wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 09:33 pm BST

PDB ID	:	5EL6 / pdb_00005el6
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and tRNALys in the A-site with a U-U mismatch in the first position and antibiotic paromomycin
Authors	:	Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on	:	2015-11-04
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

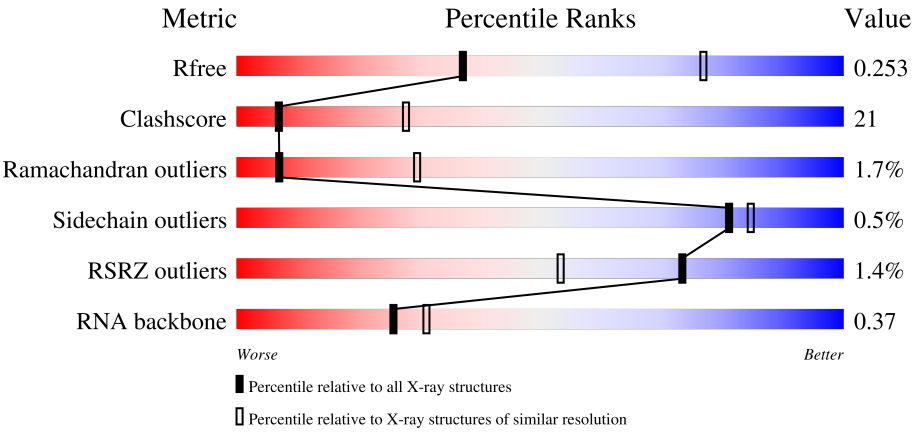
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



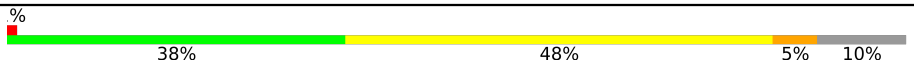
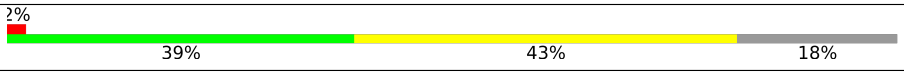
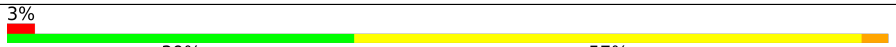
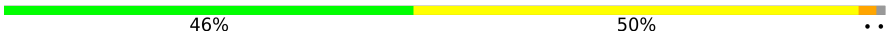
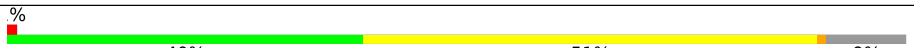
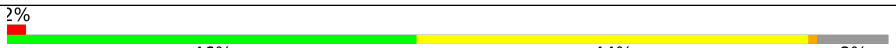
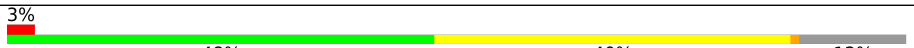
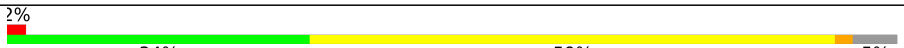
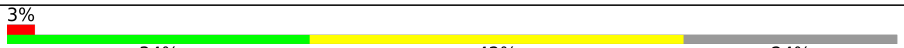
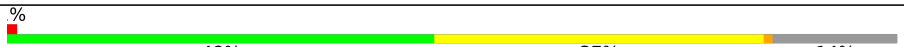
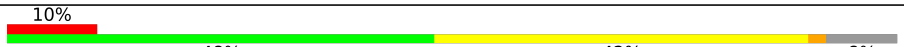
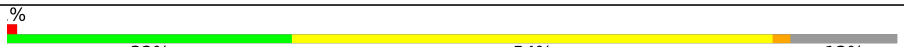
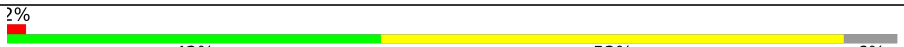
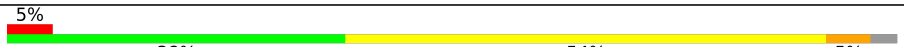
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	35% 47% 16%
1	1G	1522	32% 50% 17%
2	12	256	% 35% 43% 18%

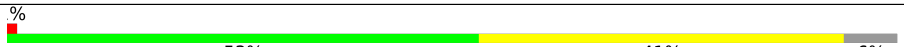
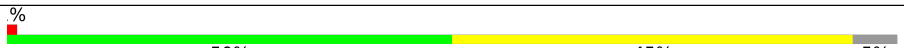
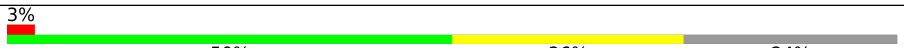
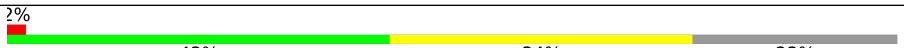
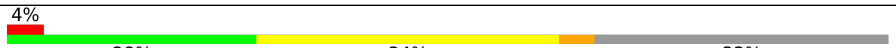
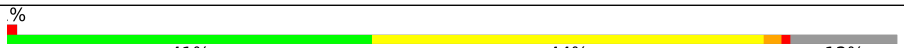
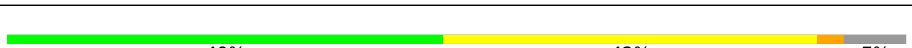
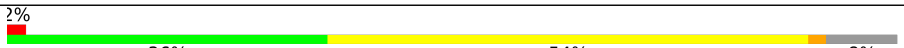
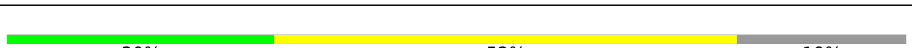
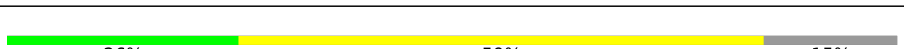
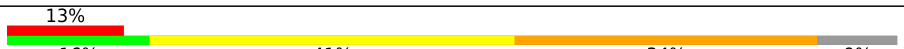
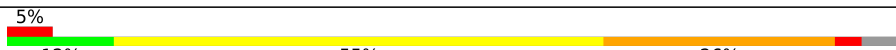
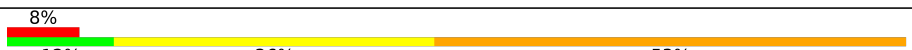
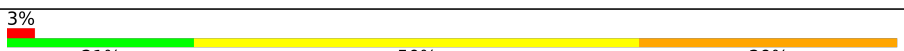
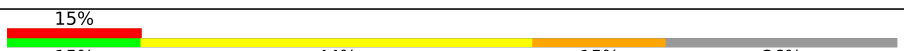
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Mol	Chain	Length	Quality of chain
2	1E	256	
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	

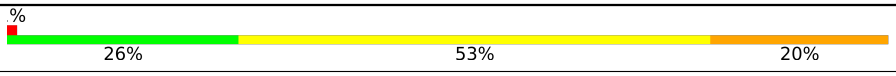
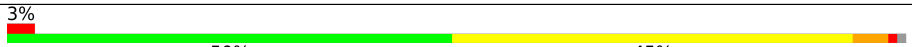
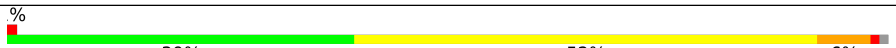
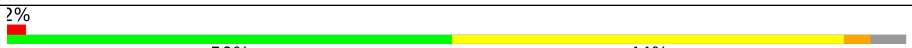
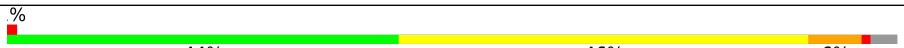
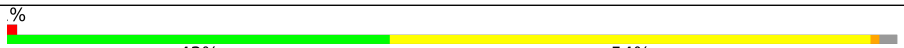
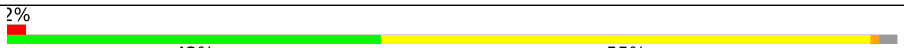
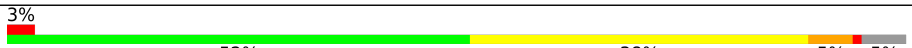
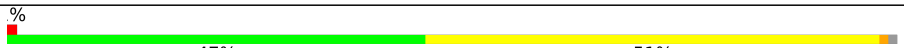
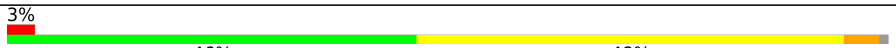
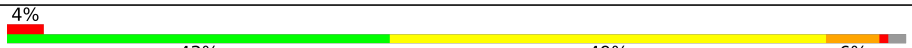
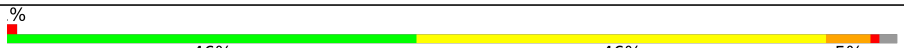
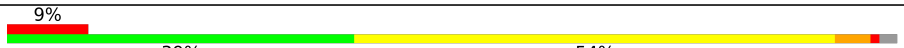
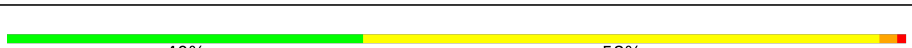
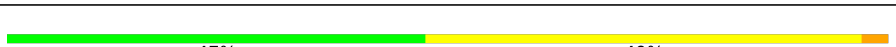
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Mol	Chain	Length	Quality of chain
15	6A	89	
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	

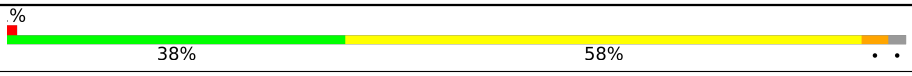
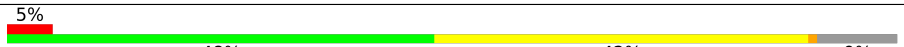
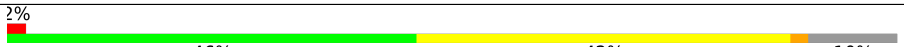
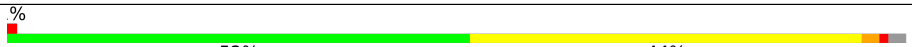
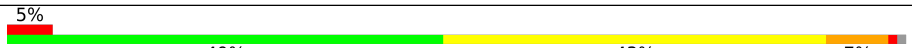
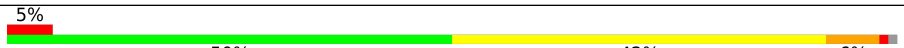
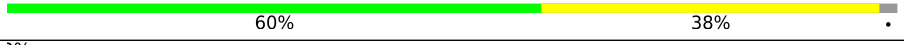
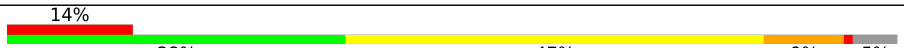
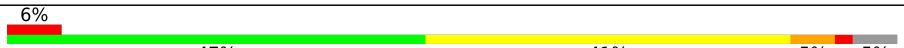
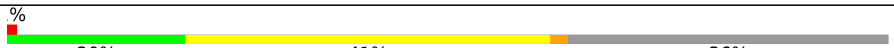
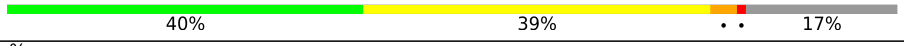
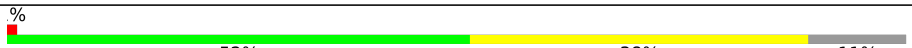
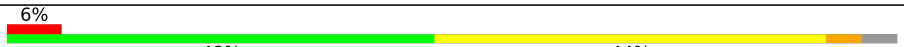
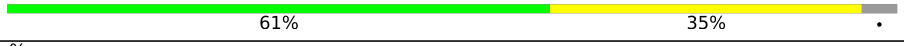
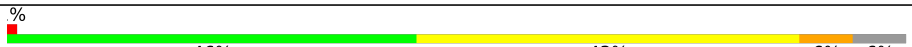
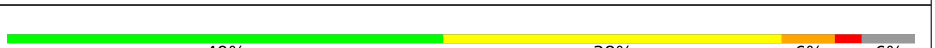
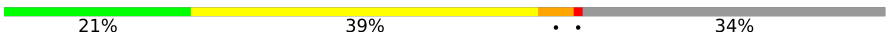
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Mol	Chain	Length	Quality of chain
27	1J	122	
28	71	229	
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	

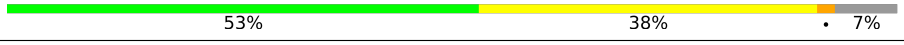
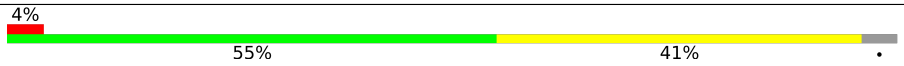
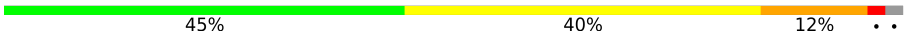
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Mol	Chain	Length	Quality of chain
40	65	112	
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	

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Mol	Chain	Length	Quality of chain
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1702	-	-	-	X
56	MG	14	3039	-	-	-	X
56	MG	14	3287	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3291	-	-	-	X
58	SF4	32	301	-	-	X	-
58	SF4	3E	302	-	-	X	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 294257 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1A	80	Total C N O 646 403 129 114	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	2I	111	Total C N O S 823 512 154 154 3	0	0	0
11	2A	113	Total C N O S 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
12	3I	122	Total C N O S 956 603 193 159 1	0	0	0
12	3A	122	Total C N O S 956 603 193 159 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	5I	60	Total C N O S 491 312 104 71 4	0	0	0
14	5A	59	Total C N O S 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
15	6I	87	Total C N O S 729 457 146 124 2	0	0	0
15	6A	87	Total C N O S 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
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			658	419	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total 1477	C 662	N 257	O 488	P 69	S 1	0	0	0
22	1L	73	Total 1563	C 700	N 271	O 518	P 73	S 1	0	0	0

- Molecule 23 is a RNA chain called E. coli tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total 1611	C 721	N 281	O 534	P 75	0	0	0
24	3L	76	Total 1611	C 721	N 281	O 534	P 75	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total 439	C 197	N 91	O 131	P 20	0	0	0
25	4L	18	Total 395	C 177	N 81	O 119	P 18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total 61028	C 27159	N 11418	O 19618	P 2833	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	69	Total	C	N	O		0	0	0
			539	339	109	91				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	132	Total 1101	C 686	N 227	O 188		0	0	0
41	75	133	Total 1109	C 691	N 228	O 189	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total 890	C 560	N 175	O 153	S 2	0	0	0
44	A5	111	Total 886	C 558	N 174	O 152	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total 743	C 482	N 134	O 126	S 1	0	0	0

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	G8	105	Total C N O S 796 513 150 128 5	0	0	0
46	C5	105	Total C N O S 799 513 153 128 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	H8	171	Total C N O S 1373 876 247 247 3	0	0	0
47	D5	132	Total C N O S 1074 691 193 188 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	J8	94	Total C N O S 737 463 146 127 1	0	0	0
49	F5	94	Total C N O S 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
50	K8	68	Total C N O S 568 352 115 100 1	0	0	0
50	G5	68	Total C N O S 568 352 115 100 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

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

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

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	131	Total	Mg	0	0
			131	131		

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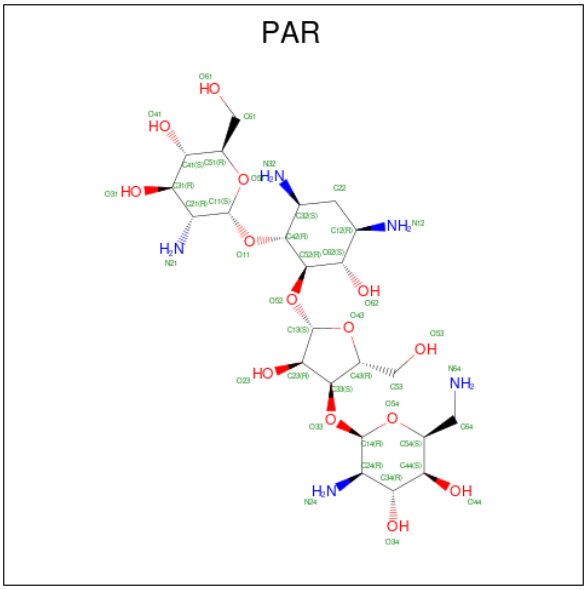
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	3E	1	Total Mg 1 1	0	0
56	5E	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	5I	1	Total Mg 1 1	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	3	Total Mg 3 3	0	0
56	3K	1	Total Mg 1 1	0	0
56	4K	1	Total Mg 1 1	0	0
56	1H	429	Total Mg 429 429	0	0
56	16	11	Total Mg 11 11	0	0
56	21	2	Total Mg 2 2	0	0
56	41	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	88	2	Total Mg 2 2	0	0
56	I8	3	Total Mg 3 3	0	0
56	L8	1	Total Mg 1 1	0	0
56	P8	1	Total Mg 1 1	0	0
56	Q8	1	Total Mg 1 1	0	0
56	1G	81	Total Mg 81 81	0	0
56	2L	3	Total Mg 3 3	0	0
56	14	382	Total Mg 382 382	0	0

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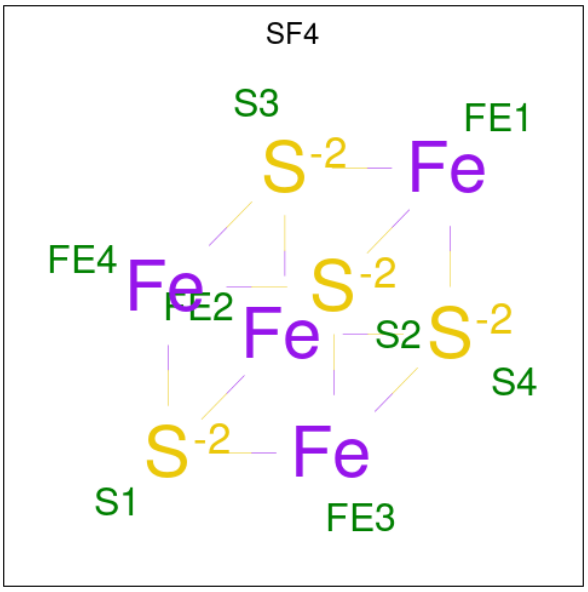
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1J	5	Total Mg 5 5	0	0
56	29	1	Total Mg 1 1	0	0
56	39	1	Total Mg 1 1	0	0
56	35	1	Total Mg 1 1	0	0
56	45	3	Total Mg 3 3	0	0
56	85	1	Total Mg 1 1	0	0
56	C5	1	Total Mg 1 1	0	0
56	E5	1	Total Mg 1 1	0	0

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	13	144	Total O 144 144	0	0
60	3E	2	Total O 2 2	0	0
60	1I	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	2	Total O 2 2	0	0
60	6I	1	Total O 1 1	0	0
60	7I	1	Total O 1 1	0	0
60	BI	1	Total O 1 1	0	0
60	3K	1	Total O 1 1	0	0
60	4K	3	Total O 3 3	0	0
60	1H	540	Total O 540 540	0	0
60	16	22	Total O 22 22	0	0
60	11	10	Total O 10 10	0	0
60	31	7	Total O 7 7	0	0
60	58	2	Total O 2 2	0	0
60	78	4	Total O 4 4	0	0
60	98	1	Total O 1 1	0	0
60	G8	1	Total O 1 1	0	0
60	I8	2	Total O 2 2	0	0
60	L8	3	Total O 3 3	0	0
60	P8	1	Total O 1 1	0	0
60	1G	68	Total O 68 68	0	0
60	32	2	Total O 2 2	0	0
60	14	367	Total O 367 367	0	0
60	1J	12	Total O 12 12	0	0

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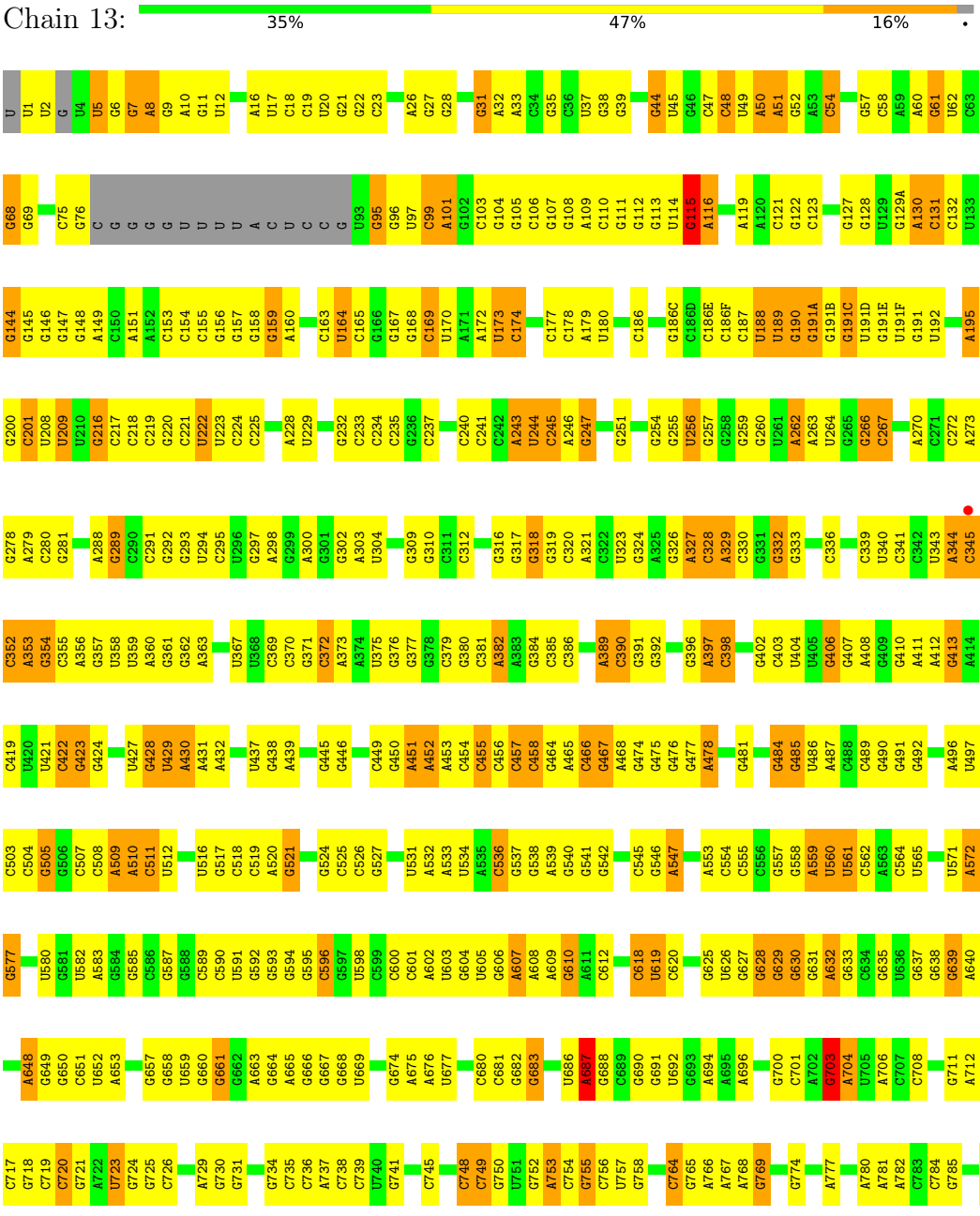
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	19	8	Total O 8 8	0	0
60	29	2	Total O 2 2	0	0
60	39	3	Total O 3 3	0	0
60	35	2	Total O 2 2	0	0
60	55	2	Total O 2 2	0	0
60	H5	1	Total O 1 1	0	0
60	L5	1	Total O 1 1	0	0

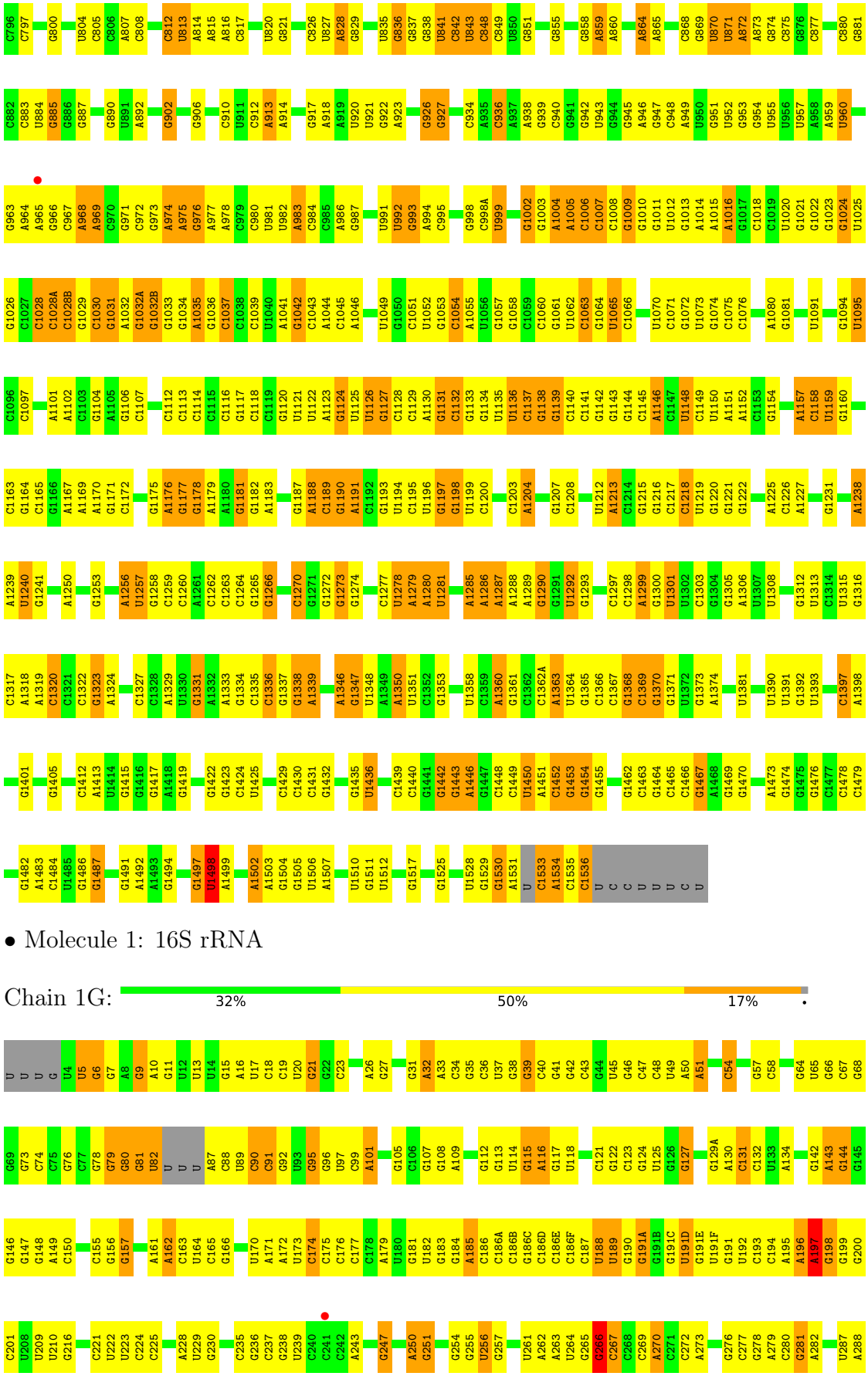
3 Residue-property plots (i)

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 rRNA

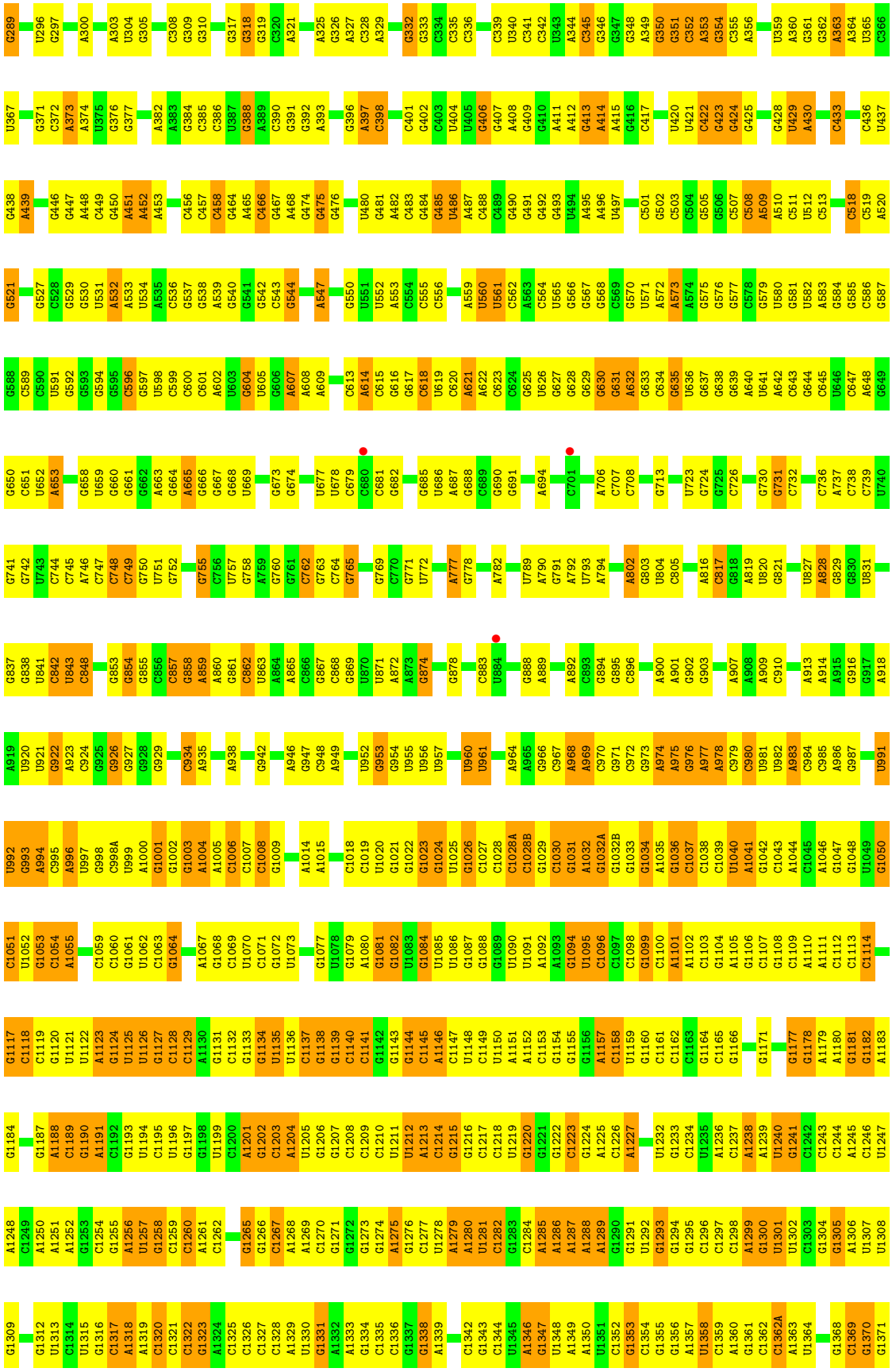
Chain 13:

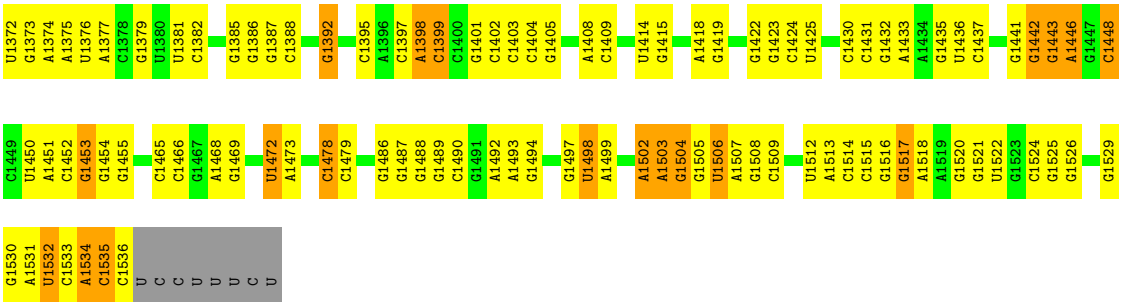




• Molecule 1: 16S rRNA

Chain 1G:

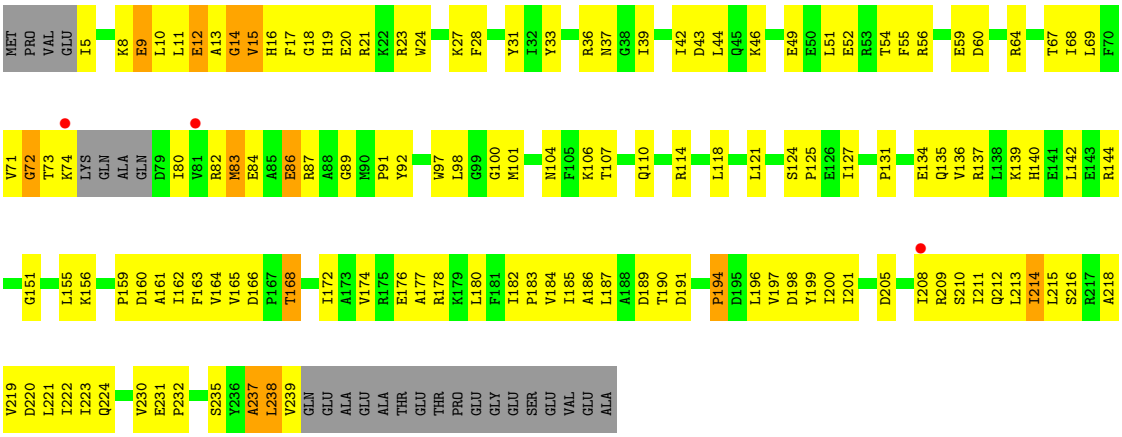




• Molecule 2: 30S ribosomal protein S2

Chain 1E:

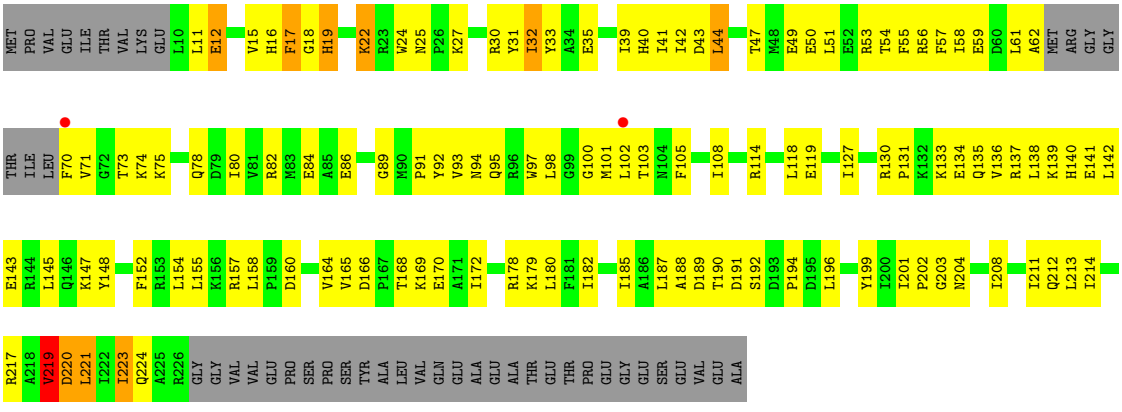




• Molecule 2: 30S ribosomal protein S2

Chain 12:

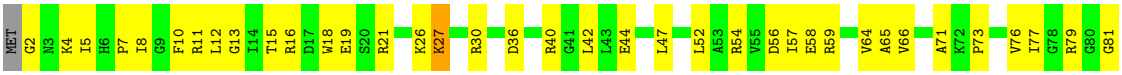


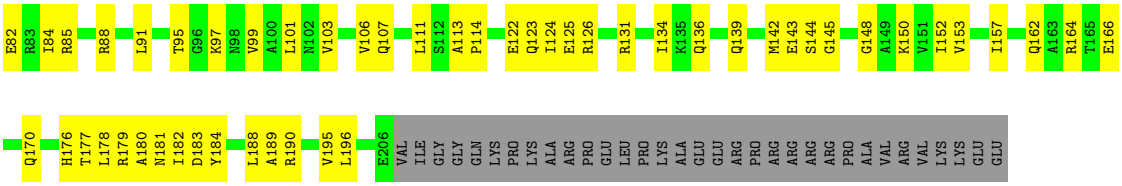


• Molecule 3: 30S ribosomal protein S3

Chain 2E:



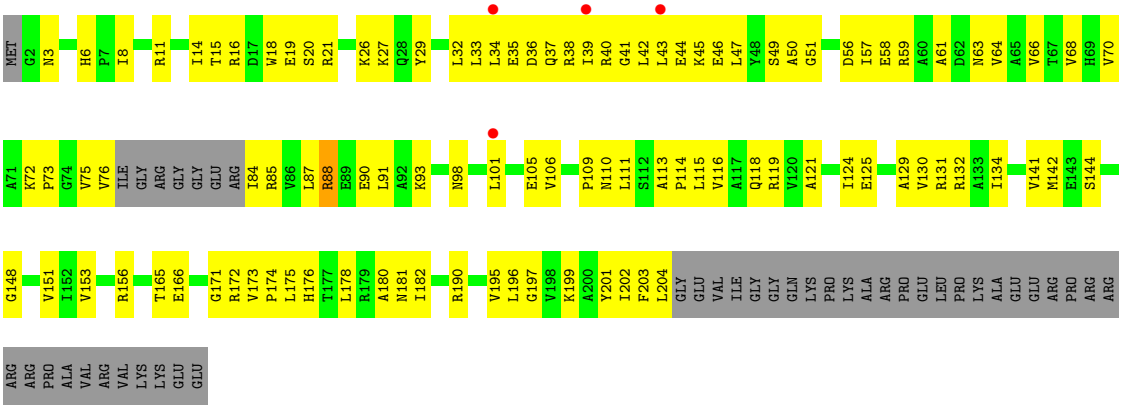




• Molecule 3: 30S ribosomal protein S3

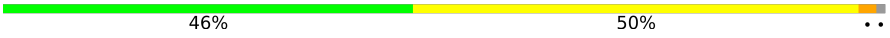
Chain 22:

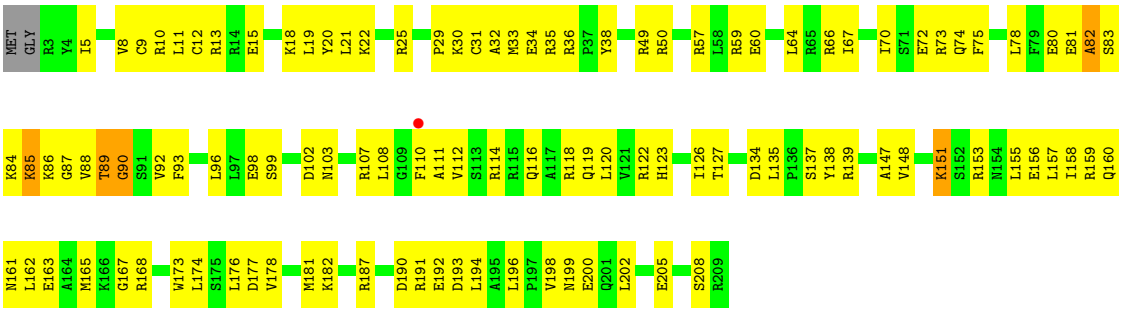




• Molecule 4: 30S ribosomal protein S4

Chain 3E:

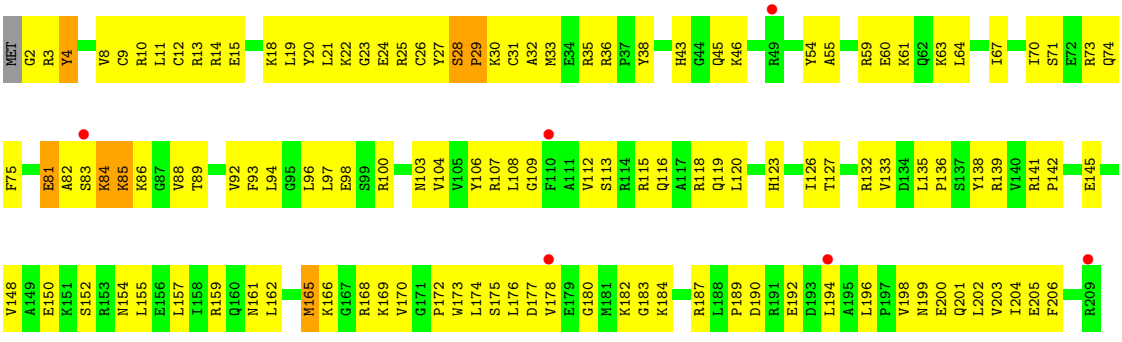




• Molecule 4: 30S ribosomal protein S4

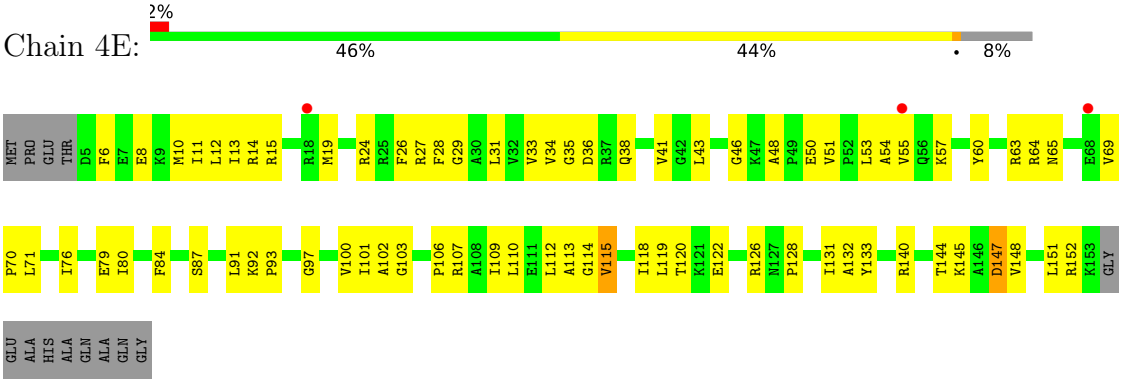
Chain 32:





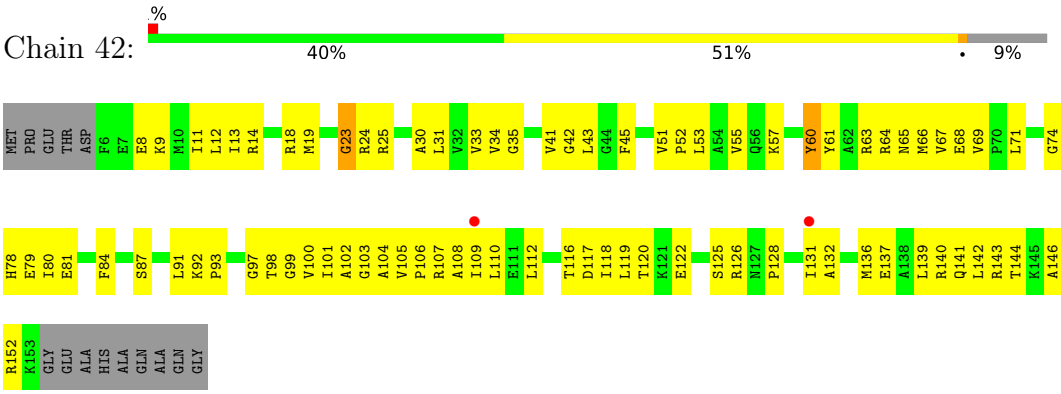
• Molecule 5: 30S ribosomal protein S5

Chain 4E:



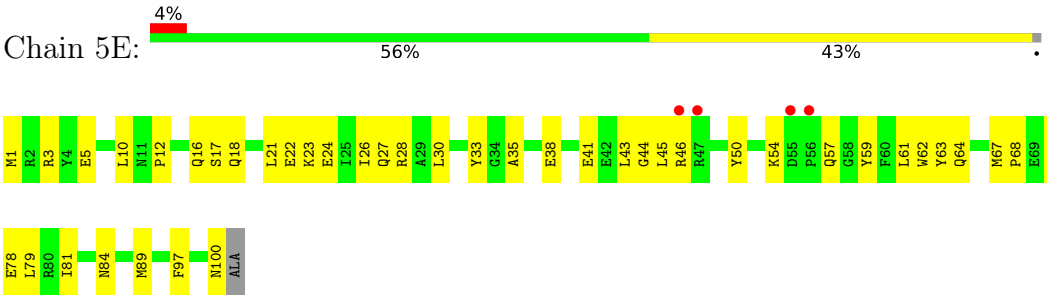
• Molecule 5: 30S ribosomal protein S5

Chain 42:



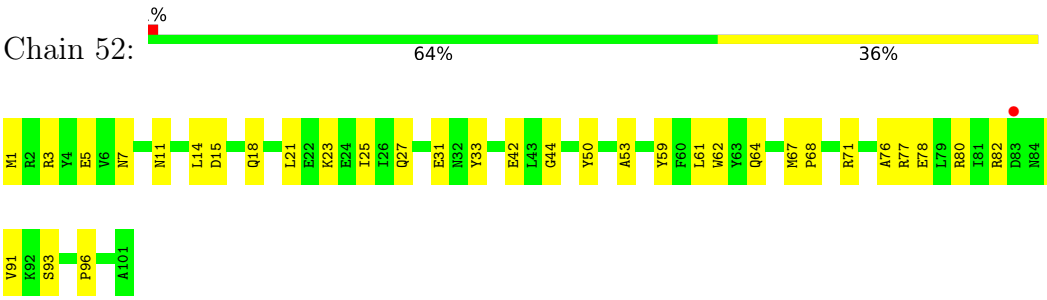
• Molecule 6: 30S ribosomal protein S6

Chain 5E:



• Molecule 6: 30S ribosomal protein S6

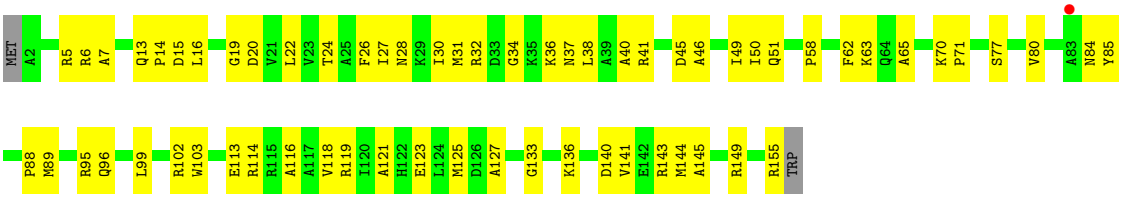
Chain 52:



• Molecule 7: 30S ribosomal protein S7

Chain 6E:

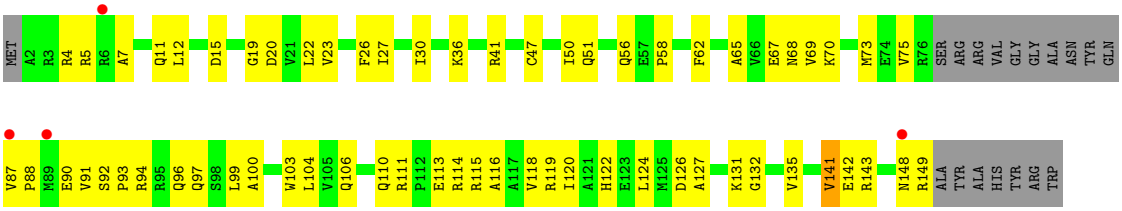




• Molecule 7: 30S ribosomal protein S7

Chain 62:

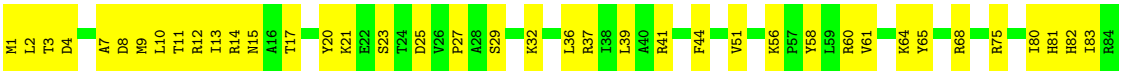




• Molecule 8: 30S ribosomal protein S8

Chain 7E:







• Molecule 8: 30S ribosomal protein S8

Chain 72:

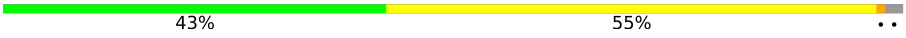




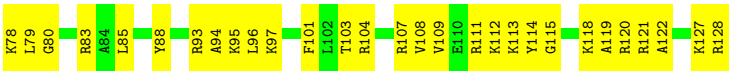


• Molecule 9: 30S ribosomal protein S9

Chain 8E:

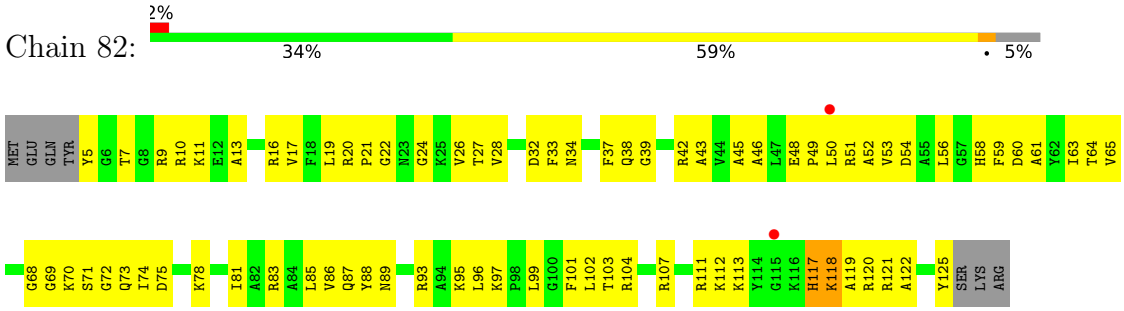






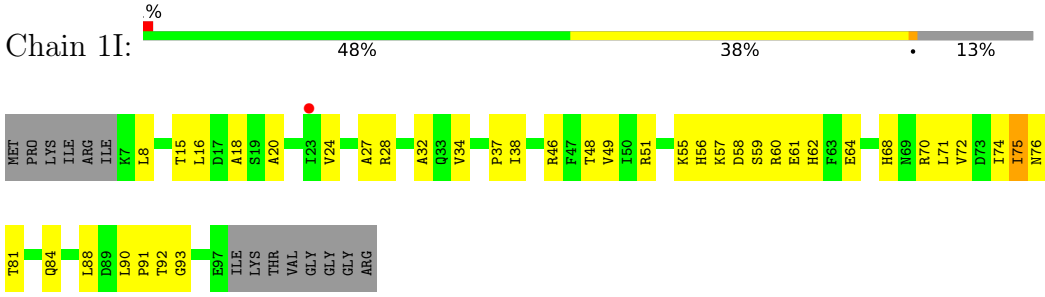
• Molecule 9: 30S ribosomal protein S9

Chain 82:



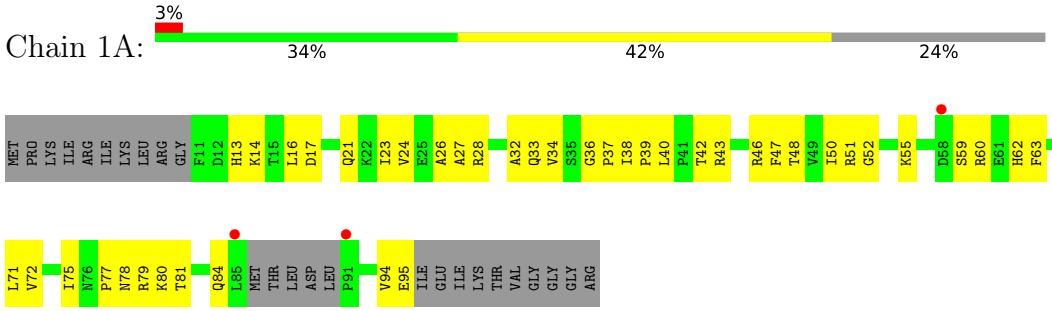
• Molecule 10: 30S ribosomal protein S10

Chain 1I:



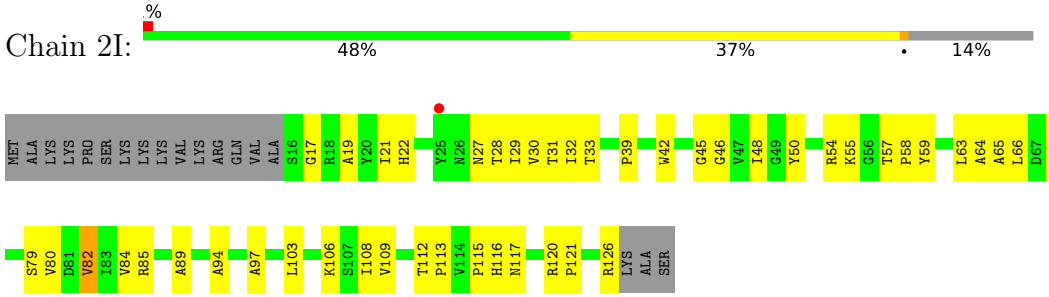
• Molecule 10: 30S ribosomal protein S10

Chain 1A:



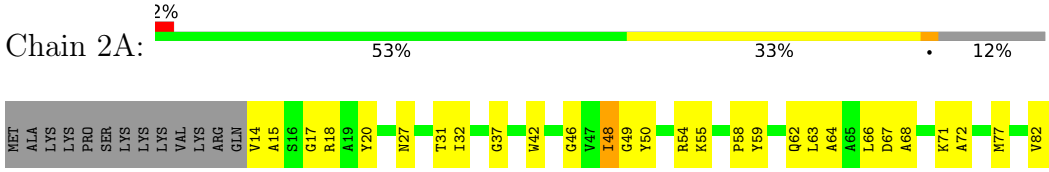
• Molecule 11: 30S ribosomal protein S11

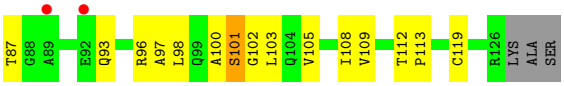
Chain 2I:



• Molecule 11: 30S ribosomal protein S11

Chain 2A:

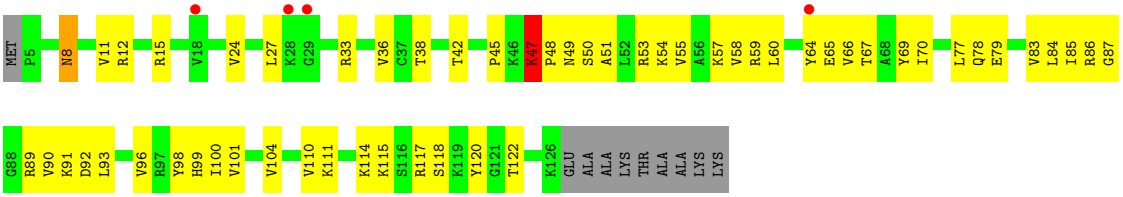




• Molecule 12: 30S ribosomal protein S12

Chain 3I:

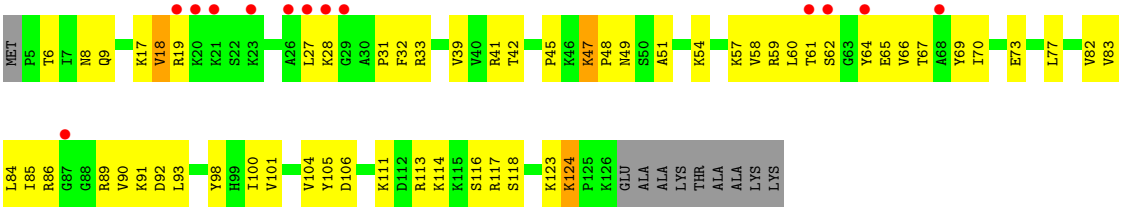




• Molecule 12: 30S ribosomal protein S12

Chain 3A:

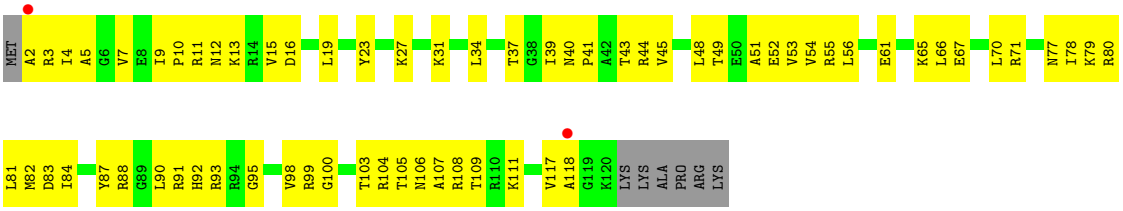




• Molecule 13: 30S ribosomal protein S13

Chain 4I:

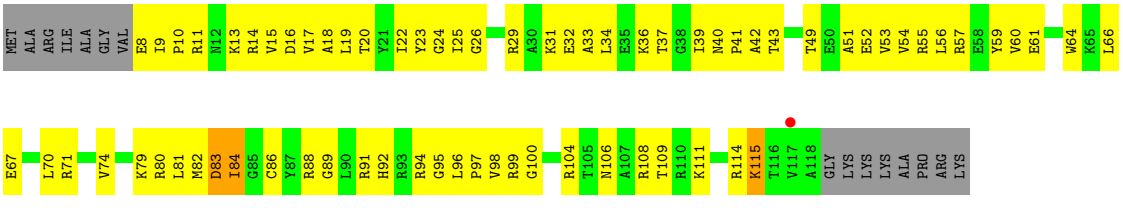




• Molecule 13: 30S ribosomal protein S13

Chain 4A:

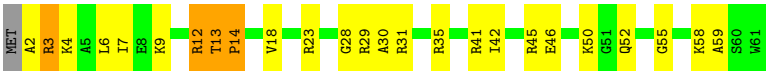




• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:

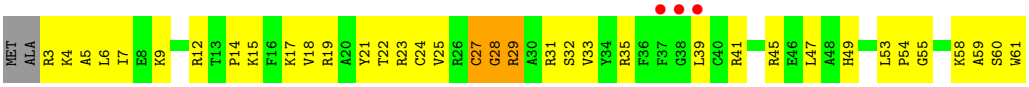




• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:





• Molecule 15: 30S ribosomal protein S15

Chain 6I:





• Molecule 15: 30S ribosomal protein S15

Chain 6A:

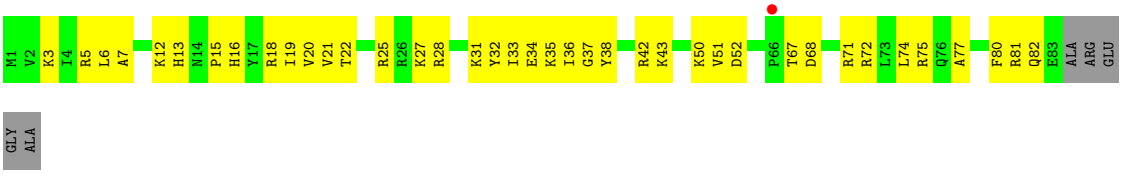




• Molecule 16: 30S ribosomal protein S16

Chain 7I:

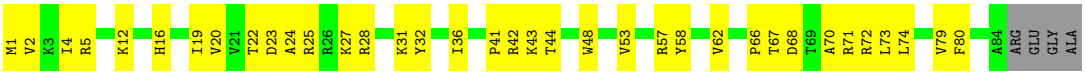




• Molecule 16: 30S ribosomal protein S16

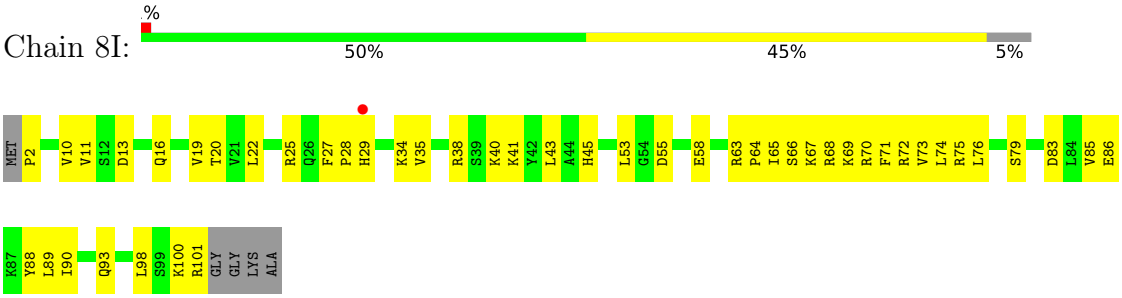
Chain 7A:





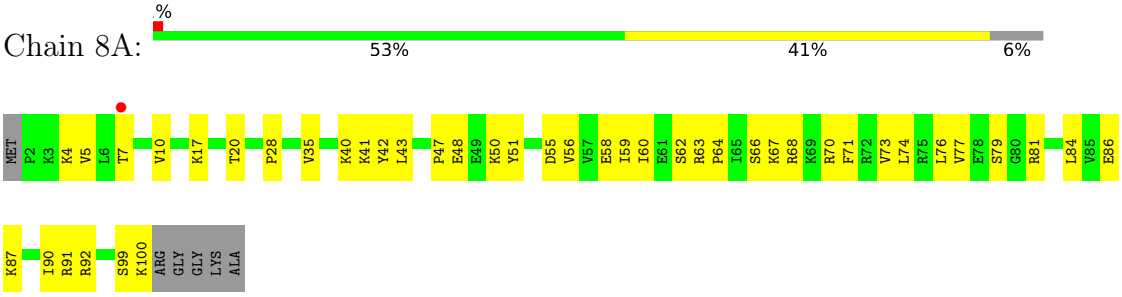
• Molecule 17: 30S ribosomal protein S17

Chain 8I:



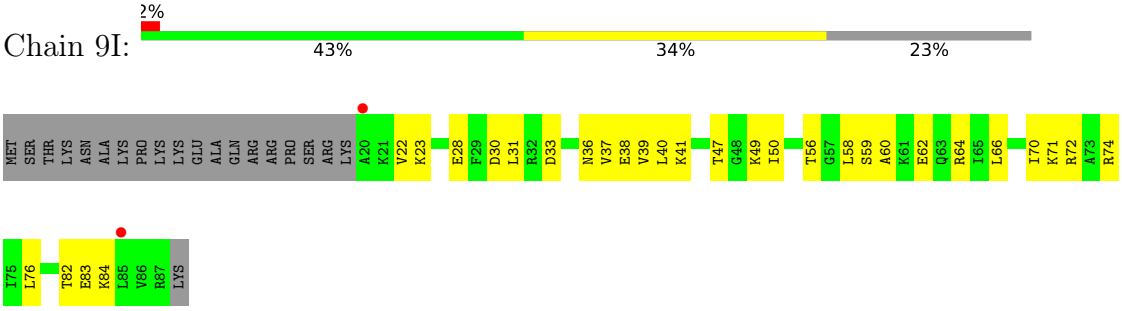
• Molecule 17: 30S ribosomal protein S17

Chain 8A:



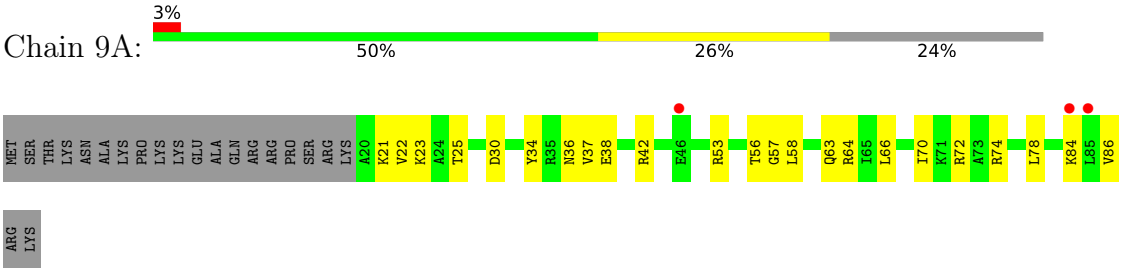
• Molecule 18: 30S ribosomal protein S18

Chain 9I:



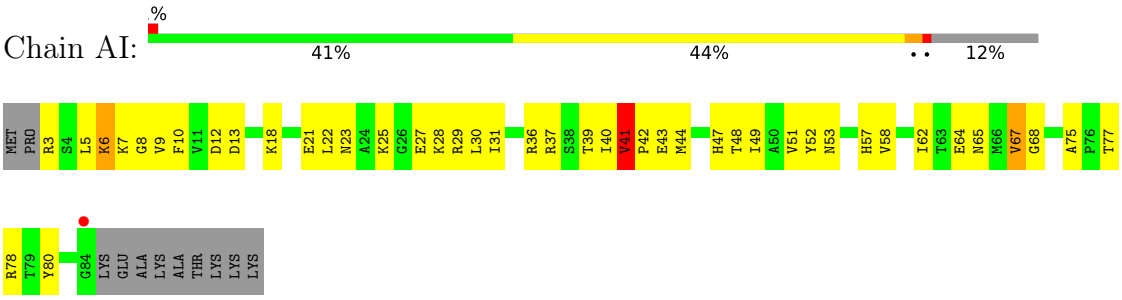
• Molecule 18: 30S ribosomal protein S18

Chain 9A:



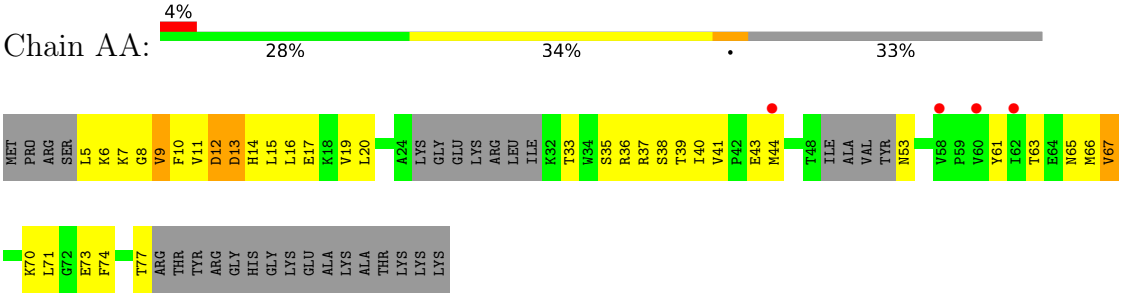
• Molecule 19: 30S ribosomal protein S19

Chain AI:



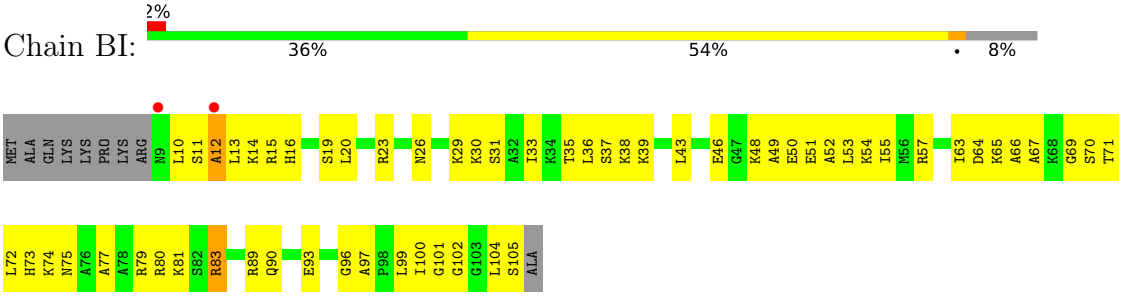
• Molecule 19: 30S ribosomal protein S19

Chain AA:



• Molecule 20: 30S ribosomal protein S20

Chain BI:



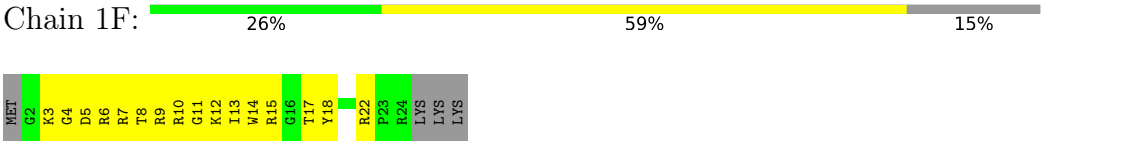
• Molecule 20: 30S ribosomal protein S20

Chain BA:



• Molecule 21: 30S ribosomal protein Thx

Chain 1F:



• Molecule 21: 30S ribosomal protein Thx

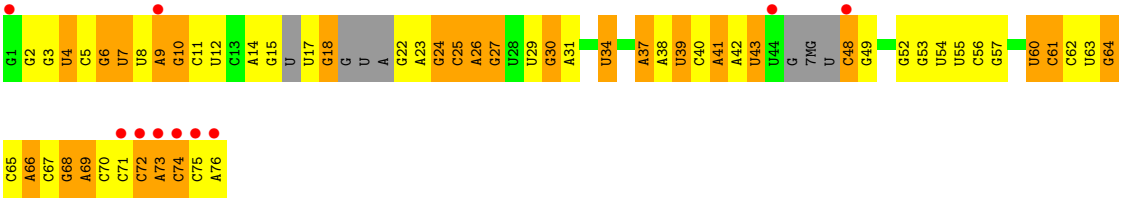
Chain 1B:



• Molecule 22: tRNALys

Chain 1K:





• Molecule 22: tRNALys

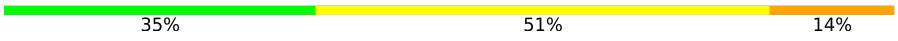
Chain 1L:

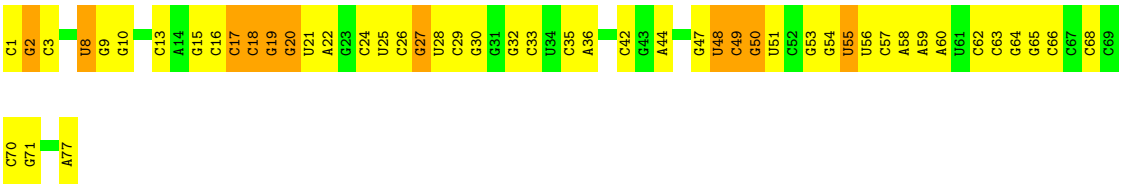




• Molecule 23: E. coli tRNAfMet

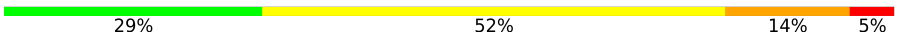
Chain 2K:





• Molecule 23: E. coli tRNAfMet

Chain 2L:

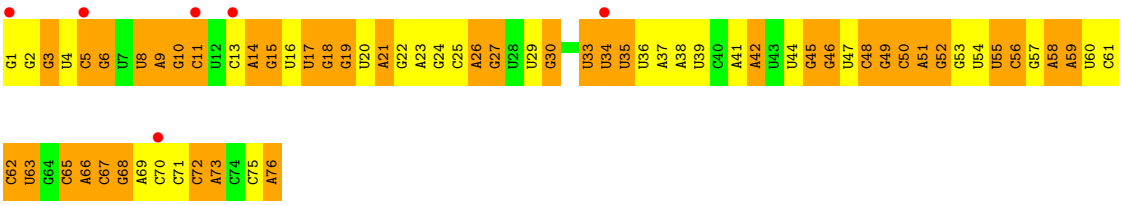




• Molecule 24: tRNALys

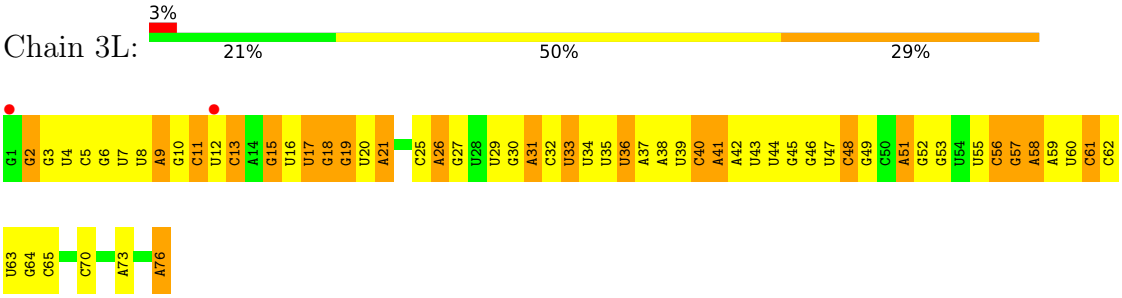
Chain 3K:





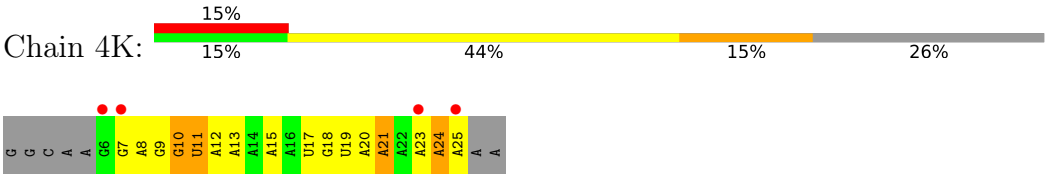
• Molecule 24: tRNALys

Chain 3L:



• Molecule 25: mRNA

Chain 4K:



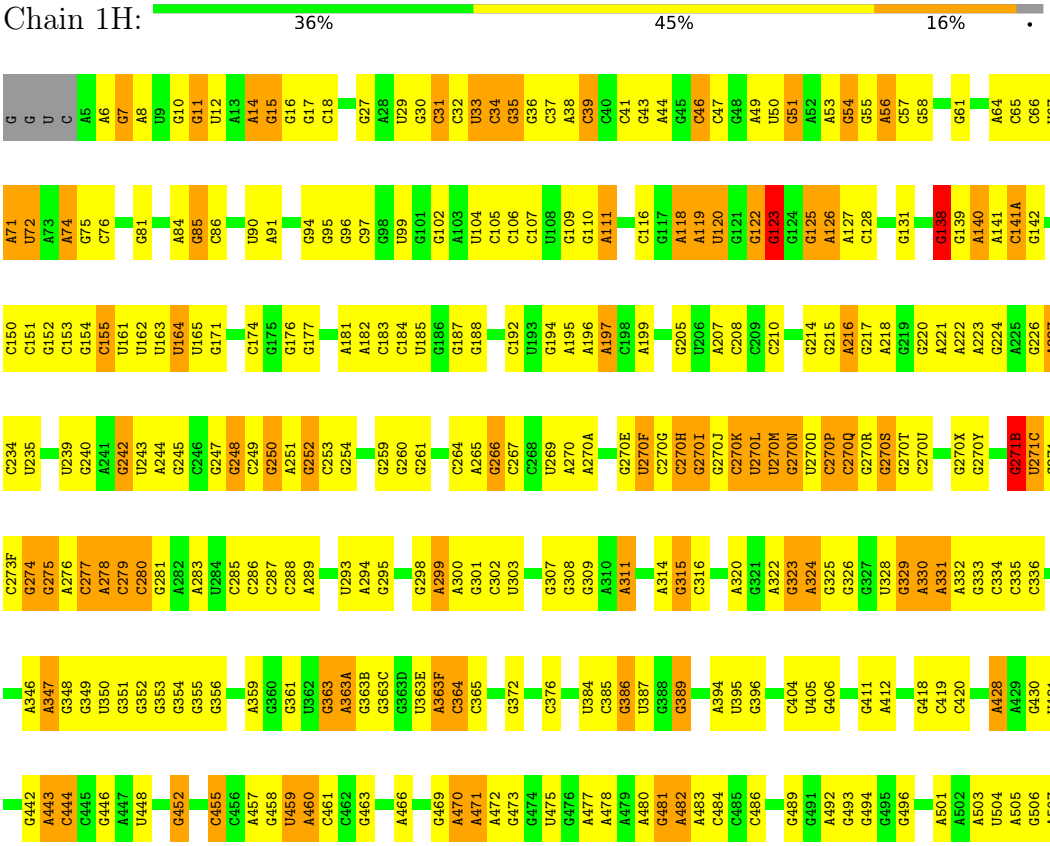
• Molecule 25: mRNA

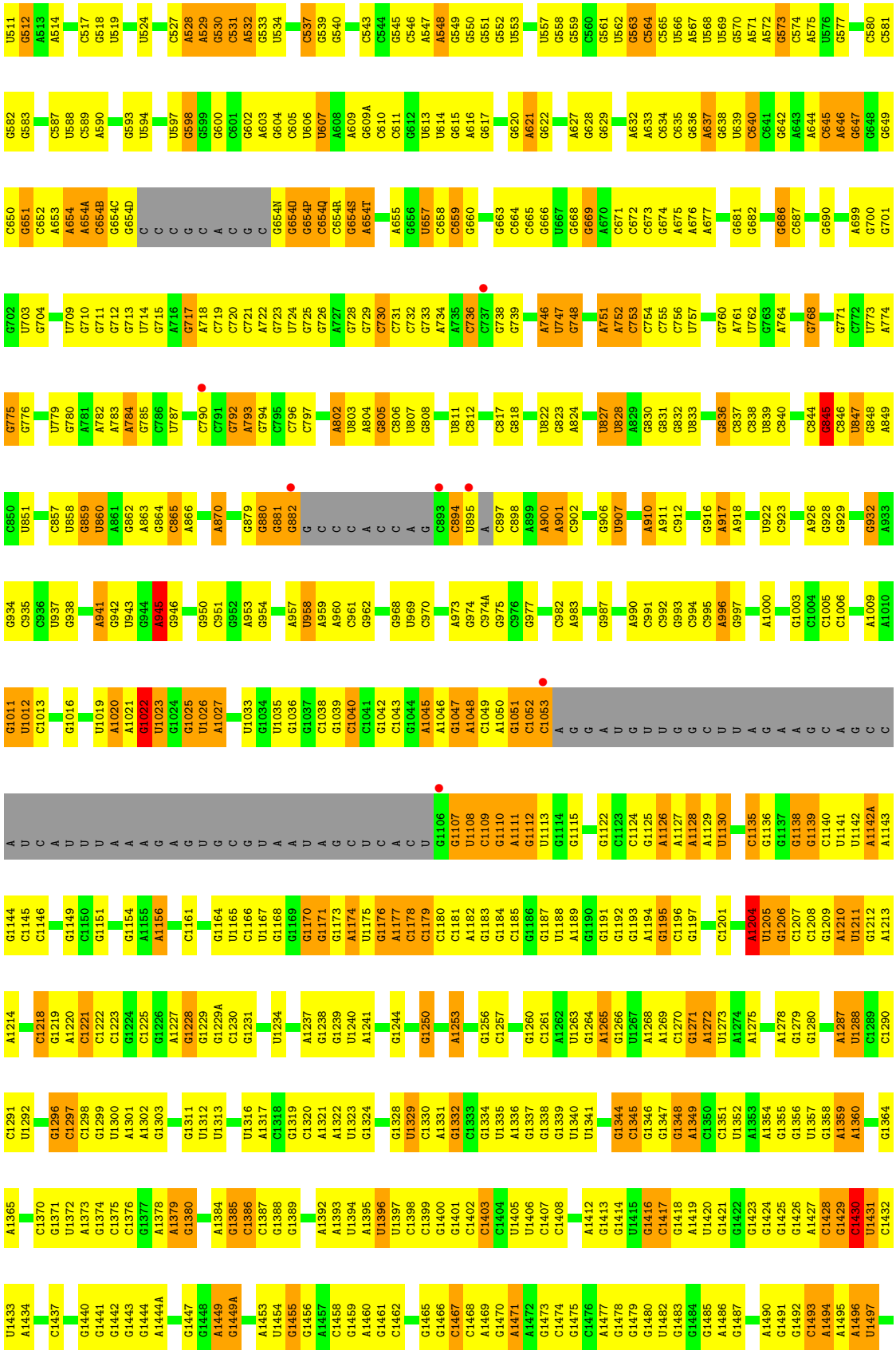
Chain 4L:

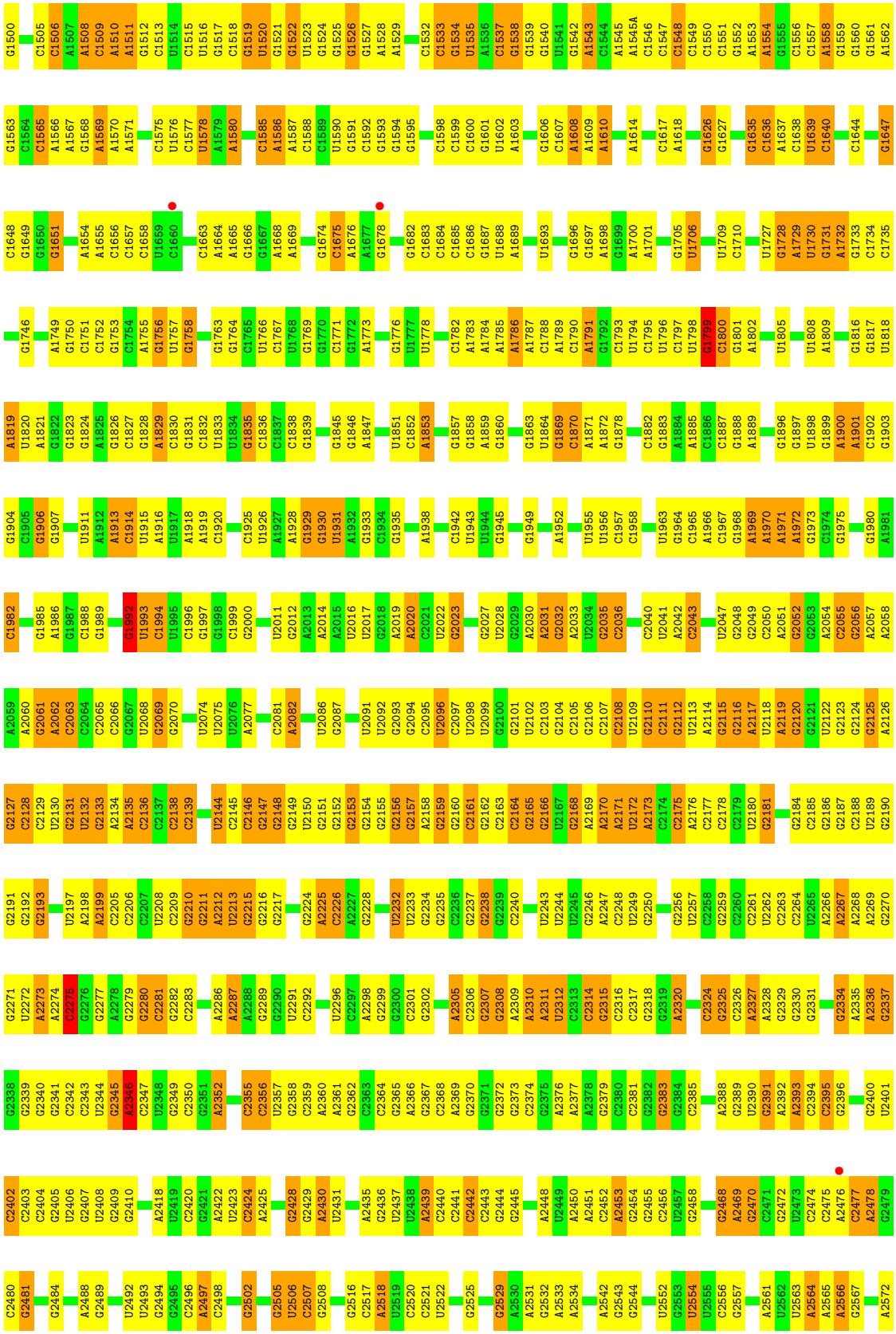


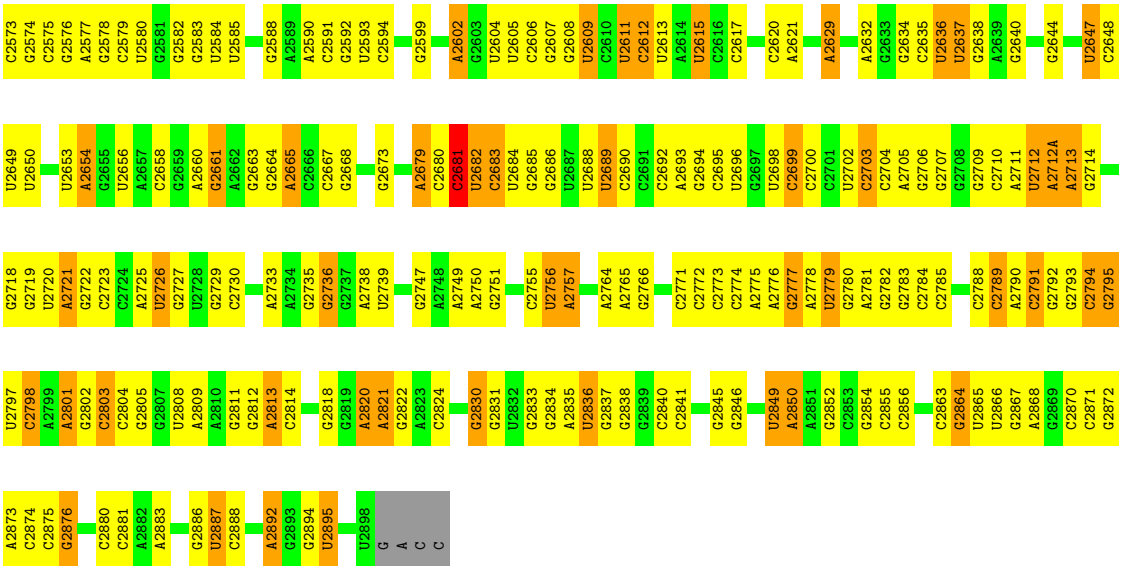
• Molecule 26: 23S rRNA

Chain 1H:





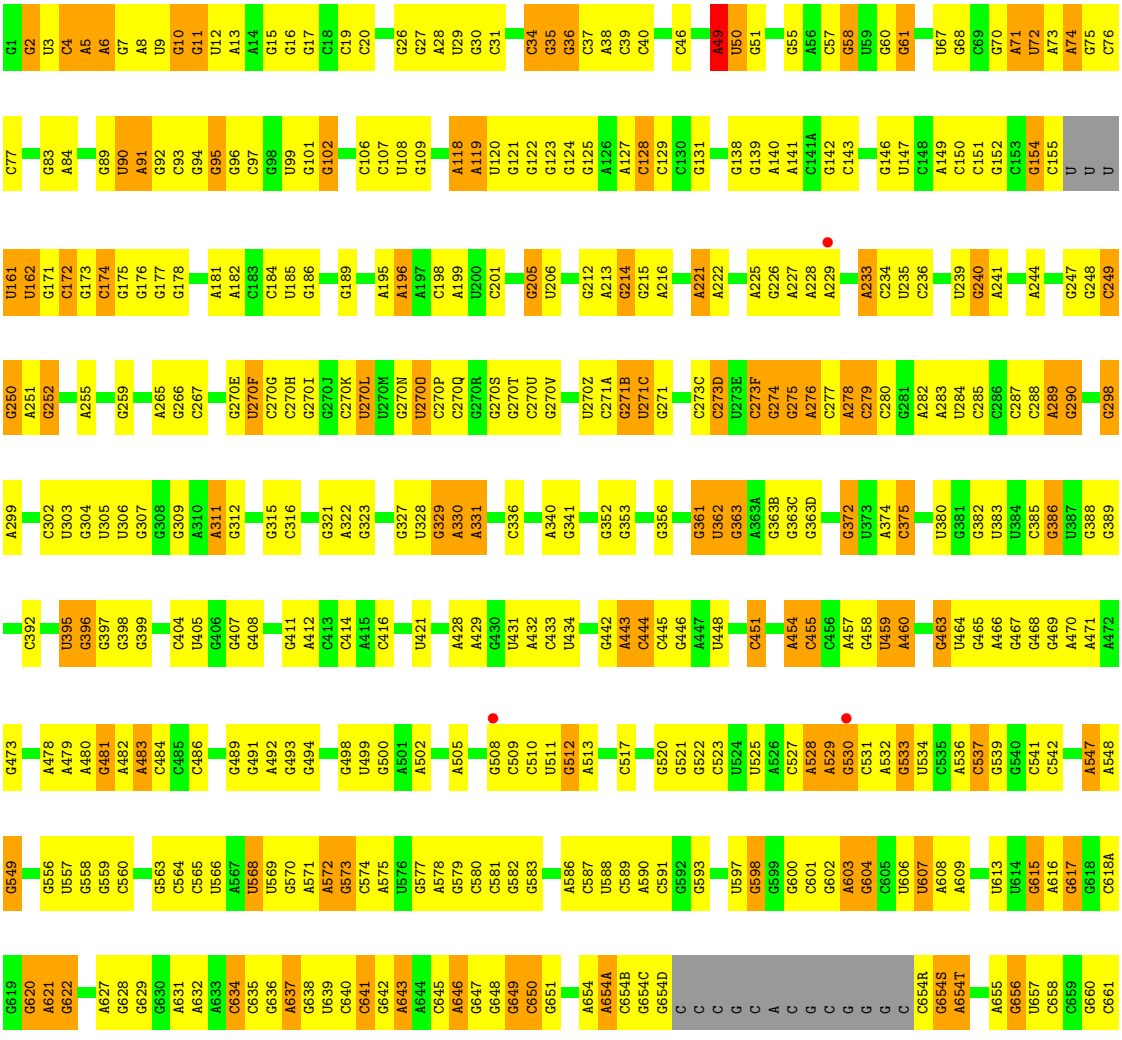




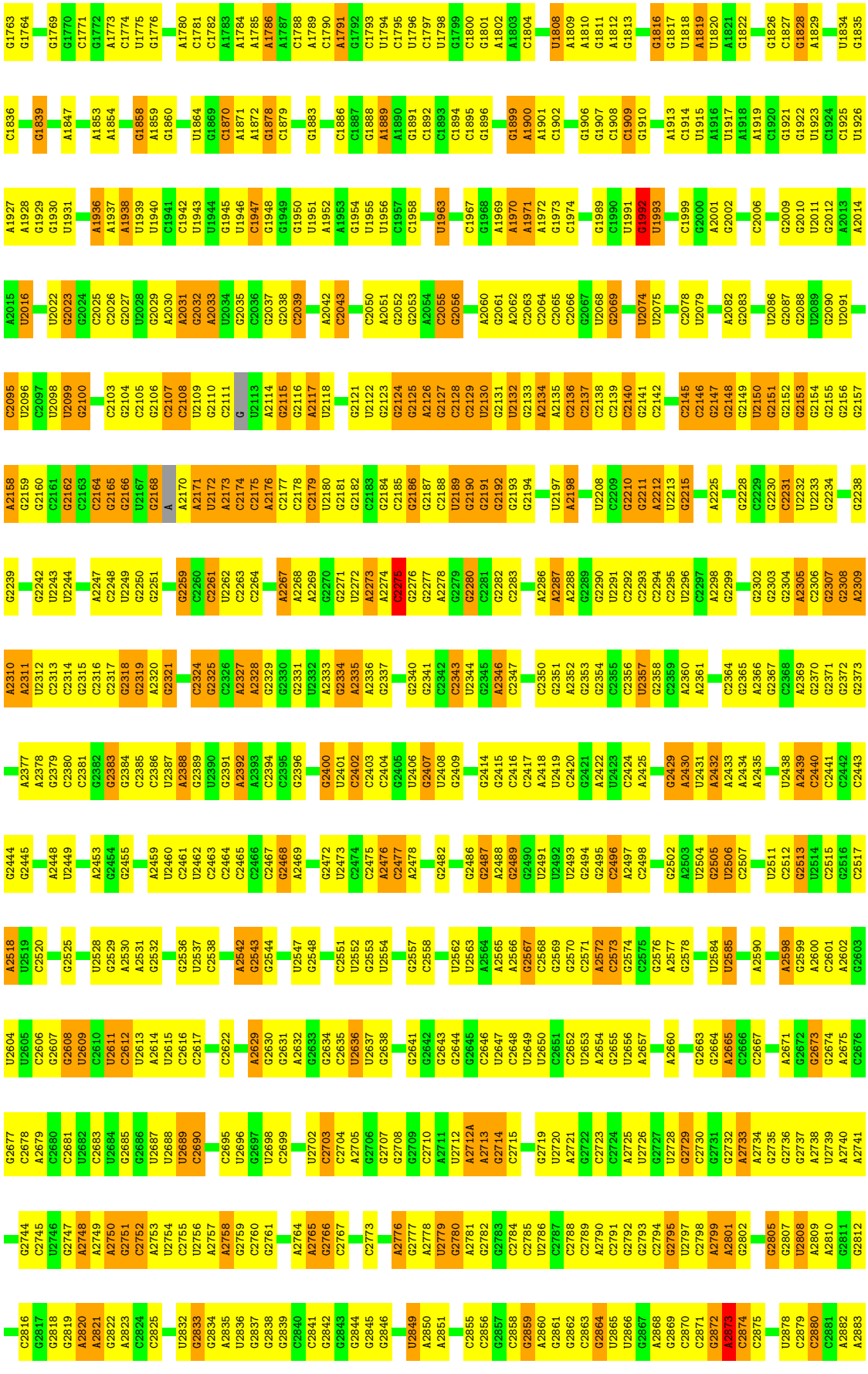
• Molecule 26: 23S rRNA

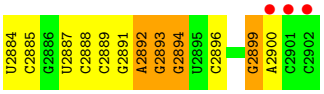
Chain 14:





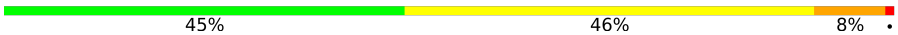
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A761 A764 G765 G769 G770 G771 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A800 G801 A804 G805 C806 U807 G808 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 A824 U827 U828 A829 G830
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U963 G966 U969 C970 C971 G972 A973 G974 C974A G975 A980 A981 C982 A983 G987 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029
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C1675 A1676 A1677 G1678 U1679 U1680 C1684 C1685 C1686 G1687 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1704 G1705 U1709 C1710 U1716 G1717 G1718 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 G1741 C1742 G1743 G1746 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1762

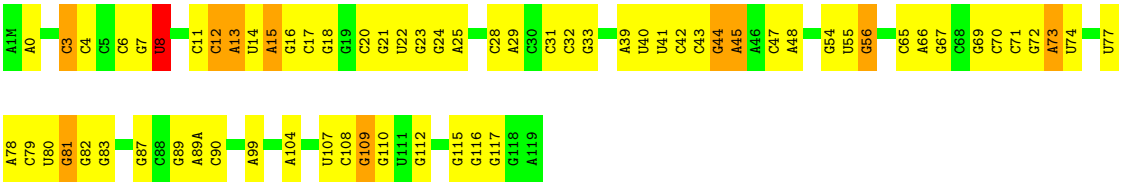




• Molecule 27: 5S rRNA

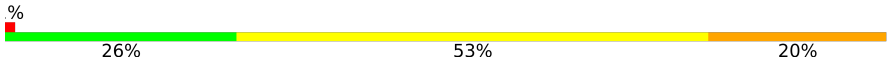
Chain 16:

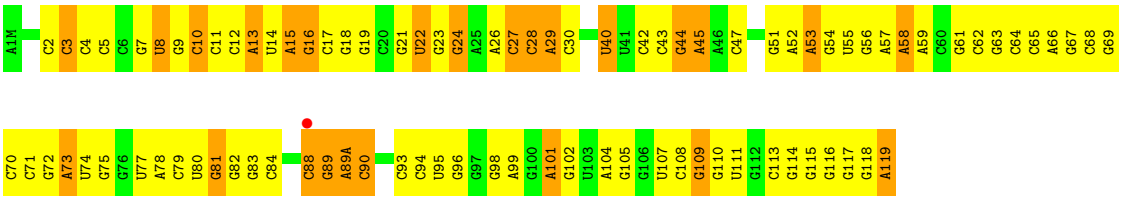




• Molecule 27: 5S rRNA

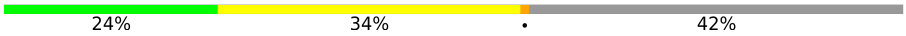
Chain 1J:

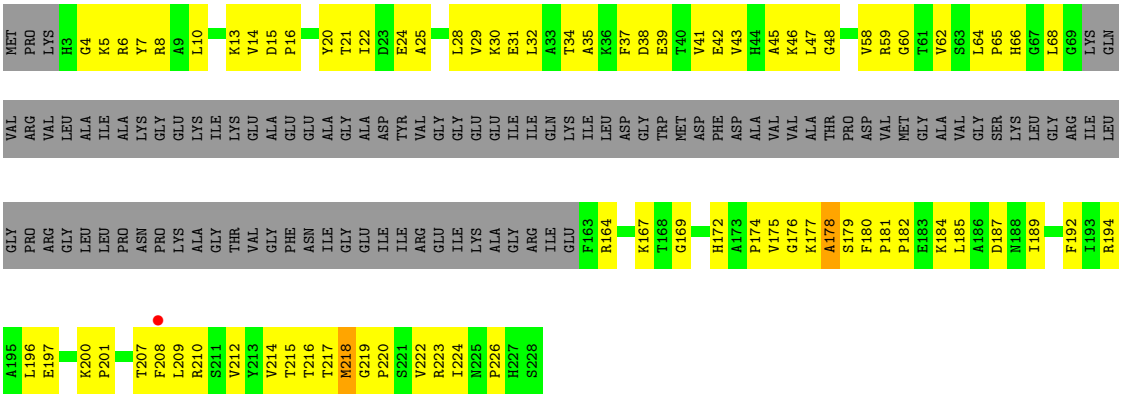




• Molecule 28: 50S ribosomal protein L1

Chain 71:

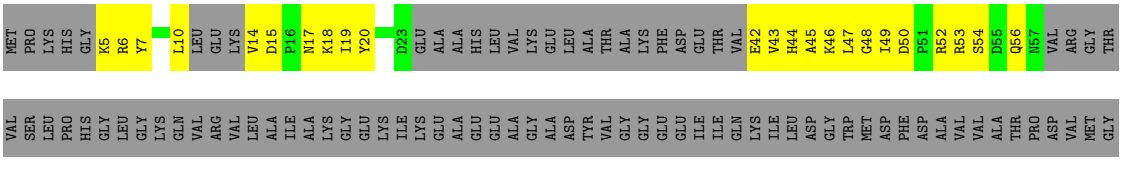


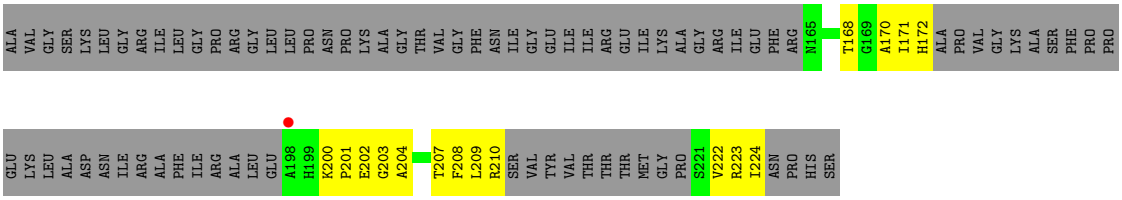


• Molecule 28: 50S ribosomal protein L1

Chain 79:

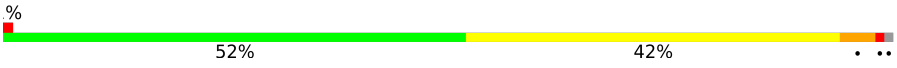


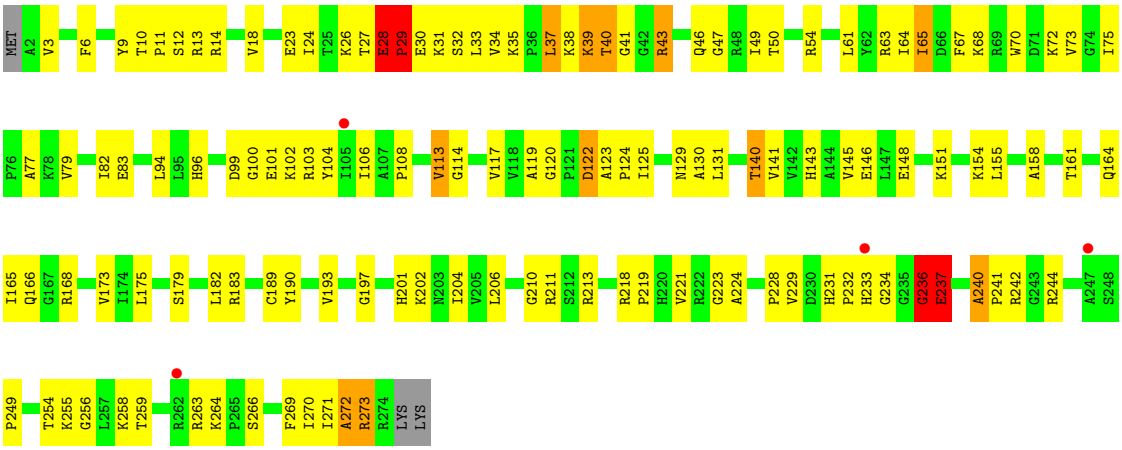




• Molecule 29: 50S ribosomal protein L2

Chain 11:

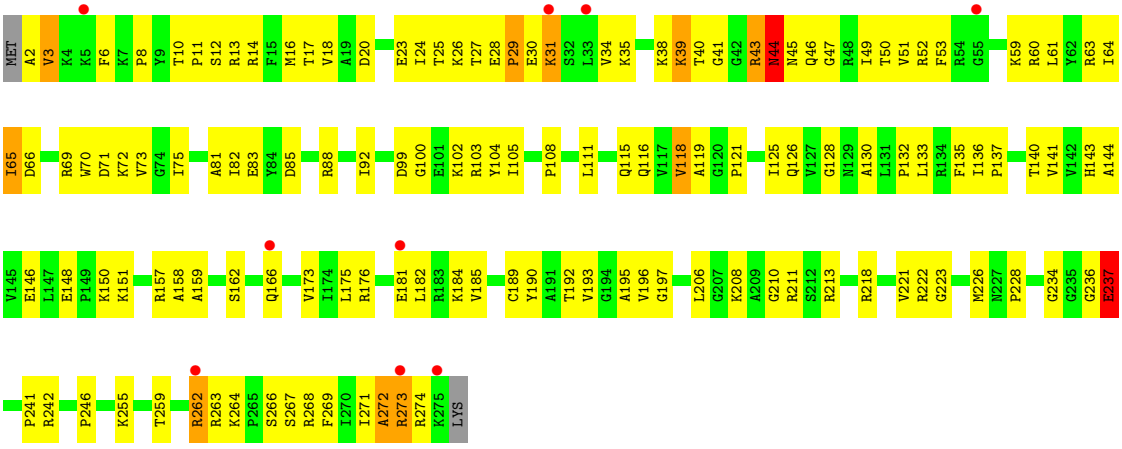




• Molecule 29: 50S ribosomal protein L2

Chain 19:

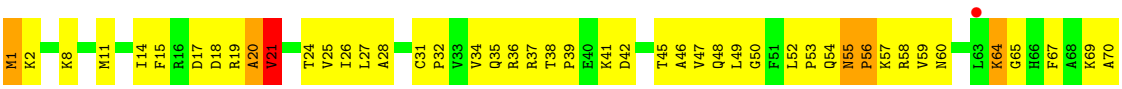


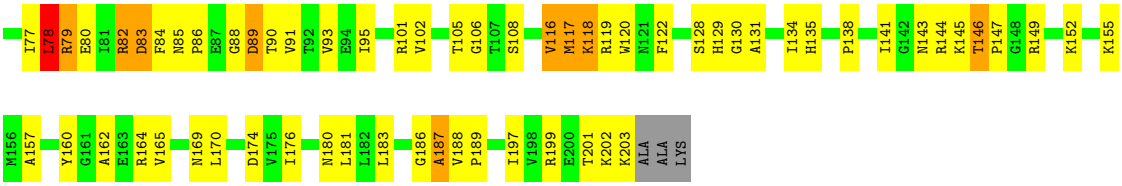


• Molecule 30: 50S ribosomal protein L3

Chain 21:





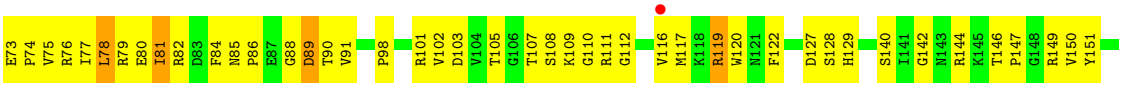


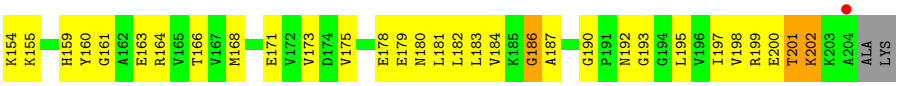
• Molecule 30: 50S ribosomal protein L3

Chain 29:





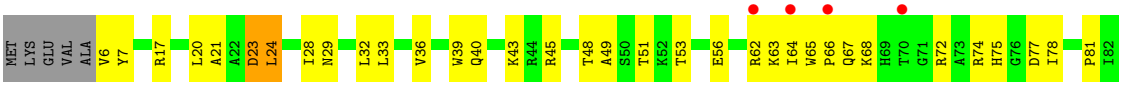


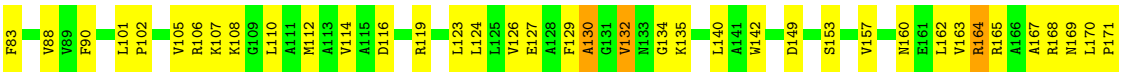


• Molecule 31: 50S ribosomal protein L4

Chain 31:







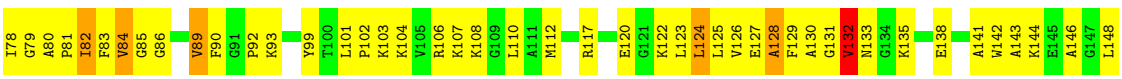


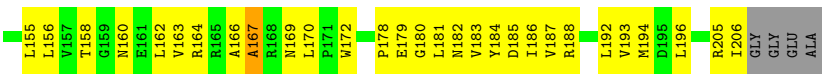
• Molecule 31: 50S ribosomal protein L4

Chain 39:



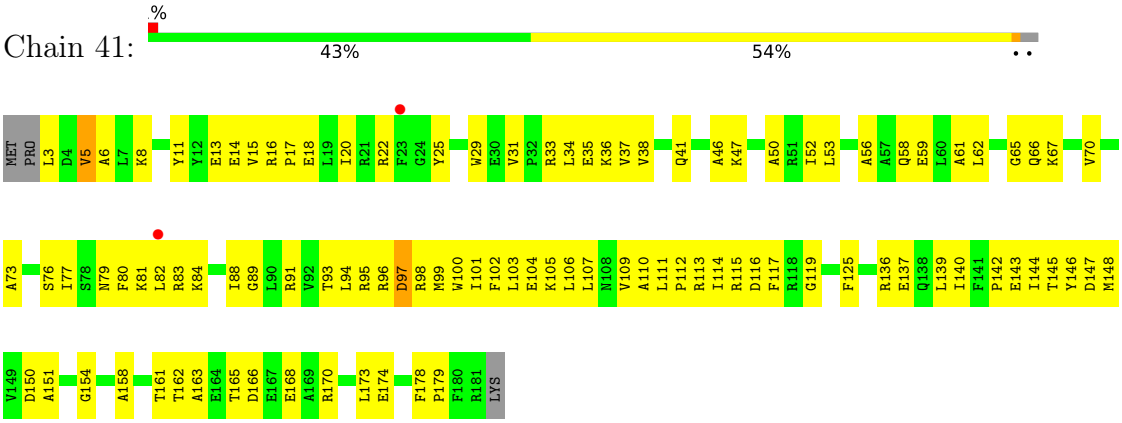






• Molecule 32: 50S ribosomal protein L5

Chain 41:



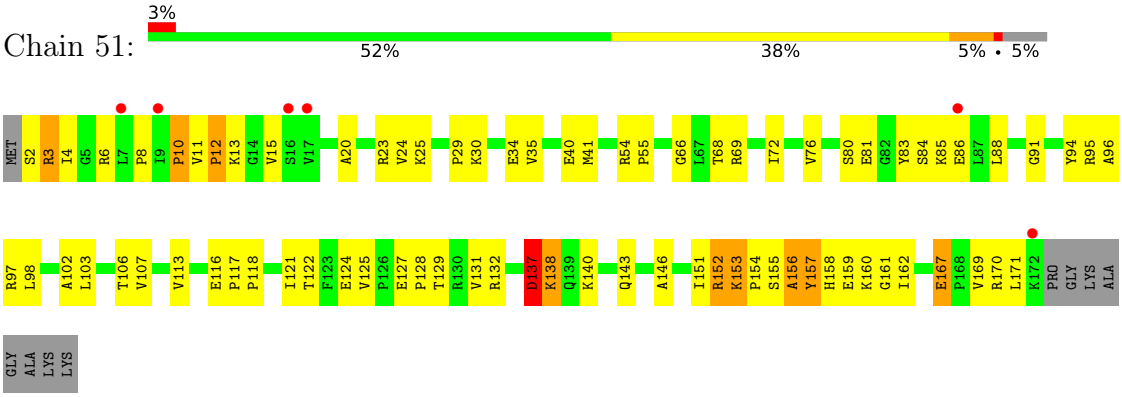
• Molecule 32: 50S ribosomal protein L5

Chain 49:



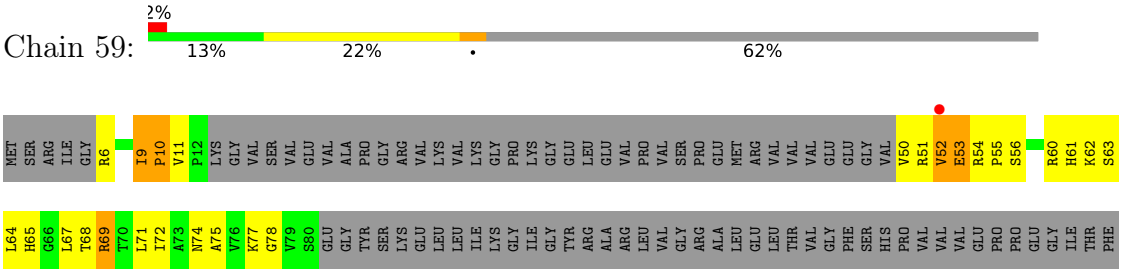
• Molecule 33: 50S ribosomal protein L6

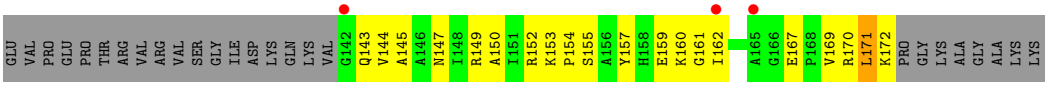
Chain 51:



• Molecule 33: 50S ribosomal protein L6

Chain 59:

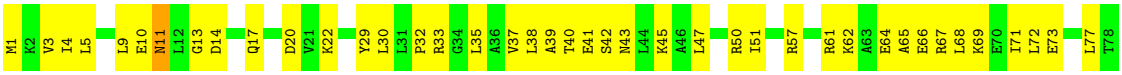


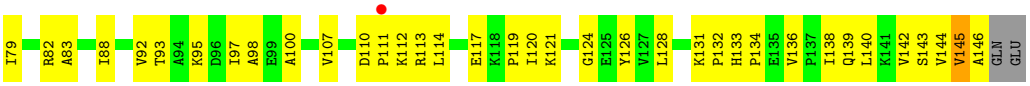


• Molecule 34: 50S ribosomal protein L9

Chain 61:



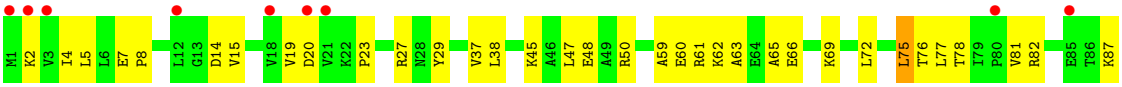




• Molecule 34: 50S ribosomal protein L9

Chain 69:





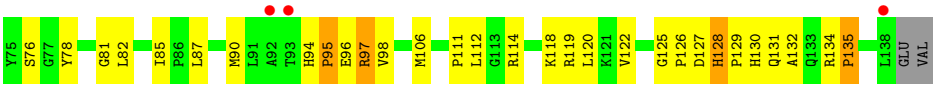


• Molecule 35: 50S ribosomal protein L13

Chain 58:



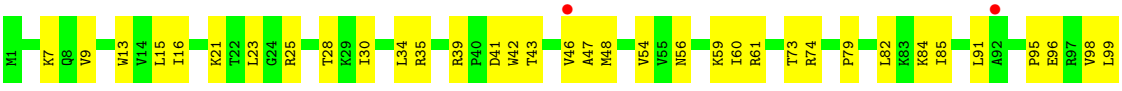




• Molecule 35: 50S ribosomal protein L13

Chain 15:



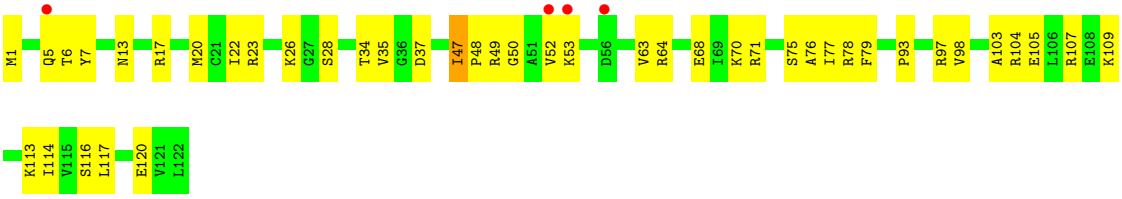




• Molecule 36: 50S ribosomal protein L14

Chain 68:





• Molecule 36: 50S ribosomal protein L14

Chain 25:

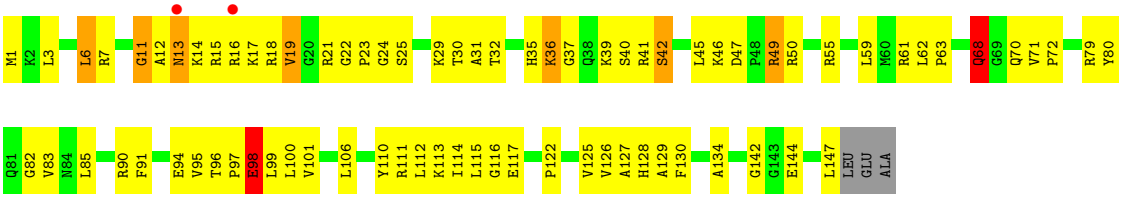




• Molecule 37: 50S ribosomal protein L15

Chain 78:

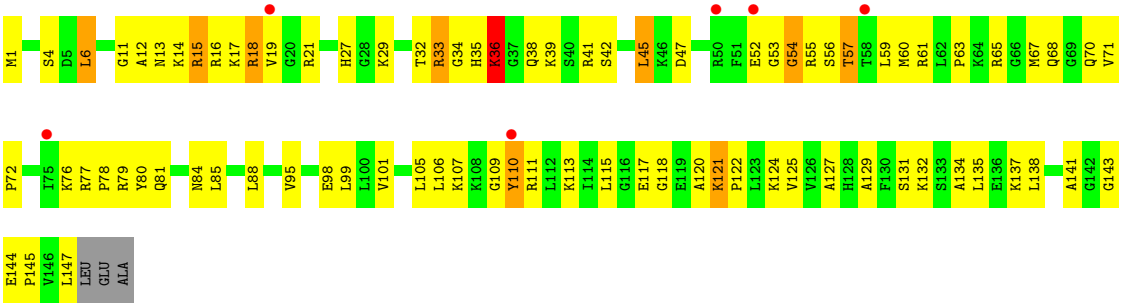




• Molecule 37: 50S ribosomal protein L15

Chain 35:

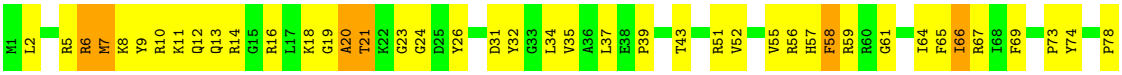




• Molecule 38: 50S ribosomal protein L16

Chain 88:



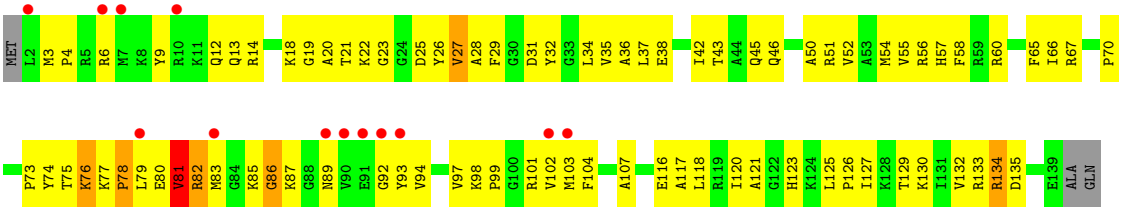




• Molecule 38: 50S ribosomal protein L16

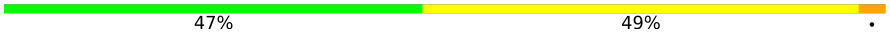
Chain 45:

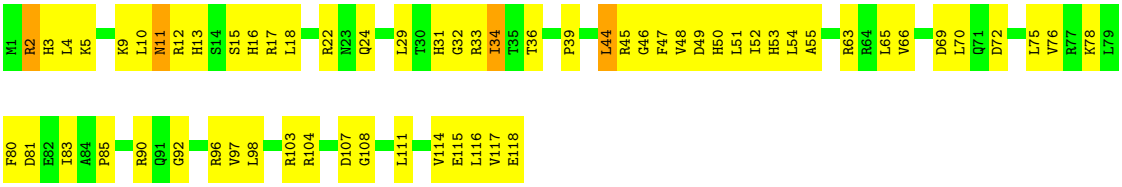




• Molecule 39: 50S ribosomal protein L17

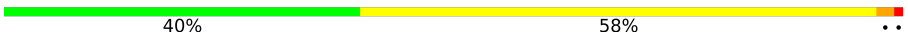
Chain 98:

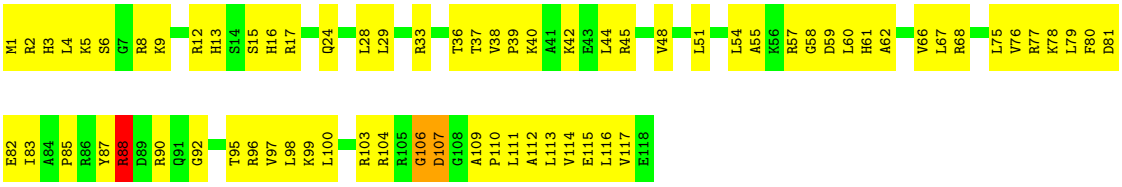




• Molecule 39: 50S ribosomal protein L17

Chain 55:





• Molecule 40: 50S ribosomal protein L18

Chain A8:

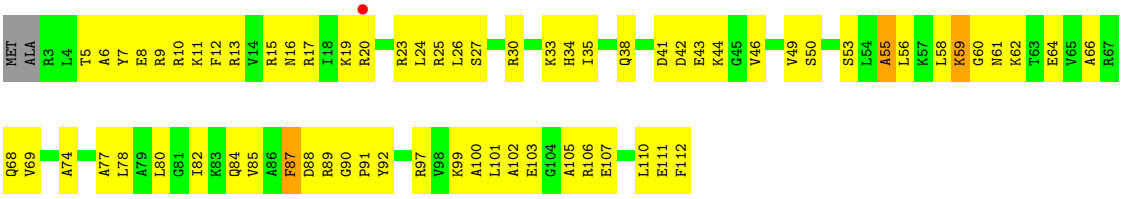




• Molecule 40: 50S ribosomal protein L18

Chain 65:

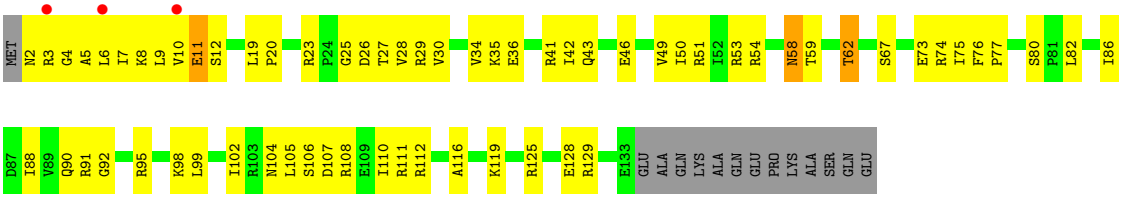




• Molecule 41: 50S ribosomal protein L19

Chain B8:

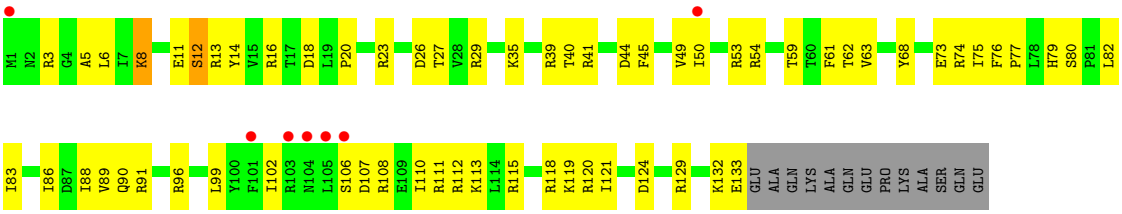




• Molecule 41: 50S ribosomal protein L19

Chain 75:

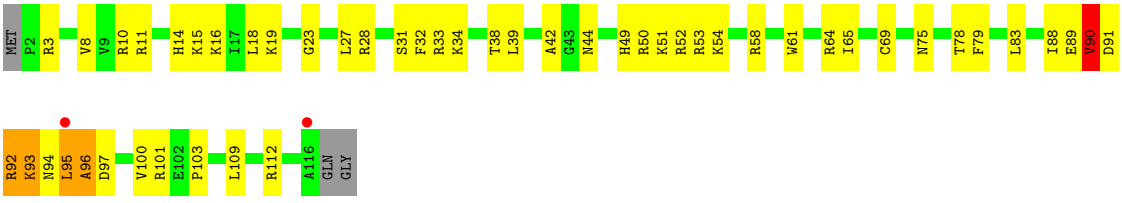




• Molecule 42: 50S ribosomal protein L20

Chain C8:

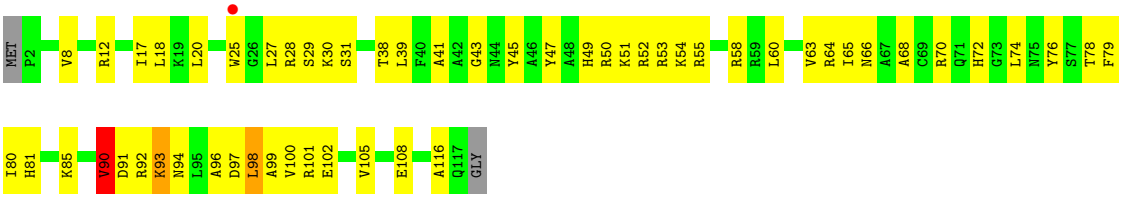




• Molecule 42: 50S ribosomal protein L20

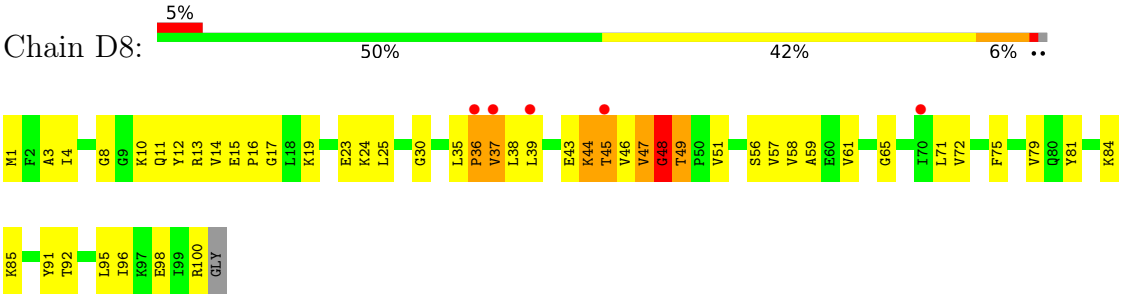
Chain 85:





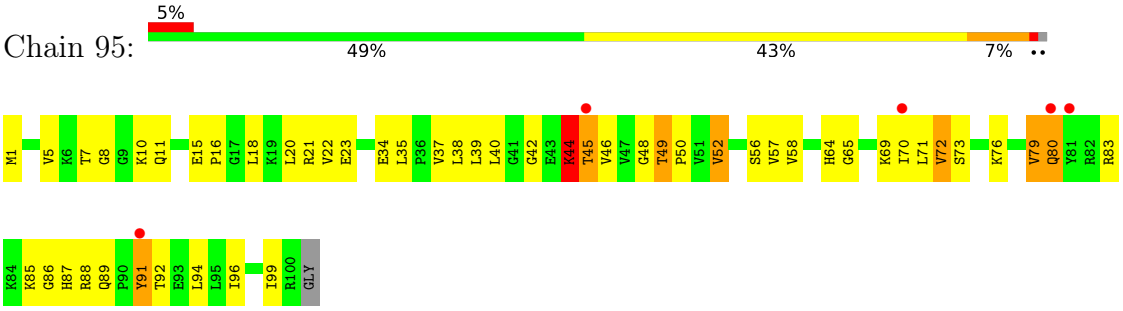
• Molecule 43: 50S ribosomal protein L21

Chain D8:



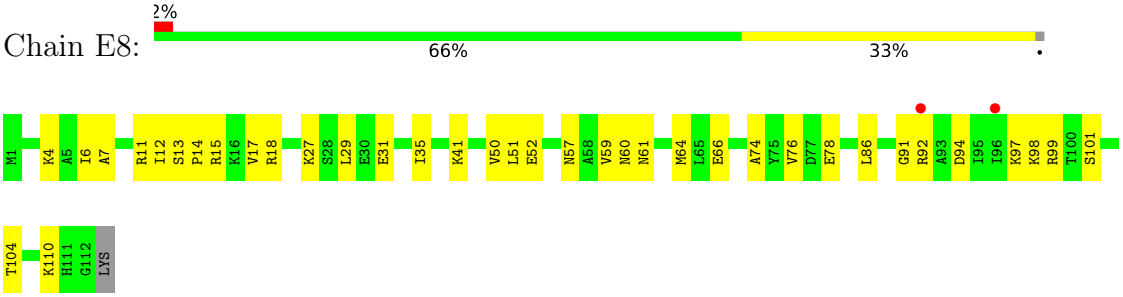
• Molecule 43: 50S ribosomal protein L21

Chain 95:



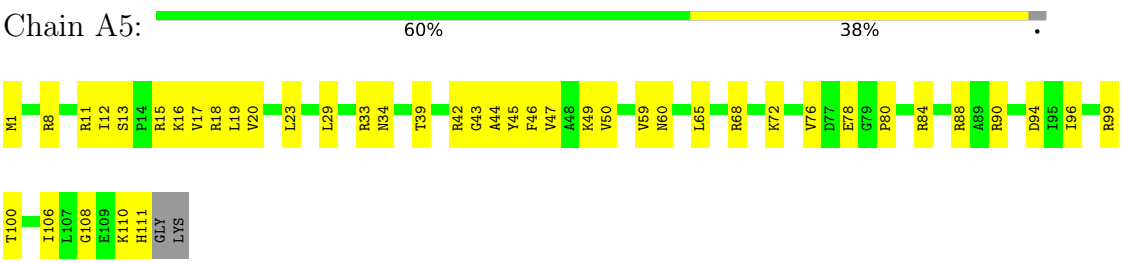
• Molecule 44: 50S ribosomal protein L22

Chain E8:



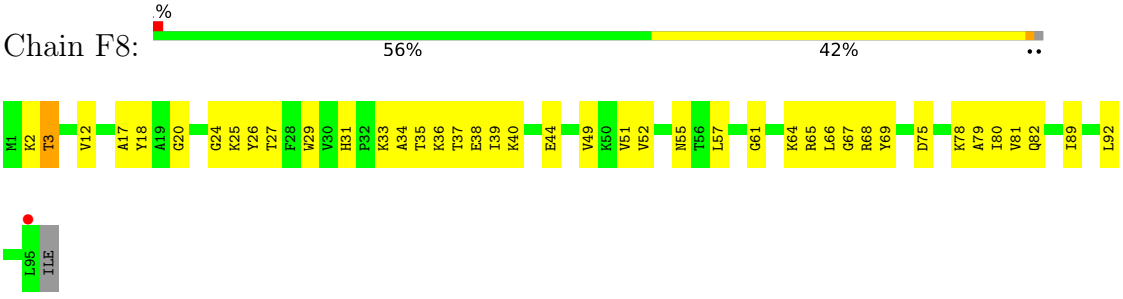
• Molecule 44: 50S ribosomal protein L22

Chain A5:



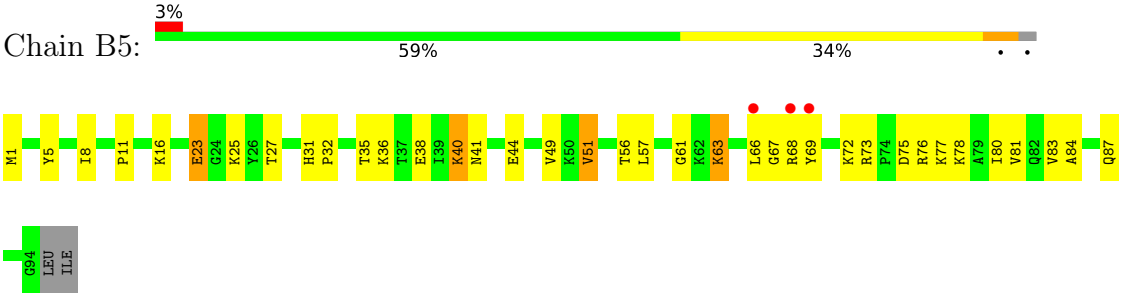
• Molecule 45: 50S ribosomal protein L23

Chain F8:



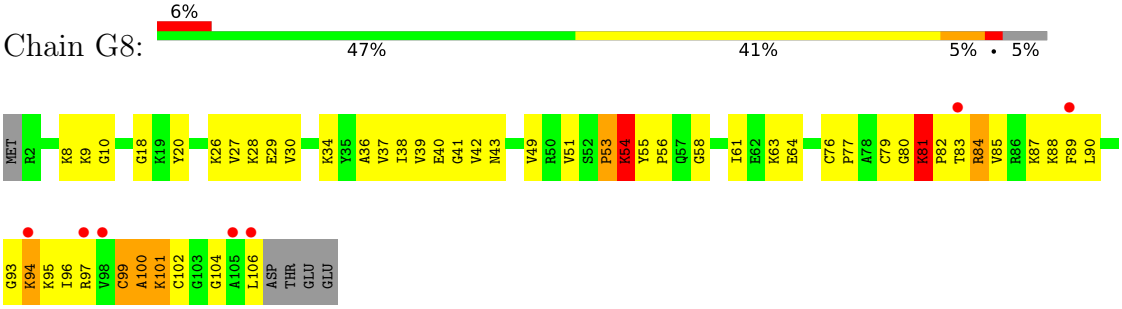
• Molecule 45: 50S ribosomal protein L23

Chain B5:



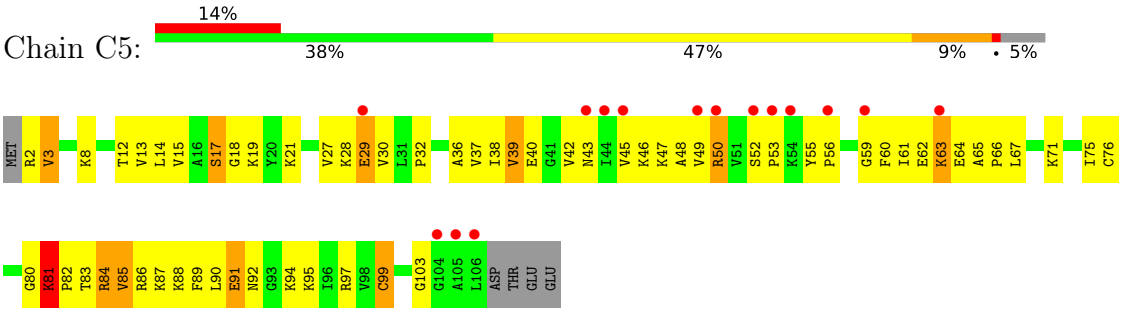
• Molecule 46: 50S ribosomal protein L24

Chain G8:



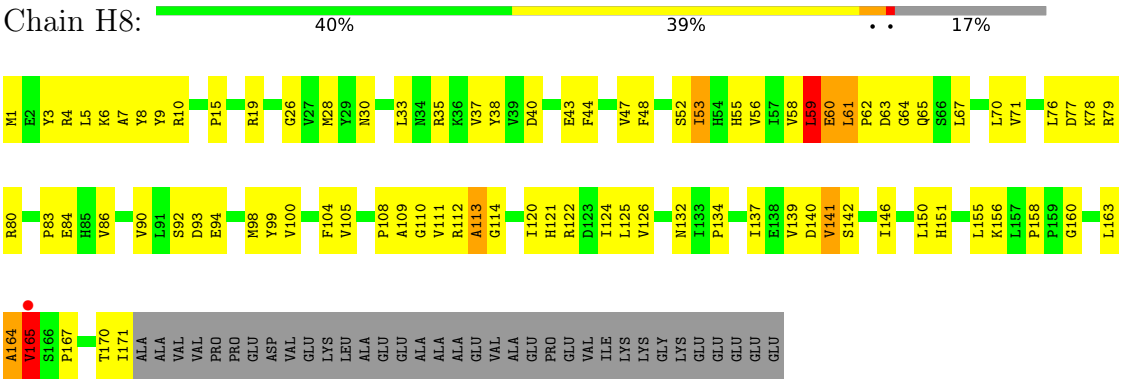
• Molecule 46: 50S ribosomal protein L24

Chain C5:



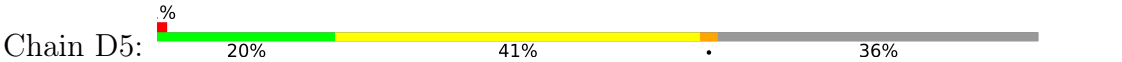
• Molecule 47: 50S ribosomal protein L25

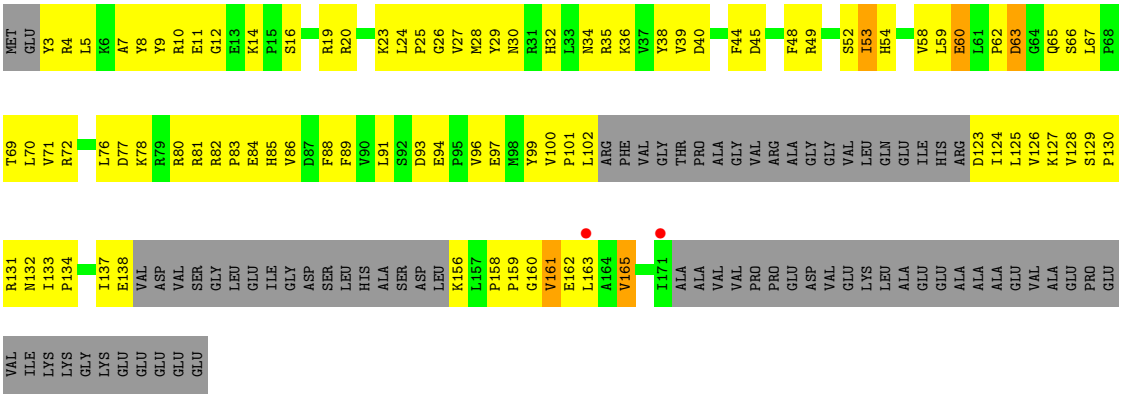
Chain H8:



• Molecule 47: 50S ribosomal protein L25

Chain D5:

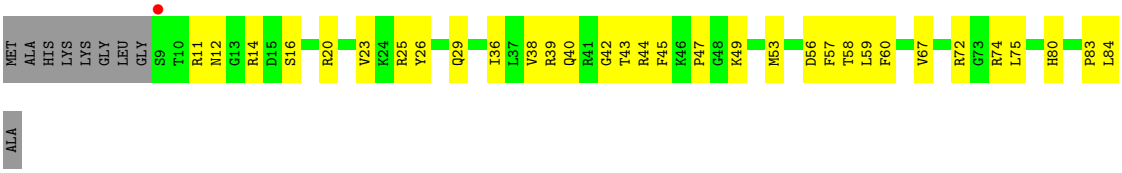




• Molecule 48: 50S ribosomal protein L27

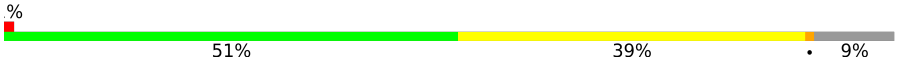
Chain I8:

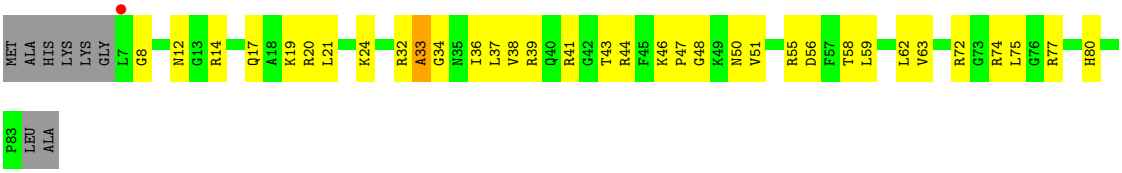




• Molecule 48: 50S ribosomal protein L27

Chain E5:

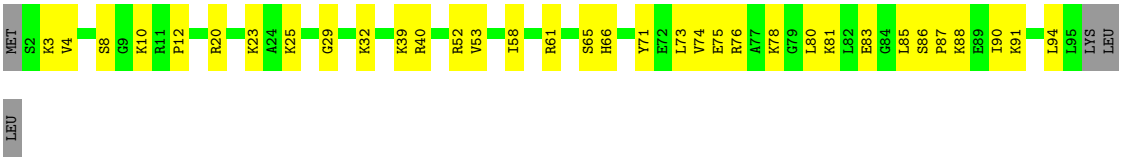




• Molecule 49: 50S ribosomal protein L28

Chain J8:

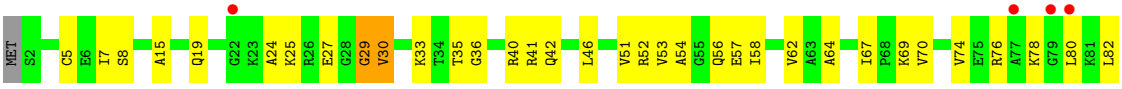




• Molecule 49: 50S ribosomal protein L28

Chain F5:



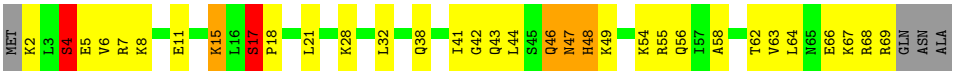




• Molecule 50: 50S ribosomal protein L29

Chain K8:

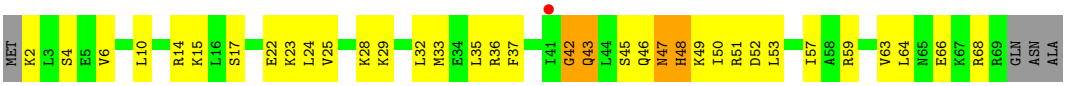




• Molecule 50: 50S ribosomal protein L29

Chain G5:





• Molecule 51: 50S ribosomal protein L30

Chain L8:

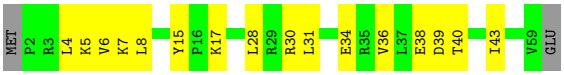




• Molecule 51: 50S ribosomal protein L30

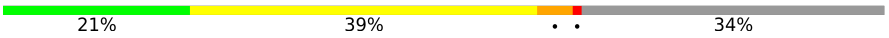
Chain H5:

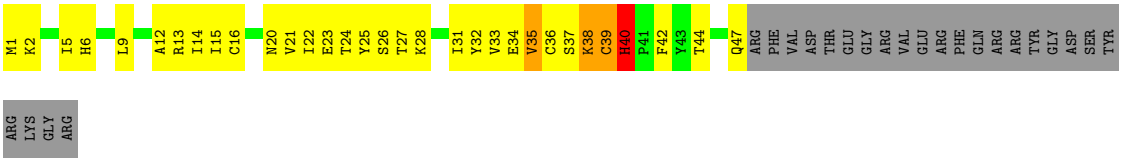




• Molecule 52: 50S ribosomal protein L31

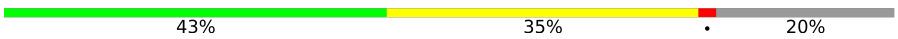
Chain M8:

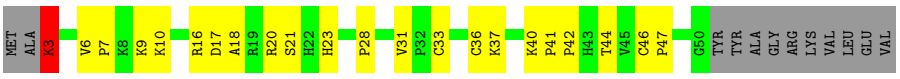




• Molecule 53: 50S ribosomal protein L32

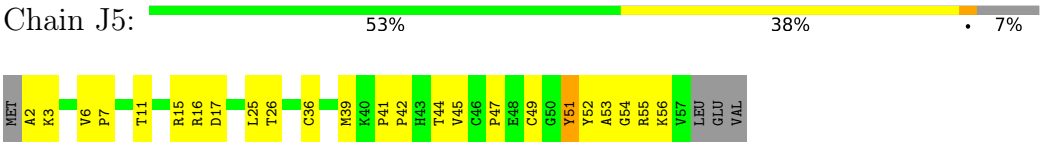
Chain N8:





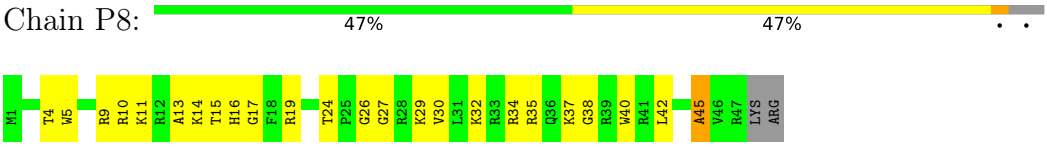
• Molecule 53: 50S ribosomal protein L32

Chain J5:



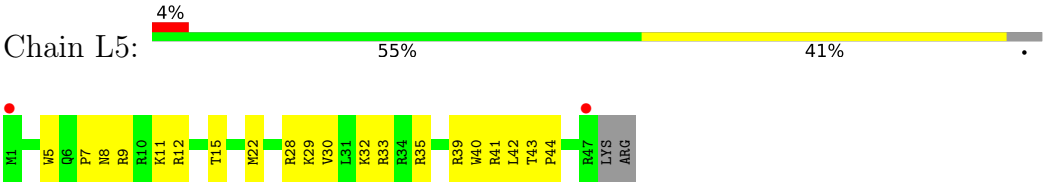
• Molecule 54: 50S ribosomal protein L34

Chain P8:



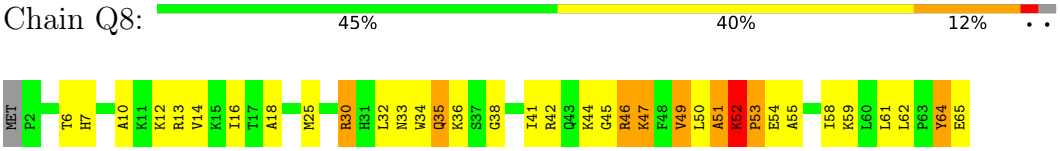
• Molecule 54: 50S ribosomal protein L34

Chain L5:



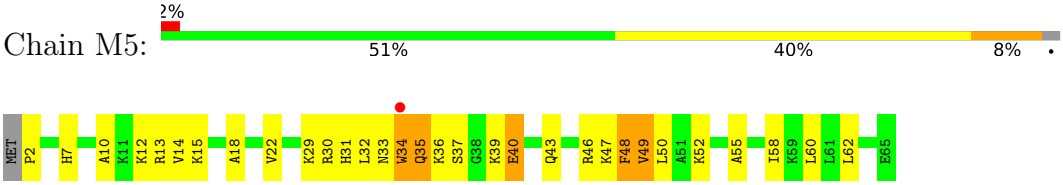
• Molecule 55: 50S ribosomal protein L35

Chain Q8:



• Molecule 55: 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	208.40Å 446.00Å 617.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.24 – 3.10 151.24 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.24-3.10) 93.3 (151.24-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.249 0.199 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	294257	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: OMC, 4SU, MG, G7M, PSU, U8U, SF4, PAR, 5MU, ZN, T6A

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	0.51	0/35994	0.76	9/56171 (0.0%)
1	1G	0.43	0/36258	0.66	4/56589 (0.0%)
2	12	0.50	0/1752	0.83	4/2360 (0.2%)
2	1E	0.43	0/1908	0.75	2/2573 (0.1%)
3	22	0.56	4/1564 (0.3%)	0.67	0/2109
3	2E	0.54	0/1629	0.71	0/2195
4	32	0.48	0/1732	0.75	0/2318
4	3E	0.55	0/1728	0.82	1/2313 (0.0%)
5	42	0.45	0/1150	0.75	0/1548
5	4E	0.53	0/1158	0.78	0/1559
6	52	0.50	0/855	0.73	0/1154
6	5E	0.60	0/850	0.73	0/1147
7	62	0.42	0/1122	0.74	3/1500 (0.2%)
7	6E	0.44	0/1259	0.63	0/1686
8	72	0.36	0/1127	0.67	0/1517
8	7E	0.69	4/1135 (0.4%)	0.77	0/1527
9	82	0.41	0/971	0.73	0/1304
9	8E	0.42	0/1019	0.79	0/1367
10	1A	0.50	0/658	0.71	0/885
10	1I	0.47	0/747	0.82	1/1006 (0.1%)
11	2A	0.42	0/850	0.68	0/1150
11	2I	0.50	0/838	0.78	2/1133 (0.2%)
12	3A	0.52	0/972	0.83	2/1301 (0.2%)
12	3I	0.71	0/972	1.07	3/1301 (0.2%)
13	4A	0.50	0/903	0.83	1/1211 (0.1%)
13	4I	0.54	0/952	0.77	0/1277
14	5A	0.43	0/495	0.90	2/657 (0.3%)
14	5I	0.54	0/500	0.86	2/664 (0.3%)
15	6A	0.45	0/740	0.67	0/987
15	6I	0.52	0/740	0.73	0/987
16	7A	0.47	0/721	0.76	0/970
16	7I	0.51	0/716	0.81	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.42	0/836	0.67	0/1117
17	8I	0.47	0/847	0.77	0/1131
18	9A	0.48	0/549	0.71	0/732
18	9I	0.59	0/554	0.84	0/739
19	AA	0.46	0/490	0.79	0/662
19	AI	0.54	1/672 (0.1%)	0.83	0/904
20	BA	0.44	0/764	0.83	0/1007
20	BI	0.50	1/748 (0.1%)	0.76	1/986 (0.1%)
21	1B	0.37	0/192	0.68	0/252
21	1F	0.46	0/203	0.64	0/266
22	1K	0.49	0/1516	0.67	0/2350
22	1L	0.44	1/1613 (0.1%)	0.57	0/2504
23	2K	0.56	1/1721 (0.1%)	0.74	0/2682
23	2L	0.46	0/1721	0.66	0/2682
24	3K	0.47	0/1777	0.65	0/2767
24	3L	0.44	0/1777	0.60	0/2767
25	4K	0.57	0/494	0.68	0/767
25	4L	0.42	0/445	0.56	0/693
26	14	0.57	0/69023	0.81	22/107740 (0.0%)
26	1H	0.66	0/68351	0.90	33/106700 (0.0%)
27	16	0.54	0/2928	0.83	1/4568 (0.0%)
27	1J	0.47	0/2928	0.72	0/4568
28	71	0.41	0/1055	0.74	0/1425
28	79	0.45	0/459	0.75	0/608
29	11	0.89	3/2170 (0.1%)	1.32	16/2926 (0.5%)
29	19	0.84	5/2175 (0.2%)	1.17	11/2933 (0.4%)
30	21	0.66	0/1591	1.07	8/2146 (0.4%)
30	29	0.68	2/1596 (0.1%)	1.06	7/2153 (0.3%)
31	31	0.71	2/1620 (0.1%)	0.96	0/2194
31	39	0.82	1/1637 (0.1%)	1.06	5/2218 (0.2%)
32	41	0.51	0/1481	0.81	0/1994
32	49	0.41	0/1482	0.72	0/1994
33	51	0.60	0/1337	1.03	6/1809 (0.3%)
33	59	0.69	1/548 (0.2%)	1.21	7/738 (0.9%)
34	61	0.51	0/1151	0.84	1/1558 (0.1%)
34	69	0.50	0/1146	0.85	4/1551 (0.3%)
35	15	0.49	0/1131	0.82	0/1525
35	58	0.59	0/1131	0.89	2/1525 (0.1%)
36	25	0.61	1/942 (0.1%)	0.82	0/1269
36	68	0.62	0/942	0.85	0/1269
37	35	0.75	2/1139 (0.2%)	1.11	5/1514 (0.3%)
37	78	0.80	2/1139 (0.2%)	1.14	5/1514 (0.3%)
38	45	0.65	1/1120 (0.1%)	0.95	3/1498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	88	0.80	1/1134 (0.1%)	1.14	6/1519 (0.4%)
39	55	0.70	2/981 (0.2%)	0.87	0/1312
39	98	0.56	0/981	0.88	0/1312
40	65	0.52	0/886	0.93	0/1180
40	A8	0.60	0/891	0.90	0/1187
41	75	0.61	0/1123	0.86	1/1500 (0.1%)
41	B8	0.69	0/1115	0.99	0/1490
42	85	0.53	0/977	0.79	0/1301
42	C8	0.64	0/968	0.90	0/1289
43	95	0.64	0/785	1.04	2/1052 (0.2%)
43	D8	0.58	0/785	0.93	2/1052 (0.2%)
44	A5	0.66	0/897	0.89	0/1204
44	E8	0.64	0/901	0.88	0/1209
45	B5	0.65	0/749	1.01	5/1007 (0.5%)
45	F8	0.72	0/757	1.17	4/1017 (0.4%)
46	C5	0.88	4/812 (0.5%)	1.14	5/1083 (0.5%)
46	G8	0.85	0/809	1.30	11/1080 (1.0%)
47	D5	0.52	0/1099	0.88	1/1490 (0.1%)
47	H8	0.49	0/1403	0.84	1/1901 (0.1%)
48	E5	0.59	0/616	0.97	0/821
48	I8	0.75	0/614	1.01	0/819
49	F5	0.61	0/744	0.99	4/989 (0.4%)
49	J8	0.68	0/744	0.95	0/989
50	G5	0.58	0/570	0.89	0/755
50	K8	0.72	0/570	1.08	3/755 (0.4%)
51	H5	0.45	0/464	0.74	0/623
51	L8	0.59	0/464	0.83	0/623
52	M8	0.55	0/375	1.09	1/507 (0.2%)
53	J5	0.59	0/448	0.84	0/606
53	N8	0.84	1/381 (0.3%)	0.97	0/516
54	L5	0.72	0/409	1.03	0/540
54	P8	0.90	0/409	1.08	1/540 (0.2%)
55	M5	0.74	0/524	1.18	3/691 (0.4%)
55	Q8	0.74	0/524	1.33	8/691 (1.2%)
All	All	0.57	40/317065 (0.0%)	0.83	231/475024 (0.0%)

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	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	5
4	32	0	6
4	3E	0	2
5	42	0	1
7	62	0	1
8	72	0	1
9	82	0	1
10	1A	0	2
11	2A	0	1
12	3I	0	2
13	4A	0	5
13	4I	0	2
14	5A	0	1
14	5I	0	1
19	AA	0	2
19	AI	0	2
20	BA	0	3
20	BI	0	2
28	71	0	3
29	11	0	8
29	19	0	4
30	21	0	10
30	29	0	6
31	31	0	2
31	39	0	9
32	49	0	3
33	51	0	6
33	59	0	5
34	61	0	4
34	69	0	4
35	58	0	1
37	35	0	4
37	78	0	7
38	45	0	6
38	88	0	3
39	55	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	1
41	B8	0	2
42	85	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	C8	0	4
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	3
46	C5	0	4
46	G8	0	7
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	3
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	191

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	39	66	PRO	N-CD	-23.05	1.15	1.47
29	19	262	ARG	CZ-NH2	-11.90	1.18	1.33
37	35	121	LYS	C-N	11.64	1.61	1.33
8	7E	102	ARG	NE-CZ	-10.12	1.22	1.33
29	11	29	PRO	N-CD	-9.47	1.34	1.47

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	11	28	GLU	CA-C-N	18.89	143.45	119.84
29	11	28	GLU	C-N-CA	18.89	143.45	119.84
29	19	196	VAL	CA-C-N	-16.44	101.47	121.85
29	19	196	VAL	C-N-CA	-16.44	101.47	121.85
45	F8	3	THR	N-CA-C	-11.35	93.69	110.48

There are no chirality outliers.

5 of 191 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
2	1E	9	GLU	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	32157	0	16234	903	0
1	1G	32391	0	16353	953	1
2	12	1721	0	1758	127	0
2	1E	1874	0	1926	130	0
3	22	1541	0	1606	94	0
3	2E	1605	0	1668	67	0
4	32	1702	0	1765	147	0
4	3E	1698	0	1760	127	0
5	42	1134	0	1200	81	0
5	4E	1142	0	1204	68	0
6	52	842	0	857	30	0
6	5E	837	0	852	47	0
7	62	1110	0	1163	64	0
7	6E	1242	0	1286	54	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	76	0
9	82	953	0	983	92	0
9	8E	1000	0	1031	64	0
10	1A	646	0	662	42	0
10	1I	734	0	761	49	0
11	2A	835	0	847	36	0
11	2I	823	0	833	42	0
12	3A	956	0	1046	70	0
12	3I	956	0	1046	49	0
13	4A	893	0	946	73	0
13	4I	942	0	997	70	0
14	5A	486	0	525	51	0
14	5I	491	0	529	30	0
15	6A	729	0	768	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	40	0
16	7A	705	0	725	46	0
16	7I	700	0	720	53	0
17	8A	823	0	891	39	0
17	8I	834	0	904	55	0
18	9A	544	0	605	23	0
18	9I	549	0	607	31	0
19	AA	481	0	468	46	0
19	AI	658	0	678	52	0
20	BA	762	0	861	45	0
20	BI	746	0	843	63	0
21	1B	188	0	195	14	0
21	1F	199	0	208	16	0
22	1K	1477	0	758	51	0
22	1L	1563	0	799	55	0
23	2K	1646	0	844	30	0
23	2L	1646	0	844	57	0
24	3K	1611	0	817	79	0
24	3L	1611	0	817	55	0
25	4K	439	0	219	11	0
25	4L	395	0	196	12	0
26	14	61630	0	31073	1539	1
26	1H	61028	0	30758	1549	0
27	16	2617	0	1328	67	0
27	1J	2617	0	1328	89	0
28	71	1033	0	1048	77	0
28	79	456	0	460	53	0
29	11	2120	0	2197	146	0
29	19	2125	0	2199	137	0
30	21	1558	0	1623	112	0
30	29	1563	0	1629	138	0
31	31	1585	0	1632	107	0
31	39	1602	0	1649	138	0
32	41	1457	0	1514	109	0
32	49	1458	0	1515	87	0
33	51	1312	0	1384	73	0
33	59	539	0	563	38	0
34	61	1136	0	1223	59	0
34	69	1131	0	1218	62	0
35	15	1104	0	1180	42	0
35	58	1104	0	1180	78	0
36	25	932	0	996	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	68	932	0	996	46	0
37	35	1122	0	1206	101	0
37	78	1122	0	1206	108	0
38	45	1099	0	1154	89	0
38	88	1113	0	1157	63	0
39	55	967	0	1033	67	0
39	98	967	0	1033	54	0
40	65	876	0	938	78	0
40	A8	881	0	943	59	0
41	75	1109	0	1170	64	0
41	B8	1101	0	1158	64	0
42	85	959	0	1019	69	0
42	C8	950	0	1011	67	0
43	95	774	0	849	66	0
43	D8	774	0	849	59	0
44	A5	886	0	948	32	0
44	E8	890	0	951	33	0
45	B5	735	0	785	39	0
45	F8	743	0	794	32	0
46	C5	799	0	888	72	0
46	G8	796	0	886	61	0
47	D5	1074	0	1087	77	0
47	H8	1373	0	1402	80	0
48	E5	608	0	622	33	0
48	I8	606	0	625	30	0
49	F5	737	0	813	51	0
49	J8	737	0	813	29	0
50	G5	568	0	614	43	0
50	K8	568	0	614	41	0
51	H5	459	0	512	11	0
51	L8	459	0	512	14	0
52	M8	366	0	370	49	0
53	J5	434	0	454	24	0
53	N8	369	0	388	24	0
54	L5	401	0	436	22	0
54	P8	401	0	436	21	0
55	M5	516	0	582	35	0
55	Q8	516	0	582	42	0
56	13	131	0	0	0	0
56	14	382	0	0	0	0
56	16	11	0	0	0	0
56	1G	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	429	0	0	0	0
56	1J	5	0	0	0	0
56	1K	1	0	0	0	0
56	21	2	0	0	0	0
56	29	1	0	0	0	0
56	2K	3	0	0	0	0
56	2L	3	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	3K	1	0	0	0	0
56	41	1	0	0	0	0
56	45	3	0	0	0	0
56	4K	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	C5	1	0	0	0	0
56	E5	1	0	0	0	0
56	I8	3	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	13	42	0	45	3	0
57	1G	42	0	45	2	0
58	32	8	0	0	3	0
58	3E	8	0	0	3	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	11	10	0	0	3	0
60	13	144	0	0	15	0
60	14	367	0	0	32	0
60	16	22	0	0	1	0
60	19	8	0	0	0	0
60	1G	68	0	0	4	0
60	1H	540	0	0	71	0
60	1I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1J	12	0	0	3	0
60	29	2	0	0	1	0
60	31	7	0	0	0	0
60	32	2	0	0	0	0
60	35	2	0	0	0	0
60	39	3	0	0	1	0
60	3E	2	0	0	1	0
60	3K	1	0	0	0	0
60	4K	3	0	0	1	0
60	55	2	0	0	2	0
60	58	2	0	0	0	0
60	5I	2	0	0	0	0
60	6I	1	0	0	0	0
60	78	4	0	0	1	0
60	7I	1	0	0	0	0
60	98	1	0	0	1	0
60	BI	1	0	0	0	0
60	G8	1	0	0	0	0
60	H5	1	0	0	0	0
60	I8	2	0	0	0	0
60	L5	1	0	0	0	0
60	L8	3	0	0	1	0
60	P8	1	0	0	0	0
All	All	294257	0	196338	9976	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 9976 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)
26:1H:943:U:OP2	37:78:36:LYS:NZ	1.64	1.30
31:39:38:ARG:NH2	31:39:99:TYR:CE1	1.96	1.30
44:E8:92:ARG:NH1	44:E8:94:ASP:OD1	1.71	1.22
35:58:49:GLY:O	35:58:119:ARG:NH1	1.77	1.16
29:11:183:ARG:NH1	29:11:269:PHE:HB2	1.61	1.15

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	206/256 (80%)	171 (83%)	30 (15%)	5 (2%)	4 22
2	1E	227/256 (89%)	188 (83%)	36 (16%)	3 (1%)	9 35
3	22	192/239 (80%)	172 (90%)	20 (10%)	0	100 100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100 100
4	32	206/209 (99%)	175 (85%)	29 (14%)	2 (1%)	12 41
4	3E	205/209 (98%)	188 (92%)	15 (7%)	2 (1%)	12 41
5	42	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18 49
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	18 49
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100 100
7	62	134/156 (86%)	122 (91%)	12 (9%)	0	100 100
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100 100
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18 49
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18 49
9	82	119/128 (93%)	111 (93%)	7 (6%)	1 (1%)	16 47
9	8E	124/128 (97%)	106 (86%)	16 (13%)	2 (2%)	7 30
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100 100
10	1I	89/105 (85%)	80 (90%)	9 (10%)	0	100 100
11	2A	111/129 (86%)	100 (90%)	9 (8%)	2 (2%)	6 28
11	2I	109/129 (84%)	98 (90%)	9 (8%)	2 (2%)	6 28
12	3A	120/132 (91%)	98 (82%)	19 (16%)	3 (2%)	4 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	3I	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	16 47
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	14 44
13	4I	117/126 (93%)	95 (81%)	22 (19%)	0	100 100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6 28
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3 16
15	6A	85/89 (96%)	78 (92%)	7 (8%)	0	100 100
15	6I	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	10 37
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100 100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100 100
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100 100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100 100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100 100
18	9I	66/88 (75%)	62 (94%)	2 (3%)	2 (3%)	3 19
19	AA	56/93 (60%)	47 (84%)	7 (12%)	2 (4%)	2 16
19	AI	80/93 (86%)	67 (84%)	10 (12%)	3 (4%)	2 15
20	BA	97/106 (92%)	86 (89%)	9 (9%)	2 (2%)	5 25
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100 100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100 100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
28	71	129/229 (56%)	119 (92%)	10 (8%)	0	100 100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100 100
29	11	271/276 (98%)	243 (90%)	19 (7%)	9 (3%)	3 17
29	19	272/276 (99%)	242 (89%)	23 (8%)	7 (3%)	4 21
30	21	201/206 (98%)	158 (79%)	35 (17%)	8 (4%)	2 13
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	2 13
31	31	200/210 (95%)	183 (92%)	14 (7%)	3 (2%)	8 32
31	39	202/210 (96%)	155 (77%)	40 (20%)	7 (4%)	3 16
32	41	177/182 (97%)	154 (87%)	21 (12%)	2 (1%)	11 39
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	11 39
33	51	169/180 (94%)	135 (80%)	25 (15%)	9 (5%)	1 10
33	59	63/180 (35%)	48 (76%)	13 (21%)	2 (3%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	61	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9 34
34	69	143/148 (97%)	114 (80%)	28 (20%)	1 (1%)	18 49
35	15	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18 49
35	58	136/140 (97%)	114 (84%)	18 (13%)	4 (3%)	3 19
36	25	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
37	35	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3 16
37	78	145/150 (97%)	117 (81%)	24 (17%)	4 (3%)	4 20
38	45	136/141 (96%)	115 (85%)	18 (13%)	3 (2%)	5 24
38	88	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3 19
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14 44
39	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	14 44
40	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	14 44
40	A8	109/112 (97%)	87 (80%)	22 (20%)	0	100 100
41	75	131/146 (90%)	121 (92%)	10 (8%)	0	100 100
41	B8	130/146 (89%)	115 (88%)	14 (11%)	1 (1%)	16 47
42	85	114/118 (97%)	105 (92%)	7 (6%)	2 (2%)	6 28
42	C8	113/118 (96%)	103 (91%)	7 (6%)	3 (3%)	4 20
43	95	98/101 (97%)	73 (74%)	20 (20%)	5 (5%)	1 10
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	2 13
44	A5	109/113 (96%)	103 (94%)	4 (4%)	2 (2%)	6 28
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100 100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	5 24
45	F8	93/96 (97%)	84 (90%)	9 (10%)	0	100 100
46	C5	103/110 (94%)	72 (70%)	24 (23%)	7 (7%)	1 5
46	G8	103/110 (94%)	87 (84%)	13 (13%)	3 (3%)	3 19
47	D5	128/206 (62%)	104 (81%)	20 (16%)	4 (3%)	3 18
47	H8	169/206 (82%)	136 (80%)	26 (15%)	7 (4%)	2 13
48	E5	75/85 (88%)	67 (89%)	5 (7%)	3 (4%)	2 13
48	I8	74/85 (87%)	69 (93%)	5 (7%)	0	100 100
49	F5	92/98 (94%)	85 (92%)	5 (5%)	2 (2%)	5 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	J8	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	11 39
50	G5	66/72 (92%)	62 (94%)	2 (3%)	2 (3%)	3 19
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	2 12
51	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100 100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100 100
52	M8	45/71 (63%)	31 (69%)	13 (29%)	1 (2%)	5 24
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	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100 100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100 100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2 11
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2 11
All	All	10971/12333 (89%)	9586 (87%)	1202 (11%)	183 (2%)	7 30

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	127	LYS
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
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	182/220 (83%)	182 (100%)	0	100 100
2	1E	200/220 (91%)	196 (98%)	4 (2%)	48 72
3	22	154/188 (82%)	154 (100%)	0	100 100
3	2E	159/188 (85%)	158 (99%)	1 (1%)	78 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	179 (99%)	1 (1%)	78	83
4	3E	180/181 (99%)	178 (99%)	2 (1%)	65	78
5	42	114/123 (93%)	114 (100%)	0	100	100
5	4E	115/123 (94%)	113 (98%)	2 (2%)	53	74
6	52	90/90 (100%)	89 (99%)	1 (1%)	65	78
6	5E	90/90 (100%)	90 (100%)	0	100	100
7	62	114/127 (90%)	114 (100%)	0	100	100
7	6E	125/127 (98%)	125 (100%)	0	100	100
8	72	118/119 (99%)	118 (100%)	0	100	100
8	7E	119/119 (100%)	119 (100%)	0	100	100
9	82	92/99 (93%)	92 (100%)	0	100	100
9	8E	97/99 (98%)	96 (99%)	1 (1%)	68	79
10	1A	71/92 (77%)	71 (100%)	0	100	100
10	1I	81/92 (88%)	81 (100%)	0	100	100
11	2A	85/99 (86%)	85 (100%)	0	100	100
11	2I	84/99 (85%)	84 (100%)	0	100	100
12	3A	103/109 (94%)	102 (99%)	1 (1%)	68	79
12	3I	103/109 (94%)	102 (99%)	1 (1%)	68	79
13	4A	91/101 (90%)	90 (99%)	1 (1%)	65	78
13	4I	94/101 (93%)	94 (100%)	0	100	100
14	5A	49/50 (98%)	49 (100%)	0	100	100
14	5I	49/50 (98%)	49 (100%)	0	100	100
15	6A	79/80 (99%)	79 (100%)	0	100	100
15	6I	79/80 (99%)	79 (100%)	0	100	100
16	7A	72/74 (97%)	72 (100%)	0	100	100
16	7I	72/74 (97%)	72 (100%)	0	100	100
17	8A	94/97 (97%)	94 (100%)	0	100	100
17	8I	95/97 (98%)	95 (100%)	0	100	100
18	9A	58/77 (75%)	58 (100%)	0	100	100
18	9I	58/77 (75%)	58 (100%)	0	100	100
19	AA	52/80 (65%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	71/80 (89%)	71 (100%)	0	100	100
20	BA	76/82 (93%)	76 (100%)	0	100	100
20	BI	75/82 (92%)	75 (100%)	0	100	100
21	1B	17/22 (77%)	17 (100%)	0	100	100
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	71	109/181 (60%)	109 (100%)	0	100	100
28	79	48/181 (26%)	48 (100%)	0	100	100
29	11	214/218 (98%)	214 (100%)	0	100	100
29	19	214/218 (98%)	212 (99%)	2 (1%)	70	80
30	21	165/166 (99%)	165 (100%)	0	100	100
30	29	165/166 (99%)	164 (99%)	1 (1%)	78	83
31	31	161/166 (97%)	161 (100%)	0	100	100
31	39	163/166 (98%)	163 (100%)	0	100	100
32	41	153/156 (98%)	152 (99%)	1 (1%)	76	82
32	49	153/156 (98%)	153 (100%)	0	100	100
33	51	142/148 (96%)	141 (99%)	1 (1%)	76	82
33	59	56/148 (38%)	56 (100%)	0	100	100
34	61	122/124 (98%)	122 (100%)	0	100	100
34	69	122/124 (98%)	121 (99%)	1 (1%)	73	81
35	15	117/119 (98%)	117 (100%)	0	100	100
35	58	117/119 (98%)	116 (99%)	1 (1%)	70	80
36	25	100/100 (100%)	99 (99%)	1 (1%)	68	79
36	68	100/100 (100%)	99 (99%)	1 (1%)	68	79
37	35	114/116 (98%)	114 (100%)	0	100	100
37	78	114/116 (98%)	112 (98%)	2 (2%)	51	73
38	45	109/111 (98%)	109 (100%)	0	100	100
38	88	109/111 (98%)	109 (100%)	0	100	100
39	55	101/101 (100%)	99 (98%)	2 (2%)	48	72
39	98	101/101 (100%)	100 (99%)	1 (1%)	68	79
40	65	87/88 (99%)	87 (100%)	0	100	100
40	A8	87/88 (99%)	86 (99%)	1 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	75	117/127 (92%)	117 (100%)	0	100 100
41	B8	116/127 (91%)	114 (98%)	2 (2%)	53 74
42	85	93/94 (99%)	93 (100%)	0	100 100
42	C8	92/94 (98%)	92 (100%)	0	100 100
43	95	82/82 (100%)	81 (99%)	1 (1%)	63 78
43	D8	82/82 (100%)	82 (100%)	0	100 100
44	A5	91/92 (99%)	89 (98%)	2 (2%)	45 71
44	E8	91/92 (99%)	90 (99%)	1 (1%)	65 78
45	B5	74/78 (95%)	74 (100%)	0	100 100
45	F8	75/78 (96%)	75 (100%)	0	100 100
46	C5	85/91 (93%)	85 (100%)	0	100 100
46	G8	85/91 (93%)	85 (100%)	0	100 100
47	D5	118/179 (66%)	117 (99%)	1 (1%)	73 81
47	H8	152/179 (85%)	152 (100%)	0	100 100
48	E5	61/67 (91%)	61 (100%)	0	100 100
48	I8	61/67 (91%)	61 (100%)	0	100 100
49	F5	79/83 (95%)	79 (100%)	0	100 100
49	J8	79/83 (95%)	79 (100%)	0	100 100
50	G5	62/67 (92%)	62 (100%)	0	100 100
50	K8	62/67 (92%)	61 (98%)	1 (2%)	55 75
51	H5	50/52 (96%)	50 (100%)	0	100 100
51	L8	50/52 (96%)	50 (100%)	0	100 100
52	M8	42/63 (67%)	42 (100%)	0	100 100
53	J5	48/52 (92%)	46 (96%)	2 (4%)	26 58
53	N8	43/52 (83%)	42 (98%)	1 (2%)	44 70
54	L5	38/42 (90%)	37 (97%)	1 (3%)	40 68
54	P8	38/42 (90%)	37 (97%)	1 (3%)	40 68
55	M5	54/55 (98%)	54 (100%)	0	100 100
55	Q8	54/55 (98%)	54 (100%)	0	100 100
All	All	9272/10193 (91%)	9229 (100%)	43 (0%)	81 85

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	4A	115	LYS
39	55	88	ARG
29	19	31	LYS
34	69	108	THR
44	A5	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
15	6A	53	HIS
36	25	5	GLN
18	9A	36	ASN
31	39	8	GLN
45	B5	87	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	349 (23%)	32 (2%)
1	1G	1505/1522 (98%)	385 (25%)	30 (1%)
22	1K	66/76 (86%)	31 (46%)	3 (4%)
22	1L	71/76 (93%)	32 (45%)	5 (7%)
23	2K	76/77 (98%)	23 (30%)	1 (1%)
23	2L	76/77 (98%)	19 (25%)	2 (2%)
24	3K	75/76 (98%)	45 (60%)	3 (4%)
24	3L	75/76 (98%)	33 (44%)	0
25	4K	18/27 (66%)	11 (61%)	1 (5%)
25	4L	17/27 (62%)	10 (58%)	0
26	14	2852/2912 (97%)	738 (25%)	51 (1%)
26	1H	2828/2912 (97%)	735 (25%)	51 (1%)
27	16	121/122 (99%)	17 (14%)	2 (1%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
All	All	9394/9624 (97%)	2461 (26%)	183 (1%)

5 of 2461 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

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Mol	Chain	Res	Type
1	13	8	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1139	G
26	14	791	C
1	1G	1300	G
26	14	34	C
26	14	1396	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	5MU	1L	54	22	19,22,23	3.96	5 (26%)	28,32,35	3.36	9 (32%)
24	PSU	3K	39	24	18,21,22	1.26	1 (5%)	22,30,33	1.82	7 (31%)
23	OMC	2K	33	23	19,22,23	1.73	3 (15%)	26,31,34	1.14	2 (7%)
22	5MU	1K	54	22	19,22,23	3.70	5 (26%)	28,32,35	2.98	6 (21%)
22	U8U	1K	34	22	19,24,25	2.55	7 (36%)	23,34,37	1.05	2 (8%)
23	G7M	2L	47	23	23,26,27	2.65	8 (34%)	35,39,42	1.75	7 (20%)
23	4SU	2L	8	23	18,21,22	1.78	3 (16%)	26,30,33	2.60	4 (15%)
23	G7M	2K	47	23	23,26,27	2.52	9 (39%)	35,39,42	1.59	10 (28%)
22	T6A	1L	37	22	31,34,35	2.21	5 (16%)	44,49,52	2.29	14 (31%)
23	PSU	2K	56	23	18,21,22	1.23	2 (11%)	22,30,33	1.73	3 (13%)
23	4SU	2K	8	23	18,21,22	1.90	5 (27%)	26,30,33	2.73	8 (30%)
22	T6A	1K	37	22	31,34,35	2.30	8 (25%)	44,49,52	2.03	11 (25%)
23	PSU	2L	56	23	18,21,22	1.21	1 (5%)	22,30,33	1.83	4 (18%)
23	5MU	2L	55	23	19,22,23	3.86	5 (26%)	28,32,35	3.46	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	U8U	1L	34	25,22	19,24,25	2.57	7 (36%)	23,34,37	0.91	2 (8%)
23	5MU	2K	55	23	19,22,23	3.69	5 (26%)	28,32,35	3.41	7 (25%)
22	PSU	1K	55	22	18,21,22	1.15	1 (5%)	22,30,33	1.50	4 (18%)
22	PSU	1L	55	22	18,21,22	1.13	1 (5%)	22,30,33	1.57	4 (18%)
24	PSU	3L	39	24	18,21,22	1.16	1 (5%)	22,30,33	1.43	2 (9%)
22	PSU	1K	39	22	18,21,22	0.92	1 (5%)	22,30,33	1.54	3 (13%)
23	OMC	2L	33	23	19,22,23	1.82	4 (21%)	26,31,34	1.27	2 (7%)
22	PSU	1L	39	22	18,21,22	1.10	1 (5%)	22,30,33	1.61	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	1L	54	22	-	3/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	22	-	0/9/28/29	0/2/2/2
23	G7M	2L	47	23	-	3/7/25/26	0/3/3/3
23	4SU	2L	8	23	-	1/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	1/7/25/26	0/3/3/3
22	T6A	1L	37	22	-	5/23/41/42	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/23/41/42	0/3/3/3
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
22	U8U	1L	34	25,22	-	4/9/28/29	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	3/9/27/28	0/2/2/2
22	PSU	1L	39	22	-	1/7/25/26	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	12.96	1.59	1.38
23	2L	55	5MU	C2-N1	12.45	1.58	1.38
22	1K	54	5MU	C2-N1	11.70	1.57	1.38
23	2K	55	5MU	C2-N1	11.53	1.56	1.38
22	1L	37	T6A	C10-N11	7.10	1.50	1.35

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	C5-C4-N3	11.33	124.98	115.31
23	2L	55	5MU	C5-C4-N3	10.65	124.40	115.31
22	1K	54	5MU	C5-C4-N3	10.44	124.22	115.31
22	1L	54	5MU	C5-C4-N3	10.32	124.12	115.31
23	2L	8	4SU	C4-N3-C2	-8.55	119.04	127.34

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	34	U8U	N-C-C5-C4
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10
22	1L	54	5MU	O4'-C4'-C5'-O5'
23	2L	47	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1L	54	5MU	2	0
22	1K	34	U8U	1	0
23	2L	47	G7M	1	0
23	2L	8	4SU	4	0
22	1K	37	T6A	2	0
23	2L	55	5MU	3	0
22	1L	34	U8U	1	0
23	2K	55	5MU	3	0
22	1L	55	PSU	2	0
22	1K	39	PSU	1	0
23	2L	33	OMC	3	0
22	1L	39	PSU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1081 ligands modelled in this entry, 1077 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	32	301	4	0,12,12	-	-	-		
58	SF4	3E	302	4	0,12,12	-	-	-		
57	PAR	13	1730	-	45,45,45	0.87	1 (2%)	64,67,67	2.10	21 (32%)
57	PAR	1G	1681	-	45,45,45	0.82	1 (2%)	64,67,67	1.71	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	32	301	4	-	-	0/6/5/5
58	SF4	3E	302	4	-	-	0/6/5/5
57	PAR	13	1730	-	-	6/18/94/94	0/4/4/4
57	PAR	1G	1681	-	-	4/18/94/94	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1681	PAR	C31-C21	-2.75	1.50	1.53
57	13	1730	PAR	O54-C14	2.13	1.47	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1G	1681	PAR	O52-C13-O43	-6.13	104.79	111.43
57	13	1730	PAR	O52-C13-O43	-5.61	105.35	111.43
57	13	1730	PAR	C32-C22-C12	-4.88	101.16	111.18
57	1G	1681	PAR	C14-O54-C54	4.67	122.86	113.69
57	1G	1681	PAR	C13-O52-C52	-4.49	106.84	117.96

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	13	1730	PAR	O54-C54-C64-N64
57	1G	1681	PAR	O51-C51-C61-O61
57	1G	1681	PAR	C41-C51-C61-O61
57	13	1730	PAR	C41-C51-C61-O61
57	1G	1681	PAR	O51-C11-O11-C42

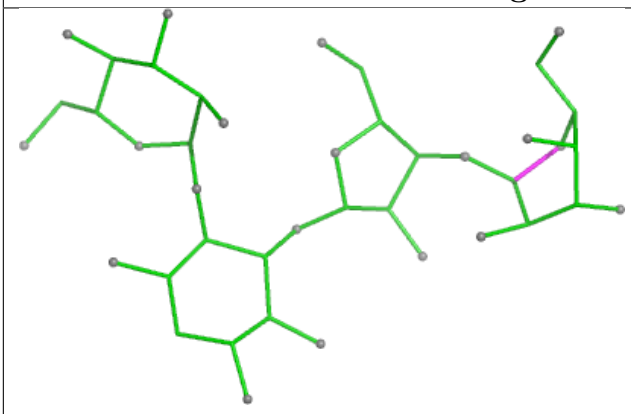
There are no ring outliers.

4 monomers are involved in 11 short contacts:

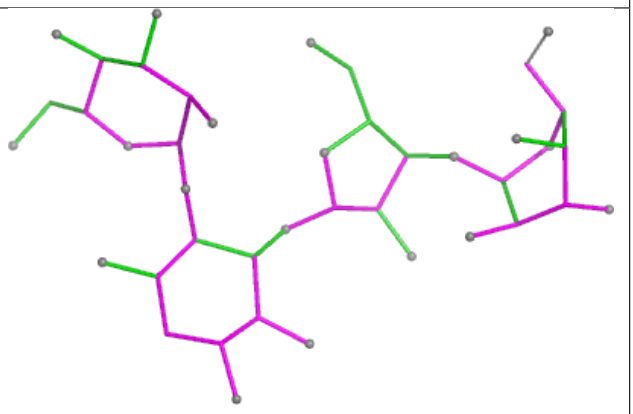
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	32	301	SF4	3	0
58	3E	302	SF4	3	0
57	13	1730	PAR	3	0
57	1G	1681	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

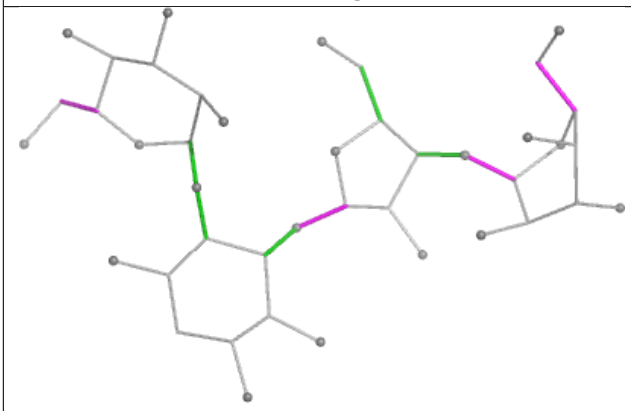
Ligand PAR 13 1730



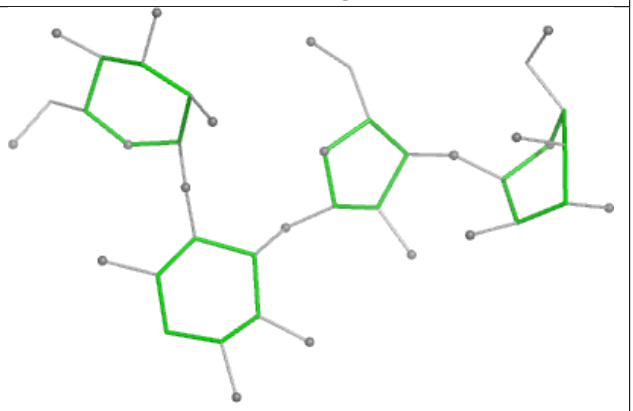
Bond lengths



Bond angles

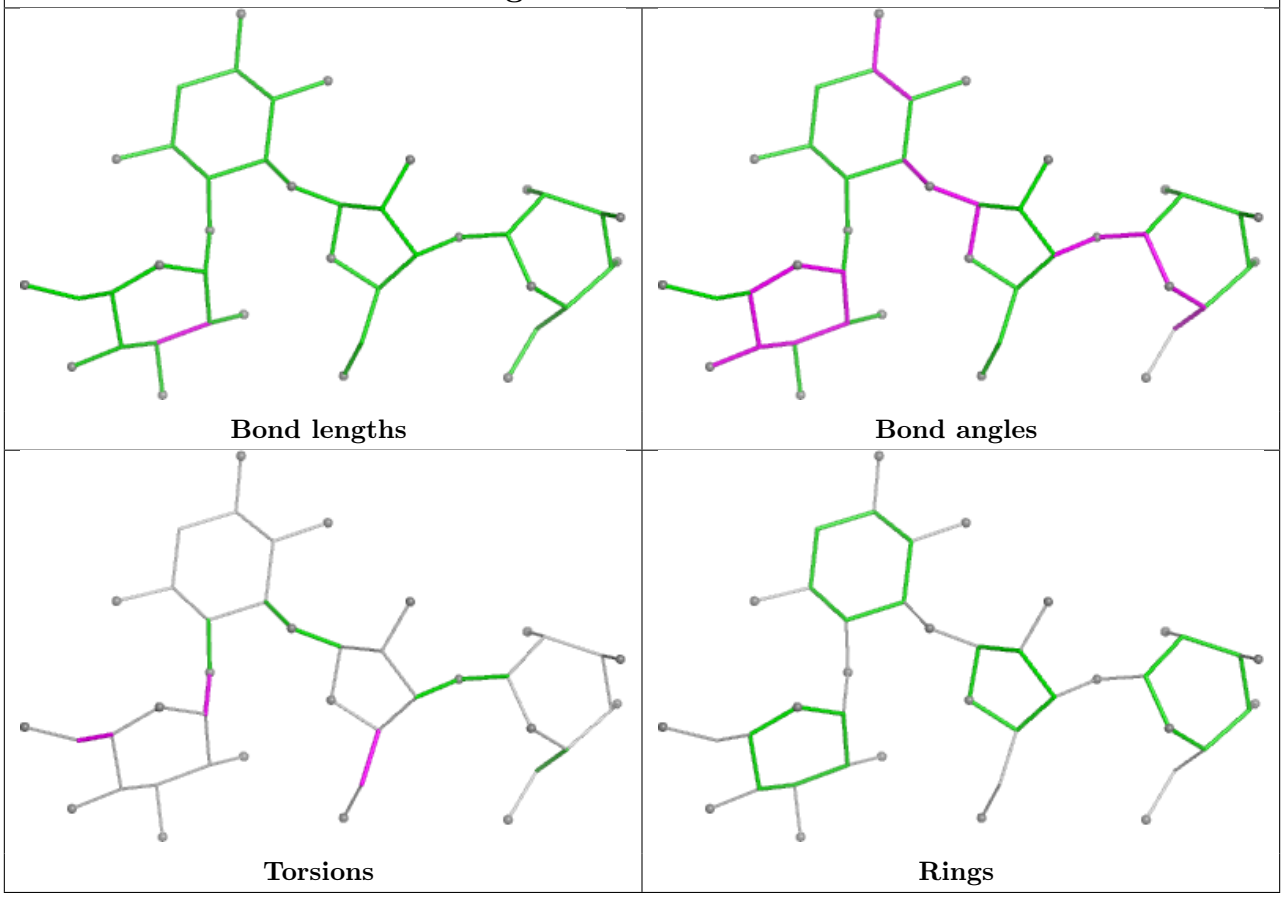


Torsions



Rings

Ligand PAR 1G 1681



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
25	4K	1
37	35	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3'	25:A	P	4.27
1	35	121:LYS	C	122:PRO	N	1.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1496/1522 (98%)	-0.74	2 (0%) 92 86	64, 104, 160, 189	0
1	1G	1507/1522 (99%)	-0.71	4 (0%) 90 80	78, 123, 164, 193	0
2	12	210/256 (82%)	0.10	2 (0%) 79 61	121, 148, 157, 163	0
2	1E	231/256 (90%)	0.01	3 (1%) 75 56	112, 136, 153, 161	0
3	22	196/239 (82%)	0.12	4 (2%) 65 44	128, 141, 155, 161	0
3	2E	205/239 (85%)	-0.38	0 100 100	90, 109, 133, 144	0
4	32	208/209 (99%)	0.28	6 (2%) 53 32	101, 123, 139, 150	0
4	3E	207/209 (99%)	-0.09	1 (0%) 87 73	88, 106, 126, 133	0
5	42	148/162 (91%)	0.22	2 (1%) 73 53	110, 128, 140, 145	0
5	4E	149/162 (91%)	0.07	3 (2%) 65 44	80, 101, 118, 130	0
6	52	101/101 (100%)	-0.07	1 (0%) 79 61	96, 111, 126, 136	0
6	5E	100/101 (99%)	0.01	4 (4%) 42 23	84, 102, 119, 129	0
7	62	138/156 (88%)	-0.03	4 (2%) 53 32	120, 131, 141, 145	0
7	6E	154/156 (98%)	-0.16	1 (0%) 85 70	105, 124, 144, 159	0
8	72	137/138 (99%)	-0.31	0 100 100	111, 131, 141, 147	0
8	7E	138/138 (100%)	0.21	2 (1%) 73 53	92, 110, 121, 130	0
9	82	121/128 (94%)	-0.04	2 (1%) 69 48	115, 146, 155, 160	0
9	8E	126/128 (98%)	-0.22	0 100 100	93, 132, 149, 152	0
10	1A	80/105 (76%)	0.16	3 (3%) 44 25	125, 141, 153, 156	0
10	1I	91/105 (86%)	-0.23	1 (1%) 78 59	84, 125, 153, 158	0
11	2A	113/129 (87%)	0.18	2 (1%) 67 47	90, 119, 128, 133	0
11	2I	111/129 (86%)	0.24	1 (0%) 81 63	82, 112, 129, 144	0
12	3A	122/132 (92%)	0.55	13 (10%) 11 6	88, 112, 132, 146	0
12	3I	122/132 (92%)	-0.15	4 (3%) 49 29	73, 82, 106, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	0.03	1 (0%) 81 63	124, 141, 150, 165	0
13	4I	119/126 (94%)	-0.25	2 (1%) 69 48	94, 120, 135, 146	0
14	5A	59/61 (96%)	0.21	3 (5%) 33 18	130, 140, 148, 150	0
14	5I	60/61 (98%)	-0.53	0 100 100	88, 100, 112, 125	0
15	6A	87/89 (97%)	-0.59	0 100 100	93, 117, 132, 135	0
15	6I	87/89 (97%)	-0.24	0 100 100	84, 103, 120, 126	0
16	7A	84/88 (95%)	-0.08	0 100 100	93, 111, 130, 141	0
16	7I	83/88 (94%)	0.07	1 (1%) 76 58	102, 112, 135, 147	0
17	8A	99/105 (94%)	-0.38	1 (1%) 79 61	108, 120, 133, 138	0
17	8I	100/105 (95%)	-0.07	1 (1%) 79 61	89, 111, 126, 131	0
18	9A	67/88 (76%)	-0.12	3 (4%) 38 20	106, 117, 135, 139	0
18	9I	68/88 (77%)	0.18	2 (2%) 53 32	89, 105, 124, 127	0
19	AA	62/93 (66%)	0.38	4 (6%) 25 13	123, 149, 157, 163	0
19	AI	82/93 (88%)	-0.17	1 (1%) 76 58	99, 118, 134, 142	0
20	BA	99/106 (93%)	-0.45	0 100 100	94, 116, 141, 150	0
20	BI	97/106 (91%)	-0.09	2 (2%) 63 42	114, 126, 144, 148	0
21	1B	22/27 (81%)	-0.07	0 100 100	124, 136, 143, 147	0
21	1F	23/27 (85%)	-0.74	0 100 100	99, 109, 116, 120	0
22	1K	64/76 (84%)	0.77	10 (15%) 5 2	93, 158, 171, 173	0
22	1L	68/76 (89%)	0.17	4 (5%) 28 15	125, 171, 178, 184	0
23	2K	72/77 (93%)	-0.29	0 100 100	77, 104, 130, 146	0
23	2L	72/77 (93%)	-0.35	0 100 100	84, 122, 150, 165	0
24	3K	75/76 (98%)	0.46	6 (8%) 18 10	81, 170, 184, 189	0
24	3L	75/76 (98%)	0.06	2 (2%) 56 35	89, 167, 182, 188	0
25	4K	20/27 (74%)	0.78	4 (20%) 3 1	76, 144, 177, 178	0
25	4L	18/27 (66%)	0.12	0 100 100	103, 157, 182, 183	0
26	14	2861/2912 (98%)	-0.80	9 (0%) 90 80	58, 92, 173, 197	0
26	1H	2833/2912 (97%)	-0.84	10 (0%) 88 76	50, 80, 164, 199	0
27	16	122/122 (100%)	-0.98	0 100 100	75, 98, 119, 170	0
27	1J	122/122 (100%)	-0.76	1 (0%) 82 65	93, 123, 141, 174	0
28	71	133/229 (58%)	0.12	1 (0%) 82 65	137, 169, 179, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	79	57/229 (24%)	0.17	1 (1%) 67 47	139, 160, 169, 174	0
29	11	273/276 (98%)	0.09	4 (1%) 72 52	48, 74, 92, 101	0
29	19	274/276 (99%)	0.14	9 (3%) 49 29	60, 82, 99, 116	0
30	21	203/206 (98%)	-0.07	1 (0%) 87 73	58, 95, 135, 146	0
30	29	204/206 (99%)	-0.27	2 (0%) 79 61	67, 99, 134, 144	0
31	31	202/210 (96%)	-0.26	4 (1%) 65 44	54, 85, 119, 138	0
31	39	204/210 (97%)	-0.14	2 (0%) 79 61	64, 112, 147, 163	0
32	41	179/182 (98%)	-0.39	2 (1%) 78 59	87, 107, 136, 148	0
32	49	179/182 (98%)	0.09	3 (1%) 69 48	121, 137, 156, 168	0
33	51	171/180 (95%)	-0.01	6 (3%) 47 27	89, 110, 125, 137	0
33	59	69/180 (38%)	0.55	4 (5%) 29 16	131, 151, 162, 166	0
34	61	146/148 (98%)	-0.12	1 (0%) 84 68	85, 129, 142, 149	0
34	69	145/148 (97%)	0.08	9 (6%) 26 14	91, 126, 142, 151	0
35	15	138/140 (98%)	0.20	3 (2%) 62 41	87, 114, 138, 154	0
35	58	138/140 (98%)	0.10	4 (2%) 53 32	69, 97, 124, 140	0
36	25	122/122 (100%)	0.20	0 100 100	76, 96, 112, 118	0
36	68	122/122 (100%)	0.09	4 (3%) 49 29	63, 84, 101, 110	0
37	35	147/150 (98%)	0.19	6 (4%) 41 23	65, 110, 135, 148	0
37	78	147/150 (98%)	-0.11	2 (1%) 73 53	50, 89, 113, 128	0
38	45	138/141 (97%)	0.37	13 (9%) 14 8	84, 111, 129, 137	0
38	88	141/141 (100%)	-0.17	3 (2%) 63 42	58, 84, 107, 125	0
39	55	118/118 (100%)	-0.46	0 100 100	70, 86, 108, 121	0
39	98	118/118 (100%)	-0.17	0 100 100	71, 92, 112, 126	0
40	65	110/112 (98%)	-0.32	1 (0%) 81 63	91, 116, 132, 137	0
40	A8	111/112 (99%)	-0.38	0 100 100	76, 94, 117, 123	0
41	75	133/146 (91%)	0.06	7 (5%) 32 17	86, 102, 130, 142	0
41	B8	132/146 (90%)	0.01	3 (2%) 61 39	78, 99, 128, 138	0
42	85	116/118 (98%)	0.07	1 (0%) 81 63	76, 101, 130, 139	0
42	C8	115/118 (97%)	0.12	2 (1%) 69 48	65, 83, 114, 118	0
43	95	100/101 (99%)	0.36	5 (5%) 34 18	76, 123, 139, 141	0
43	D8	100/101 (99%)	0.42	5 (5%) 34 18	64, 105, 128, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	A5	111/113 (98%)	-0.06	0 100 100	68, 84, 114, 141	0
44	E8	112/113 (99%)	0.08	2 (1%) 67 47	64, 82, 112, 142	0
45	B5	94/96 (97%)	-0.14	3 (3%) 50 30	75, 91, 115, 123	0
45	F8	95/96 (98%)	-0.24	1 (1%) 78 59	62, 79, 111, 125	0
46	C5	105/110 (95%)	0.71	15 (14%) 6 3	91, 124, 146, 152	0
46	G8	105/110 (95%)	0.26	7 (6%) 24 13	79, 101, 127, 132	0
47	D5	132/206 (64%)	-0.09	2 (1%) 72 52	115, 136, 152, 155	0
47	H8	171/206 (83%)	-0.07	1 (0%) 85 70	90, 124, 164, 168	0
48	E5	77/85 (90%)	-0.08	1 (1%) 75 56	75, 96, 113, 135	0
48	I8	76/85 (89%)	-0.27	1 (1%) 75 56	65, 78, 91, 107	0
49	F5	94/98 (95%)	0.48	6 (6%) 25 14	70, 90, 123, 133	0
49	J8	94/98 (95%)	-0.05	0 100 100	61, 81, 120, 128	0
50	G5	68/72 (94%)	-0.13	1 (1%) 72 52	88, 109, 129, 150	0
50	K8	68/72 (94%)	-0.08	0 100 100	66, 84, 104, 128	0
51	H5	58/60 (96%)	-0.18	0 100 100	85, 106, 134, 140	0
51	L8	58/60 (96%)	-0.22	0 100 100	65, 87, 115, 132	0
52	M8	47/71 (66%)	-0.14	0 100 100	111, 137, 156, 163	0
53	J5	56/60 (93%)	-0.16	0 100 100	67, 92, 137, 147	0
53	N8	48/60 (80%)	-0.30	0 100 100	61, 87, 134, 141	0
54	L5	47/49 (95%)	-0.33	2 (4%) 40 22	57, 68, 85, 103	0
54	P8	47/49 (95%)	-0.64	0 100 100	53, 60, 79, 88	0
55	M5	64/65 (98%)	0.06	1 (1%) 70 49	75, 86, 103, 126	0
55	Q8	64/65 (98%)	-0.12	0 100 100	64, 74, 92, 108	0
All	All	20598/21957 (93%)	-0.35	283 (1%) 73 53	48, 105, 159, 199	0

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	75	104	ASN	6.6
43	D8	37	VAL	6.0
41	75	106	SER	6.0
22	1K	76	A	5.9
38	45	90	VAL	5.6

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, 95^{th} 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	0.84	0.09	102,113,120,131	0
23	OMC	2L	33	21/22	0.84	0.10	105,114,118,121	0
23	G7M	2L	47	24/25	0.86	0.10	126,133,141,145	0
23	5MU	2L	55	21/22	0.86	0.08	119,131,141,145	0
23	PSU	2K	56	20/21	0.86	0.08	99,110,121,122	0
23	PSU	2L	56	20/21	0.86	0.07	115,126,131,135	0
23	4SU	2L	8	20/21	0.88	0.08	114,124,129,130	0
24	PSU	3K	39	20/21	0.88	0.09	141,151,156,159	0
24	PSU	3L	39	20/21	0.88	0.08	145,155,159,162	0
22	PSU	1L	55	20/21	0.89	0.06	129,139,149,150	0
22	U8U	1L	34	23/24	0.89	0.09	123,133,138,150	0
22	PSU	1L	39	20/21	0.90	0.08	135,144,149,150	0
22	5MU	1K	54	21/22	0.90	0.08	110,117,132,137	0
23	5MU	2K	55	21/22	0.90	0.09	106,117,125,127	0
22	5MU	1L	54	21/22	0.91	0.07	133,141,146,152	0
22	T6A	1L	37	32/33	0.92	0.10	132,140,153,154	0
23	G7M	2K	47	24/25	0.93	0.08	102,114,127,133	0
22	PSU	1K	39	20/21	0.93	0.10	98,115,125,127	0
22	U8U	1K	34	23/24	0.94	0.08	84,92,100,108	0
22	T6A	1K	37	32/33	0.95	0.11	79,94,121,123	0
23	OMC	2K	33	21/22	0.96	0.11	77,83,91,93	0
23	4SU	2K	8	20/21	0.96	0.07	91,98,107,109	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1K	101	1/1	0.19	0.40	138,138,138,138	0
56	MG	2K	102	1/1	0.20	0.35	126,126,126,126	0
56	MG	1G	1656	1/1	0.51	0.23	138,138,138,138	0
56	MG	1J	203	1/1	0.52	0.26	113,113,113,113	0
56	MG	14	3250	1/1	0.55	0.30	99,99,99,99	0
56	MG	14	3055	1/1	0.55	0.33	112,112,112,112	0
56	MG	1G	1616	1/1	0.56	0.36	96,96,96,96	0
56	MG	14	3302	1/1	0.57	0.36	110,110,110,110	0
56	MG	1G	1640	1/1	0.57	0.28	108,108,108,108	0
56	MG	14	3130	1/1	0.58	0.34	78,78,78,78	0
56	MG	16	204	1/1	0.58	0.25	98,98,98,98	0
56	MG	14	3288	1/1	0.58	0.27	109,109,109,109	0
56	MG	1G	1602	1/1	0.58	0.36	105,105,105,105	0
56	MG	1H	3284	1/1	0.58	0.28	88,88,88,88	0
56	MG	14	3220	1/1	0.59	0.28	107,107,107,107	0
56	MG	13	1681	1/1	0.59	0.28	106,106,106,106	0
56	MG	14	3287	1/1	0.59	0.41	105,105,105,105	0
56	MG	14	3229	1/1	0.60	0.28	86,86,86,86	0
56	MG	14	3181	1/1	0.60	0.36	98,98,98,98	0
56	MG	1H	3045	1/1	0.60	0.29	116,116,116,116	0
56	MG	1H	3277	1/1	0.61	0.27	100,100,100,100	0
56	MG	1J	202	1/1	0.61	0.25	104,104,104,104	0
56	MG	14	3266	1/1	0.61	0.30	90,90,90,90	0
56	MG	13	1700	1/1	0.62	0.26	111,111,111,111	0
56	MG	14	3142	1/1	0.62	0.18	111,111,111,111	0
56	MG	1H	3280	1/1	0.62	0.23	88,88,88,88	0
56	MG	1G	1664	1/1	0.62	0.27	119,119,119,119	0
56	MG	2L	102	1/1	0.62	0.28	98,98,98,98	0
56	MG	13	1608	1/1	0.62	0.28	91,91,91,91	0
56	MG	1H	3295	1/1	0.63	0.23	85,85,85,85	0
56	MG	14	3039	1/1	0.63	0.43	103,103,103,103	0
56	MG	13	1628	1/1	0.63	0.33	95,95,95,95	0
56	MG	1G	1630	1/1	0.63	0.35	108,108,108,108	0
56	MG	1G	1665	1/1	0.63	0.24	93,93,93,93	0
56	MG	13	1691	1/1	0.64	0.20	109,109,109,109	0
56	MG	14	3301	1/1	0.64	0.27	99,99,99,99	0
56	MG	14	3260	1/1	0.64	0.31	90,90,90,90	0
56	MG	1G	1629	1/1	0.64	0.29	104,104,104,104	0
56	MG	14	3172	1/1	0.64	0.24	98,98,98,98	0
56	MG	14	3280	1/1	0.65	0.37	99,99,99,99	0
56	MG	14	3110	1/1	0.65	0.30	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1702	1/1	0.65	0.45	103,103,103,103	0
56	MG	13	1692	1/1	0.65	0.28	100,100,100,100	0
56	MG	14	3255	1/1	0.65	0.33	87,87,87,87	0
56	MG	14	3303	1/1	0.65	0.35	98,98,98,98	0
56	MG	1H	3318	1/1	0.65	0.24	96,96,96,96	0
56	MG	1H	3326	1/1	0.65	0.20	91,91,91,91	0
56	MG	14	3274	1/1	0.66	0.25	99,99,99,99	0
56	MG	13	1646	1/1	0.66	0.37	95,95,95,95	0
56	MG	1H	3015	1/1	0.66	0.38	77,77,77,77	0
56	MG	1H	3319	1/1	0.66	0.26	102,102,102,102	0
56	MG	14	3299	1/1	0.66	0.23	96,96,96,96	0
56	MG	13	1679	1/1	0.67	0.22	107,107,107,107	0
56	MG	13	1671	1/1	0.67	0.22	102,102,102,102	0
56	MG	4K	101	1/1	0.67	0.25	156,156,156,156	0
56	MG	1H	3308	1/1	0.68	0.40	99,99,99,99	0
56	MG	14	3381	1/1	0.68	0.20	102,102,102,102	0
56	MG	1G	1660	1/1	0.68	0.32	97,97,97,97	0
56	MG	14	3298	1/1	0.68	0.33	94,94,94,94	0
56	MG	1H	3184	1/1	0.69	0.29	96,96,96,96	0
56	MG	14	3017	1/1	0.69	0.27	92,92,92,92	0
56	MG	13	1606	1/1	0.69	0.24	115,115,115,115	0
56	MG	1G	1662	1/1	0.69	0.21	133,133,133,133	0
56	MG	1G	1633	1/1	0.69	0.25	83,83,83,83	0
56	MG	1H	3123	1/1	0.69	0.33	77,77,77,77	0
56	MG	14	3139	1/1	0.69	0.23	93,93,93,93	0
56	MG	45	202	1/1	0.69	0.26	103,103,103,103	0
56	MG	1H	3169	1/1	0.70	0.18	95,95,95,95	0
56	MG	13	1648	1/1	0.70	0.33	82,82,82,82	0
56	MG	1H	3321	1/1	0.70	0.26	85,85,85,85	0
56	MG	1H	3189	1/1	0.70	0.25	84,84,84,84	0
56	MG	1G	1638	1/1	0.70	0.36	81,81,81,81	0
56	MG	1H	3260	1/1	0.70	0.34	88,88,88,88	0
56	MG	16	208	1/1	0.70	0.22	82,82,82,82	0
56	MG	1H	3274	1/1	0.70	0.28	85,85,85,85	0
56	MG	C5	201	1/1	0.70	0.22	109,109,109,109	0
56	MG	14	3264	1/1	0.71	0.20	92,92,92,92	0
56	MG	1G	1641	1/1	0.71	0.22	92,92,92,92	0
56	MG	14	3210	1/1	0.71	0.24	96,96,96,96	0
56	MG	1H	3297	1/1	0.71	0.19	101,101,101,101	0
56	MG	1H	3306	1/1	0.71	0.23	84,84,84,84	0
56	MG	13	1622	1/1	0.71	0.20	94,94,94,94	0
56	MG	14	3169	1/1	0.71	0.20	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1664	1/1	0.71	0.27	99,99,99,99	0
56	MG	14	3227	1/1	0.72	0.22	81,81,81,81	0
56	MG	1H	3263	1/1	0.72	0.34	94,94,94,94	0
56	MG	1H	3281	1/1	0.72	0.22	81,81,81,81	0
56	MG	1H	3223	1/1	0.72	0.27	88,88,88,88	0
56	MG	1H	3311	1/1	0.72	0.24	96,96,96,96	0
56	MG	14	3133	1/1	0.72	0.28	97,97,97,97	0
56	MG	13	1623	1/1	0.72	0.26	105,105,105,105	0
56	MG	1G	1603	1/1	0.73	0.20	101,101,101,101	0
56	MG	13	1678	1/1	0.73	0.23	83,83,83,83	0
56	MG	14	3164	1/1	0.73	0.25	83,83,83,83	0
56	MG	13	1689	1/1	0.73	0.29	92,92,92,92	0
56	MG	1H	3293	1/1	0.73	0.23	98,98,98,98	0
56	MG	14	3012	1/1	0.73	0.30	82,82,82,82	0
56	MG	14	3193	1/1	0.73	0.27	78,78,78,78	0
56	MG	1H	3270	1/1	0.73	0.31	70,70,70,70	0
56	MG	1H	3323	1/1	0.73	0.28	91,91,91,91	0
56	MG	1H	3209	1/1	0.73	0.20	82,82,82,82	0
56	MG	1H	3302	1/1	0.73	0.28	89,89,89,89	0
56	MG	14	3248	1/1	0.73	0.35	94,94,94,94	0
56	MG	14	3122	1/1	0.73	0.33	91,91,91,91	0
56	MG	14	3251	1/1	0.73	0.21	106,106,106,106	0
56	MG	1H	3032	1/1	0.73	0.20	80,80,80,80	0
56	MG	1H	3234	1/1	0.73	0.18	99,99,99,99	0
56	MG	13	1629	1/1	0.74	0.33	90,90,90,90	0
56	MG	14	3183	1/1	0.74	0.32	89,89,89,89	0
56	MG	14	3056	1/1	0.74	0.09	62,62,62,62	0
56	MG	13	1676	1/1	0.74	0.14	127,127,127,127	0
56	MG	13	1696	1/1	0.74	0.26	111,111,111,111	0
56	MG	14	3127	1/1	0.74	0.23	71,71,71,71	0
56	MG	1H	3047	1/1	0.74	0.25	92,92,92,92	0
56	MG	14	3232	1/1	0.74	0.23	127,127,127,127	0
56	MG	14	3239	1/1	0.74	0.24	79,79,79,79	0
56	MG	1H	3298	1/1	0.74	0.29	93,93,93,93	0
56	MG	1H	3300	1/1	0.74	0.22	77,77,77,77	0
56	MG	1H	3301	1/1	0.74	0.21	128,128,128,128	0
56	MG	3K	101	1/1	0.74	0.17	162,162,162,162	0
56	MG	14	3037	1/1	0.74	0.24	70,70,70,70	0
56	MG	13	1604	1/1	0.74	0.30	93,93,93,93	0
56	MG	14	3069	1/1	0.75	0.34	91,91,91,91	0
56	MG	1G	1667	1/1	0.75	0.25	100,100,100,100	0
56	MG	1H	3134	1/1	0.75	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3141	1/1	0.75	0.24	69,69,69,69	0
56	MG	1G	1658	1/1	0.75	0.23	124,124,124,124	0
56	MG	13	1685	1/1	0.75	0.40	95,95,95,95	0
56	MG	13	1647	1/1	0.75	0.24	95,95,95,95	0
56	MG	1H	3128	1/1	0.75	0.25	83,83,83,83	0
56	MG	14	3154	1/1	0.75	0.23	90,90,90,90	0
56	MG	45	201	1/1	0.75	0.21	96,96,96,96	0
56	MG	1G	1612	1/1	0.75	0.24	93,93,93,93	0
56	MG	14	3235	1/1	0.75	0.25	104,104,104,104	0
56	MG	1H	3183	1/1	0.76	0.27	90,90,90,90	0
56	MG	14	3061	1/1	0.76	0.22	97,97,97,97	0
56	MG	88	202	1/1	0.76	0.23	87,87,87,87	0
56	MG	14	3167	1/1	0.76	0.24	99,99,99,99	0
56	MG	1H	3212	1/1	0.76	0.28	89,89,89,89	0
56	MG	14	3119	1/1	0.76	0.27	86,86,86,86	0
56	MG	14	3022	1/1	0.76	0.33	83,83,83,83	0
56	MG	14	3031	1/1	0.76	0.27	76,76,76,76	0
56	MG	14	3191	1/1	0.76	0.18	76,76,76,76	0
56	MG	1G	1643	1/1	0.76	0.30	91,91,91,91	0
56	MG	1G	1651	1/1	0.76	0.37	93,93,93,93	0
56	MG	1G	1634	1/1	0.76	0.29	109,109,109,109	0
56	MG	14	3140	1/1	0.76	0.26	87,87,87,87	0
56	MG	14	3168	1/1	0.77	0.28	66,66,66,66	0
56	MG	14	3135	1/1	0.77	0.20	78,78,78,78	0
56	MG	1H	3317	1/1	0.77	0.31	105,105,105,105	0
56	MG	13	1655	1/1	0.77	0.24	103,103,103,103	0
56	MG	1H	3200	1/1	0.77	0.27	87,87,87,87	0
56	MG	14	3308	1/1	0.77	0.24	82,82,82,82	0
56	MG	1H	3081	1/1	0.77	0.24	85,85,85,85	0
56	MG	14	3277	1/1	0.77	0.32	92,92,92,92	0
56	MG	14	3243	1/1	0.77	0.17	89,89,89,89	0
56	MG	14	3286	1/1	0.77	0.23	83,83,83,83	0
56	MG	13	1660	1/1	0.77	0.30	81,81,81,81	0
56	MG	14	3101	1/1	0.77	0.27	91,91,91,91	0
56	MG	1H	3315	1/1	0.78	0.15	91,91,91,91	0
56	MG	14	3240	1/1	0.78	0.31	87,87,87,87	0
56	MG	14	3272	1/1	0.78	0.29	93,93,93,93	0
56	MG	14	3273	1/1	0.78	0.26	94,94,94,94	0
56	MG	1G	1668	1/1	0.78	0.24	106,106,106,106	0
56	MG	14	3310	1/1	0.78	0.18	120,120,120,120	0
56	MG	1G	1646	1/1	0.78	0.33	86,86,86,86	0
56	MG	1H	3194	1/1	0.78	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3307	1/1	0.78	0.21	82,82,82,82	0
56	MG	14	3252	1/1	0.78	0.19	73,73,73,73	0
56	MG	1G	1657	1/1	0.78	0.23	90,90,90,90	0
56	MG	14	3064	1/1	0.78	0.23	84,84,84,84	0
56	MG	14	3159	1/1	0.79	0.30	81,81,81,81	0
56	MG	14	3300	1/1	0.79	0.31	89,89,89,89	0
56	MG	13	1633	1/1	0.79	0.15	65,65,65,65	0
56	MG	1H	3013	1/1	0.79	0.34	89,89,89,89	0
56	MG	1H	3291	1/1	0.79	0.41	99,99,99,99	0
56	MG	14	3060	1/1	0.79	0.29	92,92,92,92	0
56	MG	14	3020	1/1	0.79	0.27	76,76,76,76	0
56	MG	14	3062	1/1	0.79	0.23	81,81,81,81	0
56	MG	78	201	1/1	0.79	0.34	75,75,75,75	0
56	MG	1G	1620	1/1	0.79	0.10	94,94,94,94	0
56	MG	14	3032	1/1	0.79	0.36	88,88,88,88	0
56	MG	14	3146	1/1	0.79	0.23	61,61,61,61	0
56	MG	1H	3052	1/1	0.79	0.54	99,99,99,99	0
56	MG	1H	3224	1/1	0.80	0.34	88,88,88,88	0
56	MG	1H	3227	1/1	0.80	0.15	50,50,50,50	0
56	MG	13	1699	1/1	0.80	0.23	81,81,81,81	0
56	MG	1H	3244	1/1	0.80	0.26	84,84,84,84	0
56	MG	1H	3044	1/1	0.80	0.40	89,89,89,89	0
56	MG	14	3259	1/1	0.80	0.24	84,84,84,84	0
56	MG	14	3221	1/1	0.80	0.15	91,91,91,91	0
56	MG	1H	3094	1/1	0.80	0.17	91,91,91,91	0
56	MG	14	3305	1/1	0.80	0.20	86,86,86,86	0
56	MG	13	1654	1/1	0.80	0.28	88,88,88,88	0
56	MG	13	1688	1/1	0.80	0.27	94,94,94,94	0
56	MG	1H	3219	1/1	0.80	0.32	89,89,89,89	0
56	MG	1H	3186	1/1	0.80	0.14	71,71,71,71	0
56	MG	14	3276	1/1	0.80	0.19	102,102,102,102	0
56	MG	39	301	1/1	0.80	0.16	80,80,80,80	0
56	MG	14	3180	1/1	0.80	0.22	79,79,79,79	0
56	MG	1G	1622	1/1	0.80	0.36	99,99,99,99	0
56	MG	14	3244	1/1	0.80	0.16	74,74,74,74	0
56	MG	1H	3097	1/1	0.81	0.17	103,103,103,103	0
56	MG	14	3131	1/1	0.81	0.28	76,76,76,76	0
56	MG	1H	3110	1/1	0.81	0.19	65,65,65,65	0
56	MG	14	3023	1/1	0.81	0.22	55,55,55,55	0
56	MG	13	1684	1/1	0.81	0.14	114,114,114,114	0
56	MG	1G	1644	1/1	0.81	0.26	86,86,86,86	0
56	MG	14	3290	1/1	0.81	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3295	1/1	0.81	0.23	114,114,114,114	0
56	MG	1H	3187	1/1	0.81	0.20	95,95,95,95	0
56	MG	1H	3254	1/1	0.81	0.35	95,95,95,95	0
56	MG	1H	3257	1/1	0.81	0.31	94,94,94,94	0
56	MG	13	1672	1/1	0.81	0.15	81,81,81,81	0
56	MG	1G	1611	1/1	0.81	0.29	108,108,108,108	0
56	MG	1H	3192	1/1	0.81	0.18	81,81,81,81	0
56	MG	13	1674	1/1	0.81	0.32	92,92,92,92	0
56	MG	1H	3039	1/1	0.81	0.30	80,80,80,80	0
56	MG	14	3068	1/1	0.81	0.12	89,89,89,89	0
56	MG	1H	3152	1/1	0.81	0.28	99,99,99,99	0
56	MG	1H	3163	1/1	0.81	0.30	48,48,48,48	0
56	MG	1H	3216	1/1	0.81	0.29	80,80,80,80	0
56	MG	1H	3167	1/1	0.81	0.22	81,81,81,81	0
56	MG	1H	3220	1/1	0.81	0.25	87,87,87,87	0
56	MG	14	3203	1/1	0.81	0.17	68,68,68,68	0
56	MG	13	1695	1/1	0.81	0.32	103,103,103,103	0
56	MG	14	3058	1/1	0.82	0.19	80,80,80,80	0
56	MG	1H	3204	1/1	0.82	0.14	100,100,100,100	0
56	MG	1H	3322	1/1	0.82	0.20	68,68,68,68	0
56	MG	14	3281	1/1	0.82	0.40	89,89,89,89	0
56	MG	1G	1642	1/1	0.82	0.24	123,123,123,123	0
56	MG	14	3150	1/1	0.82	0.26	91,91,91,91	0
56	MG	14	3003	1/1	0.82	0.26	69,69,69,69	0
56	MG	14	3238	1/1	0.82	0.25	78,78,78,78	0
56	MG	14	3291	1/1	0.82	0.31	94,94,94,94	0
56	MG	1H	3264	1/1	0.82	0.13	84,84,84,84	0
56	MG	14	3296	1/1	0.82	0.37	91,91,91,91	0
56	MG	14	3297	1/1	0.82	0.18	124,124,124,124	0
56	MG	14	3162	1/1	0.82	0.28	83,83,83,83	0
56	MG	13	1602	1/1	0.82	0.21	89,89,89,89	0
56	MG	14	3075	1/1	0.82	0.51	90,90,90,90	0
56	MG	1H	3180	1/1	0.82	0.23	76,76,76,76	0
56	MG	1H	3314	1/1	0.82	0.18	92,92,92,92	0
56	MG	1H	3055	1/1	0.82	0.28	88,88,88,88	0
56	MG	14	3120	1/1	0.82	0.21	71,71,71,71	0
56	MG	14	3307	1/1	0.82	0.24	108,108,108,108	0
56	MG	1G	1632	1/1	0.82	0.28	102,102,102,102	0
56	MG	14	3258	1/1	0.82	0.29	99,99,99,99	0
56	MG	1H	3051	1/1	0.82	0.16	84,84,84,84	0
56	MG	14	3188	1/1	0.82	0.32	92,92,92,92	0
56	MG	1H	3199	1/1	0.82	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1636	1/1	0.82	0.20	101,101,101,101	0
56	MG	14	3197	1/1	0.82	0.33	84,84,84,84	0
56	MG	1G	1637	1/1	0.82	0.27	97,97,97,97	0
56	MG	1H	3140	1/1	0.82	0.13	69,69,69,69	0
56	MG	1H	3276	1/1	0.83	0.23	85,85,85,85	0
56	MG	1H	3065	1/1	0.83	0.27	55,55,55,55	0
56	MG	1H	3217	1/1	0.83	0.23	67,67,67,67	0
56	MG	1H	3040	1/1	0.83	0.36	72,72,72,72	0
56	MG	14	3234	1/1	0.83	0.26	89,89,89,89	0
56	MG	13	1632	1/1	0.83	0.28	73,73,73,73	0
56	MG	13	1677	1/1	0.83	0.23	91,91,91,91	0
56	MG	1H	3104	1/1	0.83	0.22	71,71,71,71	0
56	MG	1H	3025	1/1	0.83	0.17	77,77,77,77	0
56	MG	1H	3048	1/1	0.83	0.20	92,92,92,92	0
56	MG	14	3070	1/1	0.83	0.18	71,71,71,71	0
56	MG	1H	3327	1/1	0.83	0.24	95,95,95,95	0
56	MG	16	202	1/1	0.83	0.23	86,86,86,86	0
56	MG	1H	3125	1/1	0.83	0.14	87,87,87,87	0
56	MG	14	3176	1/1	0.83	0.26	88,88,88,88	0
56	MG	14	3114	1/1	0.83	0.28	81,81,81,81	0
56	MG	1H	3050	1/1	0.83	0.26	78,78,78,78	0
56	MG	13	1620	1/1	0.83	0.15	82,82,82,82	0
56	MG	1H	3138	1/1	0.83	0.29	61,61,61,61	0
56	MG	14	3030	1/1	0.83	0.32	87,87,87,87	0
56	MG	1H	3035	1/1	0.83	0.13	76,76,76,76	0
56	MG	1H	3053	1/1	0.83	0.29	82,82,82,82	0
56	MG	14	3132	1/1	0.83	0.31	91,91,91,91	0
56	MG	13	1626	1/1	0.83	0.29	87,87,87,87	0
56	MG	35	201	1/1	0.83	0.23	76,76,76,76	0
56	MG	14	3214	1/1	0.83	0.35	87,87,87,87	0
56	MG	1H	3061	1/1	0.83	0.27	62,62,62,62	0
56	MG	14	3278	1/1	0.83	0.24	96,96,96,96	0
56	MG	1G	1652	1/1	0.84	0.26	88,88,88,88	0
56	MG	1G	1654	1/1	0.84	0.35	86,86,86,86	0
56	MG	1H	3010	1/1	0.84	0.33	57,57,57,57	0
56	MG	Q8	101	1/1	0.84	0.25	83,83,83,83	0
56	MG	13	1661	1/1	0.84	0.10	93,93,93,93	0
56	MG	1H	3305	1/1	0.84	0.25	68,68,68,68	0
56	MG	14	3071	1/1	0.84	0.19	84,84,84,84	0
56	MG	1G	1604	1/1	0.84	0.23	97,97,97,97	0
56	MG	14	3083	1/1	0.84	0.26	87,87,87,87	0
56	MG	1H	3158	1/1	0.84	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3261	1/1	0.84	0.13	90,90,90,90	0
56	MG	14	3113	1/1	0.84	0.18	78,78,78,78	0
56	MG	1H	3159	1/1	0.84	0.27	83,83,83,83	0
56	MG	14	3115	1/1	0.84	0.26	66,66,66,66	0
56	MG	1H	3162	1/1	0.84	0.28	87,87,87,87	0
56	MG	1H	3265	1/1	0.84	0.15	74,74,74,74	0
56	MG	13	1642	1/1	0.84	0.19	73,73,73,73	0
56	MG	14	3126	1/1	0.84	0.36	83,83,83,83	0
56	MG	14	3004	1/1	0.84	0.24	83,83,83,83	0
56	MG	1H	3101	1/1	0.84	0.17	64,64,64,64	0
56	MG	1H	3019	1/1	0.84	0.35	89,89,89,89	0
56	MG	13	1643	1/1	0.84	0.20	79,79,79,79	0
56	MG	13	1645	1/1	0.84	0.19	66,66,66,66	0
56	MG	1H	3221	1/1	0.84	0.28	78,78,78,78	0
56	MG	13	1686	1/1	0.84	0.35	73,73,73,73	0
56	MG	1H	3036	1/1	0.84	0.23	77,77,77,77	0
56	MG	13	1687	1/1	0.84	0.23	76,76,76,76	0
56	MG	14	3245	1/1	0.84	0.17	88,88,88,88	0
56	MG	14	3246	1/1	0.84	0.17	72,72,72,72	0
56	MG	14	3143	1/1	0.84	0.34	70,70,70,70	0
56	MG	13	1697	1/1	0.84	0.24	96,96,96,96	0
56	MG	16	203	1/1	0.84	0.17	91,91,91,91	0
56	MG	1H	3239	1/1	0.84	0.11	81,81,81,81	0
56	MG	16	207	1/1	0.84	0.23	76,76,76,76	0
56	MG	14	3256	1/1	0.84	0.22	76,76,76,76	0
56	MG	1H	3041	1/1	0.84	0.28	77,77,77,77	0
56	MG	1H	3246	1/1	0.84	0.28	88,88,88,88	0
56	MG	13	1656	1/1	0.85	0.23	88,88,88,88	0
56	MG	1G	1663	1/1	0.85	0.18	97,97,97,97	0
56	MG	13	1693	1/1	0.85	0.43	88,88,88,88	0
56	MG	14	3261	1/1	0.85	0.34	83,83,83,83	0
56	MG	1H	3132	1/1	0.85	0.30	78,78,78,78	0
56	MG	14	3086	1/1	0.85	0.35	82,82,82,82	0
56	MG	14	3271	1/1	0.85	0.17	74,74,74,74	0
56	MG	14	3096	1/1	0.85	0.23	60,60,60,60	0
56	MG	3E	301	1/1	0.85	0.33	94,94,94,94	0
56	MG	1H	3137	1/1	0.85	0.16	73,73,73,73	0
56	MG	2L	101	1/1	0.85	0.26	72,72,72,72	0
56	MG	1G	1631	1/1	0.85	0.23	91,91,91,91	0
56	MG	1H	3072	1/1	0.85	0.20	72,72,72,72	0
56	MG	14	3199	1/1	0.85	0.23	59,59,59,59	0
56	MG	14	3201	1/1	0.85	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	5E	201	1/1	0.85	0.22	84,84,84,84	0
56	MG	1H	3236	1/1	0.85	0.35	91,91,91,91	0
56	MG	1G	1635	1/1	0.85	0.18	93,93,93,93	0
56	MG	1H	3093	1/1	0.85	0.18	72,72,72,72	0
56	MG	1H	3198	1/1	0.85	0.20	67,67,67,67	0
56	MG	14	3128	1/1	0.85	0.23	73,73,73,73	0
56	MG	13	1605	1/1	0.85	0.23	75,75,75,75	0
56	MG	14	3230	1/1	0.85	0.19	72,72,72,72	0
56	MG	14	3024	1/1	0.85	0.25	74,74,74,74	0
56	MG	14	3233	1/1	0.85	0.39	80,80,80,80	0
56	MG	1H	3248	1/1	0.85	0.21	83,83,83,83	0
56	MG	1H	3299	1/1	0.85	0.34	86,86,86,86	0
56	MG	1H	3250	1/1	0.85	0.24	87,87,87,87	0
56	MG	13	1673	1/1	0.85	0.20	102,102,102,102	0
56	MG	14	3304	1/1	0.85	0.23	90,90,90,90	0
56	MG	13	1690	1/1	0.85	0.38	81,81,81,81	0
56	MG	14	3242	1/1	0.85	0.10	70,70,70,70	0
56	MG	1H	3258	1/1	0.85	0.11	72,72,72,72	0
56	MG	1G	1649	1/1	0.85	0.27	96,96,96,96	0
56	MG	1H	3206	1/1	0.85	0.29	94,94,94,94	0
56	MG	13	1669	1/1	0.85	0.23	72,72,72,72	0
56	MG	1H	3038	1/1	0.85	0.22	81,81,81,81	0
56	MG	14	3157	1/1	0.85	0.32	66,66,66,66	0
56	MG	1G	1610	1/1	0.85	0.16	102,102,102,102	0
56	MG	1H	3114	1/1	0.85	0.16	67,67,67,67	0
56	MG	1H	3007	1/1	0.85	0.27	80,80,80,80	0
56	MG	1G	1614	1/1	0.85	0.25	93,93,93,93	0
56	MG	14	3033	1/1	0.86	0.29	84,84,84,84	0
56	MG	1H	3088	1/1	0.86	0.13	54,54,54,54	0
56	MG	14	3206	1/1	0.86	0.22	82,82,82,82	0
56	MG	13	1636	1/1	0.86	0.36	85,85,85,85	0
56	MG	14	3212	1/1	0.86	0.29	69,69,69,69	0
56	MG	14	3053	1/1	0.86	0.30	61,61,61,61	0
56	MG	14	3217	1/1	0.86	0.15	87,87,87,87	0
56	MG	13	1644	1/1	0.86	0.22	84,84,84,84	0
56	MG	1G	1626	1/1	0.86	0.15	95,95,95,95	0
56	MG	14	3222	1/1	0.86	0.24	80,80,80,80	0
56	MG	13	1667	1/1	0.86	0.18	85,85,85,85	0
56	MG	1H	3099	1/1	0.86	0.24	75,75,75,75	0
56	MG	1H	3262	1/1	0.86	0.30	77,77,77,77	0
56	MG	14	3231	1/1	0.86	0.22	84,84,84,84	0
56	MG	13	1694	1/1	0.86	0.18	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3294	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3028	1/1	0.86	0.32	72,72,72,72	0
56	MG	14	3149	1/1	0.86	0.32	92,92,92,92	0
56	MG	1H	3108	1/1	0.86	0.18	62,62,62,62	0
56	MG	1H	3042	1/1	0.86	0.28	93,93,93,93	0
56	MG	13	1652	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3275	1/1	0.86	0.29	74,74,74,74	0
56	MG	14	3002	1/1	0.86	0.21	62,62,62,62	0
56	MG	14	3079	1/1	0.86	0.23	72,72,72,72	0
56	MG	14	3165	1/1	0.86	0.20	60,60,60,60	0
56	MG	I8	103	1/1	0.86	0.23	86,86,86,86	0
56	MG	1H	3309	1/1	0.86	0.21	79,79,79,79	0
56	MG	14	3306	1/1	0.86	0.19	110,110,110,110	0
56	MG	14	3007	1/1	0.86	0.29	63,63,63,63	0
56	MG	1H	3034	1/1	0.86	0.34	78,78,78,78	0
56	MG	1H	3312	1/1	0.86	0.18	67,67,67,67	0
56	MG	14	3019	1/1	0.86	0.33	84,84,84,84	0
56	MG	1J	201	1/1	0.86	0.27	90,90,90,90	0
56	MG	1H	3164	1/1	0.86	0.17	73,73,73,73	0
56	MG	1H	3046	1/1	0.86	0.33	87,87,87,87	0
56	MG	13	1653	1/1	0.86	0.17	89,89,89,89	0
56	MG	1H	3249	1/1	0.86	0.31	86,86,86,86	0
56	MG	1H	3170	1/1	0.86	0.14	81,81,81,81	0
56	MG	1G	1615	1/1	0.86	0.18	119,119,119,119	0
56	MG	1G	1653	1/1	0.86	0.17	85,85,85,85	0
56	MG	1H	3290	1/1	0.87	0.16	80,80,80,80	0
56	MG	1H	3018	1/1	0.87	0.30	78,78,78,78	0
56	MG	14	3285	1/1	0.87	0.27	72,72,72,72	0
56	MG	14	3015	1/1	0.87	0.26	63,63,63,63	0
56	MG	13	1649	1/1	0.87	0.17	75,75,75,75	0
56	MG	1H	3269	1/1	0.87	0.28	97,97,97,97	0
56	MG	I8	102	1/1	0.87	0.38	83,83,83,83	0
56	MG	14	3192	1/1	0.87	0.18	80,80,80,80	0
56	MG	14	3293	1/1	0.87	0.10	99,99,99,99	0
56	MG	14	3134	1/1	0.87	0.15	74,74,74,74	0
56	MG	1H	3296	1/1	0.87	0.26	92,92,92,92	0
56	MG	1H	3033	1/1	0.87	0.15	68,68,68,68	0
56	MG	14	3249	1/1	0.87	0.23	78,78,78,78	0
56	MG	14	3076	1/1	0.87	0.27	89,89,89,89	0
56	MG	14	3202	1/1	0.87	0.17	79,79,79,79	0
56	MG	1H	3273	1/1	0.87	0.26	84,84,84,84	0
56	MG	14	3253	1/1	0.87	0.28	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3084	1/1	0.87	0.17	82,82,82,82	0
56	MG	1H	3232	1/1	0.87	0.10	71,71,71,71	0
56	MG	1G	1609	1/1	0.87	0.23	94,94,94,94	0
56	MG	14	3097	1/1	0.87	0.19	74,74,74,74	0
56	MG	1H	3054	1/1	0.87	0.19	87,87,87,87	0
56	MG	14	3102	1/1	0.87	0.21	76,76,76,76	0
56	MG	14	3263	1/1	0.87	0.20	82,82,82,82	0
56	MG	14	3309	1/1	0.87	0.34	90,90,90,90	0
56	MG	1H	3089	1/1	0.87	0.21	74,74,74,74	0
56	MG	14	3265	1/1	0.87	0.27	89,89,89,89	0
56	MG	1H	3304	1/1	0.87	0.43	73,73,73,73	0
56	MG	14	3046	1/1	0.87	0.19	66,66,66,66	0
56	MG	1H	3043	1/1	0.87	0.28	87,87,87,87	0
56	MG	13	1675	1/1	0.87	0.14	124,124,124,124	0
56	MG	1H	3283	1/1	0.87	0.27	85,85,85,85	0
56	MG	1G	1618	1/1	0.87	0.20	101,101,101,101	0
56	MG	14	3170	1/1	0.87	0.36	81,81,81,81	0
56	MG	1H	3124	1/1	0.87	0.15	59,59,59,59	0
56	MG	13	1651	1/1	0.88	0.12	86,86,86,86	0
56	MG	14	3204	1/1	0.88	0.19	82,82,82,82	0
56	MG	5I	101	1/1	0.88	0.14	88,88,88,88	0
56	MG	1G	1647	1/1	0.88	0.19	102,102,102,102	0
56	MG	13	1698	1/1	0.88	0.28	81,81,81,81	0
56	MG	14	3213	1/1	0.88	0.16	89,89,89,89	0
56	MG	1G	1601	1/1	0.88	0.18	96,96,96,96	0
56	MG	1H	3118	1/1	0.88	0.16	61,61,61,61	0
56	MG	14	3050	1/1	0.88	0.21	73,73,73,73	0
56	MG	1H	3153	1/1	0.88	0.11	60,60,60,60	0
56	MG	1H	3225	1/1	0.88	0.32	74,74,74,74	0
56	MG	1H	3156	1/1	0.88	0.25	77,77,77,77	0
56	MG	1H	3230	1/1	0.88	0.20	73,73,73,73	0
56	MG	1H	3310	1/1	0.88	0.24	72,72,72,72	0
56	MG	1H	3191	1/1	0.88	0.15	90,90,90,90	0
56	MG	14	3289	1/1	0.88	0.17	91,91,91,91	0
56	MG	1G	1661	1/1	0.88	0.16	150,150,150,150	0
56	MG	1H	3157	1/1	0.88	0.35	83,83,83,83	0
56	MG	14	3292	1/1	0.88	0.19	86,86,86,86	0
56	MG	13	1611	1/1	0.88	0.15	61,61,61,61	0
56	MG	14	3156	1/1	0.88	0.14	62,62,62,62	0
56	MG	13	1663	1/1	0.88	0.16	75,75,75,75	0
56	MG	1H	3240	1/1	0.88	0.14	56,56,56,56	0
56	MG	1H	3241	1/1	0.88	0.29	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3058	1/1	0.88	0.12	62,62,62,62	0
56	MG	13	1621	1/1	0.88	0.19	95,95,95,95	0
56	MG	1H	3287	1/1	0.88	0.36	86,86,86,86	0
56	MG	1H	3288	1/1	0.88	0.10	94,94,94,94	0
56	MG	1H	3005	1/1	0.88	0.16	62,62,62,62	0
56	MG	14	3247	1/1	0.88	0.29	73,73,73,73	0
56	MG	14	3087	1/1	0.88	0.30	79,79,79,79	0
56	MG	1H	3067	1/1	0.88	0.20	63,63,63,63	0
56	MG	16	201	1/1	0.88	0.16	92,92,92,92	0
56	MG	14	3009	1/1	0.88	0.23	52,52,52,52	0
56	MG	1H	3207	1/1	0.88	0.28	81,81,81,81	0
56	MG	1H	3251	1/1	0.88	0.15	63,63,63,63	0
56	MG	1H	3253	1/1	0.88	0.13	60,60,60,60	0
56	MG	16	205	1/1	0.88	0.26	84,84,84,84	0
56	MG	14	3257	1/1	0.88	0.11	68,68,68,68	0
56	MG	16	206	1/1	0.88	0.13	84,84,84,84	0
56	MG	14	3117	1/1	0.88	0.34	77,77,77,77	0
56	MG	1H	3135	1/1	0.88	0.22	81,81,81,81	0
56	MG	13	1665	1/1	0.88	0.23	64,64,64,64	0
56	MG	14	3262	1/1	0.88	0.39	91,91,91,91	0
56	MG	1H	3172	1/1	0.88	0.18	82,82,82,82	0
56	MG	1H	3179	1/1	0.88	0.23	93,93,93,93	0
56	MG	E5	101	1/1	0.88	0.27	83,83,83,83	0
56	MG	14	3190	1/1	0.89	0.18	95,95,95,95	0
56	MG	14	3021	1/1	0.89	0.31	78,78,78,78	0
56	MG	1G	1606	1/1	0.89	0.21	82,82,82,82	0
56	MG	1H	3085	1/1	0.89	0.19	82,82,82,82	0
56	MG	13	1668	1/1	0.89	0.15	80,80,80,80	0
56	MG	14	3198	1/1	0.89	0.27	80,80,80,80	0
56	MG	14	3025	1/1	0.89	0.18	69,69,69,69	0
56	MG	14	3268	1/1	0.89	0.13	86,86,86,86	0
56	MG	1H	3012	1/1	0.89	0.21	79,79,79,79	0
56	MG	13	1612	1/1	0.89	0.19	79,79,79,79	0
56	MG	14	3123	1/1	0.89	0.15	82,82,82,82	0
56	MG	14	3125	1/1	0.89	0.22	54,54,54,54	0
56	MG	1H	3259	1/1	0.89	0.14	80,80,80,80	0
56	MG	1H	3014	1/1	0.89	0.39	69,69,69,69	0
56	MG	14	3211	1/1	0.89	0.27	74,74,74,74	0
56	MG	13	1683	1/1	0.89	0.26	91,91,91,91	0
56	MG	1H	3197	1/1	0.89	0.18	80,80,80,80	0
56	MG	14	3284	1/1	0.89	0.11	84,84,84,84	0
56	MG	1G	1619	1/1	0.89	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3215	1/1	0.89	0.20	83,83,83,83	0
56	MG	14	3047	1/1	0.89	0.15	57,57,57,57	0
56	MG	1H	3428	1/1	0.89	0.21	54,54,54,54	0
56	MG	14	3051	1/1	0.89	0.22	90,90,90,90	0
56	MG	1G	1621	1/1	0.89	0.26	61,61,61,61	0
56	MG	14	3224	1/1	0.89	0.26	75,75,75,75	0
56	MG	1H	3064	1/1	0.89	0.18	54,54,54,54	0
56	MG	1H	3017	1/1	0.89	0.31	77,77,77,77	0
56	MG	14	3141	1/1	0.89	0.14	90,90,90,90	0
56	MG	1G	1627	1/1	0.89	0.23	85,85,85,85	0
56	MG	13	1637	1/1	0.89	0.32	68,68,68,68	0
56	MG	1H	3202	1/1	0.89	0.24	75,75,75,75	0
56	MG	1H	3203	1/1	0.89	0.25	75,75,75,75	0
56	MG	1H	3271	1/1	0.89	0.28	94,94,94,94	0
56	MG	14	3237	1/1	0.89	0.15	62,62,62,62	0
56	MG	14	3152	1/1	0.89	0.24	91,91,91,91	0
56	MG	14	3067	1/1	0.89	0.19	74,74,74,74	0
56	MG	13	1627	1/1	0.89	0.33	81,81,81,81	0
56	MG	2L	103	1/1	0.89	0.25	79,79,79,79	0
56	MG	1H	3205	1/1	0.89	0.23	83,83,83,83	0
56	MG	14	3160	1/1	0.89	0.18	57,57,57,57	0
56	MG	1H	3173	1/1	0.89	0.34	79,79,79,79	0
56	MG	1H	3177	1/1	0.89	0.17	82,82,82,82	0
56	MG	1H	3020	1/1	0.89	0.21	60,60,60,60	0
56	MG	1H	3083	1/1	0.89	0.11	75,75,75,75	0
56	MG	14	3011	1/1	0.89	0.31	58,58,58,58	0
56	MG	1H	3115	1/1	0.89	0.24	76,76,76,76	0
56	MG	14	3013	1/1	0.89	0.25	83,83,83,83	0
56	MG	14	3091	1/1	0.89	0.42	87,87,87,87	0
56	MG	14	3014	1/1	0.89	0.21	49,49,49,49	0
56	MG	13	1662	1/1	0.89	0.23	82,82,82,82	0
56	MG	1H	3252	1/1	0.89	0.16	72,72,72,72	0
56	MG	1H	3285	1/1	0.89	0.19	72,72,72,72	0
56	MG	14	3184	1/1	0.89	0.24	86,86,86,86	0
56	MG	1H	3316	1/1	0.89	0.29	87,87,87,87	0
56	MG	1H	3278	1/1	0.90	0.27	92,92,92,92	0
56	MG	1H	3160	1/1	0.90	0.14	69,69,69,69	0
56	MG	13	1617	1/1	0.90	0.18	77,77,77,77	0
56	MG	13	1639	1/1	0.90	0.29	85,85,85,85	0
56	MG	13	1640	1/1	0.90	0.15	91,91,91,91	0
56	MG	1H	3166	1/1	0.90	0.11	68,68,68,68	0
56	MG	1H	3255	1/1	0.90	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1645	1/1	0.90	0.28	88,88,88,88	0
56	MG	1H	3256	1/1	0.90	0.15	76,76,76,76	0
56	MG	1H	3289	1/1	0.90	0.20	82,82,82,82	0
56	MG	14	3219	1/1	0.90	0.24	78,78,78,78	0
56	MG	14	3148	1/1	0.90	0.24	72,72,72,72	0
56	MG	1H	3121	1/1	0.90	0.29	53,53,53,53	0
56	MG	14	3081	1/1	0.90	0.26	62,62,62,62	0
56	MG	14	3223	1/1	0.90	0.24	83,83,83,83	0
56	MG	14	3082	1/1	0.90	0.21	63,63,63,63	0
56	MG	14	3226	1/1	0.90	0.18	72,72,72,72	0
56	MG	1H	3098	1/1	0.90	0.13	69,69,69,69	0
56	MG	14	3228	1/1	0.90	0.23	93,93,93,93	0
56	MG	1H	3292	1/1	0.90	0.07	61,61,61,61	0
56	MG	1H	3151	1/1	0.90	0.09	52,52,52,52	0
56	MG	1H	3226	1/1	0.90	0.18	55,55,55,55	0
56	MG	14	3093	1/1	0.90	0.21	85,85,85,85	0
56	MG	14	3161	1/1	0.90	0.27	73,73,73,73	0
56	MG	14	3095	1/1	0.90	0.20	56,56,56,56	0
56	MG	1H	3171	1/1	0.90	0.20	74,74,74,74	0
56	MG	1H	3429	1/1	0.90	0.16	66,66,66,66	0
56	MG	14	3166	1/1	0.90	0.31	85,85,85,85	0
56	MG	14	3098	1/1	0.90	0.23	68,68,68,68	0
56	MG	14	3028	1/1	0.90	0.34	79,79,79,79	0
56	MG	1H	3009	1/1	0.90	0.23	66,66,66,66	0
56	MG	1G	1659	1/1	0.90	0.27	85,85,85,85	0
56	MG	1H	3231	1/1	0.90	0.25	56,56,56,56	0
56	MG	1G	1625	1/1	0.90	0.32	76,76,76,76	0
56	MG	14	3179	1/1	0.90	0.41	84,84,84,84	0
56	MG	13	1625	1/1	0.90	0.38	82,82,82,82	0
56	MG	14	3116	1/1	0.90	0.24	63,63,63,63	0
56	MG	14	3182	1/1	0.90	0.21	73,73,73,73	0
56	MG	1H	3155	1/1	0.90	0.21	86,86,86,86	0
56	MG	1H	3178	1/1	0.90	0.18	74,74,74,74	0
56	MG	1H	3126	1/1	0.90	0.15	72,72,72,72	0
56	MG	1G	1666	1/1	0.90	0.24	85,85,85,85	0
56	MG	14	3254	1/1	0.90	0.27	78,78,78,78	0
56	MG	13	1607	1/1	0.90	0.30	85,85,85,85	0
56	MG	14	3124	1/1	0.90	0.15	70,70,70,70	0
56	MG	1H	3182	1/1	0.90	0.18	77,77,77,77	0
56	MG	13	1731	1/1	0.90	0.19	94,94,94,94	0
56	MG	1H	3090	1/1	0.90	0.31	72,72,72,72	0
56	MG	14	3057	1/1	0.90	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3213	1/1	0.90	0.47	84,84,84,84	0
56	MG	1H	3215	1/1	0.90	0.36	81,81,81,81	0
56	MG	14	3099	1/1	0.91	0.21	62,62,62,62	0
56	MG	1H	3142	1/1	0.91	0.19	68,68,68,68	0
56	MG	14	3044	1/1	0.91	0.26	68,68,68,68	0
56	MG	14	3103	1/1	0.91	0.16	66,66,66,66	0
56	MG	14	3107	1/1	0.91	0.15	87,87,87,87	0
56	MG	14	3163	1/1	0.91	0.30	76,76,76,76	0
56	MG	1H	3147	1/1	0.91	0.10	72,72,72,72	0
56	MG	1G	1628	1/1	0.91	0.13	98,98,98,98	0
56	MG	13	1722	1/1	0.91	0.10	93,93,93,93	0
56	MG	14	3283	1/1	0.91	0.17	80,80,80,80	0
56	MG	1H	3049	1/1	0.91	0.08	65,65,65,65	0
56	MG	1H	3303	1/1	0.91	0.23	73,73,73,73	0
56	MG	13	1670	1/1	0.91	0.20	95,95,95,95	0
56	MG	1H	3030	1/1	0.91	0.24	69,69,69,69	0
56	MG	21	302	1/1	0.91	0.12	78,78,78,78	0
56	MG	14	3173	1/1	0.91	0.13	82,82,82,82	0
56	MG	14	3236	1/1	0.91	0.13	79,79,79,79	0
56	MG	41	201	1/1	0.91	0.18	71,71,71,71	0
56	MG	1H	3243	1/1	0.91	0.06	56,56,56,56	0
56	MG	1H	3075	1/1	0.91	0.10	79,79,79,79	0
56	MG	1H	3076	1/1	0.91	0.14	65,65,65,65	0
56	MG	1H	3210	1/1	0.91	0.20	73,73,73,73	0
56	MG	1H	3127	1/1	0.91	0.16	53,53,53,53	0
56	MG	1H	3100	1/1	0.91	0.14	56,56,56,56	0
56	MG	1H	3282	1/1	0.91	0.14	78,78,78,78	0
56	MG	1H	3185	1/1	0.91	0.19	78,78,78,78	0
56	MG	1H	3130	1/1	0.91	0.12	60,60,60,60	0
56	MG	1H	3161	1/1	0.91	0.21	84,84,84,84	0
56	MG	1H	3188	1/1	0.91	0.34	76,76,76,76	0
56	MG	14	3194	1/1	0.91	0.21	86,86,86,86	0
56	MG	2K	101	1/1	0.91	0.31	86,86,86,86	0
56	MG	14	3080	1/1	0.91	0.18	67,67,67,67	0
56	MG	1H	3008	1/1	0.91	0.12	74,74,74,74	0
56	MG	13	1601	1/1	0.91	0.18	59,59,59,59	0
56	MG	2K	103	1/1	0.91	0.17	71,71,71,71	0
56	MG	1H	3195	1/1	0.91	0.34	78,78,78,78	0
56	MG	1H	3324	1/1	0.91	0.17	69,69,69,69	0
56	MG	14	3205	1/1	0.91	0.08	80,80,80,80	0
56	MG	14	3382	1/1	0.91	0.14	100,100,100,100	0
56	MG	14	3147	1/1	0.91	0.22	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3325	1/1	0.91	0.19	76,76,76,76	0
56	MG	1H	3196	1/1	0.91	0.35	80,80,80,80	0
56	MG	1H	3112	1/1	0.91	0.19	66,66,66,66	0
56	MG	1H	3228	1/1	0.91	0.21	57,57,57,57	0
56	MG	14	3153	1/1	0.91	0.26	78,78,78,78	0
56	MG	13	1603	1/1	0.91	0.25	92,92,92,92	0
56	MG	85	201	1/1	0.91	0.54	88,88,88,88	0
56	MG	14	3155	1/1	0.91	0.13	71,71,71,71	0
56	MG	1H	3024	1/1	0.91	0.34	70,70,70,70	0
56	MG	1H	3080	1/1	0.92	0.10	86,86,86,86	0
56	MG	14	3174	1/1	0.92	0.34	81,81,81,81	0
56	MG	14	3175	1/1	0.92	0.20	96,96,96,96	0
56	MG	1H	3096	1/1	0.92	0.27	78,78,78,78	0
56	MG	14	3177	1/1	0.92	0.26	87,87,87,87	0
56	MG	14	3178	1/1	0.92	0.44	90,90,90,90	0
56	MG	1G	1617	1/1	0.92	0.11	125,125,125,125	0
56	MG	1H	3272	1/1	0.92	0.14	89,89,89,89	0
56	MG	1H	3201	1/1	0.92	0.29	70,70,70,70	0
56	MG	13	1650	1/1	0.92	0.30	79,79,79,79	0
56	MG	14	3090	1/1	0.92	0.17	70,70,70,70	0
56	MG	13	1641	1/1	0.92	0.25	75,75,75,75	0
56	MG	88	201	1/1	0.92	0.22	81,81,81,81	0
56	MG	14	3048	1/1	0.92	0.27	55,55,55,55	0
56	MG	14	3008	1/1	0.92	0.28	65,65,65,65	0
56	MG	1H	3011	1/1	0.92	0.29	71,71,71,71	0
56	MG	14	3010	1/1	0.92	0.24	54,54,54,54	0
56	MG	1H	3027	1/1	0.92	0.24	48,48,48,48	0
56	MG	14	3195	1/1	0.92	0.08	107,107,107,107	0
56	MG	14	3196	1/1	0.92	0.23	69,69,69,69	0
56	MG	14	3100	1/1	0.92	0.14	91,91,91,91	0
56	MG	1H	3150	1/1	0.92	0.10	70,70,70,70	0
56	MG	1H	3087	1/1	0.92	0.11	65,65,65,65	0
56	MG	14	3200	1/1	0.92	0.22	67,67,67,67	0
56	MG	1H	3102	1/1	0.92	0.23	55,55,55,55	0
56	MG	14	3059	1/1	0.92	0.22	55,55,55,55	0
56	MG	14	3109	1/1	0.92	0.24	72,72,72,72	0
56	MG	1H	3070	1/1	0.92	0.24	50,50,50,50	0
56	MG	14	3111	1/1	0.92	0.22	69,69,69,69	0
56	MG	1H	3107	1/1	0.92	0.24	73,73,73,73	0
56	MG	13	1610	1/1	0.92	0.15	72,72,72,72	0
56	MG	1G	1605	1/1	0.92	0.23	85,85,85,85	0
56	MG	14	3066	1/1	0.92	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3214	1/1	0.92	0.15	68,68,68,68	0
56	MG	1H	3175	1/1	0.92	0.28	70,70,70,70	0
56	MG	13	1615	1/1	0.92	0.14	85,85,85,85	0
56	MG	14	3216	1/1	0.92	0.18	70,70,70,70	0
56	MG	14	3121	1/1	0.92	0.18	84,84,84,84	0
56	MG	1H	3059	1/1	0.92	0.16	48,48,48,48	0
56	MG	29	301	1/1	0.92	0.16	63,63,63,63	0
56	MG	1H	3218	1/1	0.92	0.10	76,76,76,76	0
56	MG	14	3267	1/1	0.92	0.22	66,66,66,66	0
56	MG	14	3073	1/1	0.92	0.29	81,81,81,81	0
56	MG	14	3269	1/1	0.92	0.25	75,75,75,75	0
56	MG	45	203	1/1	0.92	0.20	73,73,73,73	0
56	MG	1G	1639	1/1	0.92	0.34	80,80,80,80	0
56	MG	14	3029	1/1	0.92	0.21	83,83,83,83	0
56	MG	1H	3113	1/1	0.92	0.12	67,67,67,67	0
56	MG	1H	3222	1/1	0.93	0.28	79,79,79,79	0
56	MG	14	3207	1/1	0.93	0.12	89,89,89,89	0
56	MG	14	3208	1/1	0.93	0.10	67,67,67,67	0
56	MG	13	1638	1/1	0.93	0.30	87,87,87,87	0
56	MG	14	3088	1/1	0.93	0.21	73,73,73,73	0
56	MG	13	1630	1/1	0.93	0.37	71,71,71,71	0
56	MG	1G	1613	1/1	0.93	0.10	100,100,100,100	0
56	MG	1H	3174	1/1	0.93	0.16	85,85,85,85	0
56	MG	14	3094	1/1	0.93	0.12	82,82,82,82	0
56	MG	14	3275	1/1	0.93	0.16	68,68,68,68	0
56	MG	1H	3062	1/1	0.93	0.21	54,54,54,54	0
56	MG	1H	3294	1/1	0.93	0.32	71,71,71,71	0
56	MG	14	3218	1/1	0.93	0.20	60,60,60,60	0
56	MG	14	3158	1/1	0.93	0.09	71,71,71,71	0
56	MG	1H	3176	1/1	0.93	0.19	68,68,68,68	0
56	MG	1H	3359	1/1	0.93	0.16	66,66,66,66	0
56	MG	14	3036	1/1	0.93	0.20	73,73,73,73	0
56	MG	1H	3380	1/1	0.93	0.08	70,70,70,70	0
56	MG	14	3038	1/1	0.93	0.18	86,86,86,86	0
56	MG	3I	201	1/1	0.93	0.12	62,62,62,62	0
56	MG	1H	3086	1/1	0.93	0.21	41,41,41,41	0
56	MG	14	3105	1/1	0.93	0.11	52,52,52,52	0
56	MG	1H	3016	1/1	0.93	0.19	48,48,48,48	0
56	MG	1G	1624	1/1	0.93	0.18	76,76,76,76	0
56	MG	1H	3106	1/1	0.93	0.16	77,77,77,77	0
56	MG	14	3049	1/1	0.93	0.11	58,58,58,58	0
56	MG	14	3171	1/1	0.93	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3268	1/1	0.93	0.26	79,79,79,79	0
56	MG	1H	3181	1/1	0.93	0.04	74,74,74,74	0
56	MG	13	1631	1/1	0.93	0.38	93,93,93,93	0
56	MG	1G	1682	1/1	0.93	0.12	91,91,91,91	0
56	MG	1H	3238	1/1	0.93	0.12	82,82,82,82	0
56	MG	1H	3208	1/1	0.93	0.22	63,63,63,63	0
56	MG	1H	3131	1/1	0.93	0.12	62,62,62,62	0
56	MG	21	301	1/1	0.93	0.17	57,57,57,57	0
56	MG	1H	3031	1/1	0.93	0.15	65,65,65,65	0
56	MG	1H	3242	1/1	0.93	0.27	64,64,64,64	0
56	MG	14	3005	1/1	0.93	0.18	44,44,44,44	0
56	MG	1H	3211	1/1	0.93	0.17	71,71,71,71	0
56	MG	1H	3133	1/1	0.93	0.23	69,69,69,69	0
56	MG	13	1624	1/1	0.93	0.11	71,71,71,71	0
56	MG	1H	3092	1/1	0.93	0.17	67,67,67,67	0
56	MG	14	3129	1/1	0.93	0.21	58,58,58,58	0
56	MG	1H	3136	1/1	0.93	0.13	68,68,68,68	0
56	MG	1H	3313	1/1	0.93	0.06	66,66,66,66	0
56	MG	1H	3002	1/1	0.93	0.17	49,49,49,49	0
56	MG	14	3072	1/1	0.93	0.17	55,55,55,55	0
56	MG	1H	3003	1/1	0.93	0.12	54,54,54,54	0
56	MG	1H	3079	1/1	0.93	0.12	61,61,61,61	0
56	MG	1H	3021	1/1	0.93	0.19	57,57,57,57	0
56	MG	14	3078	1/1	0.93	0.14	64,64,64,64	0
56	MG	14	3018	1/1	0.93	0.22	73,73,73,73	0
56	MG	1H	3119	1/1	0.93	0.27	78,78,78,78	0
56	MG	1H	3143	1/1	0.93	0.28	77,77,77,77	0
56	MG	14	3145	1/1	0.93	0.14	67,67,67,67	0
56	MG	1H	3320	1/1	0.93	0.07	68,68,68,68	0
56	MG	1G	1648	1/1	0.93	0.27	78,78,78,78	0
59	ZN	G8	201	1/1	0.93	0.19	144,144,144,144	0
56	MG	14	3189	1/1	0.94	0.25	73,73,73,73	0
56	MG	1H	3165	1/1	0.94	0.23	79,79,79,79	0
56	MG	14	3144	1/1	0.94	0.30	58,58,58,58	0
56	MG	14	3054	1/1	0.94	0.09	83,83,83,83	0
56	MG	14	3016	1/1	0.94	0.18	60,60,60,60	0
56	MG	13	1701	1/1	0.94	0.17	121,121,121,121	0
56	MG	1H	3068	1/1	0.94	0.12	56,56,56,56	0
56	MG	1H	3229	1/1	0.94	0.13	45,45,45,45	0
56	MG	1H	3146	1/1	0.94	0.19	59,59,59,59	0
56	MG	14	3104	1/1	0.94	0.10	64,64,64,64	0
56	MG	1G	1607	1/1	0.94	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1608	1/1	0.94	0.06	101,101,101,101	0
56	MG	1H	3069	1/1	0.94	0.13	60,60,60,60	0
56	MG	1H	3006	1/1	0.94	0.14	61,61,61,61	0
56	MG	1H	3071	1/1	0.94	0.16	56,56,56,56	0
56	MG	14	3112	1/1	0.94	0.18	61,61,61,61	0
56	MG	14	3026	1/1	0.94	0.26	68,68,68,68	0
56	MG	1H	3286	1/1	0.94	0.09	64,64,64,64	0
56	MG	1H	3235	1/1	0.94	0.14	85,85,85,85	0
56	MG	1H	3193	1/1	0.94	0.25	72,72,72,72	0
56	MG	13	1613	1/1	0.94	0.14	77,77,77,77	0
56	MG	1H	3074	1/1	0.94	0.20	69,69,69,69	0
56	MG	1H	3060	1/1	0.94	0.18	52,52,52,52	0
56	MG	1H	3029	1/1	0.94	0.29	69,69,69,69	0
56	MG	1H	3077	1/1	0.94	0.09	63,63,63,63	0
56	MG	14	3077	1/1	0.94	0.13	60,60,60,60	0
56	MG	1H	3095	1/1	0.94	0.15	73,73,73,73	0
56	MG	1H	3001	1/1	0.94	0.23	53,53,53,53	0
56	MG	14	3040	1/1	0.94	0.31	84,84,84,84	0
56	MG	14	3041	1/1	0.94	0.09	49,49,49,49	0
56	MG	14	3042	1/1	0.94	0.16	58,58,58,58	0
56	MG	14	3043	1/1	0.94	0.14	52,52,52,52	0
56	MG	14	3085	1/1	0.94	0.26	51,51,51,51	0
56	MG	1H	3245	1/1	0.94	0.24	74,74,74,74	0
56	MG	14	3045	1/1	0.94	0.20	64,64,64,64	0
56	MG	14	3270	1/1	0.94	0.25	84,84,84,84	0
56	MG	1G	1623	1/1	0.94	0.19	83,83,83,83	0
56	MG	1H	3117	1/1	0.94	0.18	82,82,82,82	0
56	MG	13	1619	1/1	0.94	0.16	69,69,69,69	0
56	MG	14	3136	1/1	0.94	0.13	62,62,62,62	0
56	MG	13	1616	1/1	0.94	0.29	77,77,77,77	0
56	MG	1H	3066	1/1	0.94	0.10	48,48,48,48	0
56	MG	1H	3122	1/1	0.94	0.16	50,50,50,50	0
56	MG	14	3052	1/1	0.94	0.13	71,71,71,71	0
56	MG	14	3279	1/1	0.94	0.09	73,73,73,73	0
56	MG	14	3065	1/1	0.95	0.10	68,68,68,68	0
56	MG	14	3092	1/1	0.95	0.06	75,75,75,75	0
56	MG	13	1680	1/1	0.95	0.33	87,87,87,87	0
56	MG	1H	3082	1/1	0.95	0.17	65,65,65,65	0
56	MG	14	3151	1/1	0.95	0.33	81,81,81,81	0
56	MG	1H	3129	1/1	0.95	0.07	56,56,56,56	0
56	MG	1H	3145	1/1	0.95	0.24	77,77,77,77	0
56	MG	13	1659	1/1	0.95	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3027	1/1	0.95	0.26	71,71,71,71	0
56	MG	1H	3247	1/1	0.95	0.20	73,73,73,73	0
56	MG	14	3187	1/1	0.95	0.21	75,75,75,75	0
56	MG	1H	3103	1/1	0.95	0.10	51,51,51,51	0
56	MG	1H	3148	1/1	0.95	0.11	49,49,49,49	0
56	MG	1H	3026	1/1	0.95	0.28	50,50,50,50	0
56	MG	1H	3105	1/1	0.95	0.13	64,64,64,64	0
56	MG	1H	3168	1/1	0.95	0.09	65,65,65,65	0
56	MG	14	3034	1/1	0.95	0.25	74,74,74,74	0
56	MG	14	3035	1/1	0.95	0.26	84,84,84,84	0
56	MG	14	3108	1/1	0.95	0.10	75,75,75,75	0
56	MG	1H	3057	1/1	0.95	0.18	52,52,52,52	0
56	MG	14	3138	1/1	0.95	0.18	55,55,55,55	0
56	MG	13	1682	1/1	0.95	0.07	73,73,73,73	0
56	MG	13	1666	1/1	0.95	0.05	89,89,89,89	0
56	MG	13	1618	1/1	0.95	0.07	97,97,97,97	0
56	MG	1H	3111	1/1	0.95	0.12	60,60,60,60	0
56	MG	1H	3022	1/1	0.95	0.13	52,52,52,52	0
56	MG	14	3063	1/1	0.95	0.10	77,77,77,77	0
56	MG	14	3089	1/1	0.95	0.22	54,54,54,54	0
57	PAR	13	1730	42/42	0.95	0.08	67,77,86,91	0
56	MG	1H	3421	1/1	0.95	0.09	83,83,83,83	0
56	MG	1G	1678	1/1	0.96	0.07	92,92,92,92	0
56	MG	13	1723	1/1	0.96	0.10	73,73,73,73	0
56	MG	L8	101	1/1	0.96	0.35	88,88,88,88	0
56	MG	1H	3387	1/1	0.96	0.08	72,72,72,72	0
56	MG	1H	3399	1/1	0.96	0.06	91,91,91,91	0
56	MG	14	3241	1/1	0.96	0.26	68,68,68,68	0
56	MG	1H	3414	1/1	0.96	0.07	83,83,83,83	0
56	MG	1H	3237	1/1	0.96	0.08	77,77,77,77	0
56	MG	14	3185	1/1	0.96	0.08	74,74,74,74	0
56	MG	14	3186	1/1	0.96	0.43	83,83,83,83	0
56	MG	1H	3109	1/1	0.96	0.06	59,59,59,59	0
56	MG	1H	3154	1/1	0.96	0.28	69,69,69,69	0
56	MG	14	3006	1/1	0.96	0.30	58,58,58,58	0
56	MG	13	1728	1/1	0.96	0.07	127,127,127,127	0
56	MG	14	3311	1/1	0.96	0.12	83,83,83,83	0
56	MG	14	3340	1/1	0.96	0.07	83,83,83,83	0
56	MG	14	3137	1/1	0.96	0.07	62,62,62,62	0
56	MG	1H	3139	1/1	0.96	0.13	64,64,64,64	0
56	MG	1H	3073	1/1	0.96	0.10	47,47,47,47	0
56	MG	1H	3190	1/1	0.96	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3063	1/1	0.96	0.12	55,55,55,55	0
56	MG	14	3225	1/1	0.96	0.07	71,71,71,71	0
56	MG	1H	3004	1/1	0.96	0.11	41,41,41,41	0
56	MG	13	1614	1/1	0.96	0.03	81,81,81,81	0
56	MG	1H	3056	1/1	0.96	0.15	40,40,40,40	0
56	MG	1H	3078	1/1	0.96	0.07	57,57,57,57	0
56	MG	13	1634	1/1	0.96	0.16	53,53,53,53	0
56	MG	13	1635	1/1	0.96	0.07	54,54,54,54	0
56	MG	1H	3149	1/1	0.96	0.33	65,65,65,65	0
56	MG	13	1657	1/1	0.96	0.09	80,80,80,80	0
56	MG	13	1658	1/1	0.96	0.04	82,82,82,82	0
57	PAR	1G	1681	42/42	0.96	0.07	79,90,98,101	0
56	MG	1H	3374	1/1	0.96	0.08	88,88,88,88	0
56	MG	14	3282	1/1	0.97	0.43	84,84,84,84	0
56	MG	14	3074	1/1	0.97	0.13	45,45,45,45	0
56	MG	1G	1674	1/1	0.97	0.04	123,123,123,123	0
56	MG	1G	1676	1/1	0.97	0.07	111,111,111,111	0
56	MG	13	1725	1/1	0.97	0.10	102,102,102,102	0
56	MG	1G	1679	1/1	0.97	0.10	138,138,138,138	0
56	MG	14	3317	1/1	0.97	0.07	64,64,64,64	0
56	MG	14	3334	1/1	0.97	0.06	85,85,85,85	0
56	MG	14	3338	1/1	0.97	0.10	111,111,111,111	0
56	MG	1H	3344	1/1	0.97	0.09	75,75,75,75	0
56	MG	14	3341	1/1	0.97	0.05	94,94,94,94	0
56	MG	14	3358	1/1	0.97	0.04	64,64,64,64	0
56	MG	14	3365	1/1	0.97	0.04	88,88,88,88	0
56	MG	14	3367	1/1	0.97	0.06	94,94,94,94	0
56	MG	14	3370	1/1	0.97	0.05	99,99,99,99	0
56	MG	14	3371	1/1	0.97	0.04	72,72,72,72	0
56	MG	14	3379	1/1	0.97	0.10	107,107,107,107	0
56	MG	1G	1655	1/1	0.97	0.12	94,94,94,94	0
56	MG	1H	3023	1/1	0.97	0.36	57,57,57,57	0
56	MG	1H	3091	1/1	0.97	0.05	61,61,61,61	0
56	MG	1H	3266	1/1	0.97	0.09	60,60,60,60	0
56	MG	14	3084	1/1	0.97	0.15	73,73,73,73	0
56	MG	1J	205	1/1	0.97	0.10	109,109,109,109	0
56	MG	1H	3267	1/1	0.97	0.13	69,69,69,69	0
56	MG	1H	3389	1/1	0.97	0.08	64,64,64,64	0
56	MG	1H	3116	1/1	0.97	0.07	56,56,56,56	0
56	MG	1H	3408	1/1	0.97	0.04	80,80,80,80	0
56	MG	1H	3413	1/1	0.97	0.06	107,107,107,107	0
56	MG	13	1732	1/1	0.97	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3037	1/1	0.97	0.34	63,63,63,63	0
56	MG	1G	1650	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3423	1/1	0.97	0.09	147,147,147,147	0
56	MG	13	1707	1/1	0.97	0.04	85,85,85,85	0
56	MG	14	3118	1/1	0.97	0.06	66,66,66,66	0
56	MG	1G	1671	1/1	0.97	0.07	90,90,90,90	0
59	ZN	C5	202	1/1	0.97	0.06	165,165,165,165	0
56	MG	1H	3418	1/1	0.98	0.05	88,88,88,88	0
56	MG	1H	3330	1/1	0.98	0.04	60,60,60,60	0
56	MG	14	3352	1/1	0.98	0.04	78,78,78,78	0
56	MG	P8	101	1/1	0.98	0.04	78,78,78,78	0
56	MG	14	3360	1/1	0.98	0.04	75,75,75,75	0
56	MG	1H	3343	1/1	0.98	0.05	65,65,65,65	0
56	MG	14	3366	1/1	0.98	0.08	92,92,92,92	0
56	MG	1G	1672	1/1	0.98	0.10	121,121,121,121	0
56	MG	1H	3424	1/1	0.98	0.06	89,89,89,89	0
56	MG	1H	3427	1/1	0.98	0.04	84,84,84,84	0
56	MG	13	1705	1/1	0.98	0.04	94,94,94,94	0
56	MG	1H	3348	1/1	0.98	0.07	100,100,100,100	0
56	MG	1H	3358	1/1	0.98	0.06	68,68,68,68	0
56	MG	13	1609	1/1	0.98	0.08	73,73,73,73	0
56	MG	1H	3373	1/1	0.98	0.04	82,82,82,82	0
56	MG	1H	3144	1/1	0.98	0.03	54,54,54,54	0
56	MG	1J	204	1/1	0.98	0.09	99,99,99,99	0
56	MG	1H	3120	1/1	0.98	0.10	41,41,41,41	0
56	MG	1H	3386	1/1	0.98	0.04	52,52,52,52	0
56	MG	13	1724	1/1	0.98	0.04	108,108,108,108	0
56	MG	1H	3388	1/1	0.98	0.06	63,63,63,63	0
56	MG	1H	3279	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3391	1/1	0.98	0.03	107,107,107,107	0
56	MG	13	1714	1/1	0.98	0.04	104,104,104,104	0
56	MG	13	1727	1/1	0.98	0.05	115,115,115,115	0
56	MG	14	3106	1/1	0.98	0.37	69,69,69,69	0
56	MG	1H	3409	1/1	0.98	0.04	86,86,86,86	0
56	MG	1H	3233	1/1	0.98	0.05	50,50,50,50	0
56	MG	14	3209	1/1	0.98	0.11	67,67,67,67	0
56	MG	14	3336	1/1	0.98	0.04	77,77,77,77	0
56	MG	1H	3328	1/1	0.98	0.04	52,52,52,52	0
56	MG	1H	3367	1/1	0.99	0.04	71,71,71,71	0
56	MG	1H	3369	1/1	0.99	0.03	69,69,69,69	0
56	MG	1H	3372	1/1	0.99	0.04	53,53,53,53	0
56	MG	13	1708	1/1	0.99	0.04	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1709	1/1	0.99	0.03	94,94,94,94	0
56	MG	1H	3376	1/1	0.99	0.03	60,60,60,60	0
56	MG	1H	3377	1/1	0.99	0.05	77,77,77,77	0
56	MG	1H	3378	1/1	0.99	0.03	68,68,68,68	0
56	MG	1G	1669	1/1	0.99	0.05	82,82,82,82	0
56	MG	1G	1670	1/1	0.99	0.03	88,88,88,88	0
56	MG	1H	3379	1/1	0.99	0.02	61,61,61,61	0
56	MG	13	1726	1/1	0.99	0.03	82,82,82,82	0
56	MG	1G	1673	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3381	1/1	0.99	0.04	59,59,59,59	0
56	MG	1G	1675	1/1	0.99	0.04	116,116,116,116	0
56	MG	1H	3382	1/1	0.99	0.02	60,60,60,60	0
56	MG	1G	1677	1/1	0.99	0.04	119,119,119,119	0
56	MG	1H	3383	1/1	0.99	0.03	65,65,65,65	0
56	MG	1H	3384	1/1	0.99	0.04	109,109,109,109	0
56	MG	1G	1680	1/1	0.99	0.03	120,120,120,120	0
56	MG	1H	3385	1/1	0.99	0.04	78,78,78,78	0
56	MG	13	1711	1/1	0.99	0.05	92,92,92,92	0
56	MG	13	1712	1/1	0.99	0.03	78,78,78,78	0
56	MG	13	1729	1/1	0.99	0.05	103,103,103,103	0
56	MG	14	3001	1/1	0.99	0.02	51,51,51,51	0
56	MG	13	1713	1/1	0.99	0.02	88,88,88,88	0
56	MG	1H	3390	1/1	0.99	0.04	88,88,88,88	0
56	MG	13	1703	1/1	0.99	0.09	70,70,70,70	0
56	MG	1H	3392	1/1	0.99	0.03	71,71,71,71	0
56	MG	1H	3393	1/1	0.99	0.06	70,70,70,70	0
56	MG	1H	3395	1/1	0.99	0.03	74,74,74,74	0
56	MG	1H	3396	1/1	0.99	0.02	58,58,58,58	0
56	MG	1H	3397	1/1	0.99	0.03	71,71,71,71	0
56	MG	1H	3398	1/1	0.99	0.03	83,83,83,83	0
56	MG	13	1715	1/1	0.99	0.03	100,100,100,100	0
56	MG	1H	3404	1/1	0.99	0.08	64,64,64,64	0
56	MG	1H	3405	1/1	0.99	0.06	52,52,52,52	0
56	MG	1H	3406	1/1	0.99	0.04	65,65,65,65	0
56	MG	1H	3407	1/1	0.99	0.03	86,86,86,86	0
56	MG	14	3313	1/1	0.99	0.04	64,64,64,64	0
56	MG	14	3314	1/1	0.99	0.04	73,73,73,73	0
56	MG	14	3316	1/1	0.99	0.02	67,67,67,67	0
56	MG	13	1717	1/1	0.99	0.05	74,74,74,74	0
56	MG	14	3318	1/1	0.99	0.06	71,71,71,71	0
56	MG	14	3319	1/1	0.99	0.07	62,62,62,62	0
56	MG	14	3320	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3321	1/1	0.99	0.05	73,73,73,73	0
56	MG	14	3322	1/1	0.99	0.04	72,72,72,72	0
56	MG	14	3324	1/1	0.99	0.05	77,77,77,77	0
56	MG	14	3329	1/1	0.99	0.03	55,55,55,55	0
56	MG	14	3330	1/1	0.99	0.03	65,65,65,65	0
56	MG	14	3332	1/1	0.99	0.05	64,64,64,64	0
56	MG	14	3333	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3329	1/1	0.99	0.04	59,59,59,59	0
56	MG	1H	3410	1/1	0.99	0.04	53,53,53,53	0
56	MG	14	3337	1/1	0.99	0.05	79,79,79,79	0
56	MG	1H	3411	1/1	0.99	0.03	100,100,100,100	0
56	MG	1H	3412	1/1	0.99	0.04	68,68,68,68	0
56	MG	13	1718	1/1	0.99	0.04	67,67,67,67	0
56	MG	14	3342	1/1	0.99	0.05	94,94,94,94	0
56	MG	14	3344	1/1	0.99	0.04	95,95,95,95	0
56	MG	14	3345	1/1	0.99	0.07	118,118,118,118	0
56	MG	14	3347	1/1	0.99	0.06	77,77,77,77	0
56	MG	14	3348	1/1	0.99	0.03	83,83,83,83	0
56	MG	14	3349	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3350	1/1	0.99	0.06	76,76,76,76	0
56	MG	1H	3333	1/1	0.99	0.07	63,63,63,63	0
56	MG	14	3353	1/1	0.99	0.06	69,69,69,69	0
56	MG	14	3354	1/1	0.99	0.08	87,87,87,87	0
56	MG	14	3355	1/1	0.99	0.04	92,92,92,92	0
56	MG	14	3357	1/1	0.99	0.08	77,77,77,77	0
56	MG	1H	3415	1/1	0.99	0.04	94,94,94,94	0
56	MG	1H	3416	1/1	0.99	0.09	104,104,104,104	0
56	MG	14	3361	1/1	0.99	0.04	60,60,60,60	0
56	MG	14	3362	1/1	0.99	0.04	77,77,77,77	0
56	MG	14	3364	1/1	0.99	0.05	73,73,73,73	0
56	MG	1H	3334	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3419	1/1	0.99	0.02	73,73,73,73	0
56	MG	1H	3420	1/1	0.99	0.10	76,76,76,76	0
56	MG	14	3369	1/1	0.99	0.11	84,84,84,84	0
56	MG	1H	3335	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3422	1/1	0.99	0.05	100,100,100,100	0
56	MG	14	3373	1/1	0.99	0.03	87,87,87,87	0
56	MG	14	3374	1/1	0.99	0.04	129,129,129,129	0
56	MG	14	3375	1/1	0.99	0.05	111,111,111,111	0
56	MG	14	3376	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3377	1/1	0.99	0.05	60,60,60,60	0
56	MG	14	3378	1/1	0.99	0.02	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3338	1/1	0.99	0.03	59,59,59,59	0
56	MG	14	3380	1/1	0.99	0.02	83,83,83,83	0
56	MG	1H	3341	1/1	0.99	0.03	57,57,57,57	0
56	MG	1H	3425	1/1	0.99	0.04	92,92,92,92	0
56	MG	13	1719	1/1	0.99	0.05	86,86,86,86	0
56	MG	13	1720	1/1	0.99	0.13	115,115,115,115	0
56	MG	1H	3345	1/1	0.99	0.05	58,58,58,58	0
56	MG	1H	3346	1/1	0.99	0.08	63,63,63,63	0
56	MG	13	1721	1/1	0.99	0.03	79,79,79,79	0
56	MG	1H	3350	1/1	0.99	0.05	72,72,72,72	0
56	MG	1H	3352	1/1	0.99	0.05	71,71,71,71	0
56	MG	1H	3354	1/1	0.99	0.11	65,65,65,65	0
56	MG	1H	3356	1/1	0.99	0.03	61,61,61,61	0
56	MG	1H	3357	1/1	0.99	0.03	58,58,58,58	0
56	MG	13	1706	1/1	0.99	0.05	87,87,87,87	0
56	MG	16	209	1/1	0.99	0.04	64,64,64,64	0
56	MG	16	210	1/1	0.99	0.09	81,81,81,81	0
56	MG	16	211	1/1	0.99	0.06	85,85,85,85	0
56	MG	13	1704	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3360	1/1	0.99	0.02	57,57,57,57	0
58	SF4	3E	302	8/8	0.99	0.05	76,86,96,96	0
58	SF4	32	301	8/8	0.99	0.03	92,113,120,129	0
56	MG	1H	3364	1/1	0.99	0.04	56,56,56,56	0
59	ZN	5A	101	1/1	0.99	0.04	139,139,139,139	0
56	MG	1H	3365	1/1	0.99	0.03	54,54,54,54	0
56	MG	14	3356	1/1	1.00	0.05	98,98,98,98	0
56	MG	13	1716	1/1	1.00	0.02	88,88,88,88	0
56	MG	1H	3400	1/1	1.00	0.05	52,52,52,52	0
56	MG	14	3359	1/1	1.00	0.03	55,55,55,55	0
56	MG	14	3315	1/1	1.00	0.06	71,71,71,71	0
56	MG	1H	3401	1/1	1.00	0.03	55,55,55,55	0
56	MG	1H	3402	1/1	1.00	0.04	60,60,60,60	0
56	MG	14	3363	1/1	1.00	0.01	51,51,51,51	0
56	MG	1H	3403	1/1	1.00	0.03	61,61,61,61	0
56	MG	1H	3355	1/1	1.00	0.02	58,58,58,58	0
56	MG	1H	3342	1/1	1.00	0.04	59,59,59,59	0
56	MG	13	1710	1/1	1.00	0.03	72,72,72,72	0
56	MG	14	3368	1/1	1.00	0.04	49,49,49,49	0
56	MG	1H	3331	1/1	1.00	0.02	51,51,51,51	0
56	MG	14	3323	1/1	1.00	0.03	66,66,66,66	0
56	MG	1H	3336	1/1	1.00	0.04	49,49,49,49	0
56	MG	14	3372	1/1	1.00	0.02	87,87,87,87	0

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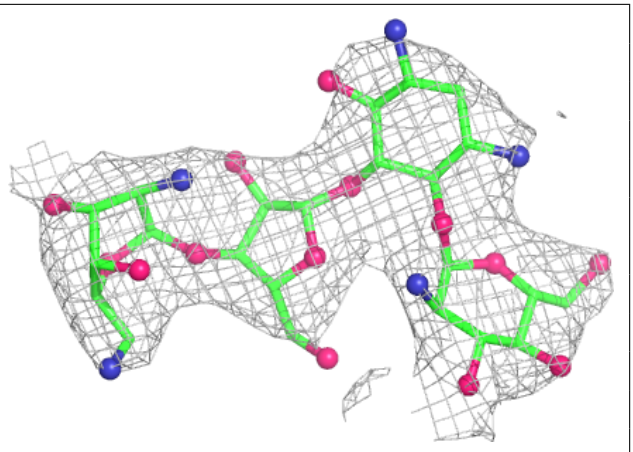
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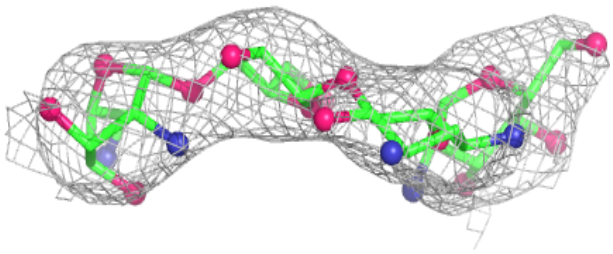
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3325	1/1	1.00	0.03	76,76,76,76	0
56	MG	14	3326	1/1	1.00	0.02	61,61,61,61	0
56	MG	14	3327	1/1	1.00	0.02	84,84,84,84	0
56	MG	14	3328	1/1	1.00	0.05	64,64,64,64	0
56	MG	1H	3337	1/1	1.00	0.05	55,55,55,55	0
56	MG	1H	3361	1/1	1.00	0.03	82,82,82,82	0
56	MG	14	3331	1/1	1.00	0.06	63,63,63,63	0
56	MG	1H	3362	1/1	1.00	0.02	64,64,64,64	0
56	MG	1H	3363	1/1	1.00	0.03	69,69,69,69	0
56	MG	1H	3347	1/1	1.00	0.02	78,78,78,78	0
56	MG	14	3335	1/1	1.00	0.02	63,63,63,63	0
56	MG	1H	3332	1/1	1.00	0.02	66,66,66,66	0
56	MG	1H	3366	1/1	1.00	0.11	59,59,59,59	0
56	MG	1H	3349	1/1	1.00	0.03	74,74,74,74	0
56	MG	14	3339	1/1	1.00	0.02	64,64,64,64	0
56	MG	1H	3417	1/1	1.00	0.01	62,62,62,62	0
56	MG	I8	101	1/1	1.00	0.04	59,59,59,59	0
56	MG	1H	3368	1/1	1.00	0.04	57,57,57,57	0
56	MG	14	3343	1/1	1.00	0.02	71,71,71,71	0
56	MG	1H	3339	1/1	1.00	0.02	70,70,70,70	0
56	MG	1H	3370	1/1	1.00	0.01	76,76,76,76	0
56	MG	14	3346	1/1	1.00	0.01	64,64,64,64	0
56	MG	1H	3371	1/1	1.00	0.02	63,63,63,63	0
56	MG	1H	3394	1/1	1.00	0.05	60,60,60,60	0
56	MG	1H	3351	1/1	1.00	0.02	73,73,73,73	0
56	MG	1H	3340	1/1	1.00	0.03	58,58,58,58	0
56	MG	14	3351	1/1	1.00	0.02	65,65,65,65	0
56	MG	1H	3353	1/1	1.00	0.03	53,53,53,53	0
59	ZN	5I	102	1/1	1.00	0.02	99,99,99,99	0
56	MG	1H	3426	1/1	1.00	0.03	54,54,54,54	0
56	MG	1H	3375	1/1	1.00	0.02	67,67,67,67	0
56	MG	14	3312	1/1	1.00	0.05	70,70,70,70	0

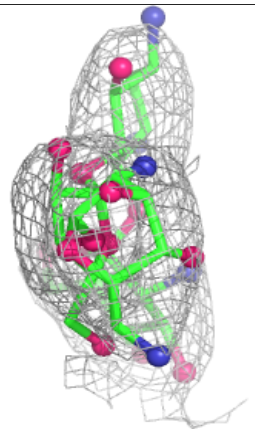
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR 13 1730:

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

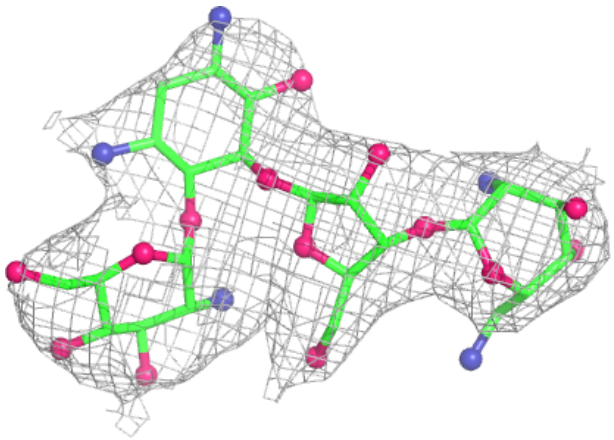


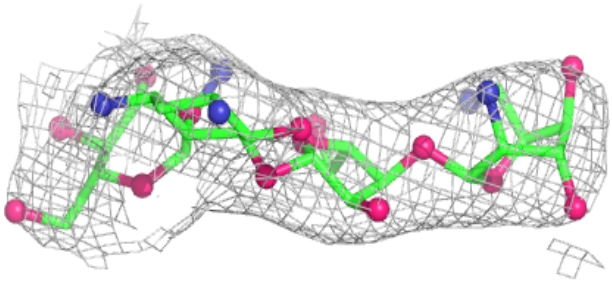


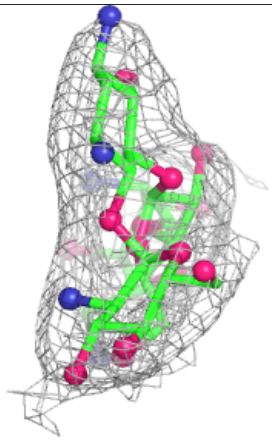


Electron density around PAR 1G 1681:

$2mF_o$-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

There are no such residues in this entry.