124,125	0
23	OMC	2L	33	21/22	0.90	0.19	94,103,107,109	0
23	PSU	2L	56	20/21	0.91	0.10	109,121,126,126	0
23	7MG	2L	47	24/25	0.92	0.14	118,128,137,141	0
23	PSU	2K	56	20/21	0.92	0.12	91,101,110,117	0
22	5MU	1K	54	21/22	0.92	0.16	104,125,133,143	0
22	PSU	1K	39	20/21	0.93	0.21	94,112,118,120	0
22	T6A	1K	37	32/33	0.94	0.20	81,92,114,116	0
23	5MU	2L	55	21/22	0.94	0.14	115,122,127,130	0
23	4SU	2K	8	20/21	0.94	0.17	89,95,101,103	0
23	7MG	2K	47	24/25	0.94	0.15	96,101,113,116	0
23	5MU	2K	55	21/22	0.95	0.14	98,105,112,114	0
23	OMC	2K	33	21/22	0.96	0.21	73,79,82,94	0
22	U8U	1K	34	23/24	0.96	0.17	83,98,108,110	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
57	MG	13	1678	1/1	0.02	0.16	112,112,112,112	0
57	MG	1H	3445	1/1	0.18	0.12	92,92,92,92	0
57	MG	1H	3081	1/1	0.19	0.45	83,83,83,83	0
57	MG	13	1704	1/1	0.32	0.13	106,106,106,106	0
57	MG	14	3393	1/1	0.32	0.08	165,165,165,165	0
57	MG	1G	1673	1/1	0.34	0.14	115,115,115,115	0
57	MG	1H	3180	1/1	0.34	0.42	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3350	1/1	0.39	0.16	101,101,101,101	0
57	MG	14	3115	1/1	0.40	0.78	87,87,87,87	0
57	MG	14	3377	1/1	0.47	0.10	131,131,131,131	0
57	MG	1H	3113	1/1	0.48	0.26	81,81,81,81	0
57	MG	1G	1609	1/1	0.50	0.87	92,92,92,92	0
57	MG	14	3163	1/1	0.51	0.38	93,93,93,93	0
57	MG	14	3422	1/1	0.52	0.24	108,108,108,108	0
57	MG	1H	3154	1/1	0.53	0.23	58,58,58,58	0
57	MG	13	1709	1/1	0.54	0.26	99,99,99,99	0
57	MG	1H	3157	1/1	0.54	0.38	89,89,89,89	0
57	MG	1H	3454	1/1	0.54	0.07	111,111,111,111	0
57	MG	1H	3520	1/1	0.54	0.10	105,105,105,105	0
57	MG	1G	1642	1/1	0.55	0.28	99,99,99,99	0
57	MG	1H	3145	1/1	0.56	0.53	80,80,80,80	0
57	MG	14	3127	1/1	0.56	1.02	87,87,87,87	0
57	MG	14	3355	1/1	0.56	0.10	104,104,104,104	0
57	MG	1G	1686	1/1	0.57	0.13	106,106,106,106	0
57	MG	13	1679	1/1	0.57	0.30	99,99,99,99	0
57	MG	1H	3237	1/1	0.57	0.46	81,81,81,81	0
57	MG	1G	1678	1/1	0.58	0.11	111,111,111,111	0
57	MG	14	3154	1/1	0.58	0.40	95,95,95,95	0
57	MG	13	1643	1/1	0.59	0.23	101,101,101,101	0
57	MG	13	1739	1/1	0.59	0.06	121,121,121,121	0
57	MG	1H	3141	1/1	0.59	0.29	83,83,83,83	0
57	MG	1H	3007	1/1	0.59	0.31	81,81,81,81	0
57	MG	1H	3050	1/1	0.59	0.38	72,72,72,72	0
57	MG	1H	3230	1/1	0.60	0.36	82,82,82,82	0
57	MG	1H	3120	1/1	0.60	0.18	88,88,88,88	0
57	MG	14	3008	1/1	0.60	0.21	77,77,77,77	0
57	MG	E5	101	1/1	0.60	0.58	89,89,89,89	0
57	MG	1H	3150	1/1	0.61	0.70	98,98,98,98	0
57	MG	14	3208	1/1	0.61	0.95	88,88,88,88	0
57	MG	14	3132	1/1	0.61	0.44	82,82,82,82	0
57	MG	14	3430	1/1	0.61	0.19	107,107,107,107	0
57	MG	1H	3339	1/1	0.61	0.12	106,106,106,106	0
57	MG	1H	3205	1/1	0.62	0.60	79,79,79,79	0
57	MG	1H	3500	1/1	0.62	0.14	94,94,94,94	0
57	MG	14	3384	1/1	0.63	0.14	78,78,78,78	0
57	MG	1H	3442	1/1	0.64	0.09	103,103,103,103	0
57	MG	14	3114	1/1	0.64	0.22	70,70,70,70	0
57	MG	1H	3503	1/1	0.64	0.12	91,91,91,91	0
57	MG	14	3347	1/1	0.64	0.10	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1685	1/1	0.64	0.16	90,90,90,90	0
57	MG	14	3433	1/1	0.64	0.26	114,114,114,114	0
57	MG	13	1738	1/1	0.64	0.10	133,133,133,133	0
57	MG	14	3332	1/1	0.65	0.09	102,102,102,102	0
57	MG	14	3064	1/1	0.65	0.48	63,63,63,63	0
57	MG	14	3166	1/1	0.65	0.46	79,79,79,79	0
57	MG	14	3426	1/1	0.65	0.16	104,104,104,104	0
57	MG	1H	3451	1/1	0.65	0.08	102,102,102,102	0
57	MG	14	3376	1/1	0.65	0.23	102,102,102,102	0
57	MG	1J	208	1/1	0.65	0.10	103,103,103,103	0
57	MG	C5	201	1/1	0.65	0.10	113,113,113,113	0
57	MG	14	3266	1/1	0.65	0.08	107,107,107,107	0
57	MG	1H	3079	1/1	0.66	0.34	63,63,63,63	0
57	MG	1H	3204	1/1	0.66	0.20	91,91,91,91	0
57	MG	1H	3388	1/1	0.66	0.13	55,55,55,55	0
57	MG	14	3344	1/1	0.66	0.09	93,93,93,93	0
57	MG	14	3135	1/1	0.66	0.32	79,79,79,79	0
57	MG	14	3152	1/1	0.66	0.17	78,78,78,78	0
57	MG	14	3434	1/1	0.66	0.12	110,110,110,110	0
57	MG	13	1671	1/1	0.66	0.51	79,79,79,79	0
57	MG	1H	3211	1/1	0.66	0.46	78,78,78,78	0
57	MG	13	1723	1/1	0.66	0.07	128,128,128,128	0
57	MG	1H	3423	1/1	0.67	0.18	84,84,84,84	0
57	MG	14	3429	1/1	0.67	0.30	95,95,95,95	0
57	MG	1H	3496	1/1	0.67	0.16	89,89,89,89	0
57	MG	14	3176	1/1	0.67	0.20	82,82,82,82	0
57	MG	14	3387	1/1	0.67	0.14	83,83,83,83	0
57	MG	14	3122	1/1	0.67	0.37	75,75,75,75	0
57	MG	14	3395	1/1	0.67	0.10	118,118,118,118	0
57	MG	1H	3004	1/1	0.67	0.51	89,89,89,89	0
57	MG	14	3277	1/1	0.68	0.16	84,84,84,84	0
57	MG	1H	3511	1/1	0.68	0.16	101,101,101,101	0
57	MG	13	1729	1/1	0.68	0.11	110,110,110,110	0
57	MG	1H	3499	1/1	0.68	0.09	112,112,112,112	0
57	MG	14	3017	1/1	0.68	0.34	119,119,119,119	0
57	MG	1H	3234	1/1	0.68	0.20	79,79,79,79	0
57	MG	1H	3487	1/1	0.68	0.11	85,85,85,85	0
57	MG	31	301	1/1	0.69	0.13	63,63,63,63	0
57	MG	1H	3085	1/1	0.69	0.28	70,70,70,70	0
57	MG	1H	3065	1/1	0.69	0.53	65,65,65,65	0
57	MG	13	1662	1/1	0.69	0.50	89,89,89,89	0
57	MG	13	1673	1/1	0.69	0.40	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3216	1/1	0.69	0.27	82,82,82,82	0
57	MG	35	201	1/1	0.69	0.22	75,75,75,75	0
57	MG	14	3407	1/1	0.69	0.12	123,123,123,123	0
57	MG	1H	3422	1/1	0.69	0.33	65,65,65,65	0
57	MG	14	3173	1/1	0.70	0.45	79,79,79,79	0
57	MG	1H	3177	1/1	0.70	0.90	82,82,82,82	0
57	MG	16	208	1/1	0.70	0.39	85,85,85,85	0
57	MG	14	3212	1/1	0.70	0.32	75,75,75,75	0
57	MG	1H	3428	1/1	0.70	0.09	89,89,89,89	0
57	MG	14	3385	1/1	0.70	0.16	67,67,67,67	0
57	MG	14	3435	1/1	0.70	0.20	92,92,92,92	0
57	MG	1H	3130	1/1	0.70	0.47	63,63,63,63	0
57	MG	4I	200	1/1	0.70	0.23	95,95,95,95	0
57	MG	1H	3419	1/1	0.70	0.15	86,86,86,86	0
57	MG	13	1668	1/1	0.70	0.29	66,66,66,66	0
57	MG	14	3110	1/1	0.71	0.24	69,69,69,69	0
57	MG	14	3161	1/1	0.71	0.41	78,78,78,78	0
57	MG	14	3264	1/1	0.71	0.14	93,93,93,93	0
57	MG	1G	1635	1/1	0.71	0.20	105,105,105,105	0
57	MG	14	3164	1/1	0.71	0.33	78,78,78,78	0
57	MG	14	3330	1/1	0.71	0.14	94,94,94,94	0
57	MG	1H	3135	1/1	0.71	0.49	79,79,79,79	0
57	MG	14	3138	1/1	0.71	0.67	78,78,78,78	0
57	MG	14	3109	1/1	0.71	0.43	67,67,67,67	0
57	MG	14	3207	1/1	0.71	0.37	70,70,70,70	0
57	MG	1H	3168	1/1	0.72	0.49	80,80,80,80	0
57	MG	1H	3195	1/1	0.72	0.31	55,55,55,55	0
57	MG	14	3291	1/1	0.72	0.21	85,85,85,85	0
57	MG	1G	1682	1/1	0.72	0.05	123,123,123,123	0
57	MG	1H	3006	1/1	0.72	0.28	74,74,74,74	0
57	MG	1H	3225	1/1	0.72	0.43	71,71,71,71	0
57	MG	1H	3227	1/1	0.72	0.28	72,72,72,72	0
57	MG	14	3252	1/1	0.72	0.18	90,90,90,90	0
57	MG	14	3409	1/1	0.72	0.22	88,88,88,88	0
57	MG	1G	1671	1/1	0.72	0.17	112,112,112,112	0
57	MG	14	3406	1/1	0.73	0.12	101,101,101,101	0
57	MG	13	1669	1/1	0.73	0.53	95,95,95,95	0
57	MG	14	3181	1/1	0.73	0.30	75,75,75,75	0
57	MG	14	3417	1/1	0.73	0.12	108,108,108,108	0
57	MG	14	3185	1/1	0.73	0.41	86,86,86,86	0
57	MG	1H	3171	1/1	0.73	0.38	73,73,73,73	0
57	MG	14	3023	1/1	0.73	0.27	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3366	1/1	0.73	0.23	82,82,82,82	0
57	MG	1H	3172	1/1	0.73	0.30	83,83,83,83	0
57	MG	13	1737	1/1	0.73	0.11	99,99,99,99	0
57	MG	1H	3458	1/1	0.73	0.10	82,82,82,82	0
57	MG	16	205	1/1	0.73	0.18	69,69,69,69	0
57	MG	1H	3075	1/1	0.73	0.29	76,76,76,76	0
57	MG	1H	3267	1/1	0.73	0.10	56,56,56,56	0
57	MG	7A	101	1/1	0.73	0.26	114,114,114,114	0
57	MG	4L	101	1/1	0.74	0.32	131,131,131,131	0
57	MG	1H	3444	1/1	0.74	0.11	74,74,74,74	0
57	MG	14	3151	1/1	0.74	0.29	70,70,70,70	0
57	MG	1H	3396	1/1	0.74	0.22	59,59,59,59	0
57	MG	13	1660	1/1	0.74	0.23	88,88,88,88	0
57	MG	1G	1644	1/1	0.74	0.20	106,106,106,106	0
57	MG	14	3073	1/1	0.74	0.31	78,78,78,78	0
57	MG	1G	1668	1/1	0.74	0.09	124,124,124,124	0
57	MG	13	1637	1/1	0.74	0.32	74,74,74,74	0
57	MG	1H	3226	1/1	0.74	0.31	71,71,71,71	0
57	MG	1H	3476	1/1	0.74	0.21	82,82,82,82	0
57	MG	14	3118	1/1	0.74	0.44	61,61,61,61	0
57	MG	13	1714	1/1	0.74	0.09	122,122,122,122	0
57	MG	13	1674	1/1	0.74	0.36	92,92,92,92	0
57	MG	14	3128	1/1	0.74	0.41	89,89,89,89	0
57	MG	14	3211	1/1	0.74	0.09	81,81,81,81	0
57	MG	P8	101	1/1	0.74	0.56	71,71,71,71	0
57	MG	1H	3217	1/1	0.75	0.64	82,82,82,82	0
57	MG	1H	3395	1/1	0.75	0.14	68,68,68,68	0
57	MG	1H	3522	1/1	0.75	0.14	110,110,110,110	0
57	MG	16	203	1/1	0.75	0.21	82,82,82,82	0
57	MG	1G	1699	1/1	0.75	0.07	133,133,133,133	0
57	MG	1H	3063	1/1	0.75	0.27	100,100,100,100	0
57	MG	1H	3415	1/1	0.75	0.14	72,72,72,72	0
57	MG	1H	3118	1/1	0.75	0.15	69,69,69,69	0
61	SPE	14	3436	13/13	0.75	0.25	83,88,93,94	0
57	MG	1G	1675	1/1	0.76	0.08	103,103,103,103	0
57	MG	1H	3479	1/1	0.76	0.10	83,83,83,83	0
57	MG	1G	1618	1/1	0.76	0.69	78,78,78,78	0
57	MG	14	3197	1/1	0.76	0.61	77,77,77,77	0
57	MG	14	3080	1/1	0.76	0.25	68,68,68,68	0
57	MG	14	3098	1/1	0.76	0.35	77,77,77,77	0
57	MG	14	3100	1/1	0.76	0.27	71,71,71,71	0
57	MG	14	3432	1/1	0.76	0.13	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3103	1/1	0.76	0.43	96,96,96,96	0
57	MG	13	1727	1/1	0.76	0.13	90,90,90,90	0
57	MG	1H	3374	1/1	0.76	0.11	83,83,83,83	0
57	MG	1H	3053	1/1	0.76	0.46	75,75,75,75	0
57	MG	1H	3243	1/1	0.76	0.17	82,82,82,82	0
57	MG	1H	3196	1/1	0.76	0.38	77,77,77,77	0
57	MG	14	3398	1/1	0.76	0.13	76,76,76,76	0
57	MG	1H	3414	1/1	0.76	0.14	105,105,105,105	0
57	MG	1H	3516	1/1	0.77	0.14	102,102,102,102	0
57	MG	1H	3153	1/1	0.77	0.44	77,77,77,77	0
57	MG	14	3060	1/1	0.77	0.30	98,98,98,98	0
57	MG	1H	3277	1/1	0.77	0.16	71,71,71,71	0
57	MG	13	1706	1/1	0.77	0.08	117,117,117,117	0
57	MG	1H	3352	1/1	0.77	0.12	57,57,57,57	0
57	MG	14	3428	1/1	0.77	0.29	119,119,119,119	0
57	MG	1H	3363	1/1	0.77	0.12	96,96,96,96	0
57	MG	1H	3488	1/1	0.77	0.28	105,105,105,105	0
57	MG	13	1676	1/1	0.77	0.47	93,93,93,93	0
57	MG	1H	3123	1/1	0.77	0.37	65,65,65,65	0
57	MG	14	3379	1/1	0.77	0.14	84,84,84,84	0
57	MG	14	3156	1/1	0.77	0.17	87,87,87,87	0
57	MG	14	3258	1/1	0.77	0.07	79,79,79,79	0
57	MG	1H	3389	1/1	0.77	0.14	88,88,88,88	0
57	MG	1H	3003	1/1	0.77	0.37	65,65,65,65	0
57	MG	14	3274	1/1	0.77	0.05	85,85,85,85	0
57	MG	1H	3203	1/1	0.77	0.24	74,74,74,74	0
57	MG	1H	3129	1/1	0.78	0.20	76,76,76,76	0
57	MG	14	3342	1/1	0.78	0.09	113,113,113,113	0
57	MG	1H	3163	1/1	0.78	0.44	91,91,91,91	0
57	MG	1H	3518	1/1	0.78	0.11	96,96,96,96	0
57	MG	14	3348	1/1	0.78	0.11	96,96,96,96	0
57	MG	14	3067	1/1	0.78	0.23	78,78,78,78	0
57	MG	1H	3206	1/1	0.78	0.56	93,93,93,93	0
57	MG	1H	3309	1/1	0.78	0.23	54,54,54,54	0
57	MG	14	3257	1/1	0.78	0.16	69,69,69,69	0
57	MG	1H	3089	1/1	0.78	0.20	38,38,38,38	0
57	MG	1H	3105	1/1	0.78	0.23	72,72,72,72	0
57	MG	14	3382	1/1	0.78	0.12	66,66,66,66	0
57	MG	14	3168	1/1	0.78	0.24	89,89,89,89	0
57	MG	14	3134	1/1	0.78	0.33	85,85,85,85	0
57	MG	13	1661	1/1	0.78	0.19	90,90,90,90	0
57	MG	1H	3241	1/1	0.78	0.22	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3326	1/1	0.78	0.09	77,77,77,77	0
57	MG	14	3139	1/1	0.78	0.31	68,68,68,68	0
57	MG	13	1647	1/1	0.79	0.47	88,88,88,88	0
57	MG	14	3421	1/1	0.79	0.10	97,97,97,97	0
57	MG	1G	1680	1/1	0.79	0.07	123,123,123,123	0
57	MG	14	3276	1/1	0.79	0.10	120,120,120,120	0
57	MG	1H	3170	1/1	0.79	0.34	80,80,80,80	0
57	MG	14	3381	1/1	0.79	0.31	79,79,79,79	0
57	MG	14	3187	1/1	0.79	0.25	117,117,117,117	0
57	MG	1H	3198	1/1	0.79	0.23	79,79,79,79	0
57	MG	1G	1688	1/1	0.79	0.24	113,113,113,113	0
57	MG	1G	1694	1/1	0.79	0.12	113,113,113,113	0
57	MG	1H	3434	1/1	0.79	0.17	95,95,95,95	0
57	MG	1J	207	1/1	0.79	0.15	97,97,97,97	0
57	MG	52	201	1/1	0.79	0.15	129,129,129,129	0
57	MG	19	301	1/1	0.79	0.42	48,48,48,48	0
57	MG	1H	3111	1/1	0.79	0.61	79,79,79,79	0
57	MG	1G	1632	1/1	0.79	0.09	91,91,91,91	0
57	MG	1G	1634	1/1	0.79	0.72	85,85,85,85	0
57	MG	14	3175	1/1	0.79	0.21	88,88,88,88	0
57	MG	13	1711	1/1	0.80	0.16	74,74,74,74	0
57	MG	1G	1663	1/1	0.80	0.23	98,98,98,98	0
57	MG	1H	3043	1/1	0.80	0.40	75,75,75,75	0
57	MG	1H	3421	1/1	0.80	0.06	82,82,82,82	0
57	MG	14	3142	1/1	0.80	0.29	80,80,80,80	0
57	MG	14	3146	1/1	0.80	0.28	75,75,75,75	0
57	MG	14	3271	1/1	0.80	0.06	94,94,94,94	0
57	MG	1H	3368	1/1	0.80	0.12	69,69,69,69	0
57	MG	1H	3224	1/1	0.80	0.33	85,85,85,85	0
57	MG	14	3069	1/1	0.80	0.46	86,86,86,86	0
57	MG	13	1664	1/1	0.80	0.46	78,78,78,78	0
57	MG	1H	3497	1/1	0.80	0.10	107,107,107,107	0
57	MG	1H	3329	1/1	0.80	0.08	85,85,85,85	0
57	MG	1H	3391	1/1	0.80	0.13	89,89,89,89	0
57	MG	14	3339	1/1	0.80	0.10	107,107,107,107	0
57	MG	1H	3332	1/1	0.80	0.16	102,102,102,102	0
57	MG	14	3108	1/1	0.80	0.28	72,72,72,72	0
57	MG	1G	1690	1/1	0.80	0.06	117,117,117,117	0
57	MG	1G	1693	1/1	0.80	0.07	129,129,129,129	0
57	MG	1H	3144	1/1	0.80	0.61	102,102,102,102	0
57	MG	1H	3405	1/1	0.80	0.09	66,66,66,66	0
57	MG	1G	1704	1/1	0.80	0.20	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1636	1/1	0.80	0.33	90,90,90,90	0
57	MG	1G	1637	1/1	0.80	0.16	103,103,103,103	0
57	MG	1H	3350	1/1	0.80	0.11	74,74,74,74	0
57	MG	14	3007	1/1	0.80	0.26	60,60,60,60	0
57	MG	14	3133	1/1	0.80	1.00	88,88,88,88	0
57	MG	1G	1605	1/1	0.81	0.39	104,104,104,104	0
57	MG	14	3285	1/1	0.81	0.06	108,108,108,108	0
57	MG	1H	3074	1/1	0.81	0.38	64,64,64,64	0
57	MG	1H	3386	1/1	0.81	0.18	42,42,42,42	0
57	MG	14	3131	1/1	0.81	0.29	64,64,64,64	0
57	MG	1H	3106	1/1	0.81	0.23	87,87,87,87	0
57	MG	14	3183	1/1	0.81	0.30	103,103,103,103	0
57	MG	1H	3470	1/1	0.81	0.08	83,83,83,83	0
57	MG	1H	3125	1/1	0.81	0.20	56,56,56,56	0
57	MG	1H	3341	1/1	0.81	0.12	78,78,78,78	0
57	MG	14	3202	1/1	0.81	0.49	84,84,84,84	0
57	MG	14	3074	1/1	0.81	0.27	69,69,69,69	0
57	MG	1H	3486	1/1	0.81	0.07	95,95,95,95	0
57	MG	14	3091	1/1	0.81	0.09	78,78,78,78	0
57	MG	1H	3083	1/1	0.81	0.84	83,83,83,83	0
57	MG	1G	1697	1/1	0.81	0.09	128,128,128,128	0
57	MG	13	1675	1/1	0.81	0.47	101,101,101,101	0
57	MG	1H	3401	1/1	0.81	0.09	64,64,64,64	0
57	MG	1H	3308	1/1	0.81	0.14	50,50,50,50	0
57	MG	1G	1669	1/1	0.81	0.09	105,105,105,105	0
57	MG	1G	1670	1/1	0.81	0.06	134,134,134,134	0
57	MG	41	201	1/1	0.81	0.12	69,69,69,69	0
57	MG	1H	3055	1/1	0.81	0.18	48,48,48,48	0
57	MG	14	3404	1/1	0.82	0.16	97,97,97,97	0
57	MG	1H	3367	1/1	0.82	0.08	66,66,66,66	0
57	MG	14	3221	1/1	0.82	0.20	62,62,62,62	0
57	MG	1H	3197	1/1	0.82	0.51	77,77,77,77	0
57	MG	14	3412	1/1	0.82	0.10	97,97,97,97	0
57	MG	14	3345	1/1	0.82	0.16	99,99,99,99	0
57	MG	1H	3408	1/1	0.82	0.12	67,67,67,67	0
57	MG	13	1628	1/1	0.82	0.32	91,91,91,91	0
57	MG	14	3262	1/1	0.82	0.14	83,83,83,83	0
57	MG	1H	3201	1/1	0.82	0.75	104,104,104,104	0
57	MG	1H	3222	1/1	0.82	0.14	69,69,69,69	0
57	MG	1H	3456	1/1	0.82	0.06	94,94,94,94	0
57	MG	13	1649	1/1	0.82	0.42	75,75,75,75	0
57	MG	1H	3119	1/1	0.82	0.39	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3072	1/1	0.82	0.27	94,94,94,94	0
57	MG	1H	3020	1/1	0.82	0.14	73,73,73,73	0
57	MG	1J	205	1/1	0.82	0.15	73,73,73,73	0
57	MG	14	3155	1/1	0.82	0.16	78,78,78,78	0
57	MG	14	3295	1/1	0.82	0.10	60,60,60,60	0
57	MG	14	3386	1/1	0.82	0.09	74,74,74,74	0
57	MG	39	302	1/1	0.82	0.20	74,74,74,74	0
57	MG	14	3298	1/1	0.82	0.11	86,86,86,86	0
57	MG	1H	3038	1/1	0.82	0.32	50,50,50,50	0
57	MG	14	3075	1/1	0.82	0.16	73,73,73,73	0
57	MG	1H	3431	1/1	0.82	0.09	98,98,98,98	0
61	SPE	14	3437	13/13	0.82	0.29	59,68,73,74	0
57	MG	14	3368	1/1	0.83	0.09	88,88,88,88	0
57	MG	13	1670	1/1	0.83	0.30	82,82,82,82	0
57	MG	14	3204	1/1	0.83	0.22	72,72,72,72	0
57	MG	1H	3483	1/1	0.83	0.17	91,91,91,91	0
57	MG	1H	3485	1/1	0.83	0.06	77,77,77,77	0
57	MG	1H	3066	1/1	0.83	0.26	60,60,60,60	0
57	MG	1H	3347	1/1	0.83	0.10	67,67,67,67	0
57	MG	14	3214	1/1	0.83	0.70	80,80,80,80	0
57	MG	14	3003	1/1	0.83	0.27	78,78,78,78	0
57	MG	14	3225	1/1	0.83	0.07	73,73,73,73	0
57	MG	14	3391	1/1	0.83	0.23	99,99,99,99	0
57	MG	14	3230	1/1	0.83	0.17	63,63,63,63	0
57	MG	14	3243	1/1	0.83	0.15	58,58,58,58	0
57	MG	14	3005	1/1	0.83	0.26	54,54,54,54	0
57	MG	1H	3229	1/1	0.83	0.49	90,90,90,90	0
57	MG	1H	3071	1/1	0.83	0.22	79,79,79,79	0
57	MG	1H	3176	1/1	0.83	0.14	83,83,83,83	0
57	MG	1H	3236	1/1	0.83	0.31	67,67,67,67	0
57	MG	1H	3134	1/1	0.83	0.14	57,57,57,57	0
57	MG	1H	3156	1/1	0.83	0.15	83,83,83,83	0
57	MG	1H	3504	1/1	0.83	0.07	109,109,109,109	0
57	MG	1H	3376	1/1	0.83	0.15	66,66,66,66	0
57	MG	1H	3191	1/1	0.83	0.27	58,58,58,58	0
57	MG	14	3278	1/1	0.83	0.09	102,102,102,102	0
57	MG	1H	3517	1/1	0.83	0.07	91,91,91,91	0
57	MG	5I	101	1/1	0.83	0.10	79,79,79,79	0
57	MG	1G	1674	1/1	0.83	0.08	107,107,107,107	0
57	MG	1H	3220	1/1	0.83	0.45	89,89,89,89	0
57	MG	1H	3298	1/1	0.83	0.11	51,51,51,51	0
57	MG	1H	3523	1/1	0.83	0.11	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3453	1/1	0.83	0.12	93,93,93,93	0
57	MG	1G	1683	1/1	0.83	0.13	121,121,121,121	0
57	MG	1H	3161	1/1	0.83	0.38	67,67,67,67	0
57	MG	1H	3223	1/1	0.83	0.43	85,85,85,85	0
57	MG	13	1728	1/1	0.83	0.05	117,117,117,117	0
57	MG	14	3184	1/1	0.83	0.26	78,78,78,78	0
57	MG	1H	3049	1/1	0.83	0.25	62,62,62,62	0
57	MG	88	203	1/1	0.83	0.33	79,79,79,79	0
57	MG	1H	3407	1/1	0.83	0.09	72,72,72,72	0
57	MG	14	3198	1/1	0.83	0.43	81,81,81,81	0
57	MG	1G	1657	1/1	0.84	0.06	121,121,121,121	0
57	MG	1H	3178	1/1	0.84	0.43	63,63,63,63	0
57	MG	1H	3162	1/1	0.84	0.29	60,60,60,60	0
57	MG	1H	3420	1/1	0.84	0.12	69,69,69,69	0
57	MG	14	3099	1/1	0.84	0.18	78,78,78,78	0
57	MG	14	3318	1/1	0.84	0.12	89,89,89,89	0
57	MG	1H	3147	1/1	0.84	0.39	84,84,84,84	0
57	MG	14	3153	1/1	0.84	0.59	90,90,90,90	0
57	MG	1H	3274	1/1	0.84	0.14	97,97,97,97	0
57	MG	14	3414	1/1	0.84	0.12	97,97,97,97	0
57	MG	14	3213	1/1	0.84	0.71	87,87,87,87	0
57	MG	14	3418	1/1	0.84	0.07	90,90,90,90	0
57	MG	14	3107	1/1	0.84	0.36	54,54,54,54	0
57	MG	14	3343	1/1	0.84	0.06	80,80,80,80	0
57	MG	14	3215	1/1	0.84	1.26	86,86,86,86	0
57	MG	14	3427	1/1	0.84	0.08	65,65,65,65	0
57	MG	1H	3506	1/1	0.84	0.08	106,106,106,106	0
57	MG	13	1724	1/1	0.84	0.11	117,117,117,117	0
57	MG	1H	3136	1/1	0.84	0.41	116,116,116,116	0
57	MG	1G	1610	1/1	0.84	0.23	91,91,91,91	0
57	MG	1H	3140	1/1	0.84	0.20	54,54,54,54	0
57	MG	14	3256	1/1	0.84	0.13	83,83,83,83	0
57	MG	1H	3084	1/1	0.84	0.20	62,62,62,62	0
57	MG	1H	3406	1/1	0.84	0.08	85,85,85,85	0
57	MG	14	3063	1/1	0.84	0.24	67,67,67,67	0
57	MG	1H	3373	1/1	0.84	0.09	80,80,80,80	0
57	MG	13	1627	1/1	0.84	0.48	71,71,71,71	0
57	MG	14	3267	1/1	0.84	0.06	82,82,82,82	0
57	MG	1H	3525	1/1	0.84	0.22	68,68,68,68	0
57	MG	1G	1691	1/1	0.84	0.05	133,133,133,133	0
57	MG	16	201	1/1	0.84	0.25	62,62,62,62	0
57	MG	13	1732	1/1	0.84	0.08	114,114,114,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3389	1/1	0.84	0.07	93,93,93,93	0
57	MG	14	3157	1/1	0.85	0.32	92,92,92,92	0
57	MG	1H	3482	1/1	0.85	0.09	94,94,94,94	0
57	MG	1H	3242	1/1	0.85	0.47	90,90,90,90	0
57	MG	1G	1641	1/1	0.85	0.59	103,103,103,103	0
57	MG	13	1733	1/1	0.85	0.11	101,101,101,101	0
57	MG	32	301	1/1	0.85	0.47	113,113,113,113	0
57	MG	14	3170	1/1	0.85	0.58	81,81,81,81	0
57	MG	1H	3433	1/1	0.85	0.14	72,72,72,72	0
57	MG	1G	1647	1/1	0.85	0.10	97,97,97,97	0
57	MG	14	3399	1/1	0.85	0.09	123,123,123,123	0
57	MG	14	3111	1/1	0.85	0.19	58,58,58,58	0
57	MG	1G	1654	1/1	0.85	0.30	108,108,108,108	0
57	MG	14	3286	1/1	0.85	0.11	73,73,73,73	0
57	MG	13	1650	1/1	0.85	0.41	75,75,75,75	0
57	MG	14	3117	1/1	0.85	0.47	64,64,64,64	0
57	MG	1H	3058	1/1	0.85	0.17	60,60,60,60	0
57	MG	14	3006	1/1	0.85	0.32	75,75,75,75	0
57	MG	14	3323	1/1	0.85	0.11	81,81,81,81	0
57	MG	14	3419	1/1	0.85	0.06	110,110,110,110	0
57	MG	14	3196	1/1	0.85	0.51	71,71,71,71	0
57	MG	14	3328	1/1	0.85	0.08	81,81,81,81	0
57	MG	14	3425	1/1	0.85	0.13	91,91,91,91	0
57	MG	1H	3489	1/1	0.85	0.32	73,73,73,73	0
57	MG	16	206	1/1	0.85	0.12	77,77,77,77	0
57	MG	14	3130	1/1	0.85	0.24	66,66,66,66	0
57	MG	1H	3061	1/1	0.85	0.28	53,53,53,53	0
57	MG	1H	3128	1/1	0.85	0.42	85,85,85,85	0
57	MG	13	1665	1/1	0.85	0.69	82,82,82,82	0
57	MG	14	3061	1/1	0.85	0.31	61,61,61,61	0
57	MG	13	1654	1/1	0.85	0.41	101,101,101,101	0
57	MG	1H	3502	1/1	0.85	0.18	141,141,141,141	0
57	MG	1H	3194	1/1	0.85	0.10	63,63,63,63	0
57	MG	1G	1606	1/1	0.85	0.13	73,73,73,73	0
57	MG	1H	3164	1/1	0.85	0.41	69,69,69,69	0
57	MG	1H	3148	1/1	0.85	0.37	83,83,83,83	0
57	MG	13	1659	1/1	0.85	0.15	126,126,126,126	0
57	MG	1G	1621	1/1	0.85	0.42	82,82,82,82	0
57	MG	1H	3346	1/1	0.85	0.10	92,92,92,92	0
57	MG	14	3380	1/1	0.85	0.08	78,78,78,78	0
60	ZN	C5	202	1/1	0.85	0.06	165,165,165,165	0
57	MG	1H	3394	1/1	0.85	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3481	1/1	0.85	0.11	103,103,103,103	0
57	MG	1H	3235	1/1	0.86	0.20	71,71,71,71	0
57	MG	14	3025	1/1	0.86	0.12	80,80,80,80	0
57	MG	14	3049	1/1	0.86	1.18	83,83,83,83	0
57	MG	I8	101	1/1	0.86	0.09	85,85,85,85	0
57	MG	14	3401	1/1	0.86	0.15	110,110,110,110	0
57	MG	1H	3320	1/1	0.86	0.08	58,58,58,58	0
57	MG	14	3312	1/1	0.86	0.16	92,92,92,92	0
57	MG	1H	3457	1/1	0.86	0.16	84,84,84,84	0
57	MG	14	3408	1/1	0.86	0.13	92,92,92,92	0
57	MG	1H	3383	1/1	0.86	0.10	68,68,68,68	0
57	MG	13	1710	1/1	0.86	0.07	96,96,96,96	0
57	MG	14	3137	1/1	0.86	0.53	99,99,99,99	0
57	MG	1H	3174	1/1	0.86	0.23	55,55,55,55	0
57	MG	1H	3512	1/1	0.86	0.13	87,87,87,87	0
57	MG	1H	3513	1/1	0.86	0.15	53,53,53,53	0
57	MG	1H	3240	1/1	0.86	0.38	73,73,73,73	0
57	MG	1H	3046	1/1	0.86	0.13	33,33,33,33	0
57	MG	14	3077	1/1	0.86	0.22	52,52,52,52	0
57	MG	1H	3392	1/1	0.86	0.15	48,48,48,48	0
57	MG	13	1740	1/1	0.86	0.06	98,98,98,98	0
57	MG	1G	1695	1/1	0.86	0.23	107,107,107,107	0
57	MG	13	1622	1/1	0.86	0.26	63,63,63,63	0
57	MG	1H	3133	1/1	0.86	0.23	55,55,55,55	0
57	MG	14	3254	1/1	0.86	0.10	77,77,77,77	0
57	MG	14	3255	1/1	0.86	0.13	79,79,79,79	0
57	MG	14	3373	1/1	0.86	0.12	65,65,65,65	0
57	MG	1H	3271	1/1	0.86	0.19	51,51,51,51	0
57	MG	1J	202	1/1	0.86	0.28	92,92,92,92	0
57	MG	1H	3443	1/1	0.86	0.10	75,75,75,75	0
57	MG	1J	206	1/1	0.86	0.24	94,94,94,94	0
57	MG	1H	3005	1/1	0.86	0.21	68,68,68,68	0
57	MG	14	3165	1/1	0.86	0.66	77,77,77,77	0
57	MG	1H	3492	1/1	0.86	0.15	78,78,78,78	0
57	MG	1H	3101	1/1	0.86	0.41	78,78,78,78	0
57	MG	1H	3080	1/1	0.86	0.17	80,80,80,80	0
57	MG	1G	1667	1/1	0.86	0.11	103,103,103,103	0
57	MG	21	302	1/1	0.86	0.25	72,72,72,72	0
57	MG	1H	3498	1/1	0.86	0.20	98,98,98,98	0
57	MG	1H	3137	1/1	0.86	0.43	70,70,70,70	0
57	MG	78	201	1/1	0.86	0.10	66,66,66,66	0
57	MG	1H	3384	1/1	0.87	0.08	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3455	1/1	0.87	0.15	76,76,76,76	0
57	MG	14	3336	1/1	0.87	0.09	94,94,94,94	0
57	MG	1H	3192	1/1	0.87	0.34	75,75,75,75	0
57	MG	14	3411	1/1	0.87	0.04	105,105,105,105	0
57	MG	13	1610	1/1	0.87	0.38	82,82,82,82	0
57	MG	1H	3213	1/1	0.87	0.29	71,71,71,71	0
57	MG	14	3416	1/1	0.87	0.13	102,102,102,102	0
57	MG	1H	3348	1/1	0.87	0.10	111,111,111,111	0
57	MG	1H	3008	1/1	0.87	0.39	82,82,82,82	0
57	MG	14	3125	1/1	0.87	0.21	81,81,81,81	0
57	MG	1H	3477	1/1	0.87	0.14	83,83,83,83	0
57	MG	1H	3001	1/1	0.87	0.39	84,84,84,84	0
57	MG	1H	3002	1/1	0.87	0.21	48,48,48,48	0
57	MG	14	3177	1/1	0.87	0.45	101,101,101,101	0
57	MG	1G	1656	1/1	0.87	0.08	100,100,100,100	0
57	MG	1H	3108	1/1	0.87	0.24	64,64,64,64	0
57	MG	1G	1659	1/1	0.87	0.04	115,115,115,115	0
57	MG	14	3268	1/1	0.87	0.15	82,82,82,82	0
57	MG	14	3076	1/1	0.87	0.45	81,81,81,81	0
57	MG	1H	3314	1/1	0.87	0.08	68,68,68,68	0
57	MG	14	3275	1/1	0.87	0.10	65,65,65,65	0
57	MG	13	1616	1/1	0.87	0.48	74,74,74,74	0
57	MG	14	3084	1/1	0.87	0.27	79,79,79,79	0
57	MG	14	3088	1/1	0.87	0.49	87,87,87,87	0
57	MG	14	3200	1/1	0.87	0.15	89,89,89,89	0
57	MG	13	1683	1/1	0.87	0.05	93,93,93,93	0
57	MG	1H	3375	1/1	0.87	0.10	79,79,79,79	0
57	MG	13	1651	1/1	0.87	0.29	98,98,98,98	0
57	MG	1H	3521	1/1	0.87	0.12	82,82,82,82	0
57	MG	14	3209	1/1	0.87	0.17	83,83,83,83	0
57	MG	1G	1611	1/1	0.87	0.65	76,76,76,76	0
57	MG	1G	1615	1/1	0.87	0.21	86,86,86,86	0
57	MG	1H	3412	1/1	0.87	0.10	75,75,75,75	0
57	MG	14	3403	1/1	0.87	0.12	84,84,84,84	0
57	MG	13	1726	1/1	0.87	0.08	74,74,74,74	0
57	MG	1H	3362	1/1	0.88	0.13	100,100,100,100	0
57	MG	1H	3515	1/1	0.88	0.19	58,58,58,58	0
57	MG	1H	3410	1/1	0.88	0.10	83,83,83,83	0
57	MG	1H	3010	1/1	0.88	0.37	39,39,39,39	0
57	MG	1H	3212	1/1	0.88	0.27	65,65,65,65	0
57	MG	1H	3069	1/1	0.88	0.41	69,69,69,69	0
57	MG	1H	3142	1/1	0.88	0.29	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1696	1/1	0.88	0.05	93,93,93,93	0
57	MG	14	3143	1/1	0.88	0.17	57,57,57,57	0
57	MG	14	3210	1/1	0.88	0.29	91,91,91,91	0
57	MG	14	3413	1/1	0.88	0.15	107,107,107,107	0
57	MG	13	1700	1/1	0.88	0.12	102,102,102,102	0
57	MG	1H	3296	1/1	0.88	0.08	91,91,91,91	0
57	MG	1H	3379	1/1	0.88	0.09	73,73,73,73	0
57	MG	13	1620	1/1	0.88	0.53	86,86,86,86	0
57	MG	1G	1646	1/1	0.88	0.10	86,86,86,86	0
57	MG	16	204	1/1	0.88	0.06	59,59,59,59	0
57	MG	1G	1649	1/1	0.88	0.14	113,113,113,113	0
57	MG	14	3424	1/1	0.88	0.09	109,109,109,109	0
57	MG	13	1615	1/1	0.88	0.24	88,88,88,88	0
57	MG	14	3236	1/1	0.88	0.28	44,44,44,44	0
57	MG	14	3159	1/1	0.88	0.11	79,79,79,79	0
57	MG	2L	102	1/1	0.88	0.18	132,132,132,132	0
57	MG	13	1613	1/1	0.88	0.13	87,87,87,87	0
57	MG	13	1617	1/1	0.88	0.14	51,51,51,51	0
57	MG	14	3431	1/1	0.88	0.25	116,116,116,116	0
57	MG	1H	3126	1/1	0.88	0.43	86,86,86,86	0
57	MG	1H	3082	1/1	0.88	0.27	71,71,71,71	0
57	MG	14	3167	1/1	0.88	0.32	78,78,78,78	0
57	MG	13	1730	1/1	0.88	0.09	94,94,94,94	0
57	MG	13	1731	1/1	0.88	0.05	112,112,112,112	0
57	MG	14	3172	1/1	0.88	0.39	77,77,77,77	0
57	MG	1H	3057	1/1	0.88	0.38	75,75,75,75	0
57	MG	1H	3452	1/1	0.88	0.10	72,72,72,72	0
57	MG	13	1635	1/1	0.88	0.24	81,81,81,81	0
57	MG	14	3273	1/1	0.88	0.09	86,86,86,86	0
57	MG	13	1712	1/1	0.88	0.07	89,89,89,89	0
57	MG	1H	3165	1/1	0.88	0.29	64,64,64,64	0
57	MG	14	3390	1/1	0.88	0.22	94,94,94,94	0
57	MG	13	1713	1/1	0.88	0.08	86,86,86,86	0
57	MG	14	3129	1/1	0.88	0.42	118,118,118,118	0
61	SPE	1G	1703	13/13	0.88	0.09	90,107,113,114	0
57	MG	13	1694	1/1	0.88	0.14	82,82,82,82	0
57	MG	1G	1679	1/1	0.88	0.09	94,94,94,94	0
57	MG	13	1655	1/1	0.89	0.50	82,82,82,82	0
57	MG	14	3223	1/1	0.89	0.10	87,87,87,87	0
57	MG	1H	3181	1/1	0.89	0.24	65,65,65,65	0
57	MG	1H	3221	1/1	0.89	0.24	73,73,73,73	0
57	MG	1G	1648	1/1	0.89	0.16	115,115,115,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3241	1/1	0.89	0.05	78,78,78,78	0
57	MG	13	1684	1/1	0.89	0.08	85,85,85,85	0
57	MG	14	3070	1/1	0.89	0.22	52,52,52,52	0
57	MG	13	1719	1/1	0.89	0.04	81,81,81,81	0
57	MG	14	3346	1/1	0.89	0.08	99,99,99,99	0
57	MG	1H	3086	1/1	0.89	0.18	53,53,53,53	0
57	MG	13	1658	1/1	0.89	0.25	82,82,82,82	0
57	MG	1H	3371	1/1	0.89	0.10	56,56,56,56	0
57	MG	1H	3149	1/1	0.89	0.24	55,55,55,55	0
57	MG	1G	1664	1/1	0.89	0.05	80,80,80,80	0
57	MG	1H	3424	1/1	0.89	0.04	101,101,101,101	0
57	MG	1H	3246	1/1	0.89	0.09	55,55,55,55	0
57	MG	14	3374	1/1	0.89	0.12	92,92,92,92	0
57	MG	1H	3460	1/1	0.89	0.06	96,96,96,96	0
57	MG	16	202	1/1	0.89	0.23	82,82,82,82	0
57	MG	14	3001	1/1	0.89	0.17	57,57,57,57	0
57	MG	14	3144	1/1	0.89	0.32	102,102,102,102	0
57	MG	1G	1625	1/1	0.89	0.08	99,99,99,99	0
57	MG	14	3148	1/1	0.89	0.39	85,85,85,85	0
57	MG	1G	1629	1/1	0.89	0.52	85,85,85,85	0
57	MG	14	3203	1/1	0.89	0.53	79,79,79,79	0
57	MG	1H	3256	1/1	0.89	0.13	47,47,47,47	0
57	MG	1J	204	1/1	0.89	0.09	89,89,89,89	0
57	MG	14	3282	1/1	0.89	0.06	90,90,90,90	0
57	MG	14	3388	1/1	0.89	0.07	85,85,85,85	0
57	MG	1H	3098	1/1	0.89	0.41	46,46,46,46	0
57	MG	1G	1676	1/1	0.89	0.09	93,93,93,93	0
57	MG	1H	3215	1/1	0.89	0.13	63,63,63,63	0
57	MG	1H	3435	1/1	0.89	0.06	62,62,62,62	0
57	MG	14	3024	1/1	0.89	0.07	81,81,81,81	0
57	MG	14	3299	1/1	0.89	0.11	79,79,79,79	0
57	MG	1H	3480	1/1	0.89	0.07	87,87,87,87	0
57	MG	14	3160	1/1	0.89	0.18	65,65,65,65	0
57	MG	14	3402	1/1	0.89	0.08	78,78,78,78	0
57	MG	1H	3509	1/1	0.89	0.12	47,47,47,47	0
57	MG	13	1629	1/1	0.89	0.21	72,72,72,72	0
57	MG	14	3354	1/1	0.90	0.14	60,60,60,60	0
57	MG	13	1708	1/1	0.90	0.16	65,65,65,65	0
57	MG	14	3358	1/1	0.90	0.15	86,86,86,86	0
57	MG	1G	1639	1/1	0.90	0.54	78,78,78,78	0
57	MG	13	1725	1/1	0.90	0.04	115,115,115,115	0
57	MG	1H	3409	1/1	0.90	0.07	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1643	1/1	0.90	0.54	83,83,83,83	0
57	MG	1H	3244	1/1	0.90	0.42	74,74,74,74	0
57	MG	13	1626	1/1	0.90	0.33	84,84,84,84	0
57	MG	1H	3062	1/1	0.90	0.13	38,38,38,38	0
57	MG	1H	3013	1/1	0.90	0.27	40,40,40,40	0
57	MG	14	3009	1/1	0.90	0.34	57,57,57,57	0
57	MG	1H	3416	1/1	0.90	0.06	89,89,89,89	0
57	MG	14	3227	1/1	0.90	0.15	58,58,58,58	0
57	MG	14	3022	1/1	0.90	0.13	81,81,81,81	0
57	MG	1H	3268	1/1	0.90	0.17	59,59,59,59	0
57	MG	1H	3127	1/1	0.90	0.12	91,91,91,91	0
57	MG	1H	3484	1/1	0.90	0.09	105,105,105,105	0
57	MG	14	3245	1/1	0.90	0.14	63,63,63,63	0
57	MG	14	3042	1/1	0.90	0.19	65,65,65,65	0
57	MG	1H	3088	1/1	0.90	0.42	80,80,80,80	0
57	MG	14	3057	1/1	0.90	0.25	49,49,49,49	0
57	MG	13	1656	1/1	0.90	0.38	74,74,74,74	0
57	MG	14	3397	1/1	0.90	0.17	96,96,96,96	0
57	MG	1H	3294	1/1	0.90	0.16	54,54,54,54	0
57	MG	1H	3037	1/1	0.90	0.54	75,75,75,75	0
57	MG	14	3260	1/1	0.90	0.11	106,106,106,106	0
57	MG	13	1657	1/1	0.90	0.15	68,68,68,68	0
57	MG	14	3263	1/1	0.90	0.09	71,71,71,71	0
57	MG	1H	3490	1/1	0.90	0.07	89,89,89,89	0
57	MG	14	3405	1/1	0.90	0.07	108,108,108,108	0
57	MG	1H	3429	1/1	0.90	0.10	88,88,88,88	0
57	MG	88	202	1/1	0.90	0.32	66,66,66,66	0
57	MG	14	3158	1/1	0.90	0.24	66,66,66,66	0
57	MG	1H	3303	1/1	0.90	0.17	48,48,48,48	0
57	MG	1H	3103	1/1	0.90	0.32	61,61,61,61	0
57	MG	13	1695	1/1	0.90	0.10	106,106,106,106	0
57	MG	13	1618	1/1	0.90	0.20	48,48,48,48	0
57	MG	13	1640	1/1	0.90	0.28	92,92,92,92	0
57	MG	1H	3321	1/1	0.90	0.46	86,86,86,86	0
57	MG	1H	3109	1/1	0.90	0.31	59,59,59,59	0
57	MG	14	3279	1/1	0.90	0.08	58,58,58,58	0
57	MG	14	3083	1/1	0.90	0.15	72,72,72,72	0
57	MG	14	3420	1/1	0.90	0.07	107,107,107,107	0
57	MG	1H	3331	1/1	0.90	0.12	70,70,70,70	0
57	MG	14	3169	1/1	0.90	0.31	85,85,85,85	0
57	MG	1G	1612	1/1	0.90	0.15	106,106,106,106	0
57	MG	1G	1614	1/1	0.90	0.60	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3296	1/1	0.90	0.12	72,72,72,72	0
57	MG	1G	1687	1/1	0.90	0.08	111,111,111,111	0
57	MG	1H	3505	1/1	0.90	0.14	100,100,100,100	0
57	MG	14	3307	1/1	0.90	0.15	66,66,66,66	0
57	MG	13	1641	1/1	0.90	0.19	81,81,81,81	0
57	MG	14	3316	1/1	0.90	0.13	69,69,69,69	0
57	MG	1G	1619	1/1	0.90	0.10	102,102,102,102	0
57	MG	14	3319	1/1	0.90	0.07	95,95,95,95	0
57	MG	1G	1692	1/1	0.90	0.12	101,101,101,101	0
57	MG	1H	3508	1/1	0.90	0.10	117,117,117,117	0
57	MG	1J	201	1/1	0.90	0.29	73,73,73,73	0
57	MG	14	3327	1/1	0.90	0.09	82,82,82,82	0
57	MG	1H	3334	1/1	0.90	0.10	77,77,77,77	0
57	MG	1G	1628	1/1	0.90	0.31	113,113,113,113	0
57	MG	14	3186	1/1	0.90	0.16	108,108,108,108	0
57	MG	1H	3336	1/1	0.90	0.14	62,62,62,62	0
57	MG	14	3193	1/1	0.90	0.13	45,45,45,45	0
57	MG	13	1722	1/1	0.90	0.09	87,87,87,87	0
57	MG	1H	3404	1/1	0.90	0.13	71,71,71,71	0
57	MG	25	201	1/1	0.90	0.05	115,115,115,115	0
57	MG	1H	3115	1/1	0.90	0.10	61,61,61,61	0
57	MG	42	201	1/1	0.90	0.21	120,120,120,120	0
57	MG	14	3119	1/1	0.90	0.20	81,81,81,81	0
57	MG	14	3120	1/1	0.90	0.18	78,78,78,78	0
57	MG	14	3121	1/1	0.90	0.12	61,61,61,61	0
57	MG	14	3349	1/1	0.90	0.13	83,83,83,83	0
57	MG	13	1631	1/1	0.90	0.09	78,78,78,78	0
57	MG	13	1677	1/1	0.91	0.47	77,77,77,77	0
57	MG	14	3396	1/1	0.91	0.03	126,126,126,126	0
57	MG	14	3297	1/1	0.91	0.17	71,71,71,71	0
57	MG	13	1701	1/1	0.91	0.12	108,108,108,108	0
57	MG	13	1720	1/1	0.91	0.15	109,109,109,109	0
57	MG	16	209	1/1	0.91	0.47	76,76,76,76	0
57	MG	14	3309	1/1	0.91	0.14	55,55,55,55	0
57	MG	1G	1696	1/1	0.91	0.07	128,128,128,128	0
57	MG	14	3313	1/1	0.91	0.05	105,105,105,105	0
57	MG	2K	101	1/1	0.91	0.11	100,100,100,100	0
57	MG	1H	3093	1/1	0.91	0.09	56,56,56,56	0
57	MG	13	1735	1/1	0.91	0.07	100,100,100,100	0
57	MG	1H	3447	1/1	0.91	0.24	70,70,70,70	0
57	MG	14	3090	1/1	0.91	0.35	86,86,86,86	0
57	MG	1H	3151	1/1	0.91	0.55	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3095	1/1	0.91	0.18	62,62,62,62	0
57	MG	1G	1652	1/1	0.91	0.15	81,81,81,81	0
57	MG	1H	3132	1/1	0.91	0.23	65,65,65,65	0
57	MG	1H	3116	1/1	0.91	0.16	53,53,53,53	0
57	MG	1H	3251	1/1	0.91	0.16	48,48,48,48	0
57	MG	14	3237	1/1	0.91	0.26	51,51,51,51	0
57	MG	1G	1604	1/1	0.91	0.17	127,127,127,127	0
57	MG	1H	3185	1/1	0.91	0.49	64,64,64,64	0
57	MG	1H	3190	1/1	0.91	0.38	91,91,91,91	0
57	MG	14	3251	1/1	0.91	0.09	80,80,80,80	0
57	MG	14	3423	1/1	0.91	0.07	120,120,120,120	0
57	MG	1H	3351	1/1	0.91	0.09	68,68,68,68	0
57	MG	1H	3117	1/1	0.91	0.18	60,60,60,60	0
57	MG	1H	3270	1/1	0.91	0.15	50,50,50,50	0
57	MG	13	1645	1/1	0.91	0.28	92,92,92,92	0
57	MG	14	3011	1/1	0.91	0.18	44,44,44,44	0
57	MG	14	3015	1/1	0.91	0.29	63,63,63,63	0
57	MG	1H	3193	1/1	0.91	0.26	61,61,61,61	0
57	MG	14	3359	1/1	0.91	0.08	93,93,93,93	0
57	MG	13	1672	1/1	0.91	0.15	88,88,88,88	0
57	MG	1H	3104	1/1	0.91	0.13	43,43,43,43	0
57	MG	14	3369	1/1	0.91	0.10	91,91,91,91	0
57	MG	1H	3138	1/1	0.91	0.14	54,54,54,54	0
57	MG	14	3180	1/1	0.91	0.41	91,91,91,91	0
57	MG	1H	3122	1/1	0.91	0.09	52,52,52,52	0
57	MG	14	3039	1/1	0.91	0.71	89,89,89,89	0
57	MG	1G	1624	1/1	0.91	0.13	95,95,95,95	0
57	MG	1H	3301	1/1	0.91	0.17	45,45,45,45	0
57	MG	1H	3228	1/1	0.91	0.15	60,60,60,60	0
57	MG	13	1697	1/1	0.91	0.07	84,84,84,84	0
57	MG	14	3188	1/1	0.91	0.50	72,72,72,72	0
57	MG	39	301	1/1	0.91	0.18	89,89,89,89	0
57	MG	1G	1630	1/1	0.91	0.37	72,72,72,72	0
57	MG	1H	3427	1/1	0.91	0.10	67,67,67,67	0
57	MG	1H	3124	1/1	0.91	0.21	61,61,61,61	0
57	MG	45	202	1/1	0.91	0.44	64,64,64,64	0
57	MG	1H	3310	1/1	0.91	0.18	70,70,70,70	0
57	MG	1G	1689	1/1	0.91	0.06	116,116,116,116	0
57	MG	14	3201	1/1	0.91	0.20	88,88,88,88	0
57	MG	1H	3231	1/1	0.91	0.49	66,66,66,66	0
57	MG	14	3392	1/1	0.91	0.07	63,63,63,63	0
57	MG	1H	3202	1/1	0.91	0.45	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3095	1/1	0.92	0.17	70,70,70,70	0
57	MG	Q8	300	1/1	0.92	0.12	80,80,80,80	0
57	MG	14	3259	1/1	0.92	0.10	71,71,71,71	0
57	MG	1G	1602	1/1	0.92	0.33	106,106,106,106	0
57	MG	14	3383	1/1	0.92	0.07	90,90,90,90	0
57	MG	1H	3370	1/1	0.92	0.08	68,68,68,68	0
57	MG	1H	3494	1/1	0.92	0.08	72,72,72,72	0
57	MG	1H	3189	1/1	0.92	0.35	68,68,68,68	0
57	MG	1G	1608	1/1	0.92	0.37	93,93,93,93	0
57	MG	1H	3425	1/1	0.92	0.07	64,64,64,64	0
57	MG	13	1682	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3100	1/1	0.92	0.54	68,68,68,68	0
57	MG	1H	3299	1/1	0.92	0.13	48,48,48,48	0
57	MG	1H	3501	1/1	0.92	0.07	90,90,90,90	0
57	MG	13	1686	1/1	0.92	0.17	76,76,76,76	0
57	MG	1H	3432	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3102	1/1	0.92	0.21	60,60,60,60	0
57	MG	1H	3077	1/1	0.92	0.42	80,80,80,80	0
57	MG	1H	3078	1/1	0.92	0.28	58,58,58,58	0
57	MG	14	3178	1/1	0.92	0.73	78,78,78,78	0
57	MG	14	3400	1/1	0.92	0.05	108,108,108,108	0
57	MG	1H	3158	1/1	0.92	0.17	71,71,71,71	0
57	MG	1H	3312	1/1	0.92	0.15	44,44,44,44	0
57	MG	14	3289	1/1	0.92	0.13	74,74,74,74	0
57	MG	1H	3023	1/1	0.92	0.17	50,50,50,50	0
57	MG	1G	1701	1/1	0.92	0.03	111,111,111,111	0
57	MG	1H	3390	1/1	0.92	0.20	64,64,64,64	0
57	MG	14	3113	1/1	0.92	0.18	52,52,52,52	0
57	MG	1H	3446	1/1	0.92	0.06	98,98,98,98	0
57	MG	1H	3034	1/1	0.92	0.21	46,46,46,46	0
57	MG	14	3302	1/1	0.92	0.11	58,58,58,58	0
57	MG	14	3303	1/1	0.92	0.07	74,74,74,74	0
57	MG	14	3306	1/1	0.92	0.08	58,58,58,58	0
57	MG	14	3190	1/1	0.92	0.37	59,59,59,59	0
57	MG	13	1707	1/1	0.92	0.10	56,56,56,56	0
57	MG	3I	201	1/1	0.92	0.24	60,60,60,60	0
57	MG	13	1698	1/1	0.92	0.11	83,83,83,83	0
57	MG	1H	3519	1/1	0.92	0.18	116,116,116,116	0
57	MG	1G	1640	1/1	0.92	0.39	108,108,108,108	0
57	MG	1H	3167	1/1	0.92	0.53	98,98,98,98	0
57	MG	1H	3397	1/1	0.92	0.19	51,51,51,51	0
57	MG	1H	3064	1/1	0.92	0.07	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3403	1/1	0.92	0.07	99,99,99,99	0
57	MG	1H	3524	1/1	0.92	0.18	81,81,81,81	0
57	MG	13	1717	1/1	0.92	0.11	99,99,99,99	0
57	MG	1H	3209	1/1	0.92	0.60	76,76,76,76	0
57	MG	14	3333	1/1	0.92	0.17	50,50,50,50	0
57	MG	1H	3340	1/1	0.92	0.05	76,76,76,76	0
57	MG	14	3337	1/1	0.92	0.14	104,104,104,104	0
57	MG	13	1638	1/1	0.92	0.07	85,85,85,85	0
57	MG	14	3020	1/1	0.92	0.12	75,75,75,75	0
57	MG	1H	3345	1/1	0.92	0.06	102,102,102,102	0
57	MG	1H	3087	1/1	0.92	0.21	71,71,71,71	0
57	MG	13	1612	1/1	0.92	0.12	86,86,86,86	0
57	MG	16	207	1/1	0.92	0.33	74,74,74,74	0
57	MG	14	3141	1/1	0.92	0.28	95,95,95,95	0
57	MG	14	3224	1/1	0.92	0.24	45,45,45,45	0
57	MG	1G	1660	1/1	0.92	0.14	74,74,74,74	0
57	MG	14	3041	1/1	0.92	0.20	55,55,55,55	0
57	MG	1G	1662	1/1	0.92	0.13	91,91,91,91	0
57	MG	1H	3253	1/1	0.92	0.08	42,42,42,42	0
57	MG	14	3357	1/1	0.92	0.08	105,105,105,105	0
57	MG	1H	3051	1/1	0.92	0.11	60,60,60,60	0
57	MG	14	3149	1/1	0.92	0.28	72,72,72,72	0
57	MG	14	3360	1/1	0.92	0.07	96,96,96,96	0
57	MG	14	3361	1/1	0.92	0.05	79,79,79,79	0
57	MG	1H	3092	1/1	0.92	0.24	61,61,61,61	0
57	MG	1H	3146	1/1	0.92	0.16	52,52,52,52	0
57	MG	1H	3417	1/1	0.92	0.18	83,83,83,83	0
60	ZN	G8	201	1/1	0.92	0.14	139,139,139,139	0
57	MG	1H	3418	1/1	0.92	0.10	46,46,46,46	0
57	MG	1H	3219	1/1	0.92	0.20	71,71,71,71	0
57	MG	1H	3073	1/1	0.92	0.21	66,66,66,66	0
57	MG	1H	3094	1/1	0.92	0.15	33,33,33,33	0
57	MG	1H	3076	1/1	0.93	0.24	72,72,72,72	0
57	MG	14	3331	1/1	0.93	0.20	90,90,90,90	0
57	MG	1H	3293	1/1	0.93	0.14	73,73,73,73	0
57	MG	14	3071	1/1	0.93	0.19	74,74,74,74	0
57	MG	14	3335	1/1	0.93	0.08	81,81,81,81	0
57	MG	13	1639	1/1	0.93	0.58	70,70,70,70	0
57	MG	1H	3462	1/1	0.93	0.10	94,94,94,94	0
57	MG	14	3338	1/1	0.93	0.05	107,107,107,107	0
57	MG	1H	3468	1/1	0.93	0.24	82,82,82,82	0
57	MG	2L	101	1/1	0.93	0.40	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3160	1/1	0.93	0.18	71,71,71,71	0
57	MG	14	3410	1/1	0.93	0.06	85,85,85,85	0
57	MG	1H	3436	1/1	0.93	0.10	70,70,70,70	0
57	MG	14	3079	1/1	0.93	0.30	48,48,48,48	0
57	MG	1H	3438	1/1	0.93	0.04	62,62,62,62	0
57	MG	1H	3478	1/1	0.93	0.06	101,101,101,101	0
57	MG	14	3415	1/1	0.93	0.15	103,103,103,103	0
57	MG	1G	1677	1/1	0.93	0.17	92,92,92,92	0
57	MG	1H	3378	1/1	0.93	0.09	50,50,50,50	0
57	MG	13	1667	1/1	0.93	0.67	89,89,89,89	0
57	MG	14	3352	1/1	0.93	0.07	82,82,82,82	0
57	MG	1H	3261	1/1	0.93	0.08	63,63,63,63	0
57	MG	14	3094	1/1	0.93	0.65	73,73,73,73	0
57	MG	1G	1681	1/1	0.93	0.06	96,96,96,96	0
57	MG	1G	1645	1/1	0.93	0.14	81,81,81,81	0
57	MG	1H	3300	1/1	0.93	0.19	62,62,62,62	0
57	MG	1G	1685	1/1	0.93	0.14	110,110,110,110	0
57	MG	1H	3048	1/1	0.93	0.13	45,45,45,45	0
57	MG	14	3365	1/1	0.93	0.13	78,78,78,78	0
57	MG	14	3284	1/1	0.93	0.14	72,72,72,72	0
57	MG	1G	1613	1/1	0.93	0.76	89,89,89,89	0
57	MG	1H	3028	1/1	0.93	0.10	67,67,67,67	0
57	MG	14	3371	1/1	0.93	0.10	107,107,107,107	0
57	MG	1G	1650	1/1	0.93	0.16	101,101,101,101	0
57	MG	1H	3155	1/1	0.93	0.15	55,55,55,55	0
57	MG	1H	3067	1/1	0.93	0.21	58,58,58,58	0
57	MG	14	3112	1/1	0.93	0.20	83,83,83,83	0
57	MG	14	3378	1/1	0.93	0.13	92,92,92,92	0
57	MG	14	3220	1/1	0.93	0.12	54,54,54,54	0
57	MG	1G	1655	1/1	0.93	0.12	110,110,110,110	0
57	MG	16	210	1/1	0.93	0.11	73,73,73,73	0
57	MG	14	3043	1/1	0.93	0.29	71,71,71,71	0
57	MG	1G	1620	1/1	0.93	0.19	91,91,91,91	0
57	MG	14	3051	1/1	0.93	0.27	61,61,61,61	0
57	MG	1H	3232	1/1	0.93	0.22	48,48,48,48	0
57	MG	14	3233	1/1	0.93	0.26	65,65,65,65	0
57	MG	14	3311	1/1	0.93	0.11	67,67,67,67	0
57	MG	1H	3343	1/1	0.93	0.07	78,78,78,78	0
57	MG	1H	3430	1/1	0.93	0.08	73,73,73,73	0
57	MG	1H	3393	1/1	0.93	0.11	50,50,50,50	0
57	MG	14	3317	1/1	0.93	0.08	82,82,82,82	0
57	MG	14	3124	1/1	0.93	0.18	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	M5	101	1/1	0.93	0.18	88,88,88,88	0
57	MG	1G	1700	1/1	0.93	0.06	109,109,109,109	0
57	MG	14	3249	1/1	0.93	0.15	52,52,52,52	0
57	MG	14	3250	1/1	0.93	0.08	79,79,79,79	0
57	MG	88	201	1/1	0.93	0.19	76,76,76,76	0
57	MG	14	3068	1/1	0.93	0.41	53,53,53,53	0
57	MG	14	3238	1/1	0.94	0.20	50,50,50,50	0
57	MG	14	3362	1/1	0.94	0.06	114,114,114,114	0
57	MG	1H	3475	1/1	0.94	0.12	97,97,97,97	0
57	MG	13	1644	1/1	0.94	0.45	85,85,85,85	0
57	MG	14	3367	1/1	0.94	0.08	106,106,106,106	0
57	MG	14	3244	1/1	0.94	0.15	54,54,54,54	0
57	MG	1H	3218	1/1	0.94	0.21	37,37,37,37	0
57	MG	14	3029	1/1	0.94	0.21	57,57,57,57	0
57	MG	14	3033	1/1	0.94	0.33	80,80,80,80	0
57	MG	14	3035	1/1	0.94	0.41	58,58,58,58	0
57	MG	14	3038	1/1	0.94	0.21	52,52,52,52	0
57	MG	21	301	1/1	0.94	0.14	59,59,59,59	0
57	MG	1H	3259	1/1	0.94	0.17	54,54,54,54	0
57	MG	14	3145	1/1	0.94	0.21	90,90,90,90	0
57	MG	13	1681	1/1	0.94	0.14	59,59,59,59	0
57	MG	1G	1666	1/1	0.94	0.14	100,100,100,100	0
57	MG	14	3046	1/1	0.94	0.45	79,79,79,79	0
57	MG	14	3150	1/1	0.94	0.12	63,63,63,63	0
57	MG	1H	3266	1/1	0.94	0.08	54,54,54,54	0
57	MG	14	3050	1/1	0.94	0.20	57,57,57,57	0
57	MG	1H	3184	1/1	0.94	0.24	70,70,70,70	0
57	MG	14	3265	1/1	0.94	0.07	91,91,91,91	0
57	MG	14	3054	1/1	0.94	0.25	79,79,79,79	0
57	MG	1H	3009	1/1	0.94	0.54	71,71,71,71	0
57	MG	13	1666	1/1	0.94	0.20	85,85,85,85	0
57	MG	14	3269	1/1	0.94	0.05	78,78,78,78	0
57	MG	13	1653	1/1	0.94	0.33	73,73,73,73	0
57	MG	13	1633	1/1	0.94	0.22	73,73,73,73	0
57	MG	1H	3356	1/1	0.94	0.11	54,54,54,54	0
57	MG	1H	3357	1/1	0.94	0.12	52,52,52,52	0
57	MG	1H	3358	1/1	0.94	0.18	45,45,45,45	0
57	MG	14	3162	1/1	0.94	0.40	74,74,74,74	0
57	MG	1H	3276	1/1	0.94	0.10	78,78,78,78	0
57	MG	1H	3131	1/1	0.94	0.50	83,83,83,83	0
57	MG	1H	3491	1/1	0.94	0.10	70,70,70,70	0
57	MG	1H	3365	1/1	0.94	0.16	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3366	1/1	0.94	0.17	68,68,68,68	0
57	MG	1H	3279	1/1	0.94	0.15	48,48,48,48	0
57	MG	1H	3283	1/1	0.94	0.15	71,71,71,71	0
57	MG	1G	1684	1/1	0.94	0.06	96,96,96,96	0
57	MG	14	3292	1/1	0.94	0.12	74,74,74,74	0
57	MG	1H	3285	1/1	0.94	0.14	55,55,55,55	0
57	MG	1H	3288	1/1	0.94	0.08	54,54,54,54	0
57	MG	1H	3372	1/1	0.94	0.08	89,89,89,89	0
57	MG	1H	3021	1/1	0.94	0.17	49,49,49,49	0
57	MG	1H	3107	1/1	0.94	0.12	60,60,60,60	0
57	MG	1H	3295	1/1	0.94	0.09	89,89,89,89	0
57	MG	13	1634	1/1	0.94	0.36	75,75,75,75	0
57	MG	14	3304	1/1	0.94	0.10	74,74,74,74	0
57	MG	1H	3026	1/1	0.94	0.39	55,55,55,55	0
57	MG	1G	1623	1/1	0.94	0.21	115,115,115,115	0
57	MG	13	1715	1/1	0.94	0.06	76,76,76,76	0
57	MG	14	3097	1/1	0.94	0.26	97,97,97,97	0
57	MG	1H	3507	1/1	0.94	0.08	57,57,57,57	0
57	MG	1G	1626	1/1	0.94	0.19	83,83,83,83	0
57	MG	1H	3441	1/1	0.94	0.06	105,105,105,105	0
57	MG	1H	3030	1/1	0.94	0.10	39,39,39,39	0
57	MG	14	3104	1/1	0.94	0.18	78,78,78,78	0
57	MG	14	3105	1/1	0.94	0.14	73,73,73,73	0
57	MG	14	3321	1/1	0.94	0.08	69,69,69,69	0
57	MG	14	3106	1/1	0.94	0.41	57,57,57,57	0
57	MG	1H	3510	1/1	0.94	0.14	39,39,39,39	0
57	MG	1H	3114	1/1	0.94	0.15	71,71,71,71	0
57	MG	13	1716	1/1	0.94	0.10	71,71,71,71	0
57	MG	1H	3035	1/1	0.94	0.11	40,40,40,40	0
57	MG	13	1642	1/1	0.94	0.13	103,103,103,103	0
57	MG	13	1718	1/1	0.94	0.09	90,90,90,90	0
57	MG	14	3205	1/1	0.94	0.45	59,59,59,59	0
57	MG	1H	3449	1/1	0.94	0.10	80,80,80,80	0
57	MG	1H	3238	1/1	0.94	0.34	80,80,80,80	0
57	MG	1H	3313	1/1	0.94	0.17	47,47,47,47	0
57	MG	1H	3239	1/1	0.94	0.10	67,67,67,67	0
57	MG	1H	3041	1/1	0.94	0.28	51,51,51,51	0
57	MG	14	3340	1/1	0.94	0.09	107,107,107,107	0
57	MG	1H	3173	1/1	0.94	0.22	59,59,59,59	0
57	MG	13	1687	1/1	0.94	0.06	103,103,103,103	0
57	MG	1H	3175	1/1	0.94	0.29	64,64,64,64	0
57	MG	13	1691	1/1	0.94	0.12	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3218	1/1	0.94	0.09	65,65,65,65	0
57	MG	14	3123	1/1	0.94	0.28	83,83,83,83	0
57	MG	1H	3245	1/1	0.94	0.11	47,47,47,47	0
57	MG	13	1625	1/1	0.94	0.16	82,82,82,82	0
57	MG	14	3010	1/1	0.94	0.25	57,57,57,57	0
57	MG	1H	3337	1/1	0.94	0.05	86,86,86,86	0
57	MG	1H	3469	1/1	0.94	0.14	58,58,58,58	0
58	PAR	1G	1702	42/42	0.94	0.22	83,92,100,103	0
57	MG	1H	3099	1/1	0.94	0.44	56,56,56,56	0
57	MG	14	3232	1/1	0.94	0.14	66,66,66,66	0
57	MG	14	3018	1/1	0.94	0.14	44,44,44,44	0
57	MG	1H	3473	1/1	0.94	0.13	95,95,95,95	0
57	MG	1H	3474	1/1	0.94	0.09	93,93,93,93	0
57	MG	13	1611	1/1	0.95	0.25	70,70,70,70	0
57	MG	14	3174	1/1	0.95	0.08	89,89,89,89	0
57	MG	14	3370	1/1	0.95	0.06	97,97,97,97	0
57	MG	1G	1665	1/1	0.95	0.05	91,91,91,91	0
57	MG	1H	3159	1/1	0.95	0.13	80,80,80,80	0
57	MG	13	1636	1/1	0.95	0.28	74,74,74,74	0
57	MG	14	3272	1/1	0.95	0.09	71,71,71,71	0
57	MG	1H	3459	1/1	0.95	0.13	75,75,75,75	0
57	MG	14	3179	1/1	0.95	0.32	77,77,77,77	0
57	MG	14	3021	1/1	0.95	0.35	38,38,38,38	0
57	MG	1H	3139	1/1	0.95	0.35	71,71,71,71	0
57	MG	1H	3047	1/1	0.95	0.15	55,55,55,55	0
57	MG	1H	3467	1/1	0.95	0.03	84,84,84,84	0
57	MG	13	1721	1/1	0.95	0.17	106,106,106,106	0
57	MG	14	3281	1/1	0.95	0.16	69,69,69,69	0
57	MG	14	3028	1/1	0.95	0.33	45,45,45,45	0
57	MG	14	3283	1/1	0.95	0.07	68,68,68,68	0
57	MG	1H	3514	1/1	0.95	0.05	98,98,98,98	0
57	MG	14	3030	1/1	0.95	0.36	57,57,57,57	0
57	MG	14	3189	1/1	0.95	0.33	51,51,51,51	0
57	MG	14	3288	1/1	0.95	0.19	49,49,49,49	0
57	MG	1G	1616	1/1	0.95	0.13	94,94,94,94	0
57	MG	14	3290	1/1	0.95	0.22	59,59,59,59	0
57	MG	14	3192	1/1	0.95	0.28	74,74,74,74	0
57	MG	1G	1617	1/1	0.95	0.11	116,116,116,116	0
57	MG	14	3195	1/1	0.95	0.25	78,78,78,78	0
57	MG	14	3036	1/1	0.95	0.27	85,85,85,85	0
57	MG	1H	3249	1/1	0.95	0.13	63,63,63,63	0
57	MG	1H	3250	1/1	0.95	0.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3472	1/1	0.95	0.04	83,83,83,83	0
57	MG	14	3300	1/1	0.95	0.09	89,89,89,89	0
57	MG	2K	102	1/1	0.95	0.17	78,78,78,78	0
57	MG	1H	3143	1/1	0.95	0.37	50,50,50,50	0
57	MG	14	3126	1/1	0.95	0.28	72,72,72,72	0
57	MG	13	1646	1/1	0.95	0.17	71,71,71,71	0
57	MG	1H	3257	1/1	0.95	0.14	43,43,43,43	0
57	MG	1H	3068	1/1	0.95	0.40	72,72,72,72	0
57	MG	1H	3316	1/1	0.95	0.07	78,78,78,78	0
57	MG	14	3053	1/1	0.95	0.07	95,95,95,95	0
57	MG	1H	3260	1/1	0.95	0.19	42,42,42,42	0
57	MG	14	3315	1/1	0.95	0.12	68,68,68,68	0
57	MG	1H	3377	1/1	0.95	0.09	76,76,76,76	0
57	MG	14	3058	1/1	0.95	0.34	84,84,84,84	0
57	MG	13	1703	1/1	0.95	0.13	70,70,70,70	0
57	MG	14	3136	1/1	0.95	0.46	92,92,92,92	0
57	MG	14	3320	1/1	0.95	0.09	53,53,53,53	0
57	MG	1H	3326	1/1	0.95	0.10	62,62,62,62	0
57	MG	14	3062	1/1	0.95	0.25	59,59,59,59	0
57	MG	1H	3381	1/1	0.95	0.11	74,74,74,74	0
57	MG	1H	3052	1/1	0.95	0.18	59,59,59,59	0
57	MG	14	3065	1/1	0.95	0.10	47,47,47,47	0
57	MG	14	3329	1/1	0.95	0.06	105,105,105,105	0
57	MG	1H	3200	1/1	0.95	0.26	71,71,71,71	0
57	MG	1G	1638	1/1	0.95	0.14	127,127,127,127	0
57	MG	1H	3072	1/1	0.95	0.20	58,58,58,58	0
57	MG	1H	3269	1/1	0.95	0.16	41,41,41,41	0
57	MG	14	3334	1/1	0.95	0.10	60,60,60,60	0
57	MG	13	1624	1/1	0.95	0.32	59,59,59,59	0
57	MG	1H	3110	1/1	0.95	0.23	79,79,79,79	0
57	MG	1H	3054	1/1	0.95	0.35	52,52,52,52	0
57	MG	1H	3233	1/1	0.95	0.08	93,93,93,93	0
57	MG	1H	3017	1/1	0.95	0.29	62,62,62,62	0
57	MG	1H	3493	1/1	0.95	0.05	101,101,101,101	0
57	MG	31	302	1/1	0.95	0.16	77,77,77,77	0
57	MG	1H	3019	1/1	0.95	0.23	32,32,32,32	0
57	MG	1H	3344	1/1	0.95	0.08	103,103,103,103	0
57	MG	14	3246	1/1	0.95	0.13	61,61,61,61	0
57	MG	1J	203	1/1	0.95	0.26	73,73,73,73	0
57	MG	14	3247	1/1	0.95	0.09	52,52,52,52	0
57	MG	14	3248	1/1	0.95	0.29	47,47,47,47	0
57	MG	1H	3282	1/1	0.95	0.04	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3039	1/1	0.95	0.20	33,33,33,33	0
57	MG	14	3085	1/1	0.95	0.25	88,88,88,88	0
57	MG	14	3351	1/1	0.95	0.11	78,78,78,78	0
57	MG	14	3087	1/1	0.95	0.27	76,76,76,76	0
57	MG	14	3353	1/1	0.95	0.08	83,83,83,83	0
57	MG	1G	1653	1/1	0.95	0.11	97,97,97,97	0
57	MG	1H	3284	1/1	0.95	0.07	83,83,83,83	0
57	MG	45	201	1/1	0.95	0.13	101,101,101,101	0
57	MG	1H	3179	1/1	0.95	0.14	80,80,80,80	0
57	MG	14	3092	1/1	0.95	0.26	66,66,66,66	0
57	MG	I8	102	1/1	0.95	0.05	62,62,62,62	0
57	MG	1H	3096	1/1	0.95	0.15	64,64,64,64	0
58	PAR	13	1741	42/42	0.95	0.24	64,71,75,82	0
57	MG	1G	1658	1/1	0.95	0.06	104,104,104,104	0
57	MG	1H	3289	1/1	0.95	0.12	59,59,59,59	0
57	MG	14	3363	1/1	0.95	0.09	107,107,107,107	0
57	MG	13	1688	1/1	0.95	0.10	109,109,109,109	0
57	MG	1H	3355	1/1	0.95	0.09	59,59,59,59	0
57	MG	1H	3182	1/1	0.95	0.57	60,60,60,60	0
57	MG	1H	3323	1/1	0.96	0.17	57,57,57,57	0
57	MG	1H	3324	1/1	0.96	0.08	70,70,70,70	0
57	MG	1H	3070	1/1	0.96	0.34	75,75,75,75	0
57	MG	14	3089	1/1	0.96	0.24	54,54,54,54	0
57	MG	13	1689	1/1	0.96	0.07	88,88,88,88	0
57	MG	14	3372	1/1	0.96	0.12	86,86,86,86	0
57	MG	1H	3330	1/1	0.96	0.10	71,71,71,71	0
57	MG	13	1690	1/1	0.96	0.05	70,70,70,70	0
57	MG	1H	3199	1/1	0.96	0.12	61,61,61,61	0
57	MG	13	1604	1/1	0.96	0.15	62,62,62,62	0
57	MG	14	3096	1/1	0.96	0.20	65,65,65,65	0
57	MG	1H	3335	1/1	0.96	0.14	48,48,48,48	0
57	MG	1H	3272	1/1	0.96	0.09	63,63,63,63	0
57	MG	1H	3461	1/1	0.96	0.06	45,45,45,45	0
57	MG	14	3280	1/1	0.96	0.14	61,61,61,61	0
57	MG	1H	3399	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3182	1/1	0.96	0.36	74,74,74,74	0
57	MG	14	3102	1/1	0.96	0.56	85,85,85,85	0
57	MG	1H	3463	1/1	0.96	0.09	81,81,81,81	0
57	MG	1H	3464	1/1	0.96	0.08	63,63,63,63	0
57	MG	1H	3465	1/1	0.96	0.09	67,67,67,67	0
57	MG	14	3287	1/1	0.96	0.11	88,88,88,88	0
57	MG	1H	3400	1/1	0.96	0.12	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3012	1/1	0.96	0.32	57,57,57,57	0
57	MG	13	1705	1/1	0.96	0.17	97,97,97,97	0
57	MG	14	3016	1/1	0.96	0.38	74,74,74,74	0
57	MG	14	3394	1/1	0.96	0.05	91,91,91,91	0
57	MG	1H	3402	1/1	0.96	0.05	85,85,85,85	0
57	MG	1H	3338	1/1	0.96	0.11	66,66,66,66	0
57	MG	14	3194	1/1	0.96	0.22	80,80,80,80	0
57	MG	1H	3471	1/1	0.96	0.12	90,90,90,90	0
57	MG	1H	3275	1/1	0.96	0.18	57,57,57,57	0
57	MG	1H	3022	1/1	0.96	0.19	49,49,49,49	0
57	MG	13	1692	1/1	0.96	0.18	72,72,72,72	0
57	MG	14	3116	1/1	0.96	0.13	88,88,88,88	0
57	MG	1H	3342	1/1	0.96	0.06	86,86,86,86	0
57	MG	1H	3024	1/1	0.96	0.24	83,83,83,83	0
57	MG	14	3027	1/1	0.96	0.14	66,66,66,66	0
57	MG	1H	3025	1/1	0.96	0.35	75,75,75,75	0
57	MG	13	1693	1/1	0.96	0.07	85,85,85,85	0
57	MG	14	3310	1/1	0.96	0.15	54,54,54,54	0
57	MG	1H	3207	1/1	0.96	0.24	92,92,92,92	0
57	MG	14	3031	1/1	0.96	0.28	73,73,73,73	0
57	MG	1H	3208	1/1	0.96	0.15	72,72,72,72	0
57	MG	14	3314	1/1	0.96	0.16	69,69,69,69	0
57	MG	1H	3286	1/1	0.96	0.12	40,40,40,40	0
57	MG	1H	3287	1/1	0.96	0.08	71,71,71,71	0
57	MG	13	1608	1/1	0.96	0.08	76,76,76,76	0
57	MG	1H	3029	1/1	0.96	0.32	77,77,77,77	0
57	MG	1H	3290	1/1	0.96	0.12	55,55,55,55	0
57	MG	13	1736	1/1	0.96	0.12	101,101,101,101	0
57	MG	14	3217	1/1	0.96	0.20	56,56,56,56	0
57	MG	1H	3033	1/1	0.96	0.25	70,70,70,70	0
57	MG	14	3324	1/1	0.96	0.15	48,48,48,48	0
57	MG	14	3219	1/1	0.96	0.10	57,57,57,57	0
57	MG	14	3044	1/1	0.96	0.18	57,57,57,57	0
57	MG	1G	1603	1/1	0.96	0.14	88,88,88,88	0
57	MG	1H	3214	1/1	0.96	0.47	77,77,77,77	0
57	MG	13	1652	1/1	0.96	0.62	71,71,71,71	0
57	MG	1H	3297	1/1	0.96	0.14	49,49,49,49	0
57	MG	1H	3183	1/1	0.96	0.21	70,70,70,70	0
57	MG	1H	3426	1/1	0.96	0.05	74,74,74,74	0
57	MG	1H	3248	1/1	0.96	0.11	44,44,44,44	0
57	MG	14	3140	1/1	0.96	0.13	51,51,51,51	0
57	MG	14	3234	1/1	0.96	0.18	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1614	1/1	0.96	0.34	84,84,84,84	0
57	MG	14	3059	1/1	0.96	0.23	89,89,89,89	0
57	MG	1H	3495	1/1	0.96	0.05	97,97,97,97	0
57	MG	14	3240	1/1	0.96	0.12	73,73,73,73	0
57	MG	13	1632	1/1	0.96	0.22	78,78,78,78	0
57	MG	1H	3369	1/1	0.96	0.08	44,44,44,44	0
57	MG	1H	3188	1/1	0.96	0.41	49,49,49,49	0
57	MG	1H	3305	1/1	0.96	0.14	63,63,63,63	0
57	MG	1H	3307	1/1	0.96	0.14	44,44,44,44	0
57	MG	1H	3112	1/1	0.96	0.26	55,55,55,55	0
57	MG	13	1680	1/1	0.96	0.16	64,64,64,64	0
57	MG	13	1699	1/1	0.96	0.09	83,83,83,83	0
57	MG	1H	3258	1/1	0.96	0.11	47,47,47,47	0
57	MG	1H	3440	1/1	0.96	0.09	92,92,92,92	0
57	MG	13	1623	1/1	0.96	0.22	76,76,76,76	0
57	MG	1H	3042	1/1	0.96	0.26	65,65,65,65	0
57	MG	1H	3014	1/1	0.96	0.17	53,53,53,53	0
57	MG	1H	3317	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3318	1/1	0.96	0.15	59,59,59,59	0
57	MG	1G	1698	1/1	0.96	0.10	123,123,123,123	0
57	MG	14	3078	1/1	0.96	0.29	56,56,56,56	0
57	MG	1H	3263	1/1	0.96	0.19	46,46,46,46	0
57	MG	14	3261	1/1	0.96	0.17	59,59,59,59	0
57	MG	1G	1631	1/1	0.96	0.56	92,92,92,92	0
57	MG	14	3082	1/1	0.96	0.49	79,79,79,79	0
57	MG	14	3364	1/1	0.96	0.07	92,92,92,92	0
57	MG	1H	3166	1/1	0.96	0.43	78,78,78,78	0
57	MG	1H	3387	1/1	0.96	0.10	33,33,33,33	0
57	MG	1H	3056	1/1	0.97	0.31	49,49,49,49	0
57	MG	1H	3439	1/1	0.97	0.07	67,67,67,67	0
57	MG	14	3081	1/1	0.97	0.15	56,56,56,56	0
57	MG	1G	1601	1/1	0.97	0.20	77,77,77,77	0
57	MG	1H	3018	1/1	0.97	0.18	41,41,41,41	0
57	MG	14	3026	1/1	0.97	0.29	56,56,56,56	0
57	MG	13	1663	1/1	0.97	0.10	107,107,107,107	0
57	MG	14	3199	1/1	0.97	0.38	76,76,76,76	0
57	MG	14	3086	1/1	0.97	0.23	56,56,56,56	0
57	MG	1H	3262	1/1	0.97	0.18	43,43,43,43	0
57	MG	14	3270	1/1	0.97	0.13	67,67,67,67	0
57	MG	13	1606	1/1	0.97	0.26	72,72,72,72	0
57	MG	1H	3315	1/1	0.97	0.10	63,63,63,63	0
57	MG	1H	3411	1/1	0.97	0.07	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3032	1/1	0.97	0.41	64,64,64,64	0
57	MG	1G	1651	1/1	0.97	0.11	76,76,76,76	0
57	MG	14	3093	1/1	0.97	0.42	84,84,84,84	0
57	MG	1H	3264	1/1	0.97	0.25	50,50,50,50	0
57	MG	1H	3413	1/1	0.97	0.10	78,78,78,78	0
57	MG	14	3037	1/1	0.97	0.26	65,65,65,65	0
57	MG	1H	3448	1/1	0.97	0.07	80,80,80,80	0
57	MG	1H	3265	1/1	0.97	0.08	46,46,46,46	0
57	MG	13	1602	1/1	0.97	0.14	120,120,120,120	0
57	MG	1H	3382	1/1	0.97	0.09	49,49,49,49	0
57	MG	14	3101	1/1	0.97	0.33	87,87,87,87	0
57	MG	1H	3011	1/1	0.97	0.30	56,56,56,56	0
57	MG	1H	3090	1/1	0.97	0.21	42,42,42,42	0
57	MG	14	3045	1/1	0.97	0.20	53,53,53,53	0
57	MG	1H	3012	1/1	0.97	0.42	58,58,58,58	0
57	MG	14	3048	1/1	0.97	0.47	51,51,51,51	0
57	MG	1G	1661	1/1	0.97	0.08	95,95,95,95	0
57	MG	1H	3353	1/1	0.97	0.14	48,48,48,48	0
57	MG	14	3226	1/1	0.97	0.16	51,51,51,51	0
57	MG	14	3293	1/1	0.97	0.10	63,63,63,63	0
57	MG	1H	3354	1/1	0.97	0.17	60,60,60,60	0
57	MG	14	3052	1/1	0.97	0.23	54,54,54,54	0
57	MG	14	3231	1/1	0.97	0.23	55,55,55,55	0
57	MG	1H	3247	1/1	0.97	0.14	36,36,36,36	0
57	MG	1H	3036	1/1	0.97	0.16	37,37,37,37	0
57	MG	1H	3328	1/1	0.97	0.13	47,47,47,47	0
57	MG	13	1609	1/1	0.97	0.15	70,70,70,70	0
57	MG	14	3171	1/1	0.97	0.34	56,56,56,56	0
57	MG	1H	3361	1/1	0.97	0.07	52,52,52,52	0
57	MG	14	3239	1/1	0.97	0.17	77,77,77,77	0
57	MG	14	3375	1/1	0.97	0.07	93,93,93,93	0
57	MG	14	3002	1/1	0.97	0.37	57,57,57,57	0
57	MG	14	3308	1/1	0.97	0.10	94,94,94,94	0
57	MG	1H	3273	1/1	0.97	0.14	78,78,78,78	0
57	MG	14	3004	1/1	0.97	0.28	63,63,63,63	0
57	MG	16	211	1/1	0.97	0.11	73,73,73,73	0
57	MG	13	1605	1/1	0.97	0.20	71,71,71,71	0
57	MG	1G	1672	1/1	0.97	0.12	110,110,110,110	0
57	MG	1H	3364	1/1	0.97	0.09	44,44,44,44	0
57	MG	21	303	1/1	0.97	0.09	46,46,46,46	0
57	MG	1H	3466	1/1	0.97	0.05	72,72,72,72	0
57	MG	1H	3169	1/1	0.97	0.45	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1734	1/1	0.97	0.10	94,94,94,94	0
57	MG	14	3014	1/1	0.97	0.25	59,59,59,59	0
57	MG	14	3253	1/1	0.97	0.07	58,58,58,58	0
57	MG	1H	3304	1/1	0.97	0.10	58,58,58,58	0
57	MG	1H	3186	1/1	0.97	0.26	62,62,62,62	0
57	MG	1H	3306	1/1	0.97	0.09	75,75,75,75	0
57	MG	1H	3040	1/1	0.97	0.31	44,44,44,44	0
57	MG	1H	3027	1/1	0.97	0.19	52,52,52,52	0
57	MG	1H	3437	1/1	0.97	0.09	92,92,92,92	0
57	MG	14	3147	1/1	0.98	0.40	69,69,69,69	0
57	MG	14	3191	1/1	0.98	0.26	67,67,67,67	0
57	MG	1H	3255	1/1	0.98	0.08	49,49,49,49	0
57	MG	14	3294	1/1	0.98	0.05	75,75,75,75	0
57	MG	13	1648	1/1	0.98	0.16	67,67,67,67	0
57	MG	1H	3319	1/1	0.98	0.18	57,57,57,57	0
57	MG	14	3066	1/1	0.98	0.57	61,61,61,61	0
57	MG	1G	1622	1/1	0.98	0.20	125,125,125,125	0
57	MG	13	1619	1/1	0.98	0.21	52,52,52,52	0
57	MG	14	3356	1/1	0.98	0.06	75,75,75,75	0
57	MG	1H	3349	1/1	0.98	0.12	50,50,50,50	0
57	MG	14	3301	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3380	1/1	0.98	0.18	55,55,55,55	0
57	MG	1H	3015	1/1	0.98	0.31	51,51,51,51	0
57	MG	1G	1627	1/1	0.98	0.41	87,87,87,87	0
57	MG	14	3305	1/1	0.98	0.12	49,49,49,49	0
57	MG	1H	3322	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3187	1/1	0.98	0.42	44,44,44,44	0
57	MG	1H	3016	1/1	0.98	0.19	44,44,44,44	0
57	MG	1H	3385	1/1	0.98	0.15	25,25,25,25	0
57	MG	14	3206	1/1	0.98	0.27	85,85,85,85	0
57	MG	1H	3278	1/1	0.98	0.09	75,75,75,75	0
57	MG	14	3034	1/1	0.98	0.48	40,40,40,40	0
57	MG	1G	1633	1/1	0.98	0.21	118,118,118,118	0
57	MG	1H	3327	1/1	0.98	0.08	50,50,50,50	0
57	MG	1H	3152	1/1	0.98	0.41	70,70,70,70	0
57	MG	1H	3302	1/1	0.98	0.13	51,51,51,51	0
57	MG	1H	3280	1/1	0.98	0.15	36,36,36,36	0
57	MG	14	3040	1/1	0.98	0.25	68,68,68,68	0
57	MG	1H	3359	1/1	0.98	0.17	44,44,44,44	0
57	MG	14	3216	1/1	0.98	0.21	52,52,52,52	0
57	MG	1H	3281	1/1	0.98	0.15	61,61,61,61	0
57	MG	14	3322	1/1	0.98	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1601	1/1	0.98	0.42	80,80,80,80	0
57	MG	1H	3333	1/1	0.98	0.13	77,77,77,77	0
57	MG	14	3325	1/1	0.98	0.04	79,79,79,79	0
57	MG	1H	3097	1/1	0.98	0.06	65,65,65,65	0
57	MG	1G	1607	1/1	0.98	0.20	86,86,86,86	0
57	MG	14	3222	1/1	0.98	0.20	59,59,59,59	0
57	MG	14	3047	1/1	0.98	0.34	65,65,65,65	0
57	MG	1H	3044	1/1	0.98	0.36	67,67,67,67	0
57	MG	29	301	1/1	0.98	0.35	58,58,58,58	0
57	MG	1H	3045	1/1	0.98	0.28	46,46,46,46	0
57	MG	1H	3398	1/1	0.98	0.07	78,78,78,78	0
57	MG	13	1621	1/1	0.98	0.09	85,85,85,85	0
57	MG	14	3228	1/1	0.98	0.14	56,56,56,56	0
57	MG	14	3229	1/1	0.98	0.13	59,59,59,59	0
57	MG	13	1702	1/1	0.98	0.13	85,85,85,85	0
57	MG	1H	3311	1/1	0.98	0.09	53,53,53,53	0
57	MG	14	3013	1/1	0.98	0.23	47,47,47,47	0
57	MG	13	1603	1/1	0.98	0.24	74,74,74,74	0
57	MG	1H	3252	1/1	0.98	0.09	65,65,65,65	0
57	MG	14	3341	1/1	0.98	0.12	66,66,66,66	0
57	MG	14	3235	1/1	0.98	0.24	48,48,48,48	0
60	ZN	5A	101	1/1	0.98	0.09	146,146,146,146	0
57	MG	1H	3210	1/1	0.98	0.18	56,56,56,56	0
57	MG	1H	3292	1/1	0.98	0.21	43,43,43,43	0
57	MG	1H	3254	1/1	0.98	0.08	46,46,46,46	0
57	MG	14	3019	1/1	0.98	0.35	57,57,57,57	0
57	MG	13	1607	1/1	0.99	0.20	72,72,72,72	0
57	MG	1H	3059	1/1	0.99	0.27	56,56,56,56	0
57	MG	1H	3060	1/1	0.99	0.16	35,35,35,35	0
57	MG	14	3242	1/1	0.99	0.10	62,62,62,62	0
57	MG	1H	3091	1/1	0.99	0.15	41,41,41,41	0
57	MG	1H	3031	1/1	0.99	0.14	51,51,51,51	0
57	MG	1H	3325	1/1	0.99	0.15	46,46,46,46	0
57	MG	1H	3121	1/1	0.99	0.24	39,39,39,39	0
59	SF4	3E	301	8/8	0.99	0.21	82,91,95,98	0
59	SF4	32	302	8/8	0.99	0.17	100,109,118,124	0
60	ZN	5I	102	1/1	0.99	0.13	86,86,86,86	0
57	MG	1H	3032	1/1	0.99	0.25	47,47,47,47	0
57	MG	1H	3291	1/1	0.99	0.13	59,59,59,59	0
57	MG	13	1630	1/1	0.99	0.34	96,96,96,96	0
57	MG	1H	3360	1/1	0.99	0.09	78,78,78,78	0
57	MG	14	3055	1/1	0.99	0.30	60,60,60,60	0

Continued on next page...

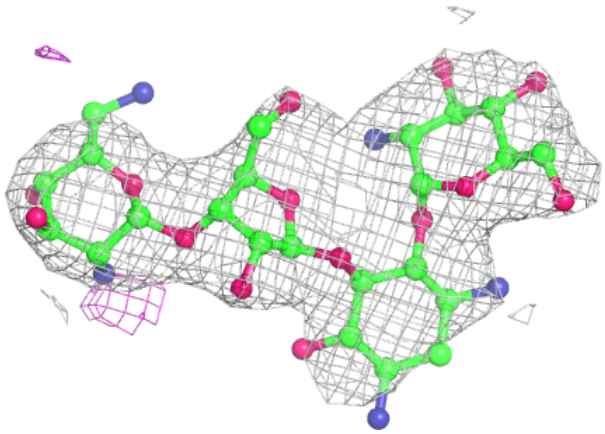
Continued from previous page...

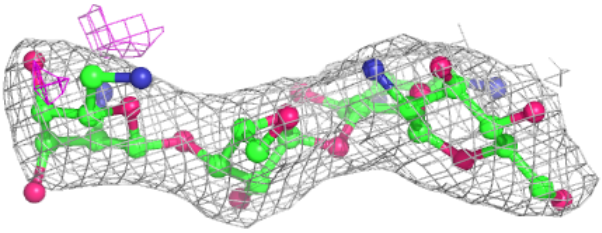
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3056	1/1	0.99	0.11	54,54,54,54	0
57	MG	1H	3450	1/1	1.00	0.06	44,44,44,44	0

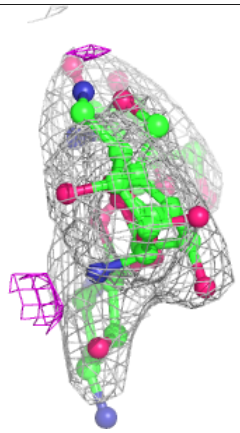
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR 1G 1702:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

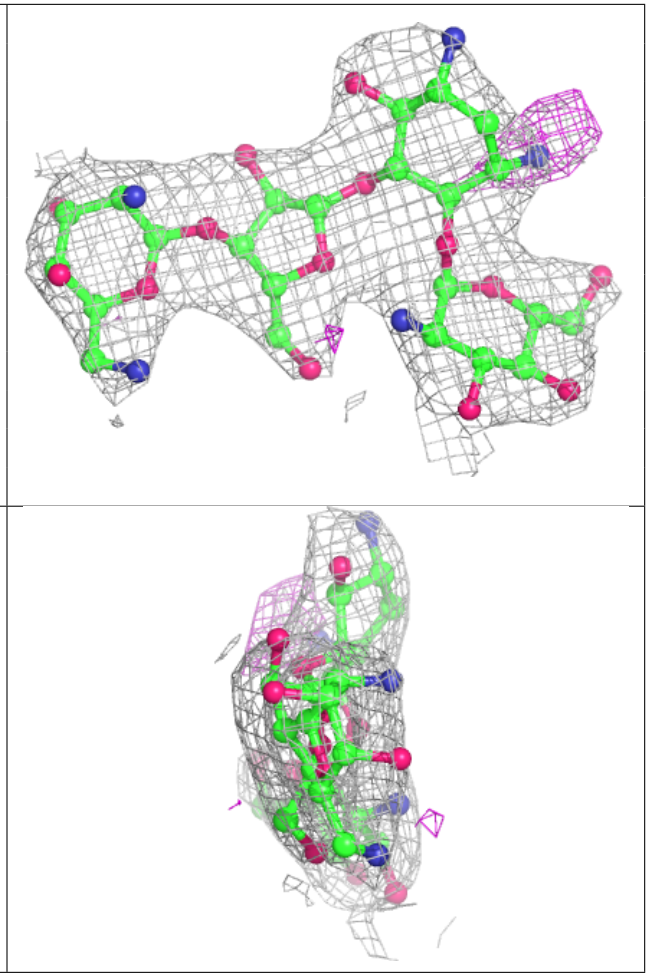






Electron density around PAR 13 1741:

$2mF_o$-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.