



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:35 AM UTC

PDB ID : 4V9O / pdb_00004v9o
Title : Control of ribosomal subunit rotation by elongation factor G
Authors : Pulk, A.; Cate, J.H.D.
Deposited on : 2013-05-03
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

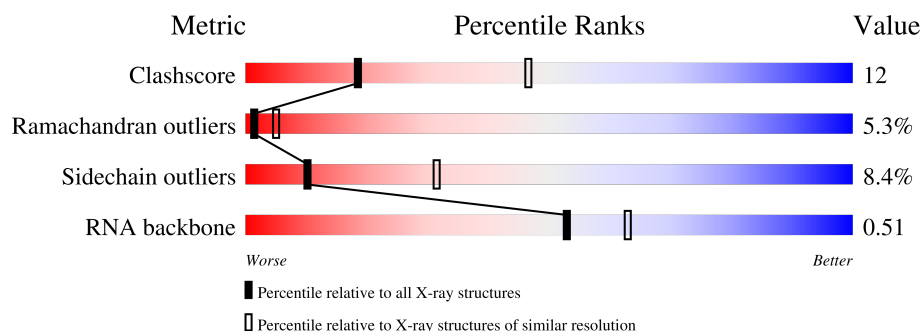
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AB	120	68% 24% 7% .
1	CB	120	61% 31% 7% .
1	EB	120	64% 24% 10% .
1	GB	120	38% 52% 9% .
2	AC	273	67% 26% 5% .
2	CC	273	67% 25% 6% ..

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Mol	Chain	Length	Quality of chain
2	EC	273	 62% 32% . . .
2	GC	273	 64% 29% 5% .
3	AA	2904	 59% 32% 7% .
3	CA	2904	 57% 34% 8% .
3	EA	2904	 60% 30% 8% .
3	GA	2904	 48% 41% 9% .
4	AD	209	 61% 29% 8% .
4	CD	209	 61% 31% 8% .
4	ED	209	 62% 28% 10%
4	GD	209	 65% 29% 6%
5	AE	201	 67% 25% 7%
5	CE	201	 68% 25% 6%
5	EE	201	 67% 26% 7%
5	GE	201	 52% 42% 5% .
6	AF	179	 64% 28% 7% .
6	CF	179	 67% 27% 5% .
6	EF	179	 55% 34% 9% .
6	GF	179	 54% 40% 6% .
7	AG	177	 63% 27% 8% . .
7	CG	177	 60% 31% 8% . .
7	EG	177	 58% 34% 6% . .
7	GG	177	 59% 34% 6% . .
8	AH	50	 54% 36% 10%
8	CH	50	 48% 48% .
8	EH	50	 58% 34% 8%

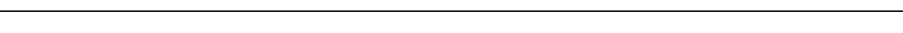
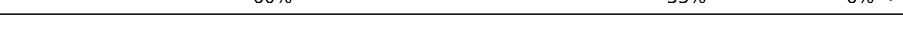
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Mol	Chain	Length	Quality of chain
8	GH	50	
9	AI	142	
9	CI	142	
9	EI	142	
9	GI	142	
10	AJ	142	
10	CJ	142	
10	EJ	142	
10	GJ	142	
11	AK	123	
11	CK	123	
11	EK	123	
11	GK	123	
12	AL	144	
12	CL	144	
12	EL	144	
12	GL	144	
13	AM	136	
13	CM	136	
13	EM	136	
13	GM	136	
14	AN	127	
14	CN	127	
14	EN	127	
14	GN	127	

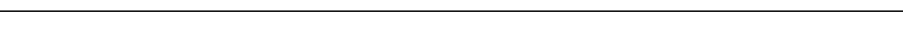
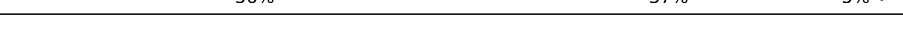
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Mol	Chain	Length	Quality of chain
15	AO	117	
15	CO	117	
15	EO	117	
15	GO	117	
16	AP	115	
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
17	EQ	118	
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
19	ES	110	
19	GS	110	
20	AT	100	
20	CT	100	
20	ET	100	
20	GT	100	
21	AU	104	

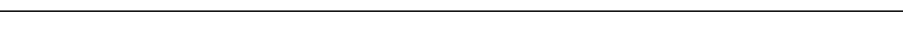
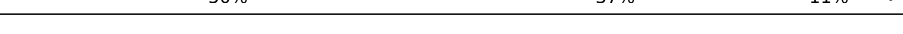
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Mol	Chain	Length	Quality of chain
21	CU	104	
21	EU	104	
21	GU	104	
22	AV	94	
22	CV	94	
22	EV	94	
22	GV	94	
23	AW	85	
23	CW	85	
23	EW	85	
23	GW	85	
24	AX	78	
24	CX	78	
24	EX	78	
24	GX	78	
25	AY	63	
25	CY	63	
25	EY	63	
25	GY	63	
26	AZ	59	
26	CZ	59	
26	EZ	59	
26	GZ	59	
27	A0	57	
27	C0	57	

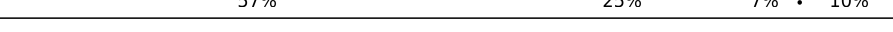
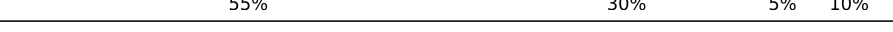
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Mol	Chain	Length	Quality of chain
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	C5	165	
32	E5	165	
33	A6	121	
34	BB	241	
34	DB	241	
34	FB	241	

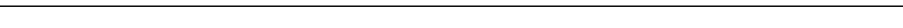
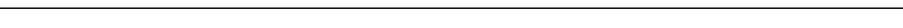
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Mol	Chain	Length	Quality of chain
34	HB	241	
35	BA	1542	
35	DA	1542	
35	FA	1542	
35	HA	1542	
36	BC	233	
36	DC	233	
36	FC	233	
36	HC	233	
37	BD	206	
37	DD	206	
37	FD	206	
37	HD	206	
38	BE	167	
38	DE	167	
38	FE	167	
38	HE	167	
39	BF	135	
39	DF	135	
39	FF	135	
39	HF	135	
40	BG	179	
40	DG	179	
40	FG	179	
40	HG	179	

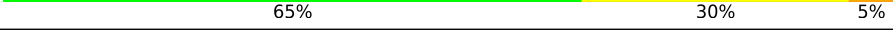
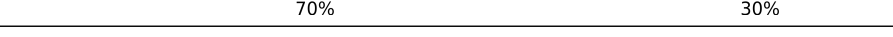
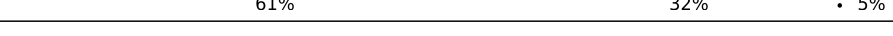
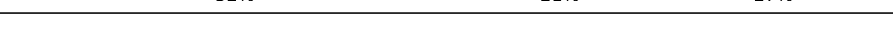
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Mol	Chain	Length	Quality of chain
41	BH	130	
41	DH	130	
41	FH	130	
41	HH	130	
42	BI	130	
42	DI	130	
42	FI	130	
42	HI	130	
43	BJ	103	
43	DJ	103	
43	FJ	103	
43	HJ	103	
44	BK	129	
44	DK	129	
44	FK	129	
44	HK	129	
45	BL	124	
45	DL	124	
45	FL	124	
45	HL	124	
46	BM	118	
46	DM	118	
46	FM	118	
46	HM	118	
47	BN	101	

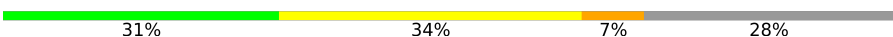
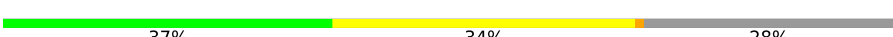
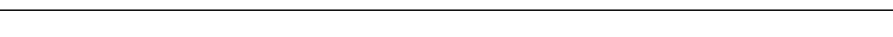
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Mol	Chain	Length	Quality of chain
47	DN	101	
47	FN	101	
47	HN	101	
48	BO	89	
48	DO	89	
48	FO	89	
48	HO	89	
49	BP	82	
49	DP	82	
49	FP	82	
49	HP	82	
50	BQ	84	
50	DQ	84	
50	FQ	84	
50	HQ	84	
51	BR	75	
51	DR	75	
51	FR	75	
51	HR	75	
52	BS	92	
52	DS	92	
52	FS	92	
52	HS	92	
53	BT	87	
53	DT	87	

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Mol	Chain	Length	Quality of chain
53	FT	87	
53	HT	87	
54	BU	71	
54	DU	71	
54	FU	71	
54	HU	71	
55	BV	704	
55	DV	704	
55	FV	704	
55	HV	704	
56	BW	6	
56	DW	6	
56	FW	6	
56	HW	6	

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	KBE	BW	1	-	X	-	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 592086 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 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	EB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	GB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	EC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	GC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	CA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	EA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	GA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	ED	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	GD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	EE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	GE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	EF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	GF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	EG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	GG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	CH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	EH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	GH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	EI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	GI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	EJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	GJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	EK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	GK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	EL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	GL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	EM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	GM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	EN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	GN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	CO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	EO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	GO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	EP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	GP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	EQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	GQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	ER	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	GR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	ES	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	GS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	ET	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	GT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	EU	102	Total	C	N	O	0	0	0
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	GU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	EV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	GV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	CW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	EW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	GW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	EX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	GX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	EY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	GY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	EZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	GZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	E0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	G0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	A1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	E1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	G1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	E2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	G2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	E3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	G3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	E4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	G4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	C5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	145	Total	C	N	O	S	0	0	0
			1101	696	193	205	7			

- Molecule 33 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A6	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	FB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	HB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	DA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	FA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	HA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
36	FC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
36	HC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	FD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	HD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	FE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	HE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	102	Total	C	N	O	S	0	0	0
			832	525	150	150	7			
39	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	FG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	HG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	FH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	HH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	FI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	HI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
43	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
43	FJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	HJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	FK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	HK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	FL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	HL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	FM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	HM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	FN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	HN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	DO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	FO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	HO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	FP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	HP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
50	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
50	FQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	HQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	DR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	FR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	HR	55	Total	C	N	O		0	0	0
			455	288	86	81				

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	FS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	HS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	FT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	HT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	FU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	HU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 55 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	690	Total	C	N	O	S	0	0	0
			5345	3369	920	1031	25			
55	DV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	FV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	HV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			

- Molecule 56 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	DW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	FW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	HW	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AB	4	Total	Mg	0	0
			4	4		
57	AC	1	Total	Mg	0	0
			1	1		
57	AA	136	Total	Mg	0	0
			136	136		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AE	1	Total 1	Mg 1	0	0
57	A4	1	Total 1	Mg 1	0	0
57	BA	40	Total 40	Mg 40	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	BV	1	Total 1	Mg 1	0	0
57	CB	4	Total 4	Mg 4	0	0
57	CA	136	Total 136	Mg 136	0	0
57	CE	1	Total 1	Mg 1	0	0
57	CN	1	Total 1	Mg 1	0	0
57	C4	1	Total 1	Mg 1	0	0
57	DA	43	Total 43	Mg 43	0	0
57	DV	1	Total 1	Mg 1	0	0
57	EA	137	Total 137	Mg 137	0	0
57	EB	4	Total 4	Mg 4	0	0
57	ED	1	Total 1	Mg 1	0	0
57	EE	1	Total 1	Mg 1	0	0
57	FA	39	Total 39	Mg 39	0	0
57	FE	1	Total 1	Mg 1	0	0
57	FN	2	Total 2	Mg 2	0	0

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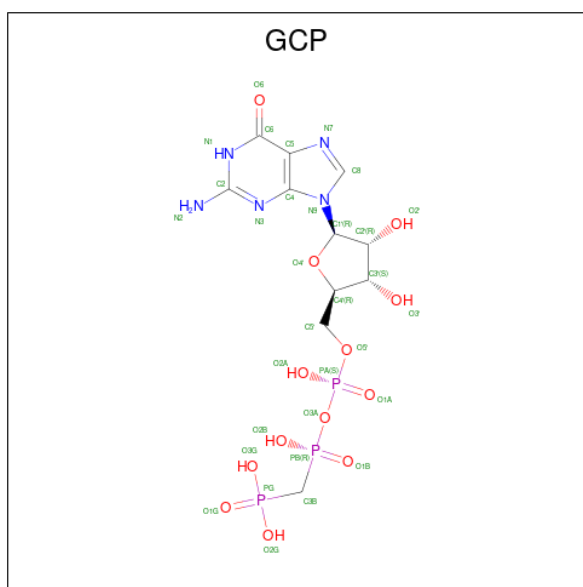
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	FU	1	Total	Mg	0	0
			1	1		
57	FV	1	Total	Mg	0	0
			1	1		
57	GB	4	Total	Mg	0	0
			4	4		
57	GA	136	Total	Mg	0	0
			136	136		
57	GC	2	Total	Mg	0	0
			2	2		
57	GL	1	Total	Mg	0	0
			1	1		
57	HA	41	Total	Mg	0	0
			41	41		
57	HE	1	Total	Mg	0	0
			1	1		
57	HK	1	Total	Mg	0	0
			1	1		
57	HV	1	Total	Mg	0	0
			1	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	A4	1	Total	Zn	0	0
			1	1		
58	C4	1	Total	Zn	0	0
			1	1		
58	E4	1	Total	Zn	0	0
			1	1		
58	G4	1	Total	Zn	0	0
			1	1		

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
59	BV	1	Total 32	C 11	N 5	O 13	P 3	0	0
59	DV	1	Total 32	C 11	N 5	O 13	P 3	0	0
59	FV	1	Total 32	C 11	N 5	O 13	P 3	0	0
59	HV	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AB	18	Total O 18 18	0	0
60	AC	6	Total O 6 6	0	0
60	AA	614	Total O 614 614	0	0
60	AD	4	Total O 4 4	0	0
60	AE	1	Total O 1 1	0	0
60	AF	1	Total O 1 1	0	0
60	AJ	1	Total O 1 1	0	0
60	AL	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AN	2	Total 2	O 2	0	0
60	AP	1	Total 1	O 1	0	0
60	AQ	2	Total 2	O 2	0	0
60	AS	1	Total 1	O 1	0	0
60	A0	2	Total 2	O 2	0	0
60	A2	1	Total 1	O 1	0	0
60	A3	1	Total 1	O 1	0	0
60	A4	1	Total 1	O 1	0	0
60	BA	202	Total 202	O 202	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	2	Total 2	O 2	0	0
60	BT	2	Total 2	O 2	0	0
60	BV	1	Total 1	O 1	0	0
60	CB	21	Total 21	O 21	0	0
60	CA	607	Total 607	O 607	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	3	Total 3	O 3	0	0
60	CE	1	Total 1	O 1	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	5	Total 5	O 5	0	0
60	CN	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CQ	1	Total 1	O 1	0	0
60	CS	2	Total 2	O 2	0	0
60	CT	2	Total 2	O 2	0	0
60	CU	1	Total 1	O 1	0	0
60	C0	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	186	Total 186	O 186	0	0
60	DC	2	Total 2	O 2	0	0
60	DD	1	Total 1	O 1	0	0
60	DE	1	Total 1	O 1	0	0
60	DG	1	Total 1	O 1	0	0
60	DK	1	Total 1	O 1	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	8	Total 8	O 8	0	0
60	DQ	1	Total 1	O 1	0	0
60	DT	4	Total 4	O 4	0	0
60	DU	1	Total 1	O 1	0	0
60	DV	1	Total 1	O 1	0	0
60	EA	610	Total 610	O 610	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	EB	18	Total 18	O 18	0	0
60	EC	9	Total 9	O 9	0	0
60	ED	3	Total 3	O 3	0	0
60	EE	2	Total 2	O 2	0	0
60	EL	4	Total 4	O 4	0	0
60	EN	3	Total 3	O 3	0	0
60	ER	1	Total 1	O 1	0	0
60	ET	2	Total 2	O 2	0	0
60	EV	2	Total 2	O 2	0	0
60	E0	1	Total 1	O 1	0	0
60	E2	1	Total 1	O 1	0	0
60	E3	2	Total 2	O 2	0	0
60	E4	2	Total 2	O 2	0	0
60	FA	197	Total 197	O 197	0	0
60	FC	1	Total 1	O 1	0	0
60	FE	2	Total 2	O 2	0	0
60	FN	3	Total 3	O 3	0	0
60	FT	4	Total 4	O 4	0	0
60	FU	1	Total 1	O 1	0	0
60	FV	1	Total 1	O 1	0	0
60	GB	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	GA	606	Total O 606 606	0	0
60	GC	10	Total O 10 10	0	0
60	GD	3	Total O 3 3	0	0
60	GE	2	Total O 2 2	0	0
60	GJ	1	Total O 1 1	0	0
60	GL	4	Total O 4 4	0	0
60	GN	4	Total O 4 4	0	0
60	GQ	1	Total O 1 1	0	0
60	GR	2	Total O 2 2	0	0
60	GS	2	Total O 2 2	0	0
60	GU	1	Total O 1 1	0	0
60	GV	1	Total O 1 1	0	0
60	G2	2	Total O 2 2	0	0
60	G3	1	Total O 1 1	0	0
60	G4	1	Total O 1 1	0	0
60	HA	193	Total O 193 193	0	0
60	HD	3	Total O 3 3	0	0
60	HE	3	Total O 3 3	0	0
60	HN	7	Total O 7 7	0	0
60	HQ	1	Total O 1 1	0	0
60	HT	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	HV	1	Total	O	0	0
			1	1		

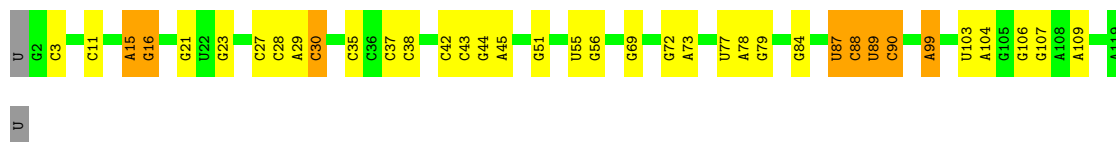
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

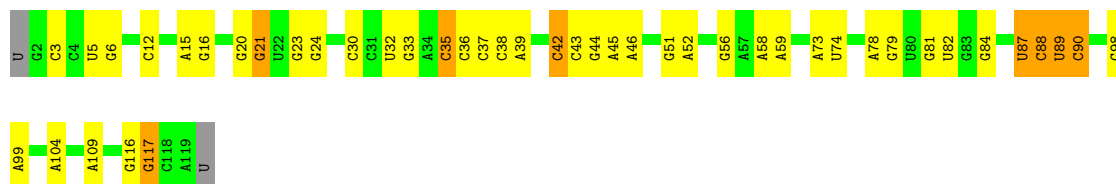
• Molecule 1: 5S rRNA

Chain AB: 



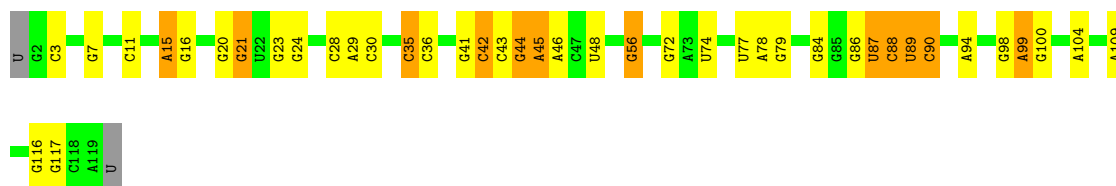
• Molecule 1: 5S rRNA

Chain CB: 

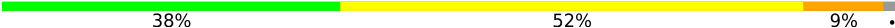


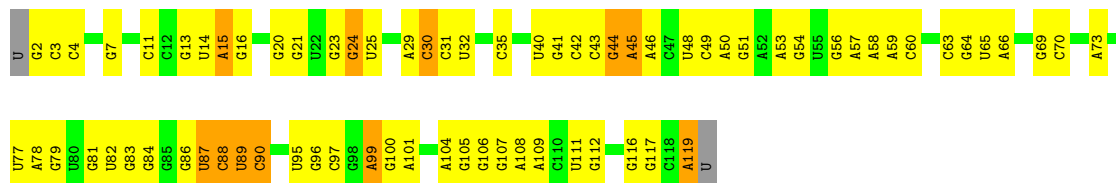
• Molecule 1: 5S rRNA

Chain EB: 

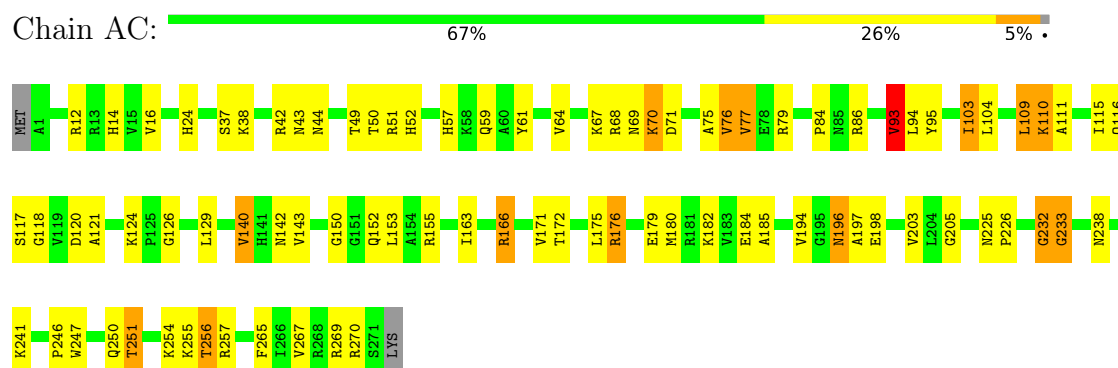


• Molecule 1: 5S rRNA

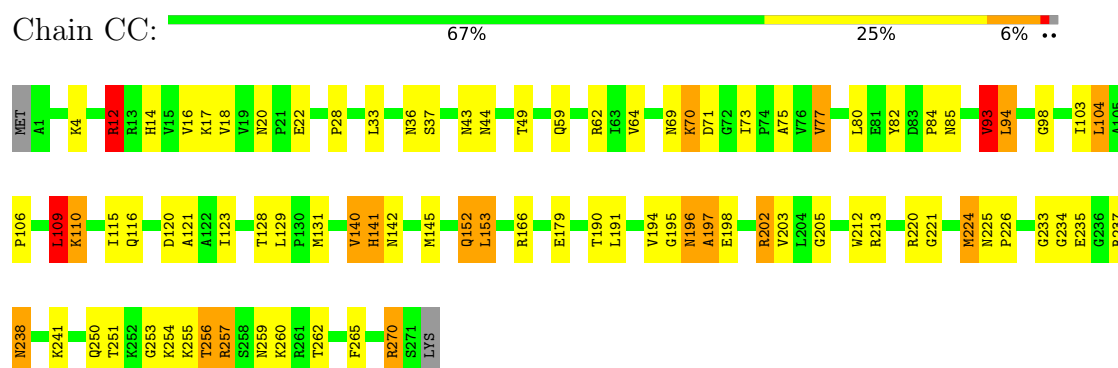
Chain GB: 



- Molecule 2: 50S ribosomal protein L2



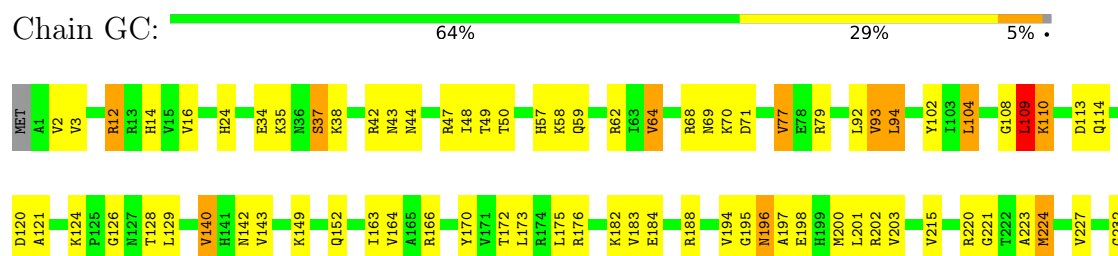
- Molecule 2: 50S ribosomal protein L2

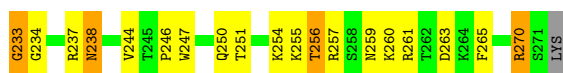


- Molecule 2: 50S ribosomal protein L2



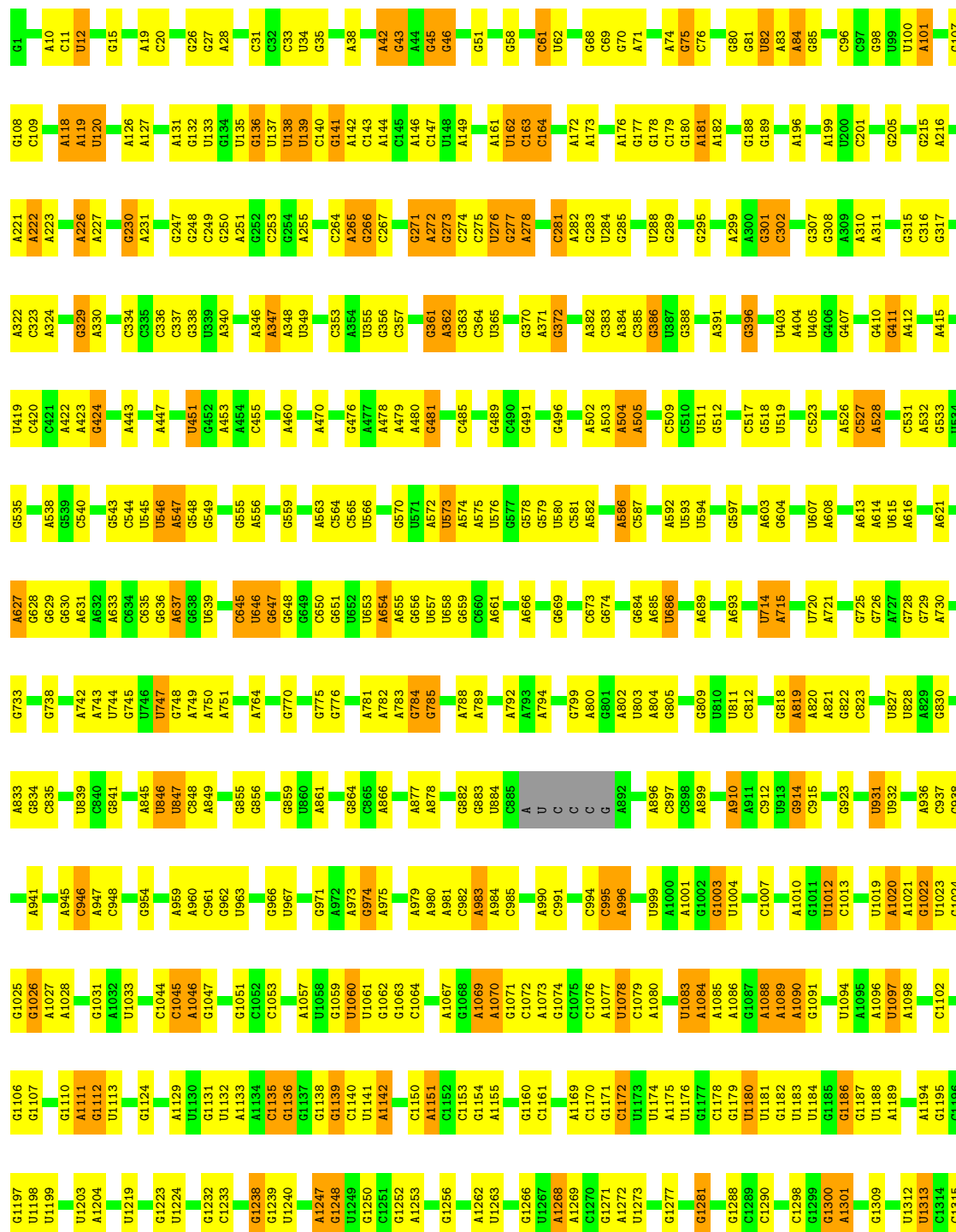
- Molecule 2: 50S ribosomal protein L2



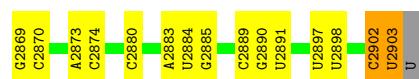


• Molecule 3: 23S rRNA

Chain AA: 59% 32% 7%

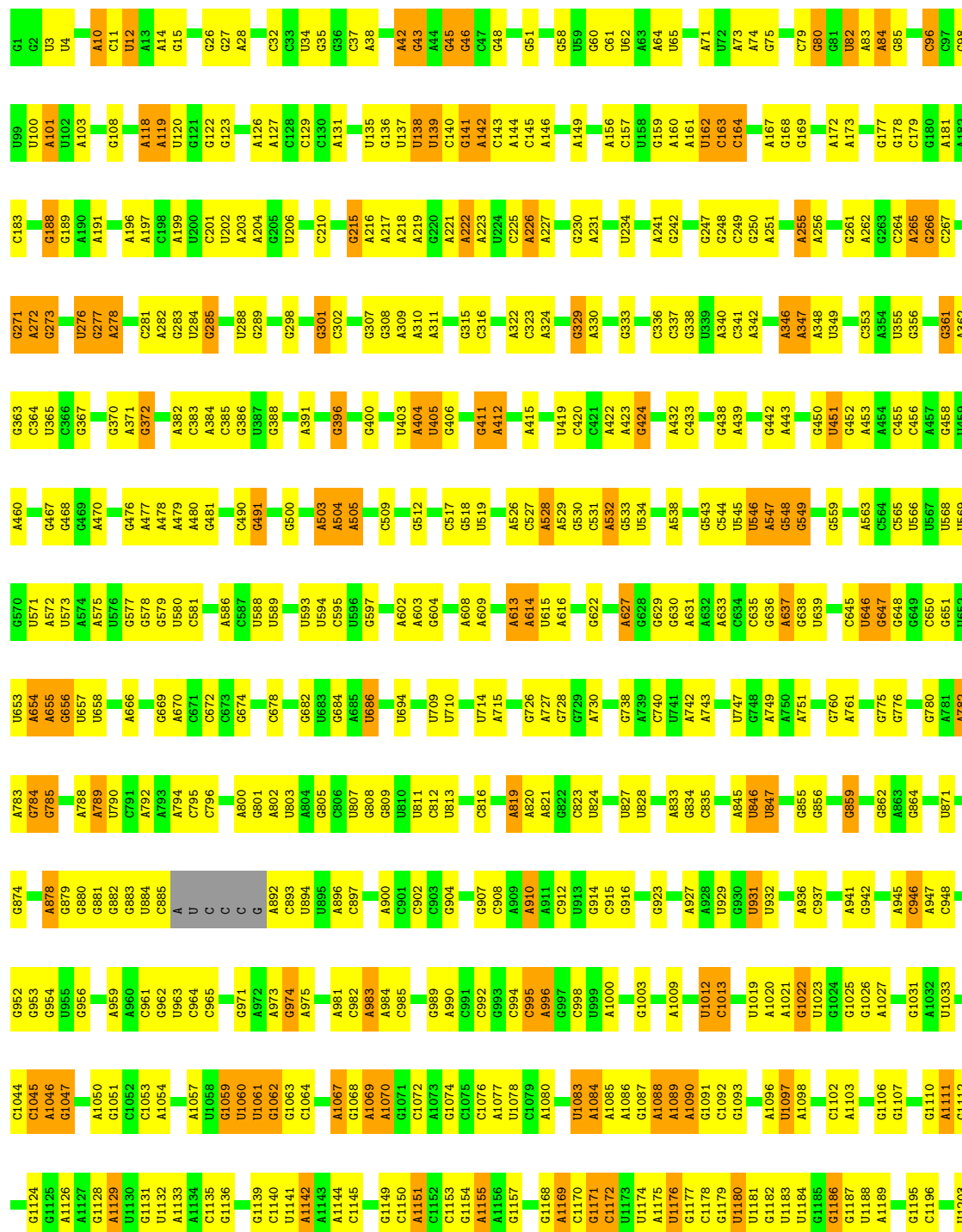




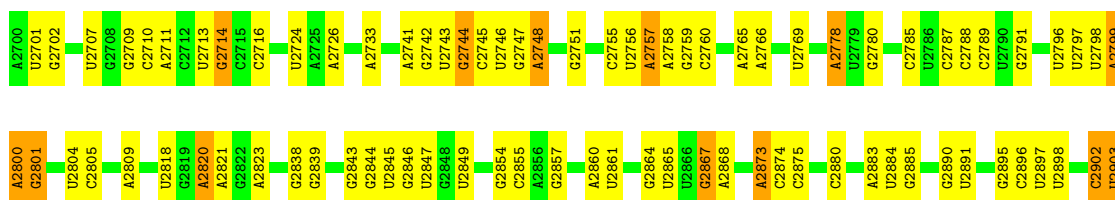


• Molecule 3: 23S rRNA

Chain CA: 57% 34% 8%



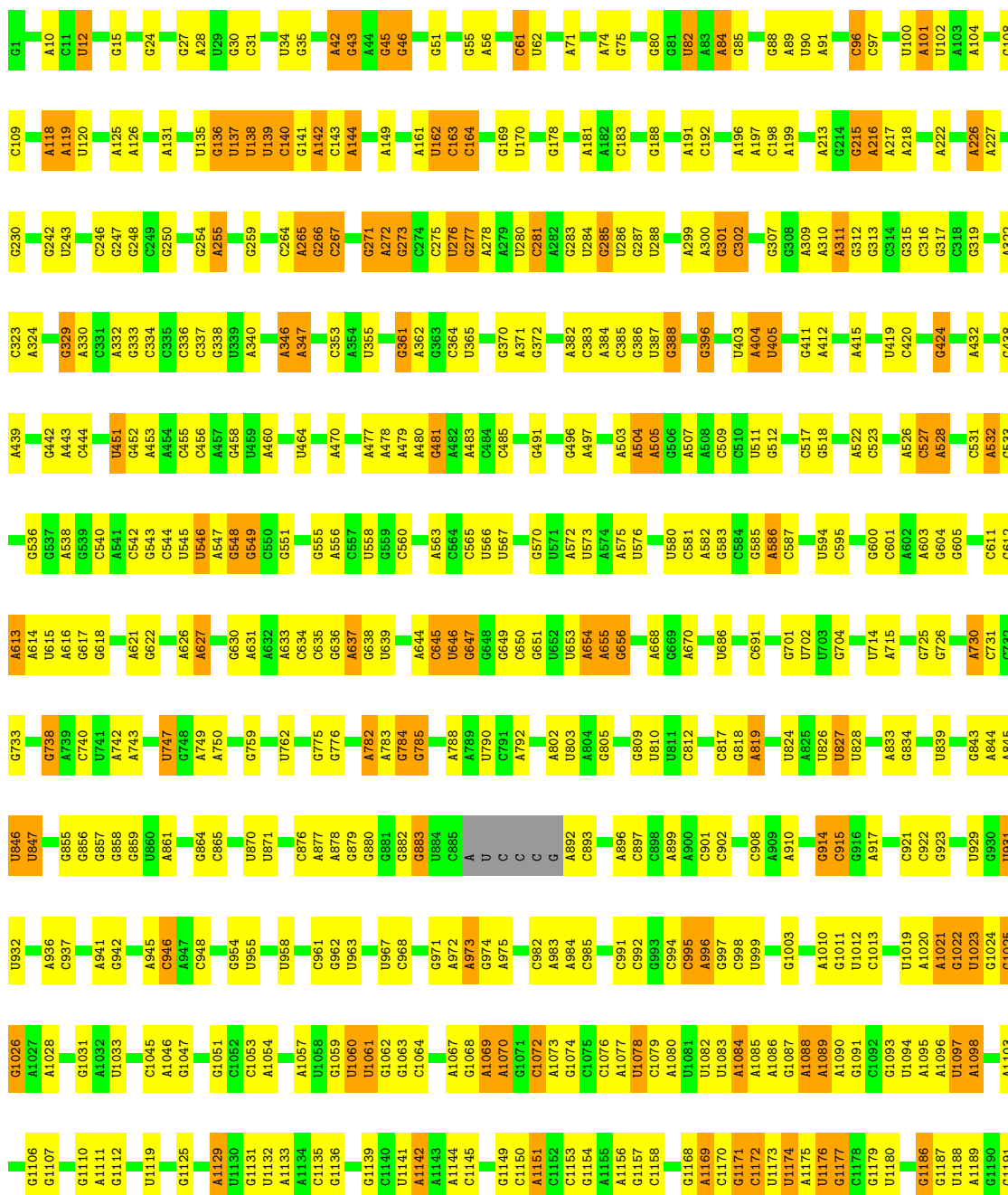
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G2602	U2604	U2393	G2507	U2194	G	G2038	U1951	U1818	G1734	A1505	A1506	U1397	C1296	C1207
G2603	G2506	C2394	G2308	U2199	C	U2039	A1952	A1819	G1737	A1616	U1506	A1403	C1297	C1208
U2609	C2507	G2400	U2311	A2198	U	C2043	U1954	A1829	G1738	A1617	C1507	U1404	U1209	U1209
U2613	A2518	U2401	U2312	A2199	U	A2051	U1955	C1833	A1739	A1618	A1508	U1405	A1301	U1217
A2614	U2522	G2402	G2204	G2204	G2133	C2055	A1960	C1837	A1744	A1626	A1509	U1406	G1300	G1220
U2615	G2529	A2406	G2209	U2210	A2135	G2056	A1966	C1838	A1745	G1627	U1513	G1410	G1309	C1221
G2618	U2533	A2407	G2210	U2211	G2136	A2060	A1967	G1839	A1746	G1628	U1514	C1414	U1313	U1224
C2619	U2533	G2408	U2321	U2212	U2137	G2061	G1968	U1841	C1748	C1638	A1515	U1415	C1315	G1225
U2629	U2533	G2409	G2323	A2212	U2139	A2062	A1969	G1842	G1753	C1638	G1524	C1417	U1317	A1230
U2632	U2539	A2412	U2324	U2213	G2140	C2063	A1970	C1843	U1758	A1641	C1533	U1418	G1318	U1231
U2636	C2540	G2415	G2325	G2214	A2142	C2064	U1971	A1847	A1759	G1642	U1534	U1419	U1317	U1230
U2637	A2541	C2416	G2326	G2215	G2143	G2065	G1972	A1848	C1760	U1647	A1535	U1420	U1326	G1238
U2638	C2417	U2219	U2327	U2216	G2144	G2069	C1974	G1873	C1761	U1648	C1536	G1421	A1327	G1239
U2639	U2422	U2220	G2330	U2221	C2145	A2070	G1975	A1888	A1762	G1649	G1537	G1428	A1328	U1242
G2642	C2423	G2221	G2331	G2221	A2147	C2072	U1976	U1864	C1764	G1653	A1548	G1435	G1331	C1243
U2647	C2424	G2225	U2332	G2226	G2148	A2071	A1977	U1865	A1773	A1654	A1549	U1439	G1332	G1245
G2648	A2425	C2226	U2333	G2226	U2149	U2079	G1983	G1869	A1774	A1655	A1553	G1444	G1338	A1246
U2653	G2426	C2227	G2334	U2233	C2150	A2080	G1989	C1870	U1775	C1688	U1563	G1445	U1338	A1247
U2654	C2427	G2228	U2335	G2233	U2151	U2081	U1989	A1871	G1776	C1688	C1564	G1446	A1342	U1248
U2657	G2428	G2233	U2336	G2234	C2152	C2091	C1990	A1872	U1779	A1684	C1565	G1447	G1343	G1250
G2660	U2429	G2234	U2337	U2235	A2154	U2092	U1991	G1873	U1780	A1684	A1566	G1448	U1344	C1251
U2661	A2430	U2236	U2338	U2236	G2155	G2093	G1992	C1874	U1781	A1668	G1567	G1449	U1352	G1252
G2663	U2435	G2237	G2339	U2237	G2156	A2094	U1993	G1875	U1782	A1669	G1568	G1450	U1352	A1253
U2665	C2436	G2238	U2348	G2239	G2157	A2095	C1997	U1883	A1783	A1673	A1569	G1451	G1360	G1256
G2671	U2440	G2239	U2349	G2240	A	C2096	A1998	G1884	A1785	C1674	A1570	G1452	G1361	A1262
U2674	A2441	G2240	U2350	U2241	C	A2097	C2006	A1899	A1786	A1676	G1573	G1458	C1362	U1267
A2675	U2448	U2242	U2351	U2242	C	G2102	G2010	G1906	A1789	A1677	U1578	G1459	G1363	A1268
C2676	U2449	U2243	U2352	U2243	A	C2103	G2011	A1913	C1790	G1681	A1579	A1469	G1364	A1265
U2680	A2450	U2244	U2353	U2244	C	G2104	U2011	C1914	A1791	C1708	A1583	U1475	A1365	G1266
C2681	U2459	U2245	U2354	U2245	C	U2105	G2012	U1915	A1794	G1684	U1584	G1476	G1368	A1268
A2682	U2469	U2246	U2355	U2246	U	G2106	A2015	U1916	C1795	C1685	C1585	U1477	G1370	A1269
C2683	G2470	A2273	U2356	U2247	C	U2107	U2016	A1916	U1796	G1707	G1588	G1479	G1371	C1271
U2684	U2473	G2277	U2357	U2248	A	A2108	U2017	A1927	G1797	C1708	U1588	G1482	A1378	A1272
U2685	U2474	G2278	U2358	U2249	C	G2110	G2018	A1928	U1798	G1708	A1602	G1483	G1379	U1273
U2688	C2475	G2279	U2359	U2250	U	U	A2019	G1929	U1799	A1713	A1593	U1484	G1380	A1276
U2689	U2476	U2283	U2360	U2251	U	G	A2020	G1930	C1800	U1714	U1594	U1485	G1381	G1277
U2690	A2477	C2283	U2361	U2252	A	U	C2021	U1931	A1801	G1715	C1595	U1486	G1382	G1280
U2696	U2478	G2284	U2362	U2253	C	G	U2022	A1932	A1805	A1722	G1601	U1487	A1383	G1280
G2697	U2479	U2285	U2363	U2254	C	G	C2023	A1933	A1806	G1723	U1602	G1492	A1384	A1285
C2699	U2482	G2286	U2364	U2255	C	A	G2024	A1937	A1808	G1723	A1603	G1493	A1385	A1286
	C2483	U2287	U2365	U2256	C	U	C2025	A1938	A1809	G1727	A1604	U1494	A1387	G1287
	U2491	U2288	U2366	U2257	C	U	A2030	U1939	A1810	G1728	C1605	A1495	A1388	A1288
	U2491	U2289	U2367	U2258	C	U	G2032	G1945	U1811	U1729	C1606	A1496	A1389	G1289
	U2491	U2290	U2368	U2259	C	U	A2033	U1946	U1812	G1730	C1607	A1497	A1392	G1290
	U2491	U2291	U2369	U2260	C	U	U2034	C1947	G1813	G1731	A1608	C1498	A1393	C1291
	U2491	U2292	U2370	U2261	C	U	G2035	G1948	C1816	G1732	A1609	G1500	A1394	C1292
	U2491	U2293	U2371	U2262	C	U	C2036	G1949					A1395	



U

• Molecule 3: 23S rRNA

Chain EA: 60% 30% 8%

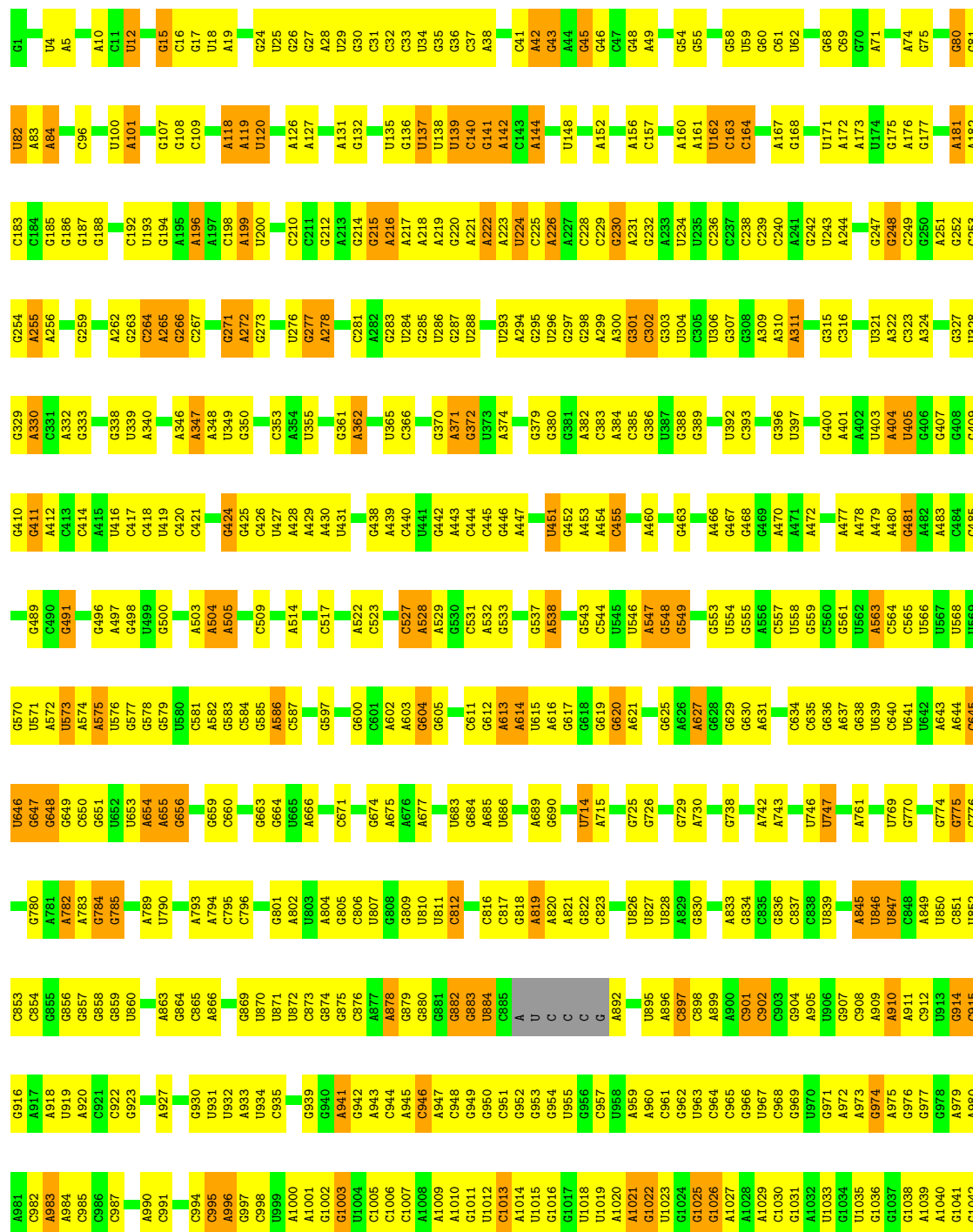


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G2714	A2598	C2499	U2384	A2297	U2185	G	G1906	A1784	A1653	A1535	A1420	G1309	U1198
C2715	G2715	C2385	U2386	G	U2186	A	U2039	A1785	C1536	G1537	G1421	U1312	A1205
C2716	A2602	U2305	A2386	U2305	U2187	G	A1913	A1786	C1536	G1537	G1422	U1313	G1220
U2720	G2603	G2308	U2387	G	G2190	C	C1914	A1787	C1536	A1544	A1427	U1314	C1221
A2721	U2609	G2502	A2388	U2390	U2194	U	A1927	A1791	G1658	A1545	C1428	U1315	U1222
G2722	C2612	U2503	G2389	A2311	U2195	U	A1928	A1794	A1664	A1548	G1429	U1316	U1223
A2726	U2606	C2505	C2196	G	C2196	U	G1929	C1795	A1665	A1549	G1430	G1317	U1224
A2733	C2394	U2506	U2197	A2314	U2198	G	G1930	G1799	G1666	U1559	U1431	U1325	G1225
U2737	C2395	C2507	A2198	G2315	A2199	C	A1936	C1800	A1667	G1435	U1436	U1326	A1226
G2742	G2396	U2511	C2200	G2316	C2200	U	A1937	A1801	A1668	G1436	C1437	A1327	G1238
U2743	U2402	U2514	G2204	A2317	G2137	U	A1938	A1802	A1669	U1566	A1438	G1332	G1245
G2744	C2403	C2515	G2204	G2138	U2137	U	U1939	C1806	U1671	C1565	A1439	U1340	A1246
C2745	U2516	C2517	U2210	G2139	G2140	U	G1948	G1807	G1674	G1567	G1445	U1341	A1247
U2746	A2406	C2517	A2211	G2141	A2142	C	U1948	A1808	C1675	U1569	C1446	U1342	G1248
G2747	G2409	A2518	A2212	C2143	C2143	U	U1985	G1811	A1676	U1578	G1450	G1343	U1249
U2748	U2519	U2519	C2214	C2144	C2145	U	G1959	G1812	A1678	A1579	G1451	U1344	U1250
C2755	G2325	C2520	C2214	C2145	C2146	U	U1960	G1813	U1678	G1582	G1452	C1350	A1253
U2756	C2326	C2521	A2225	A2147	A2147	C	U1963	C1816	U1688	G1583	G1456	C1351	G1256
A2757	U2419	U2522	C2226	G2148	G2149	U	U1966	G1817	A1700	U1584	U1457	C1352	C1257
A2758	C2328	G2526	G2230	U2149	U2149	U	A1967	U1818	U1700	C1585	U1458	A1354	A1260
G2759	U2330	G2330	U2231	C2150	C2151	U	G1968	G1824	U1712	U1594	G1459	G1355	C1261
C2760	A2331	C2331	U2231	U2151	G2152	U	U1969	G1825	U1713	C1595	U1468	C1356	A1262
A2765	C2332	C2332	G2238	C2153	C2153	U	A1969	G1827	U1714	A1596	U1468	C1357	U1263
A2766	A2333	G2333	G2239	A2154	A2154	U	U1970	U1827	G1715	U1474	U1474	G1360	A1264
U2769	A2336	A2336	G2239	U2155	U2155	U	U1971	U1828	G1723	A1603	G1475	C1265	A1265
G2777	U2340	G2340	U2249	G2156	G2157	U	G1972	A1829	C1727	G1604	G1475	G1364	G1266
A2778	A2346	C2347	G2250	G2157	G2157	U	U1991	G1831	C1728	U1482	G1482	A1365	U1267
U2779	C2347	C2347	G2251	A	A	U	G1992	G1832	U1729	C1607	U1485	G1368	A1268
G2780	U2348	U2348	G2252	C	C	U	U1993	C1833	C1730	A1608	U1486	U1372	A1269
C2788	A2352	A2352	G2252	C	C	U	C1996	U1843	G1731	A1609	U1487	U1372	C1270
U2789	G2353	G2353	U2268	G	G	U	C1997	C1843	G1732	U1610	U1487	A1272	G1271
A2790	C2354	C2354	G2269	A	A	U	C1998	A1847	G1733	G1613	C1493	C1376	U1273
G2791	U2355	U2355	A2270	C	C	U	A1998	A1848	G1733	A1614	A1494	A1377	G1277
A2792	U2356	U2356	G2271	U	U	U	A2005	A1853	G1737	C1615	A1495	C1378	C1278
C2793	G2357	G2357	C2275	U	U	U	A2013	U1858	G1738	A1618	A1504	G1380	G1279
C2794	U2358	U2358	G2276	G	G	U	A2016	A1858	A1739	G1619	A1508	G1281	G1280
U2796	A2358	A2358	G2277	A	A	U	U2017	A1866	A1744	A1508	A1508	A1383	G1281
U2797	G2361	G2361	A2278	U	U	U	G2018	G1867	U1747	A1509	G1510	A1384	A1284
U2798	A2366	A2366	G2280	A	A	U	A2019	C1868	C1748	G1626	G1510	A1385	A1285
A2799	G2367	G2367	A2281	C	C	U	A2020	G1869	G1764	A1515	A1515	A1387	G1288
U2800	C2368	C2368	C2282	C	C	U	C2021	A1870	A1773	G1516	G1517	A1394	G1292
G2801	A2369	A2369	A2283	A	A	U	U2022	A1871	A1774	A1630	A1522	A1395	C1293
C2802	G2370	G2370	A2284	C	C	U	G2024	A1872	U1775	G1631	U1523	U1407	G1298
G2803	U2375	U2375	C2285	C	C	U	A2030	G1873	G1776	A1634	A1524	G1415	C1293
U2804	G2375	G2375	G2286	U	U	U	A2031	A1876	U1647	U1648	G1524	U1415	G1300
C2805	A2378	A2378	A2287	U2180	U2180	U	G2032	A1877	G1776	U1649	A1532	U1416	A1301
G2806	G2379	G2379	A2288	G	G	U	A2033	G1878	U1779	A1650	C1533	G1303	A1302
	C2380	C2380	G2290	U	U	U							G1303

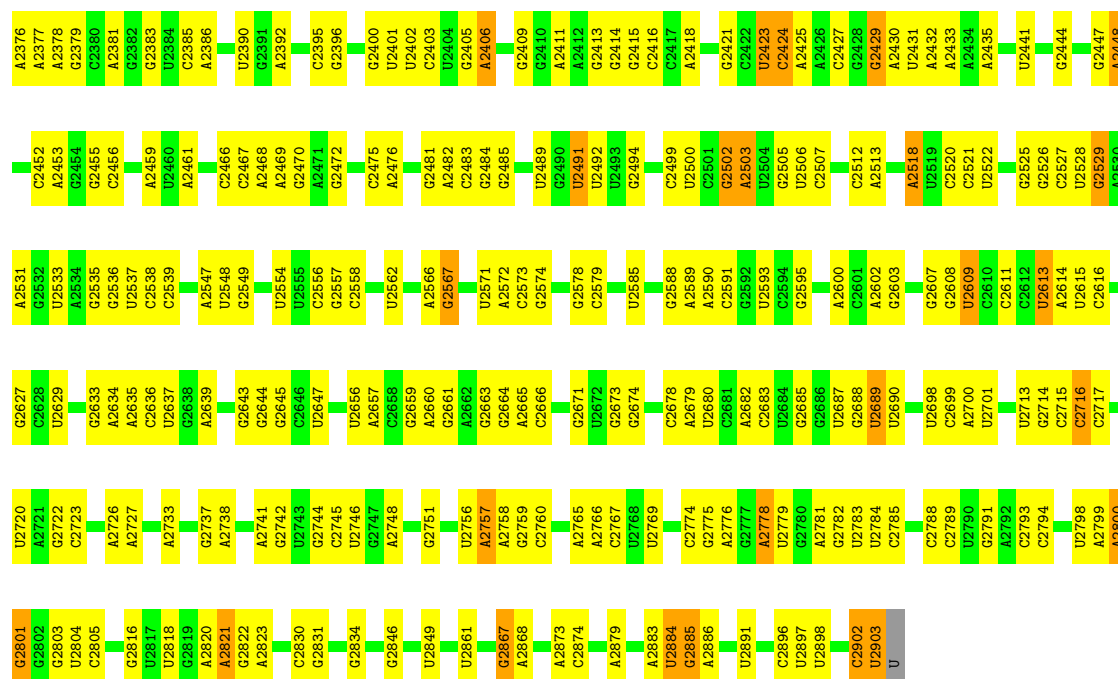


● Molecule 3: 23S rRNA

Chain GA: 48% 41% 9%

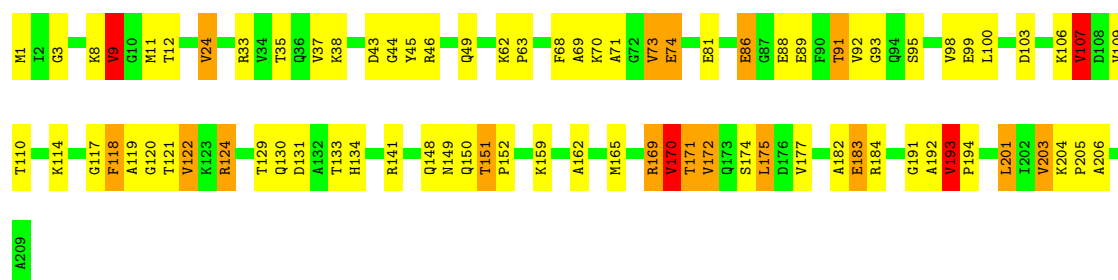


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C2310	A2227	C	A2097	G2011	C1881	U1798	G1703	C1469	C1370	C1270	G1194	C1117	A1045
C2312	G2230	G	U2011	G2012	U1882	C1800	A1713	A1474	G1371	G1271	G1195	G1046	A1046
C2313	G2230	A	A2013	G2013	U1883	A1801	A1714	U1474	C1376	A1272	G1196	A1126	G1047
A2314	G2230	C	G2104	G2014	G1884	A1802	G1715	G1475	G1377	A1273	G1197		
G2315	U2233	C	U2105	U2017	G1893	A1803	U1716		A1378	A1274	U1198		A1050
G2316	G2234	U	U2106	G2018	C1894	C1804	G1721	G1478	A1379	G1281	G1202	A1129	G1051
A2317	G2237	U	G2107	A2019	C1895	A1805	G1722	G1479	G1380	U1379	U1203	U1130	C1052
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U2320	G2240	A	G2110	U2022	G1905	A1809	G1723	G1483	A1286	A1286	C1208	A1133	A1057
U2321	G2242	A	U	G2023	G1906	A1810	G1727	U1485	A1287	A1287	U1209	C1135	U1058
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G2323	G2247	A	U	C2025	G1912	U1812	U1729	U1486	A1385	G1295	G1211	G1137	U1060
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G2326	G2250	C	G	G2027	C1914	A1816	C1730		A1387	A1214	G1215	G1139	G1062
A2327	G2251	A	G		C1914	C1816	U1735	C1493		A1214	G1215	C1140	G1063
	G2252	C	U	A2030	C1920	U1820	U1736	A1494	A1392	G3000	G1218	U1141	C1064
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G2342	A2273	C	C	G2046	A1938	G1832	U1747	G1516		G317	A1231	A1151	A1073
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G2346	G2276	U	U	A2054	C1957	G1835	A1759	G1533	U1415	G327	G1235	G1154	A1077
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G2283	C2283	A	G2133	A2060	U1966	G1846	G1763	U1534	A1420	G333	G1238	G1158	U1081
A2284	C2284	U	A2134	C2061	C1967	A1847	C1764	A1535	G1421	G334	G1239		U1082
G2285	C2285	U	A2135	A2062	G1968	A1848		C1536	G1422				U1083
G2286	C2286	U	G2136	G2066	G1969	U1848	A1772	G1537		C1243		C1170	A1084
A2287	C2287	U	U2137	G2067	A1960	U1851	A1773	C1428	C1428	G1338	A1244	G1171	
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		U	U	A2062	C1966	A1853	U1775	G1430	G1430	A1088	G1248	U1173	A1088
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		U	U	G2087	U1993	A1871	A1791	G1455	G1455	G1361	C1261	G1186	U1108
		U	U	A2088	U1997	A1872	G1792	U1584	U1458	A1365	A1262	U1188	G1109
		U	U	G2091	C1997	G1873	G1793	C1585	G1459	A1366	G1266	A1189	G1110
		U	U	U2092	A1998	G1874	C1794	U1589	G1459	A1367	U1267	G1191	A1111
		U	U		C1999	G1875	C1795						G1112



• Molecule 4: 50S ribosomal protein L3

Chain AD: 61% 29% 8% .



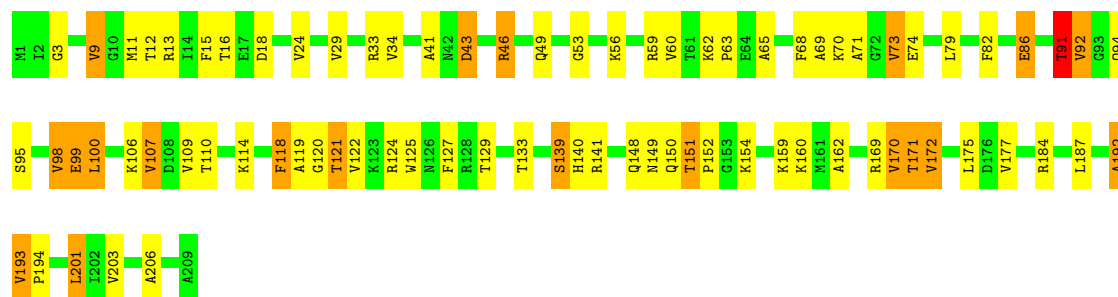
• Molecule 4: 50S ribosomal protein L3

Chain CD: 61% 31% 8% .

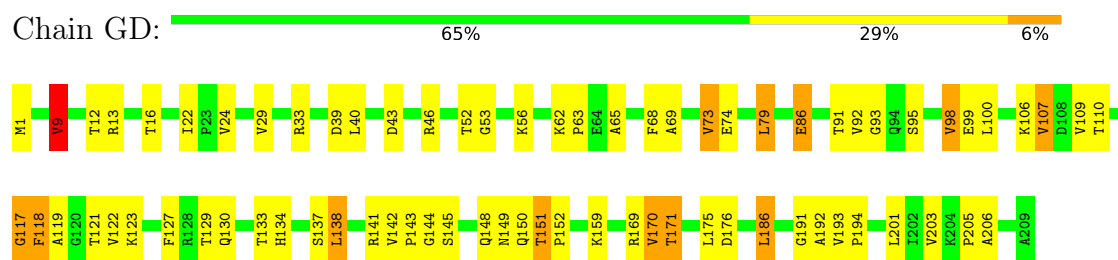


• Molecule 4: 50S ribosomal protein L3

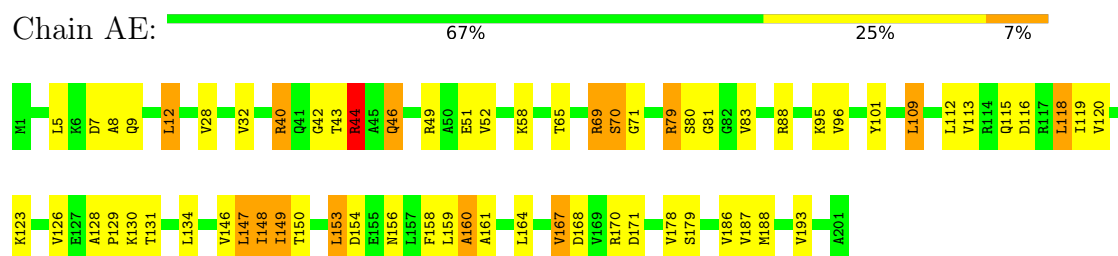
Chain ED: 62% 28% 10%



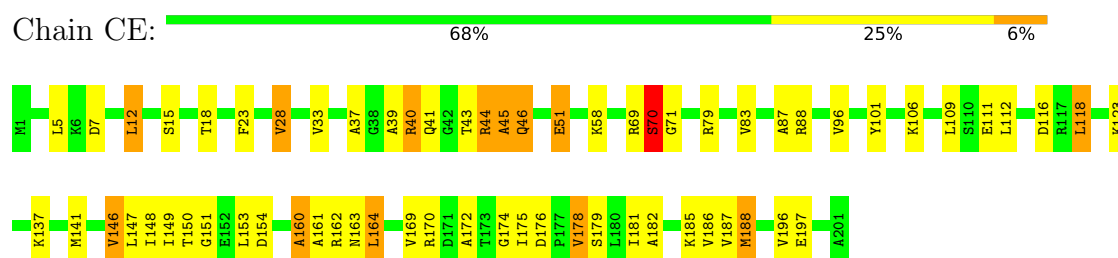
• Molecule 4: 50S ribosomal protein L3



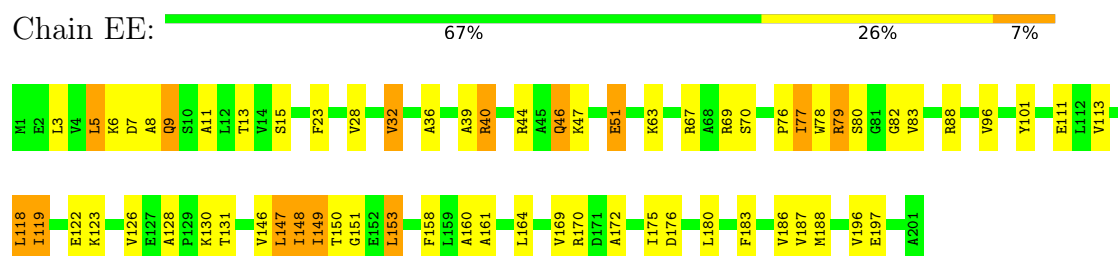
• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L4



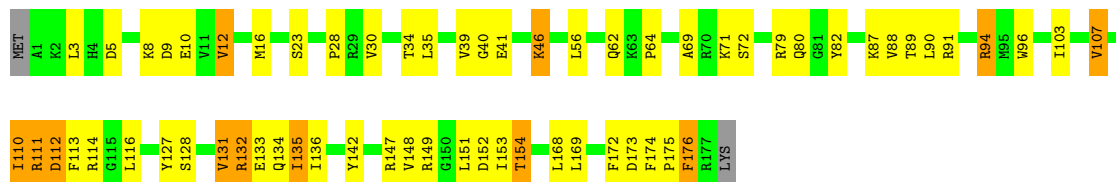
- Molecule 5: 50S ribosomal protein L4

Chain GE:  52% 42% 5% .



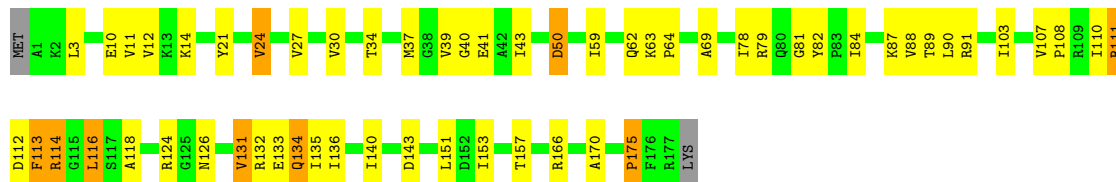
- Molecule 6: 50S ribosomal protein L5

Chain AF:  64% 28% 7% .



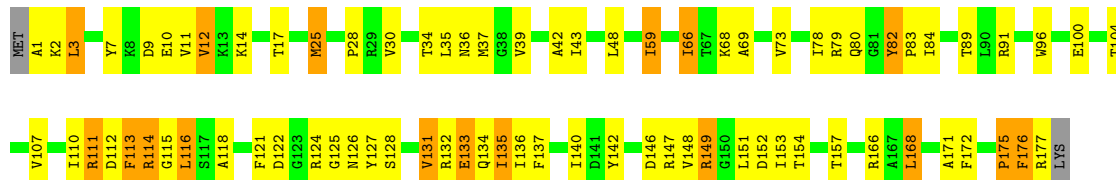
- Molecule 6: 50S ribosomal protein L5

Chain CF:  67% 27% 5% .



- Molecule 6: 50S ribosomal protein L5

Chain EF:  55% 34% 9% .



- Molecule 6: 50S ribosomal protein L5

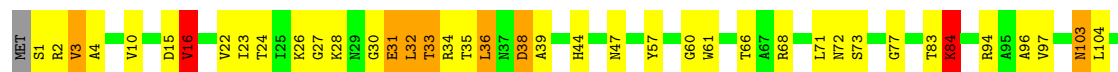
Chain GF:  54% 40% 6% .





• Molecule 7: 50S ribosomal protein L6

Chain AG: 63% 27% 8% ..



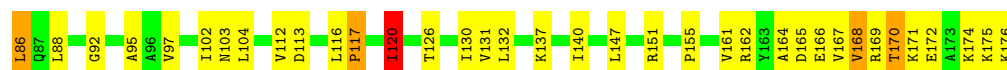
• Molecule 7: 50S ribosomal protein L6

Chain CG: 60% 31% 8% ..



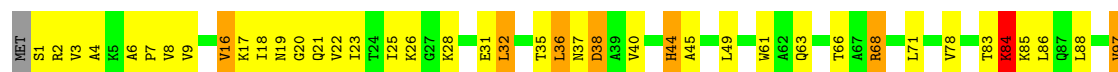
• Molecule 7: 50S ribosomal protein L6

Chain EG: 58% 34% 6% ..



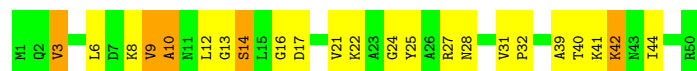
• Molecule 7: 50S ribosomal protein L6

Chain GG: 59% 34% 6% ..



• Molecule 8: 50S ribosomal protein L9

Chain AH: 54% 36% 10%



- Molecule 8: 50S ribosomal protein L9

Chain CH: 



- Molecule 8: 50S ribosomal protein L9

Chain EH: 



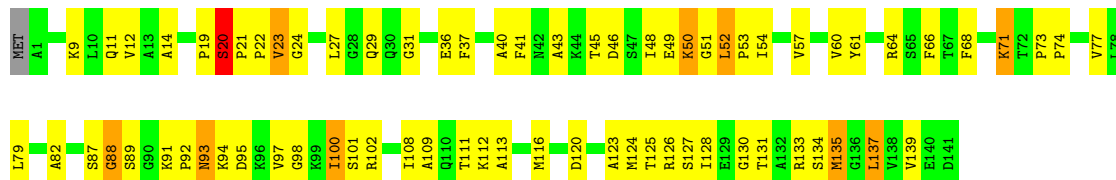
- Molecule 8: 50S ribosomal protein L9

Chain GH: 



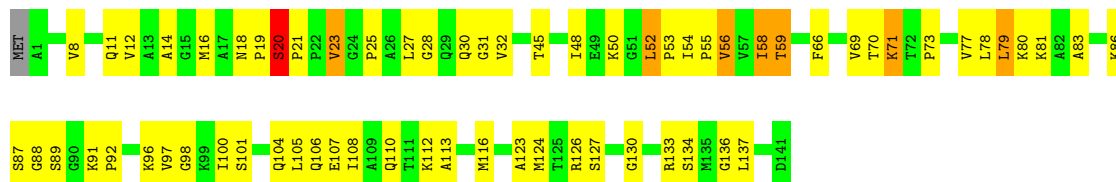
- Molecule 9: 50S ribosomal protein L11

Chain AI: 



- Molecule 9: 50S ribosomal protein L11

Chain CI: 



- Molecule 9: 50S ribosomal protein L11

Chain EI: 





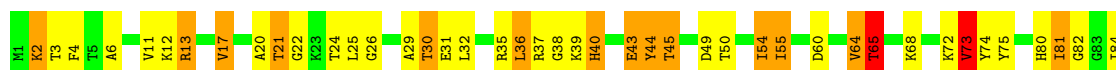
- Molecule 9: 50S ribosomal protein L11

Chain GI: 51% 39% 10% .



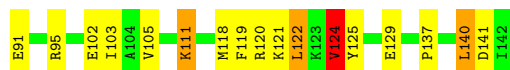
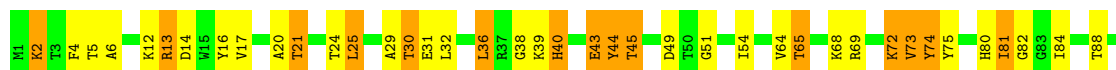
- Molecule 10: 50S ribosomal protein L13

Chain AJ: 55% 32% 11% .



- Molecule 10: 50S ribosomal protein L13

Chain CJ: 60% 27% 13% .



- Molecule 10: 50S ribosomal protein L13

Chain EJ: 56% 30% 12% .



- Molecule 10: 50S ribosomal protein L13

Chain GJ: 54% 33% 13% .

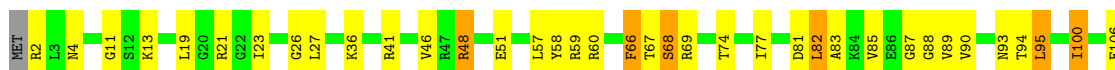






- Molecule 12: 50S ribosomal protein L15

Chain CL: 65% 29% 5% .



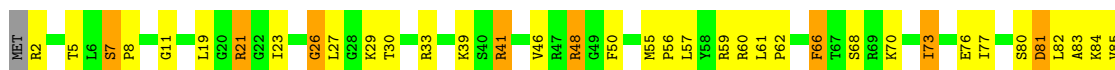
- Molecule 12: 50S ribosomal protein L15

Chain EL: 62% 31% 6% ..



- Molecule 12: 50S ribosomal protein L15

Chain GL: 59% 32% 8% .



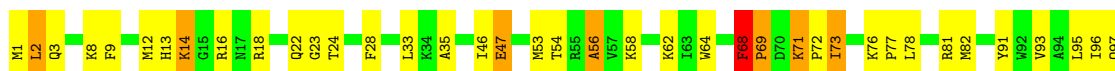
- Molecule 13: 50S ribosomal protein L16

Chain AM: 62% 29% 9% .



- Molecule 13: 50S ribosomal protein L16

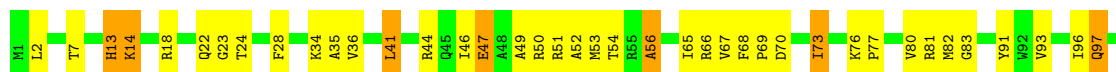
Chain CM: 62% 29% 8% .





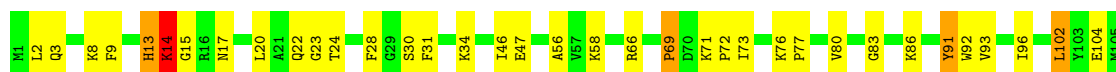
- Molecule 13: 50S ribosomal protein L16

Chain EM: 60% 34% 7%



- Molecule 13: 50S ribosomal protein L16

Chain GM: 68% 26% 6%



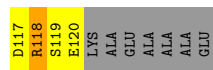
- Molecule 14: 50S ribosomal protein L17

Chain AN: 61% 28% 5% 6%



- Molecule 14: 50S ribosomal protein L17

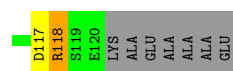
Chain CN: 65% 26% 6%



- Molecule 14: 50S ribosomal protein L17

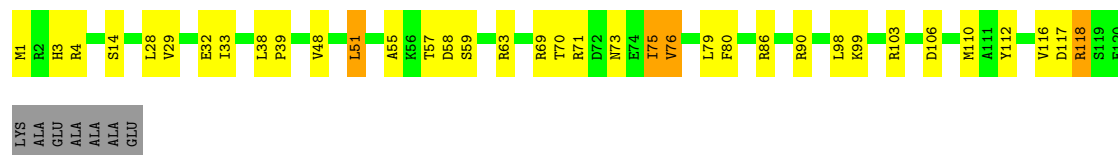
Chain EN: 66% 26% 6%





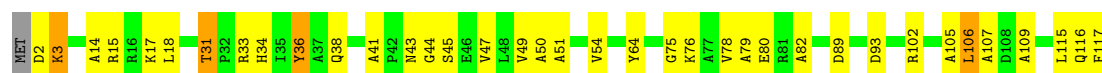
- Molecule 14: 50S ribosomal protein L17

Chain GN: 66% 25% 6%



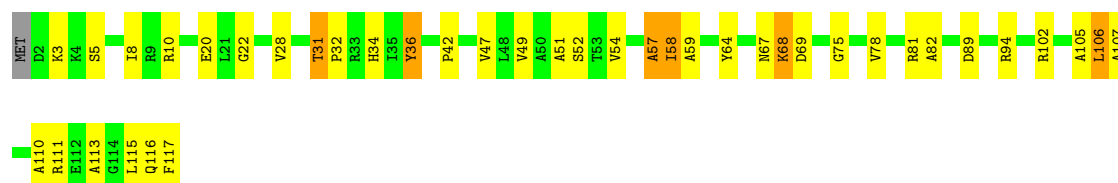
- Molecule 15: 50S ribosomal protein L18

Chain AO: 68% 28% 2%



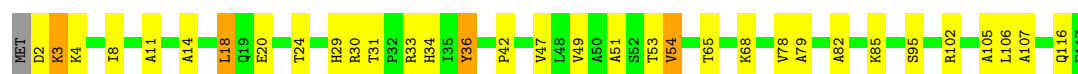
- Molecule 15: 50S ribosomal protein L18

Chain CO: 65% 29% 5%



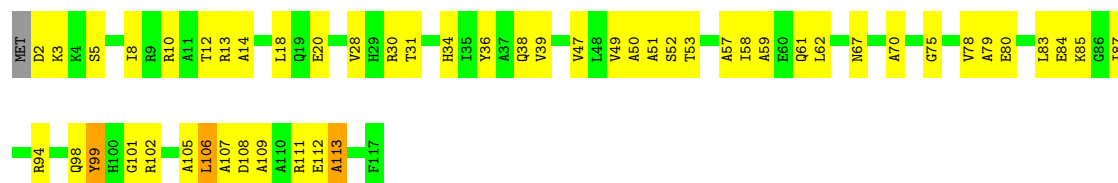
- Molecule 15: 50S ribosomal protein L18

Chain EO: 71% 25% 2%



- Molecule 15: 50S ribosomal protein L18

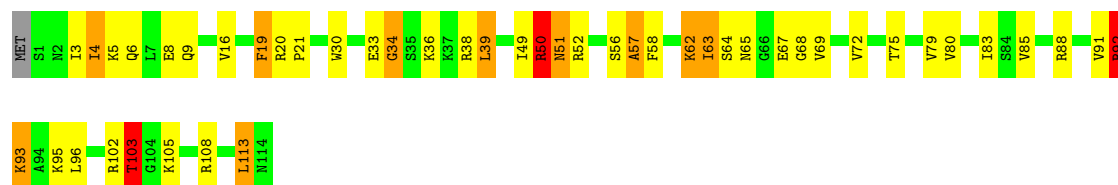
Chain GO: 56% 41% 2%



- Molecule 16: 50S ribosomal protein L19

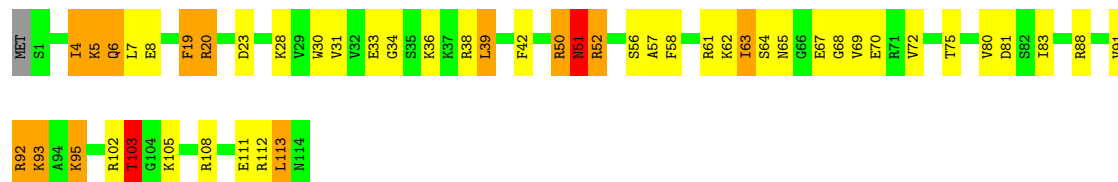
Chain AP: 58% 30% 9%





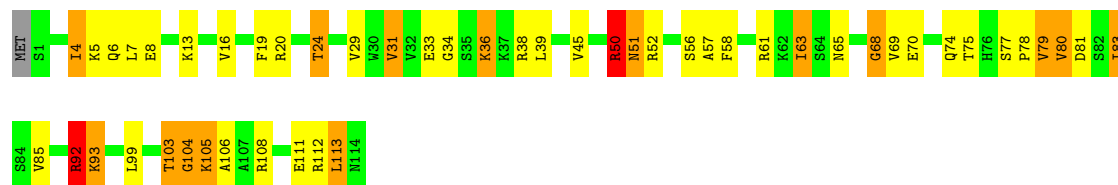
- Molecule 16: 50S ribosomal protein L19

Chain CP: 57% 30% 11% ..



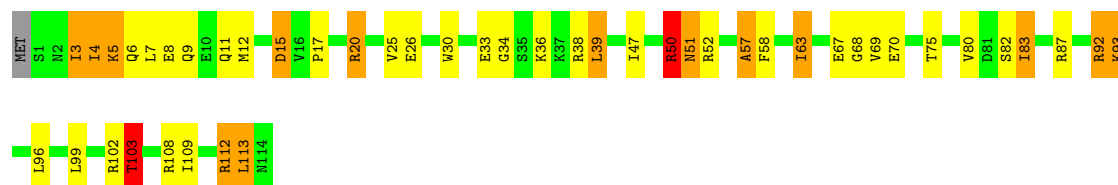
- Molecule 16: 50S ribosomal protein L19

Chain EP: 56% 29% 13% ..



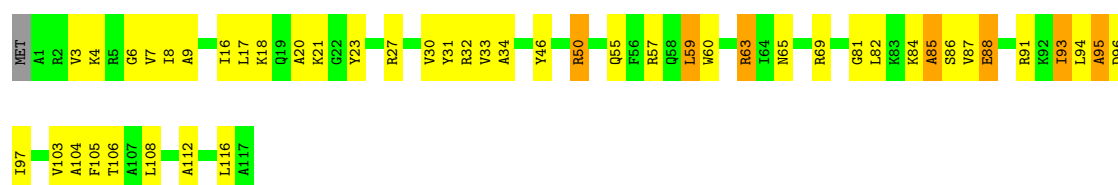
- Molecule 16: 50S ribosomal protein L19

Chain GP: 59% 26% 12% ..



- Molecule 17: 50S ribosomal protein L20

Chain AQ: 59% 34% 6% .

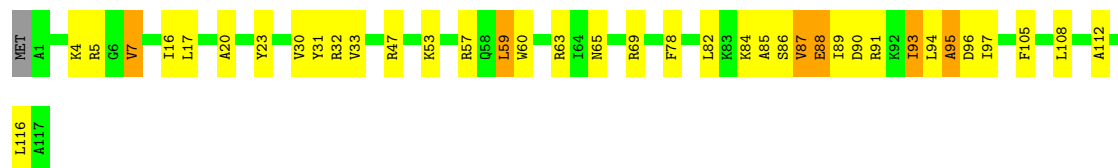


- Molecule 17: 50S ribosomal protein L20

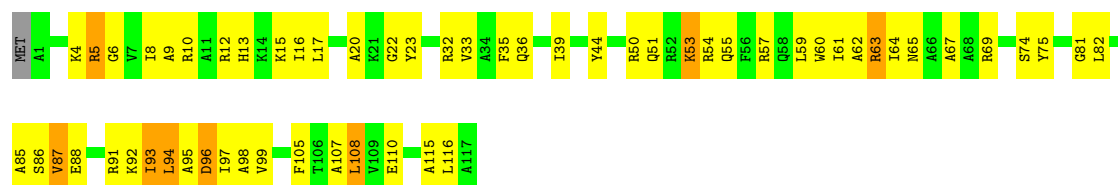
Chain CQ: 70% 23% 6% .



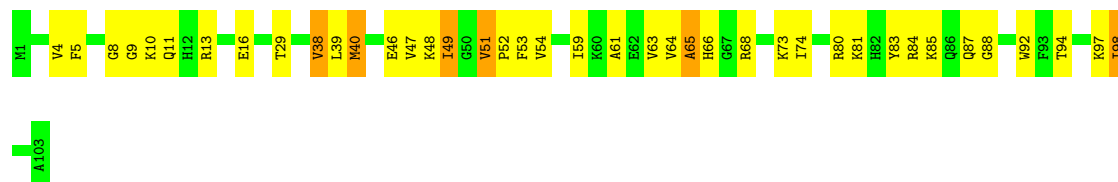
- Molecule 17: 50S ribosomal protein L20



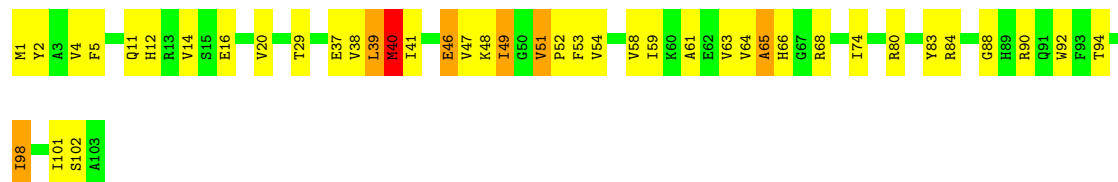
- Molecule 17: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L21



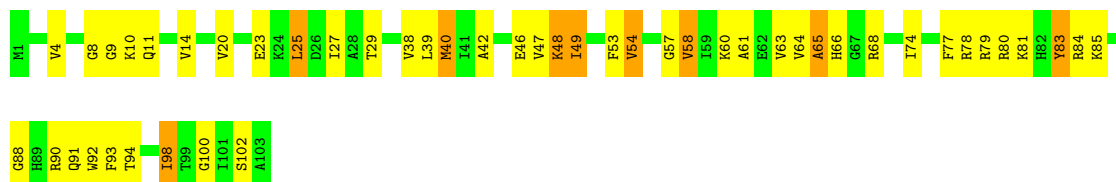
- Molecule 18: 50S ribosomal protein L21





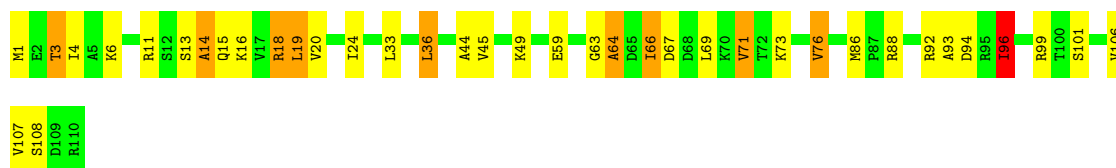
- Molecule 18: 50S ribosomal protein L21

Chain GR: 53% 38% 9%



- Molecule 19: 50S ribosomal protein L22

Chain AS: 65% 25% 8%



- Molecule 19: 50S ribosomal protein L22

Chain CS: 68% 25% 6%



- Molecule 19: 50S ribosomal protein L22

Chain ES: 69% 23% 7%



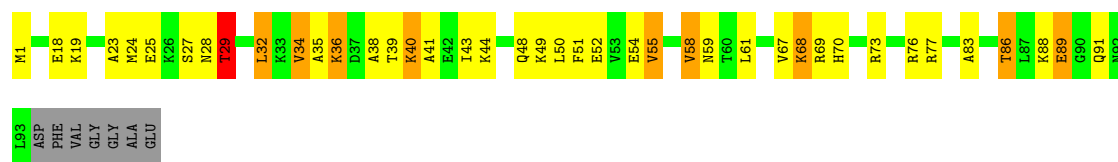
- Molecule 19: 50S ribosomal protein L22

Chain GS: 63% 32% 5%



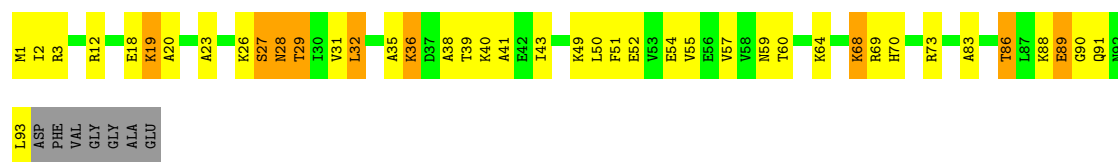
- Molecule 20: 50S ribosomal protein L23

Chain AT:  52% 31% 9% 7%

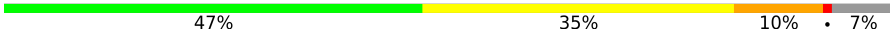


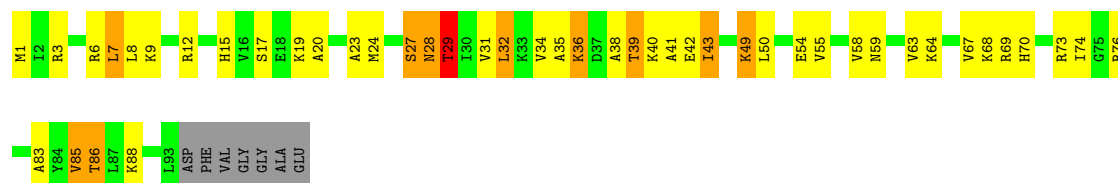
- Molecule 20: 50S ribosomal protein L23

Chain CT:  51% 33% 9% 7%



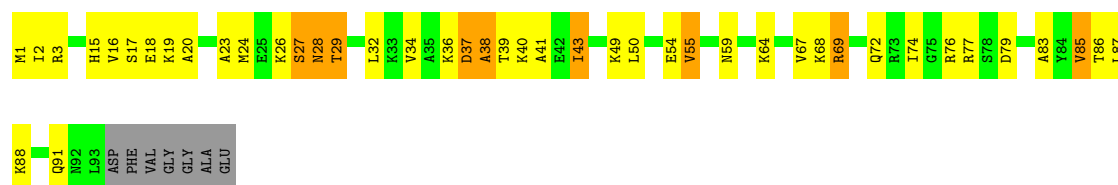
- Molecule 20: 50S ribosomal protein L23

Chain ET:  47% 35% 10% 7%



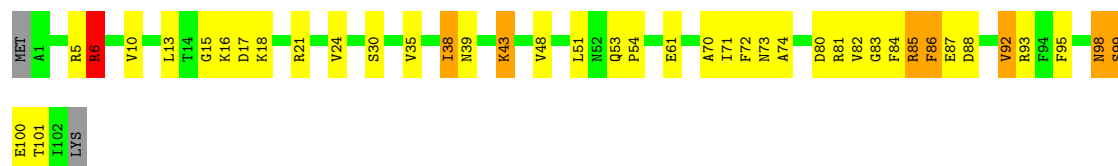
- Molecule 20: 50S ribosomal protein L23

Chain GT:  49% 35% 9% 7%



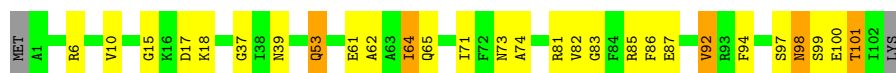
- Molecule 21: 50S ribosomal protein L24

Chain AU:  59% 32% 7% 2%

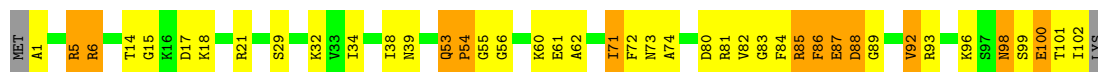


- Molecule 21: 50S ribosomal protein L24

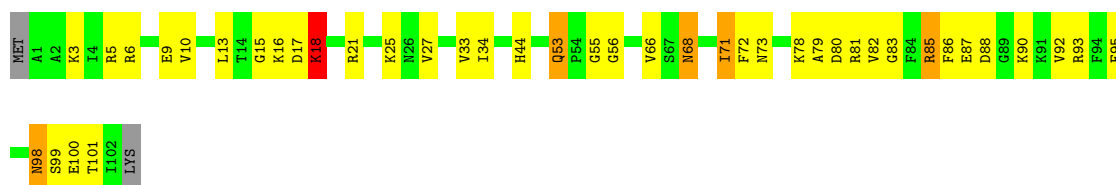
Chain CU:  71% 22% 5% 2%



- Molecule 21: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L24



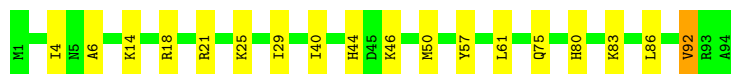
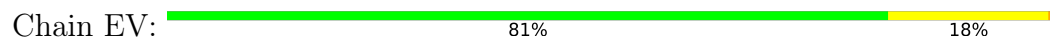
- Molecule 22: 50S ribosomal protein L25



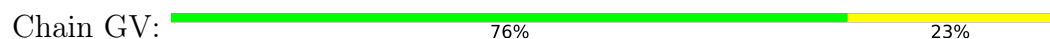
- Molecule 22: 50S ribosomal protein L25



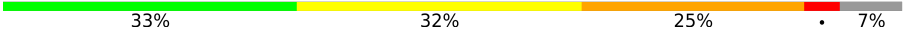
- Molecule 22: 50S ribosomal protein L25

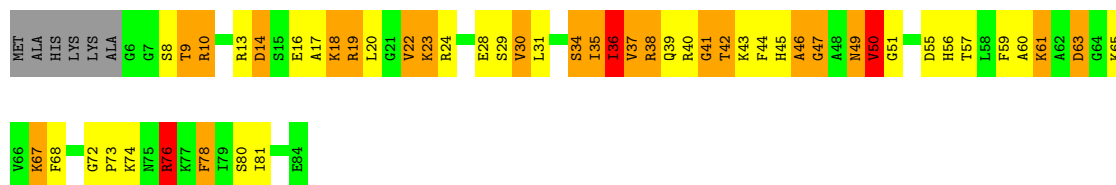


- Molecule 22: 50S ribosomal protein L25

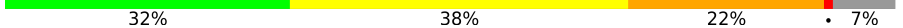


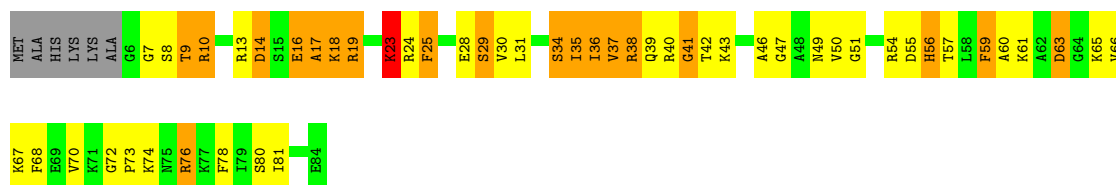
- Molecule 23: 50S ribosomal protein L27

Chain AW: 

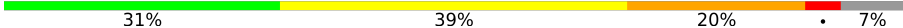


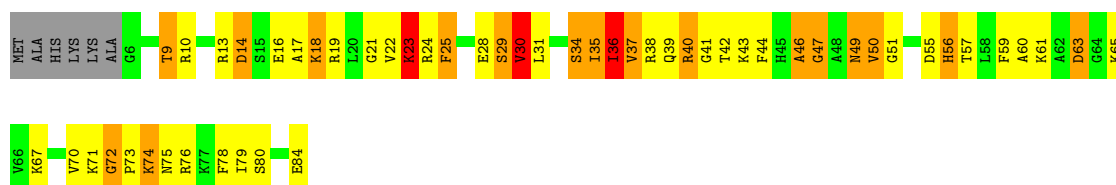
- Molecule 23: 50S ribosomal protein L27

Chain CW: 



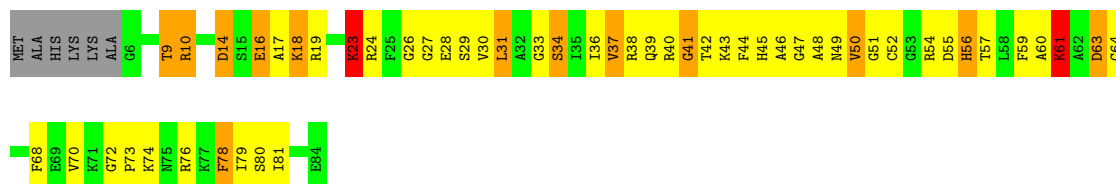
- Molecule 23: 50S ribosomal protein L27

Chain EW: 



- Molecule 23: 50S ribosomal protein L27

Chain GW: 



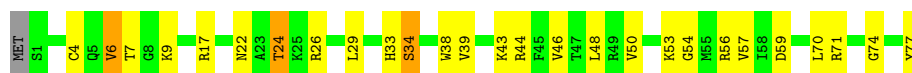
- Molecule 24: 50S ribosomal protein L28

Chain AX: 



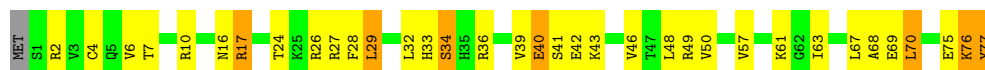
- Molecule 24: 50S ribosomal protein L28

Chain CX: 



- Molecule 24: 50S ribosomal protein L28

Chain EX: 54% 36% 9% .



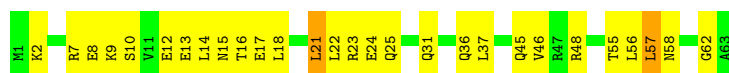
- Molecule 24: 50S ribosomal protein L28

Chain GX: 56% 37% 5% .



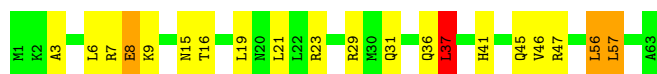
- Molecule 25: 50S ribosomal protein L29

Chain AY: 56% 41% 3% .



- Molecule 25: 50S ribosomal protein L29

Chain CY: 68% 25% 5% .



- Molecule 25: 50S ribosomal protein L29

Chain EY: 59% 29% 13% .



- Molecule 25: 50S ribosomal protein L29

Chain GY: 65% 29% 5% .



- Molecule 26: 50S ribosomal protein L30

Chain AZ: 49% 39% 10% .



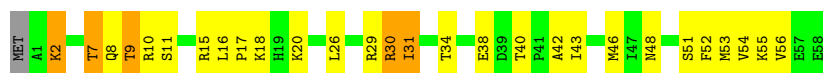
- Molecule 26: 50S ribosomal protein L30



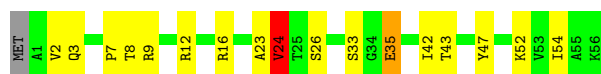
- Molecule 26: 50S ribosomal protein L30



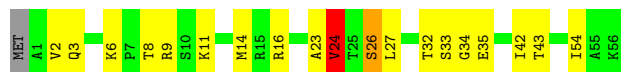
- Molecule 26: 50S ribosomal protein L30



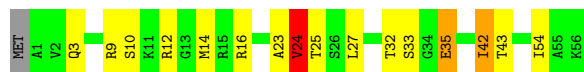
- Molecule 27: 50S ribosomal protein L32



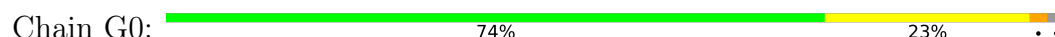
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

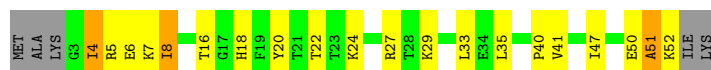


- Molecule 27: 50S ribosomal protein L32





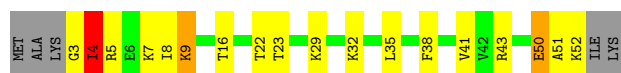
- Molecule 28: 50S ribosomal protein L33



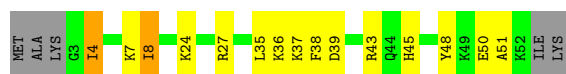
- Molecule 28: 50S ribosomal protein L33



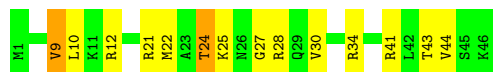
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



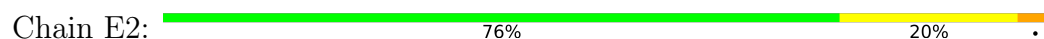
- Molecule 29: 50S ribosomal protein L34

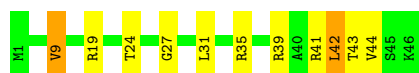


- Molecule 29: 50S ribosomal protein L34

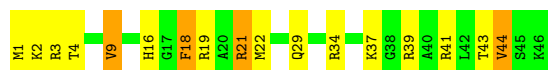


- Molecule 29: 50S ribosomal protein L34

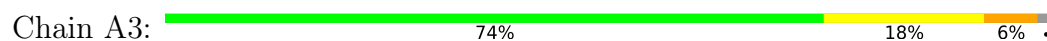




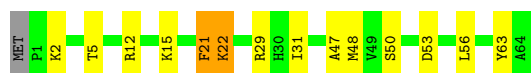
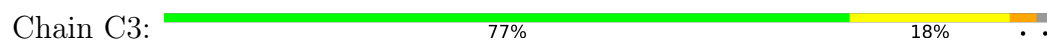
- Molecule 29: 50S ribosomal protein L34



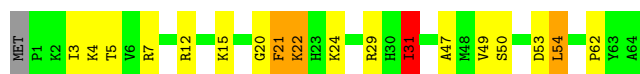
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

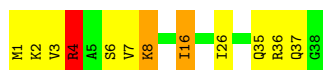


- Molecule 31: 50S ribosomal protein L36

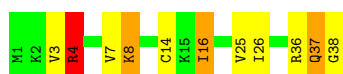




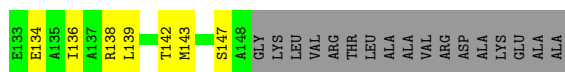
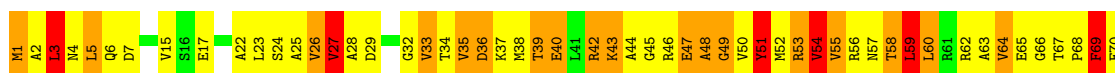
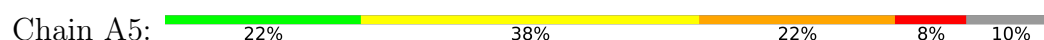
- Molecule 31: 50S ribosomal protein L36



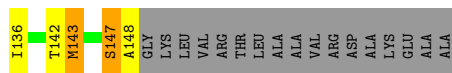
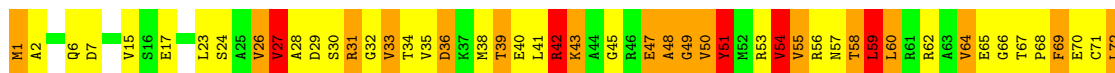
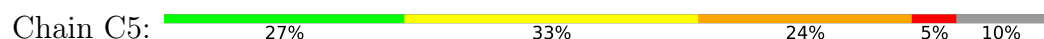
- Molecule 31: 50S ribosomal protein L36



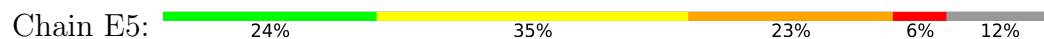
- Molecule 32: 50S ribosomal protein L10

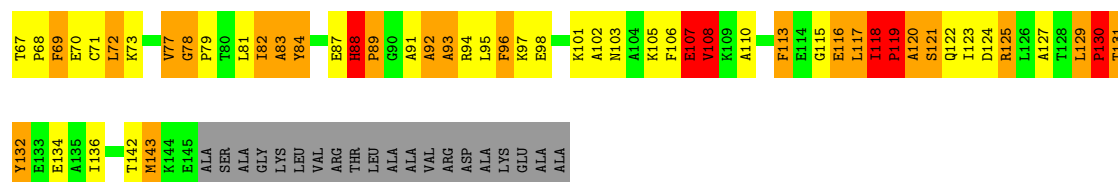


- Molecule 32: 50S ribosomal protein L10



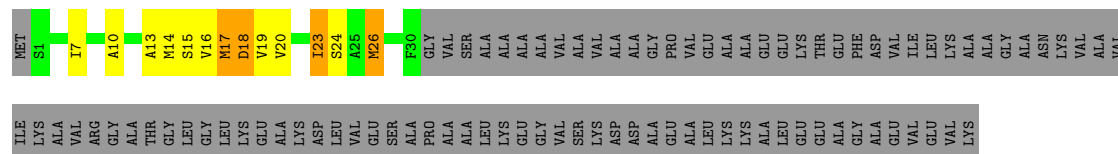
- Molecule 32: 50S ribosomal protein L10





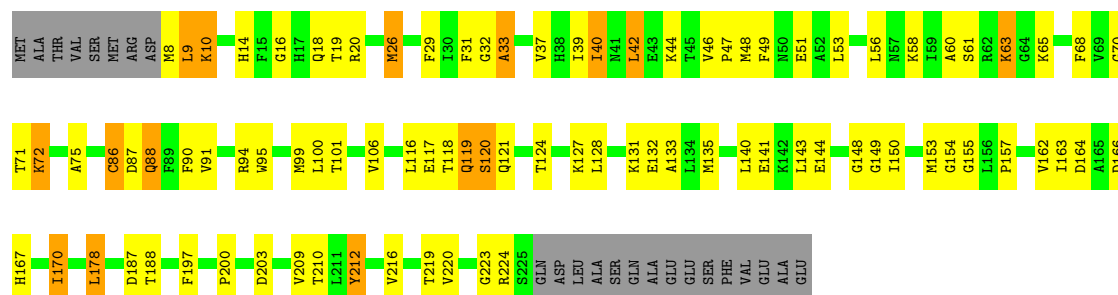
- Molecule 33: 50S ribosomal protein L7/L12

Chain A6: 14% 7% . 75%



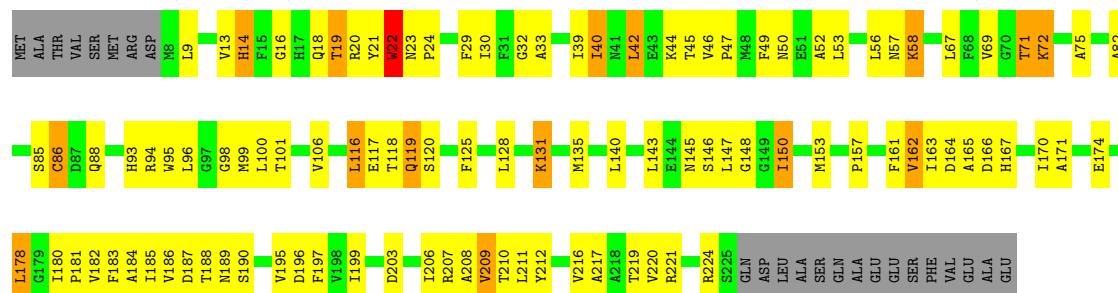
- Molecule 34: 30S ribosomal protein S2

Chain BB: 53% 31% 6% 10%



- Molecule 34: 30S ribosomal protein S2

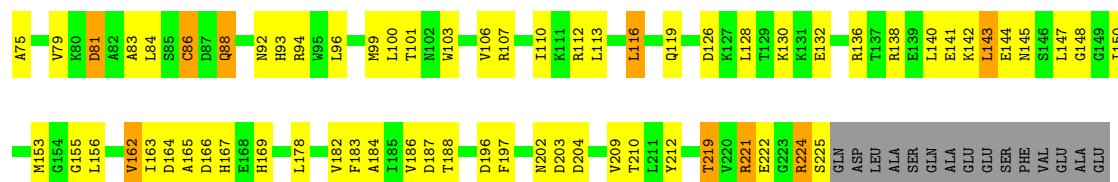
Chain DB: 47% 37% 6% 10%



- Molecule 34: 30S ribosomal protein S2

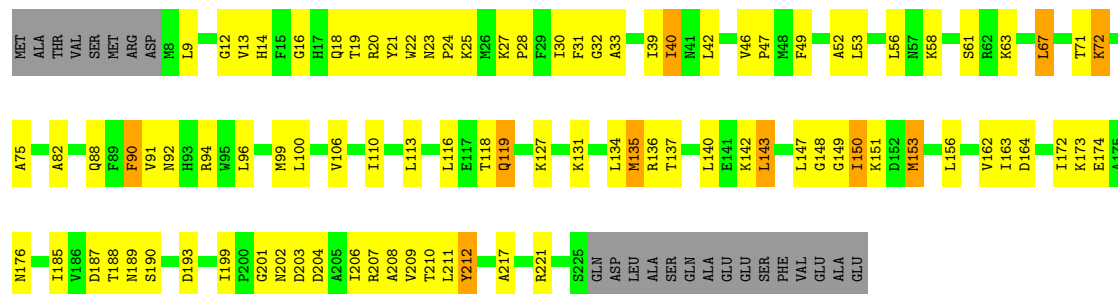
Chain FB: 48% 36% 6% 10%





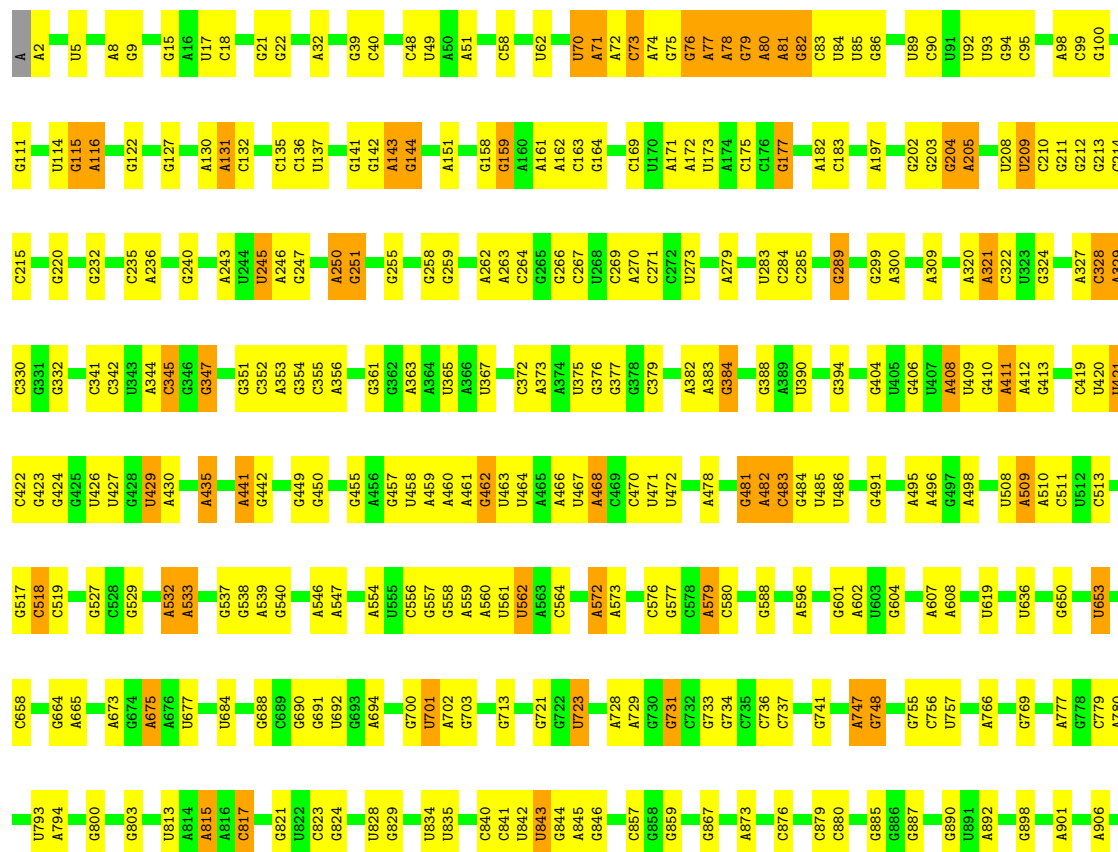
• Molecule 34: 30S ribosomal protein S2

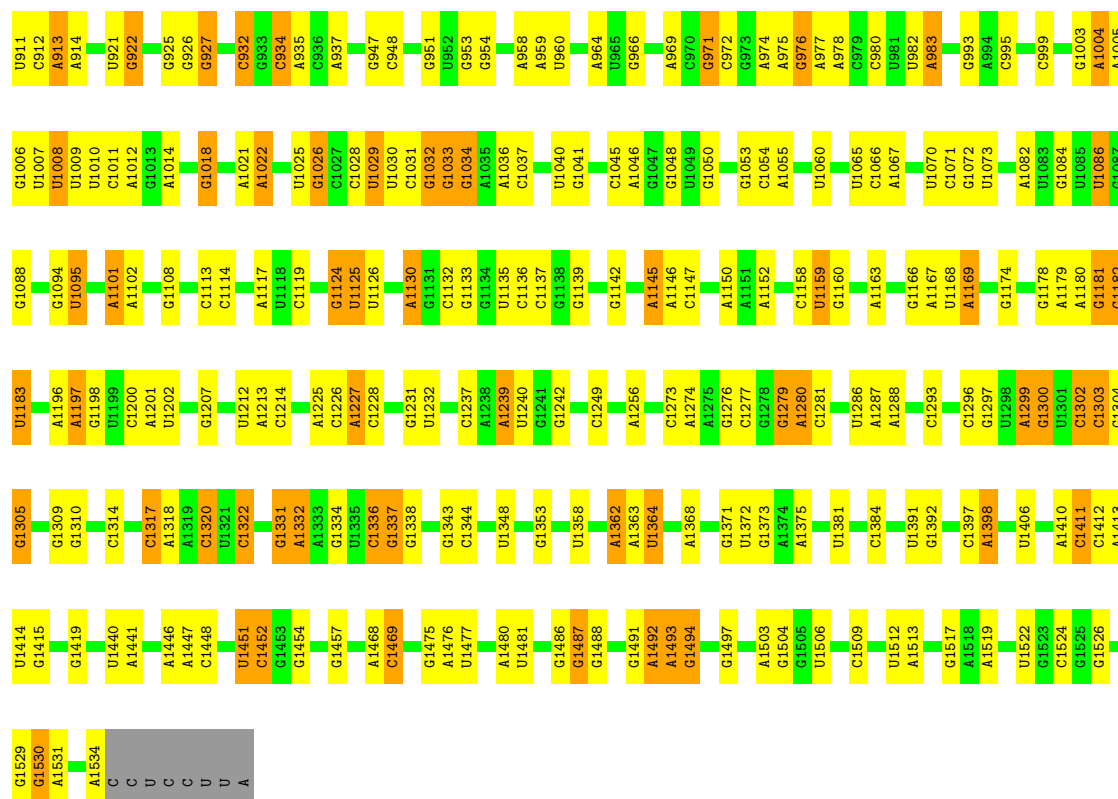
Chain HB: 52% 34% 10%



• Molecule 35: 16S rRNA

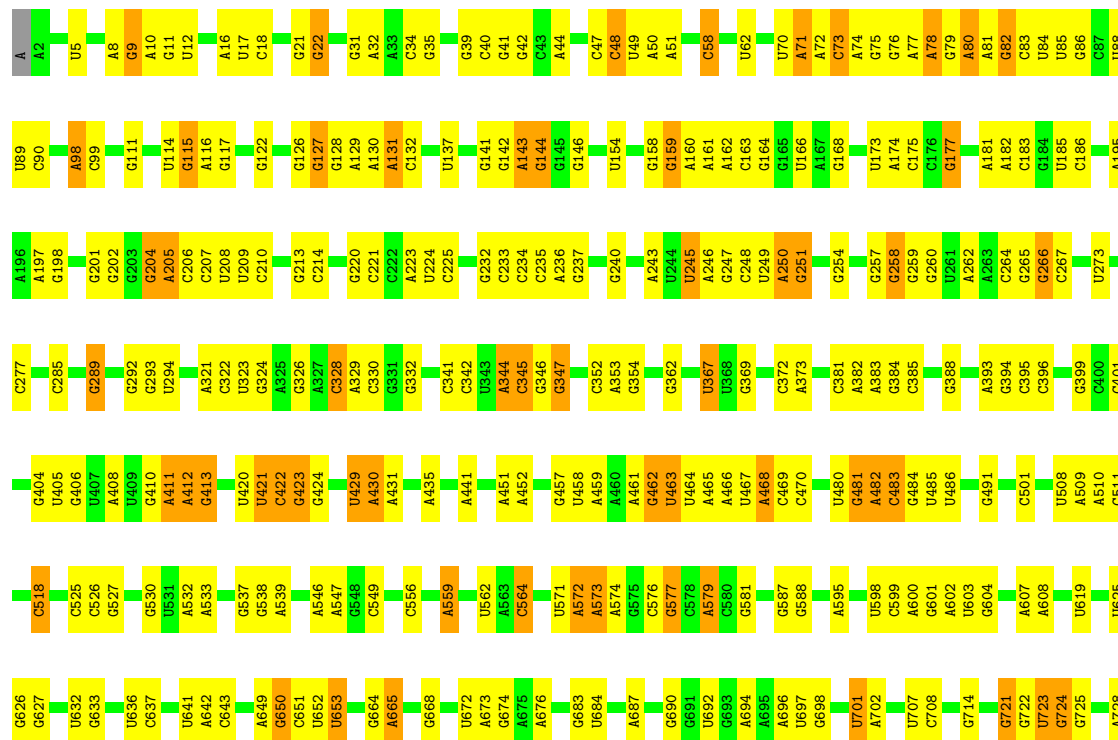
Chain BA: 63% 29% 8%





• Molecule 35: 16S rRNA

Chain DA: 53% 38% 8% .

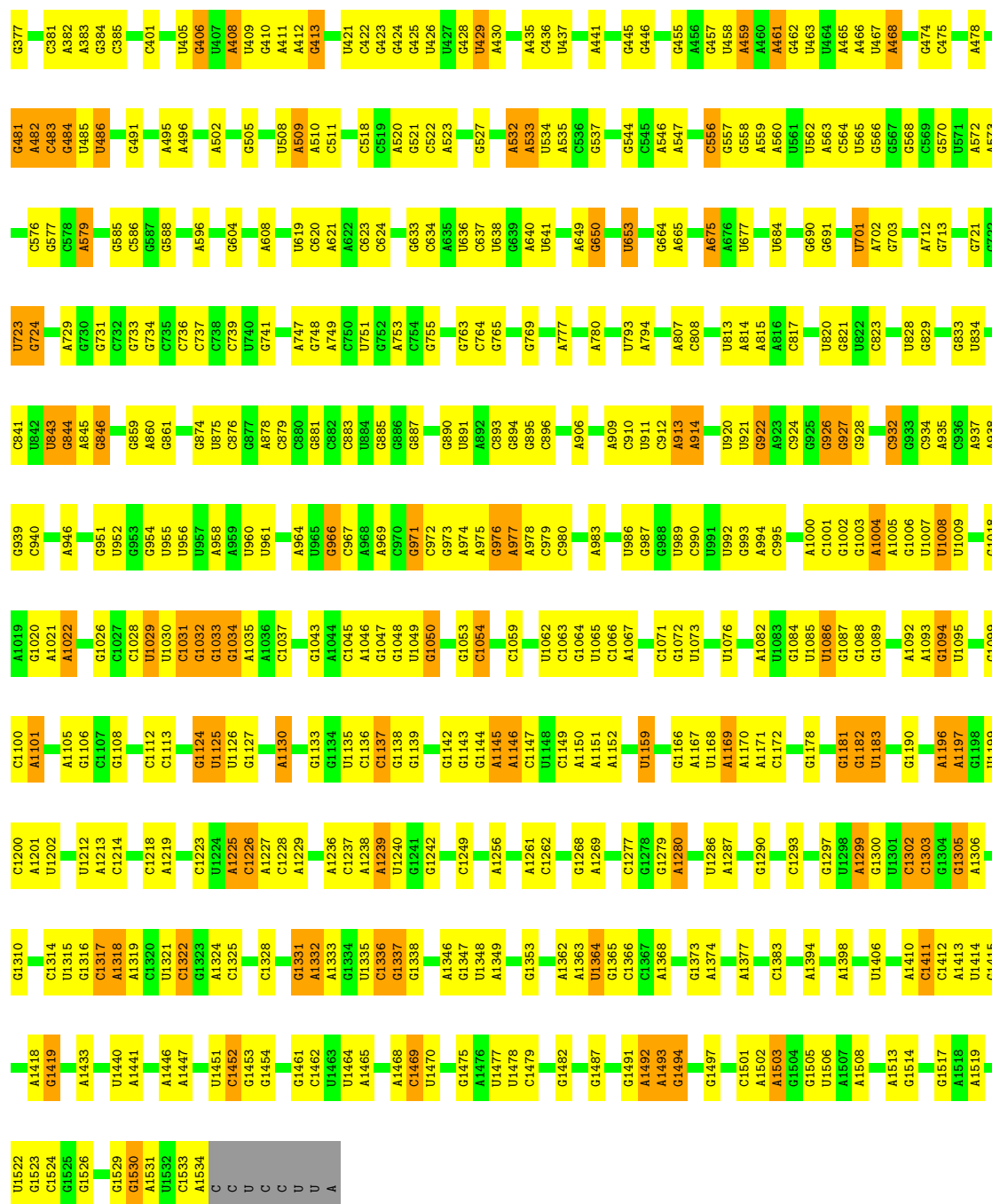


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G1491	C1383	G1312	G1241	C1147	U1072	A815	A906	G730
A1492	G1387	U1315	G1242	C1149	U1073	A816	G991	G731
A1493	C1388	G1316	G1243	C1149	G1074	C817	U992	G732
G1494	C1388	C1317	G1244	A1157	U1075	G821	C910	G733
G1497	U1391	A1318	C1245	C1158	U1076	G821	U911	G734
U1498	U1392	A1319	C1249	U1159	G1077	G735	C912	C735
A1499	U1393	C1320	G1250	C1161	A1080	G824	A913	C736
A1500	A1394	C1322	A1251	C1162	U1083	A825	A914	C737
C1501	C1395	G1323	A1254	A1163	G1084	C826	A918	C738
A1502	A1396	A1324	G1255	G1166	U1085	U827	A919	C739
A1503	C1397	C1325	A1256	A1167	U1086	U828	U920	U740
G1504	A1398	G1257	A1257	U1167	U1087	G829	U1007	G741
U1505	C1328	U1330	G1258	U1168	G1088	G833	G922	G745
U1506	G1401	A1329	C1259	A1169	U1089	U834	G926	A746
A1507	C1402	U1336	G1260	U1173	U1090	U835	G927	A747
C1508	U1406	A1331	G1266	G1174	U1091	G836	G928	G748
C1509	U1406	A1332	G1266	G1174	A1092	C841	G928	C750
C1510	U1406	A1333	G1266	G1175	A1093	G842	C932	U751
C1511	C1411	G1334	A1269	A1176	G1094	U843	G933	G752
U1512	C1412	U1335	G1270	G1177	U1095	G844	C934	A753
A1513	A1413	C1336	A1271	G1178	C1096	A845	A935	G754
G1517	G1416	G1337	G1272	A1179	C1097	G846	C936	C755
A1518	G1416	G1338	A1275	A1180	G1101	U855	A937	U757
A1519	G1417	A1339	A1275	U1181	A1102	G856	A938	G760
U1522	G1419	A1340	G1276	G1182	C1103	C857	G939	C764
G1523	C1439	U1341	C1277	U1183	G1104	G858	G945	C765
C1524	U1440	G1343	G1278	G1186	G1108	G859	A946	G769
G1525	A1441	A1346	A1280	C1192	C1109	G861	C947	C770
G1526	U1444	A1350	U1283	C1192	A1110	C862	G951	G776
C1529	U1444	A1351	C1284	A1196	U1118	C866	U952	A777
G1530	U1445	C1352	A1285	A1197	C1119	G867	G953	G778
A1531	A1446	G1353	U1286	G1198	G1120	C868	U957	C779
U1532	A1447	C1354	A1287	U1199	U1121	G869	A958	A780
C1533	C1448	U1354	A1288	C1200	U1121	U870	A959	C781
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U	U1464	A1362	G1297	A1216	U1049	G877	C970	U789
U	A1465	A1363	U1298	C1217	G1050	C878	C971	C791
A	A1468	U1364	A1299	C1218	G1133	C880	C972	A792
	C1469	G1365	G1300	A1219	U1135	C881	G973	U793
		C1366	U1301	C1136	C1053	C882	A974	A794
		C1367	C1302	G1137	G1054	C883	G975	A802
		A1368	G1303	C1225	C1055	C884	A976	C793
		C1369	G1304	C1226	G1138	C885	G977	A794
		G1370	G1305	A1227	G1139	C886	A978	A802
		G1371	A1306	C1228	C1140	C887	C979	C794
		U1372	U1307	C1237	G1141	C888	C980	C795
		G1373	U1308	C1237	G1142	C889	C981	C796
		A1374	U1309	C1238	G1143	C890	U982	C797
		A1375	G1310	A1239	G1144	C891	A983	C798
		G1376	G1311	C1240	A1145	C892	U984	C799
		C1377	G1312	C1241	C1146	C893	U985	C800
		U1378	G1313	C1242	C1147	C894	U986	C801
		C1379	G1314	C1243	C1148	C895	U987	C802
		A1380	G1315	C1244	C1149	C896	U988	C803
		G1381	G1316	C1245	C1150	C897	U989	C804
		U1382	G1317	C1246	C1151	C898	U990	C805
		C1383	G1318	C1247	C1152	C899	U991	C806
		A1384	G1319	C1248	C1153	C900	U992	C807
		U1385	G1320	C1249	C1154	C901	U993	C808
		C1386	G1321	C1250	C1155	C902	U994	C809
		G1387	G1322	C1251	C1156	C903	U995	C810
		A1388	G1323	C1252	C1157	C904	U996	C811
		U1389	G1324	C1253	C1158	C905	U997	C812
		C1390	G1325	C1254	C1159	C906	U998	C813
		A1391	G1326	C1255	C1160	C907	U999	C814
		U1392	G1327	C1256	C1161	C908	U1000	C815
		C1393	G1328	C1257	C1162	C909	U1001	C816
		A1394	G1329	C1258	C1163	C910	U1002	C817
		U1395	G1330	C1259	C1164	C911	U1003	C818
		C1396	G1331	C1260	C1165	C912	U1004	C819
		A1397	G1332	C1261	C1166	C913	U1005	C820
		U1398	G1333	C1262	C1167	C914	U1006	C821
		C1399	G1334	C1263	C1168	C915	U1007	C822
		A1400	G1335	C1264	C1169	C916	U1008	C823
		U1401	G1336	C1265	C1170	C917	U1009	C824
		C1402	G1337	C1266	C1171	C918	U1010	C825
		A1403	G1338	C1267	C1172	C919	U1011	C826
		U1404	G1339	C1268	C1173	C920	U1012	C827
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		A1406	G1341	C1270	C1175	C922	U1014	C829
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		C1408	G1343	C1272	C1177	C924	U1016	C831
		A1409	G1344	C1273	C1178	C925	U1017	C832
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		A1418	G1353	C1282	C1187	C934	U1026	C841
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		U1422	G1357	C1286	C1191	C938	U1030	C845
		C1423	G1358	C1287	C1192	C939	U1031	C846
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		U1425	G1360	C1289	C1194	C941	U1033	C848
		C1426	G1361	C1290	C1195	C942	U1034	C849
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		A1436	G1371	C1300	C1205	C952	U1044	C859
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		C1441	G1376	C1305	C1210	C957	U1049	C864
		A1442	G1377	C1306	C1211	C958	U1050	C865
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		A1450	G1386	C1315	C1220	C967	U1059	C874
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		U1460	G1396	C1325	C1230	C977	U1069	C884
		C1461	G1397	C1326	C1231	C978	U1070	C885
		A1462	G1398	C1327	C1232	C979	U1071	C886
		U1463	G1399	C1328	C1233	C980	U1072	C887
		C1464	G1400	C1329	C1234	C981	U1073	C888
		A1465	G1401	C1330	C1235	C982	U1074	C889
		U1466	G1402	C1331	C1236	C983	U1075	C890
		C1467	G1403	C1332	C1237	C984	U1076	C891
		A1468	G1404	C1333	C1238	C985	U1077	C892
		U1469	G1405	C1334	C1239	C986	U1078	C893
		C1470	G1406	C1335	C1240	C987	U1079	C894
		A1471	G1407	C1336	C1241	C988	U1080	C895
		U1472	G1408	C1337	C1242	C989	U1081	C896
		C1473	G1409	C1338	C1243	C990	U1082	C897
		A1474	G1410	C1339	C1244	C991	U1083	C898
		U1475	G1411	C1340	C1245	C992	U1084	C899
		C1476	G1412	C1341	C1246	C993	U1085	C900
		A1477	G1413	C1342	C1247	C994	U1086	C901
		U1478	G1414	C1343	C1248	C995	U1087	C902
		C1479	G1415	C1344	C1249	C996	U1088	C903
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		U1481	G1417	C1346	C1251	C998		

• Molecule 35: 16S rRNA

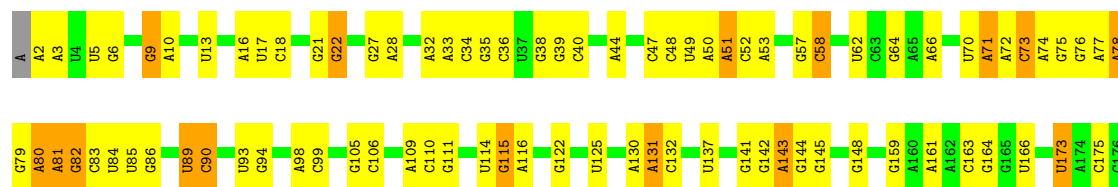
Chain FA:  58% 34% 7%

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A195	A196	G202	G203	G204	A205	C206	C207	U208	U209	C210	C211	G212	G213	C222	G227	G237	G240	A243	U244	U245	A246	G247	A250	G251	G254	G255	U256	G257	G258	G259	U261	A262	G265	G266	C267	U268	C269	A270	U273	A274	G275	G276	C277	C280	U281	A282		
U89	C90	U91	U92	U93	G94	A98	C99	G100	A109	C110	G111	U114	G115	A116	G122	U123	G127	G128	A129	A130	A131	C135	C136	U137	G138	G141	G142	A143	G144	G145	G146	G147	G158	A159	A160	A161	A162	C163	G164	U173	A174	C175	A176	G177	A182	C183	U188	A189
A	A2	U5	G6	A7	A8	G9	A16	U17	C18	G21	G22	A32	A33	C34	G35	G39	C40	G41	G42	C48	U49	A50	A51	C52	A53	G57	C58	G61	U62	A66	C67	U70	A71	A72	C73	A74	G75	G76	A77	A80	A81	G82	C83	U84	U85	G86	C87	U88

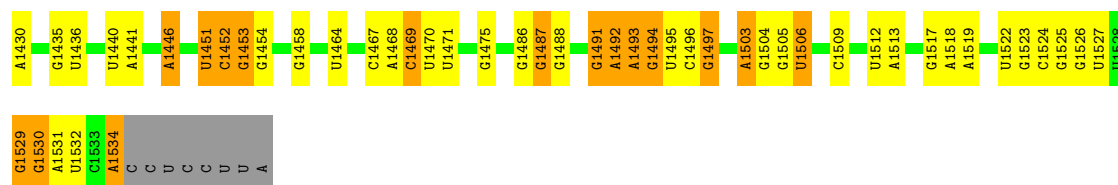


• Molecule 35: 16S rRNA

Chain HA: 48% 43% 8%

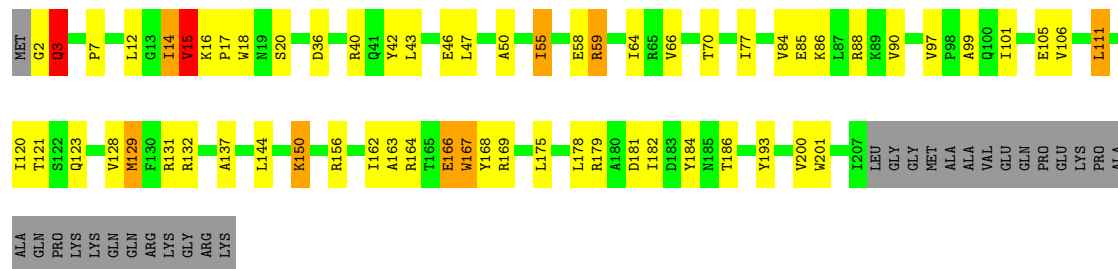


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G1347	A1280	G1133	U1056	U982	A913	G821	A747	G671	A563	G474	C387	C271	C178
A1348	C1281	G1134	G1057	A983	C984	U822	G748	U672	C564	U480	U399	U272	A179
U1349	C1282	U1135	G1058	C985	A915	C823	A749	A673	U565	U481	C392	U273	U180
A1350	U1283	C1136	C1059	C986	U916	U827	C750	G674	G566	U482	A397	C265	A181
U1351	C1284	U1214	U1060	U986	U917	U828	U751	A675	A481	A482	U398	G289	A182
C1352	A1285	G1138	G1061	C987	G917	U829	G752	A676	C483	C484	U399	G297	C183
G1353	U1286	C1139	U1062	G988	A918	U830	A753	U677	A572	U485	C400	G298	C188
U1354	C1287	G1140	C1063	G989	U919	U835	G754	U678	A573	U486	C401	G299	A189
G1355	A1288	C1141	U1064	C990	U921	U836	G755	C679	C576	U490	C402	A300	A196
U1358	G1292	G1143	C1066	C995	G922	U837	A759	G683	C577	G491	C403	G194	C194
C1359	A1290	G1144	A1067	C1001	G926	C838	G761	U684	A579	U498	C404	A301	A197
A1360	C1293	A1145	C1071	G1002	G927	C841	U762	G685	C580	C501	U405	G301	A195
G1361	U1295	C1147	G1072	G1003	G928	U842	G763	U686	G581	U502	C406	C316	A196
U1364	C1296	U1148	U1073	C929	G929	U843	C764	A687	C582	A501	U407	U317	G204
G1365	G1297	A1225	U1074	A1004	C930	C844	G765	G688	A583	C503	A408	G326	A205
C1366	A1298	C1150	G1074	A1005	C931	A845	A766	C689	G584	C504	U409	A321	C206
G1367	U1299	C1158	G1077	U1008	C932	C846	G769	G690	G587	G505	C410	G328	G207
C1369	C1302	U1159	U1078	C1011	G933	G851	G774	U692	G588	G506	A412	A327	U208
G1370	G1304	G1166	A1079	A1012	C934	C852	G775	G691	C589	C507	C413	U209	U209
A1306	G1305	A1167	G1084	G1013	A935	G858	G776	U697	A596	A508	A414	G327	G211
U1307	C1236	U1168	U1085	G1015	C936	C859	A777	C699	U597	A510	C415	A329	G212
C1308	C1237	A1169	U1086	A1016	G939	G860	G778	G700	U598	C511	C416	G213	G213
G1309	A1238	A1170	G1087	U1017	G940	A864	C779	U701	G604	C512	C419	U216	U216
U1310	C1239	C1171	U1088	A1018	G942	A865	A780	A702	C615	C513	U420	G332	C217
C1311	U1240	C1172	G1089	C1018	U943	C866	A781	G703	G615	G517	U421	A344	G220
U1314	C1243	G1177	G1094	A1021	G944	C867	A784	U707	U619	C518	C422	C345	U224
G1315	G1244	C1178	U1095	A1022	G945	C868	G785	G714	C620	G526	C423	G346	C225
C1316	C1245	A1179	C1096	G1023	A946	C869	C796	A715	A621	G527	G428	G347	U239
A1318	A1250	G1180	C1097	U1025	C948	A872	G791	A716	C622	G530	U429	C352	G232
U1319	C1251	G1181	C1098	G1026	U952	C874	A792	U717	C623	U531	A430	A353	G237
G1392	U1256	U1183	C1099	C1028	U958	G877	U793	C720	G626	A532	A435	G354	A238
C1397	A1257	G1187	A1101	U1029	A968	A878	C795	G721	G627	A533	U439	A356	G240
A1398	G1258	A1188	G1104	U1030	A969	C879	C796	U722	A640	U534	C440	G360	U245
G1401	C1259	U1189	A1105	C1031	U960	G885	U798	G723	U641	A535	A441	G361	G246
C1402	G1260	G1190	G1106	G1032	U961	C886	G799	G724	A642	C536	A451	G362	A247
A1403	U1261	A1191	C1107	G1033	C962	C887	G800	C726	C643	G537	A452	U367	A250
C1404	C1262	C1192	G1108	G1034	G963	G888	U801	G727	U644	A539	G457	C372	G254
G1405	G1263	G1193	C1109	A1035	A964	U901	A814	C741	G650	G540	U458	A373	G258
U1406	U1264	U1194	A1110	A1036	U965	G902	A815	G742	G651	U543	A459	A374	G259
C1411	C1265	C1195	C1113	C1037	G966	G903	A816	A743	U652	C545	A460	U375	G260
A1412	G1266	A1196	G1114	C1038	A969	C892	C808	C736	C653	U544	A461	C379	U261
U1413	C1267	U1197	U1115	G1039	C970	G895	C811	G733	U653	C546	A462	A381	A262
C1414	A1269	U1199	U1118	C1045	G971	C896	C812	G734	G654	A547	U463	C382	G380
G1415	G1270	C1200	C1119	A1046	C972	C897	U813	C735	A655	A547	U464	A383	A384
C1416	A1271	U1201	G1124	G1047	G973	G898	A814	C736	U656	U552	A465	C381	G381
G1417	G1272	U1202	U1125	A1048	A974	U901	A815	C741	C658	C556	A466	A382	G382
A1418	C1273	C1203	U1125	U1049	A975	G902	A816	G742	A663	G557	U467	A383	G383
G1419	A1274	A1204	G1050	C1061	G976	G903	A817	A743	A664	G558	A468	G384	G384
C1423	U1275	U1205	C1128	U1052	A977	U905	A818	G745	A665	A559	C469	C267	C267
U1424	G1276	G1206	C1129	A1053	A978	C979	C818	C744	A666	A559	C469	C267	C267
C1343	C1277	C1207	A1300	G1053	A979	U905	G819	G745	A666	A559	C469	C267	C267
U1345	G1278	C1208	G1131	C1054	C980	U905	A819	G745	A666	A559	C469	C267	C267



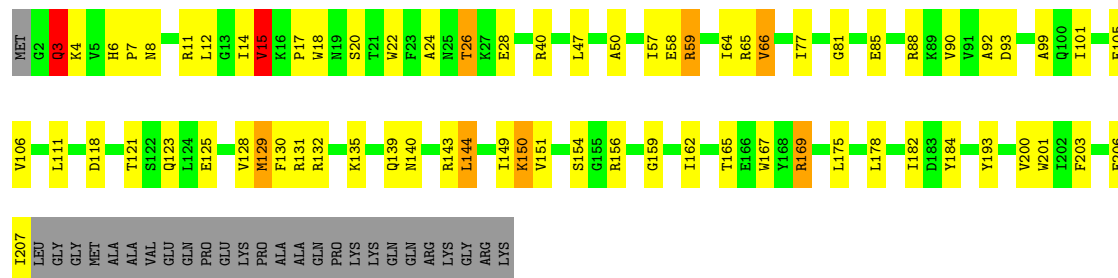
- Molecule 36: 30S ribosomal protein S3

Chain BC: 61% 23% 12%



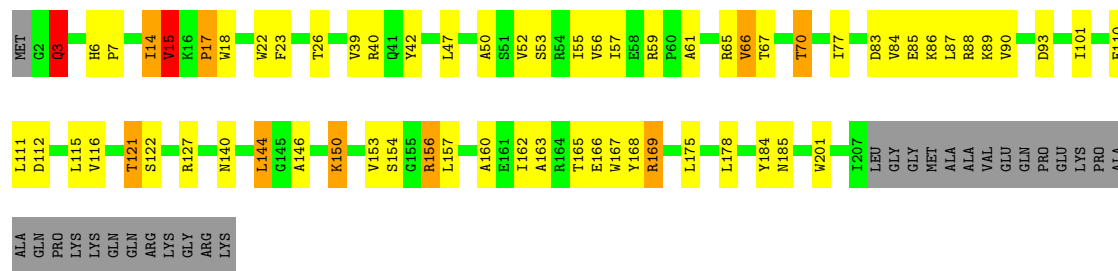
- Molecule 36: 30S ribosomal protein S3

Chain DC: 58% 27% 12%



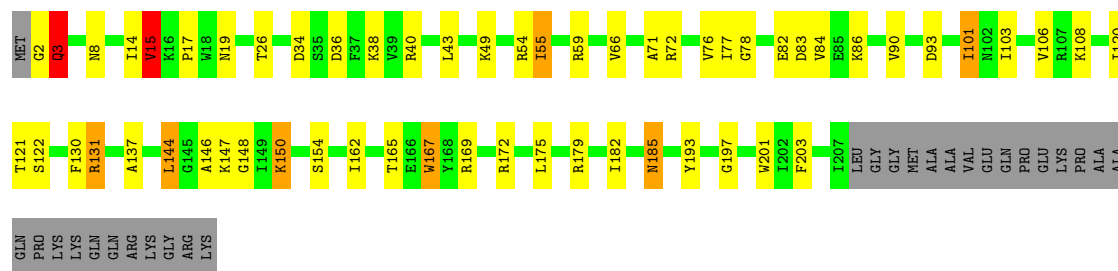
- Molecule 36: 30S ribosomal protein S3

Chain FC: 60% 24% 12%



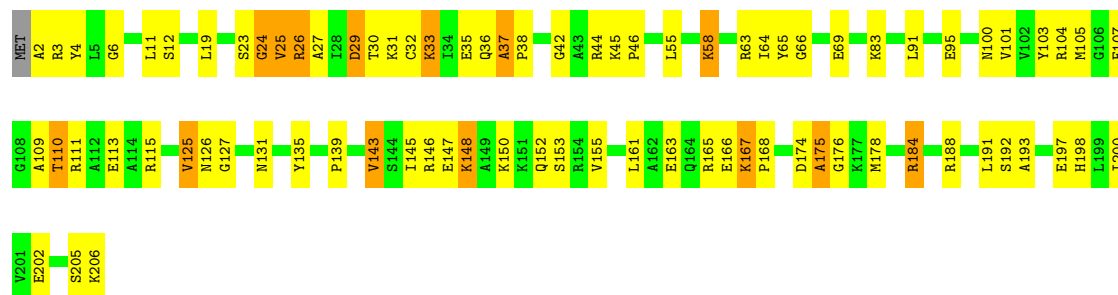
- Molecule 36: 30S ribosomal protein S3

Chain HC: 64% 21% 12%



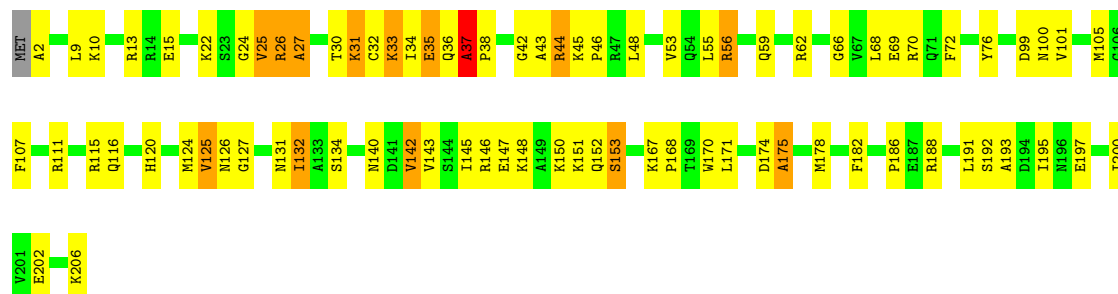
- Molecule 37: 30S ribosomal protein S4

Chain BD: 60% 33% 7%



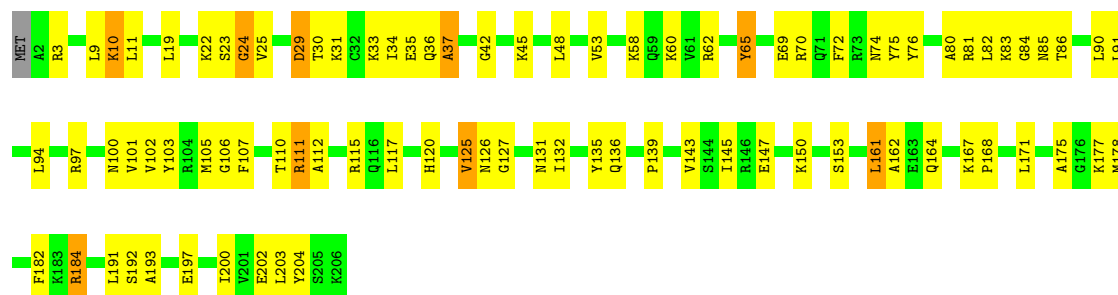
- Molecule 37: 30S ribosomal protein S4

Chain DD: 60% 33% 6%



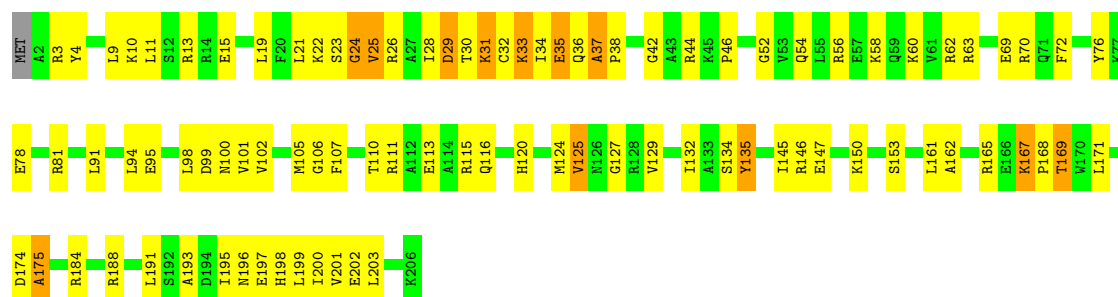
- Molecule 37: 30S ribosomal protein S4

Chain FD: 57% 38% .



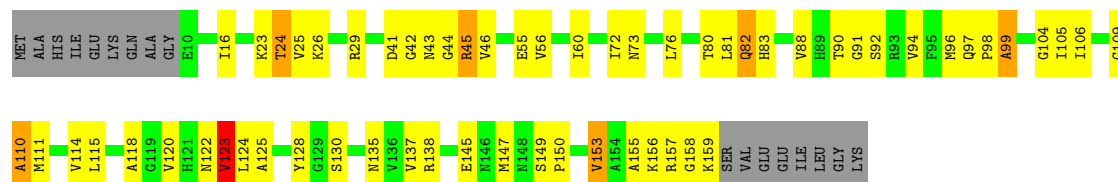
- Molecule 37: 30S ribosomal protein S4

Chain HD: 



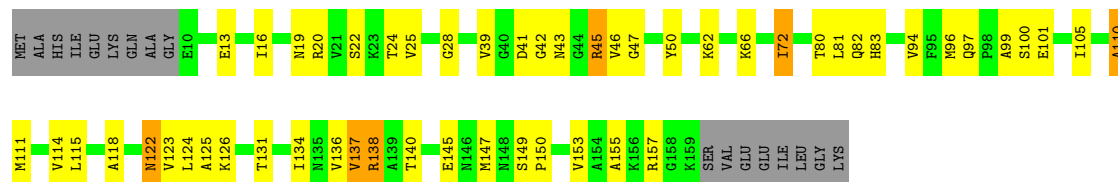
- Molecule 38: 30S ribosomal protein S5

Chain BE: 



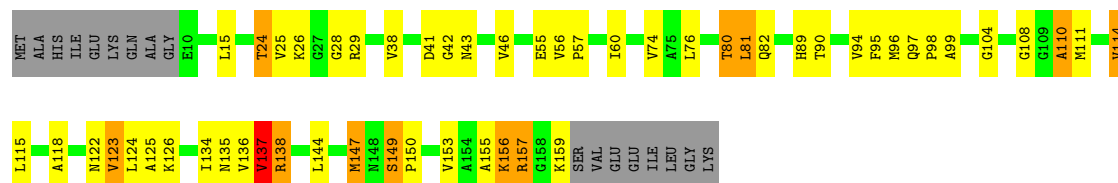
- Molecule 38: 30S ribosomal protein S5

Chain DE: 



- Molecule 38: 30S ribosomal protein S5

Chain FE: 



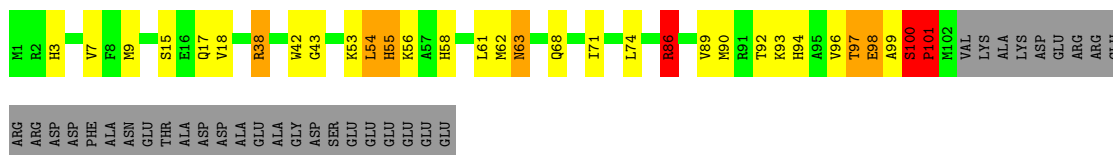
- Molecule 38: 30S ribosomal protein S5

Chain HE: 

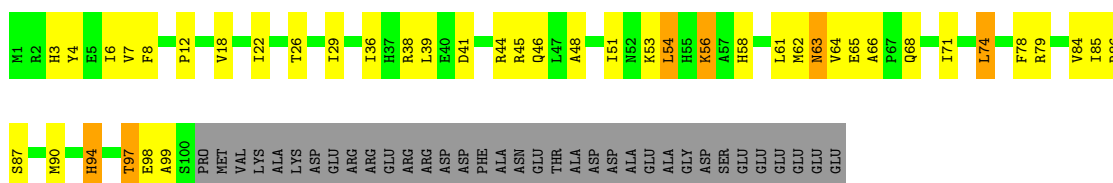




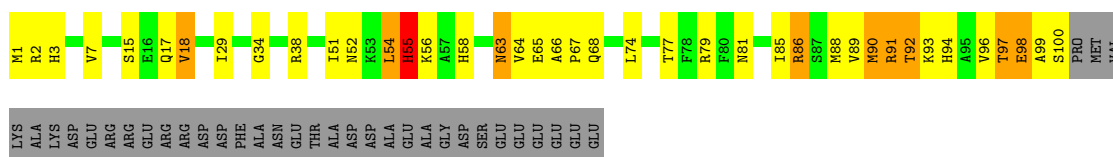
- Molecule 39: 30S ribosomal protein S6



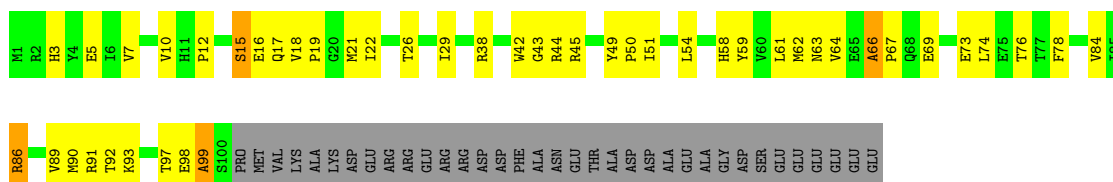
- Molecule 39: 30S ribosomal protein S6



- Molecule 39: 30S ribosomal protein S6



- Molecule 39: 30S ribosomal protein S6

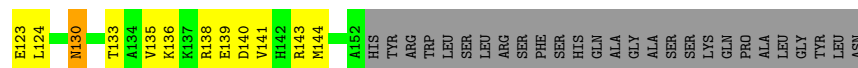


- Molecule 40: 30S ribosomal protein S7

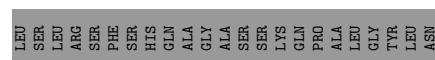




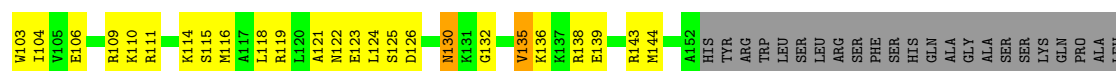
- Molecule 40: 30S ribosomal protein S7



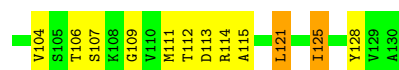
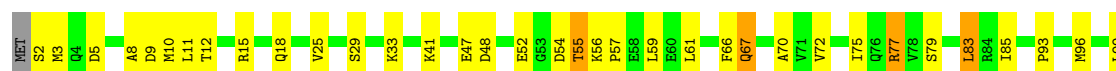
- Molecule 40: 30S ribosomal protein S7



- Molecule 40: 30S ribosomal protein S7

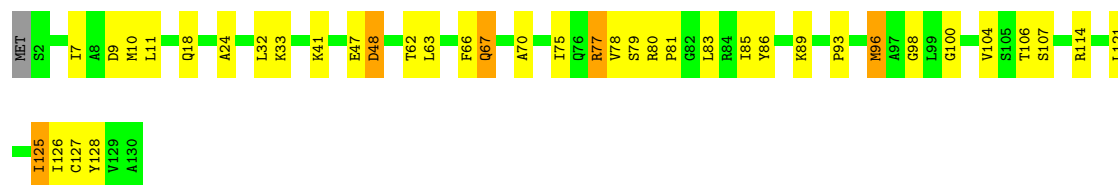


- Molecule 41: 30S ribosomal protein S8



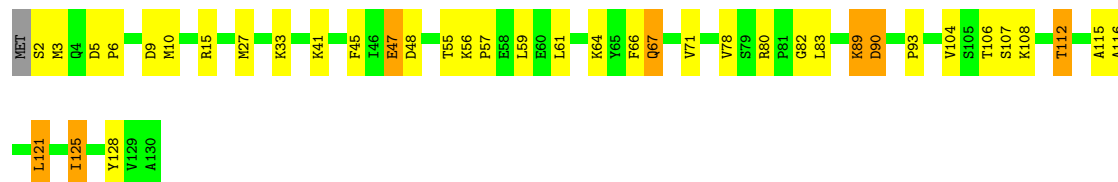
- Molecule 41: 30S ribosomal protein S8





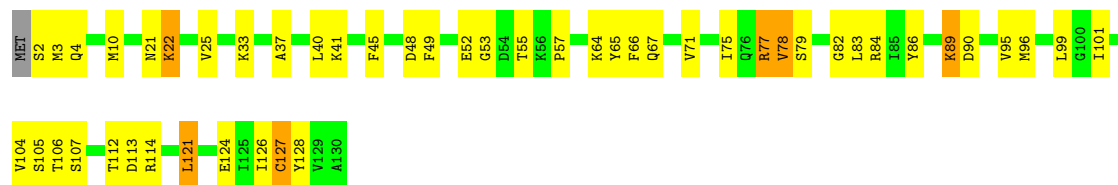
- Molecule 41: 30S ribosomal protein S8

Chain FH: 69% 25% 5% .



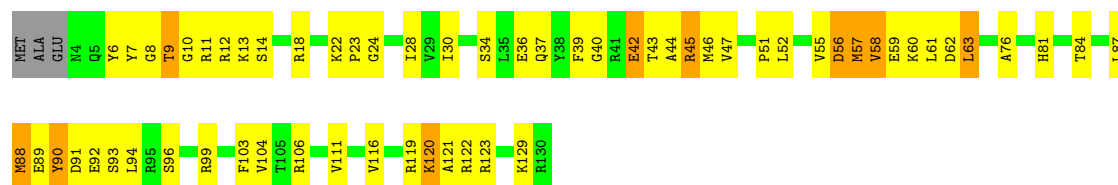
- Molecule 41: 30S ribosomal protein S8

Chain HH: 62% 33% 5% .



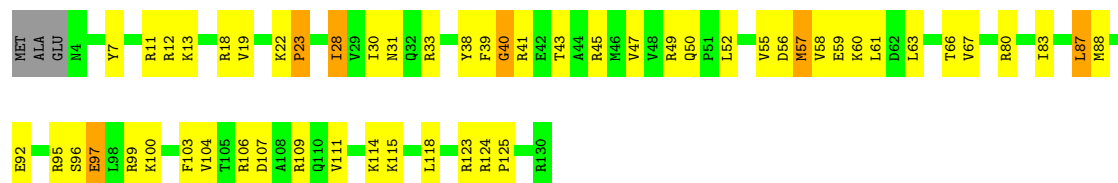
- Molecule 42: 30S ribosomal protein S9

Chain BI: 51% 39% 8% .



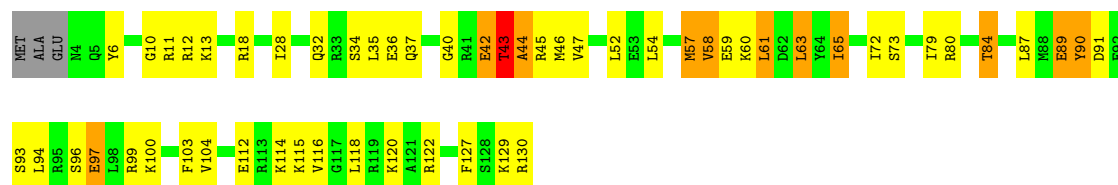
- Molecule 42: 30S ribosomal protein S9

Chain DI: 56% 37% 5% .



- Molecule 42: 30S ribosomal protein S9

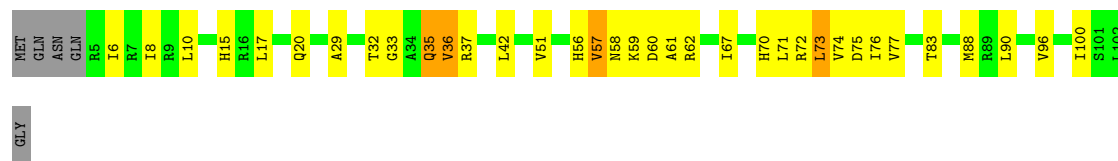
Chain FI: 55% 33% 8% ..



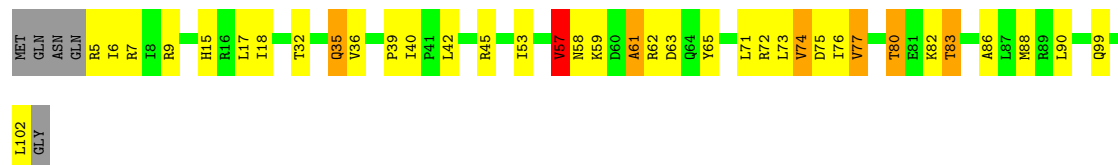
- Molecule 42: 30S ribosomal protein S9



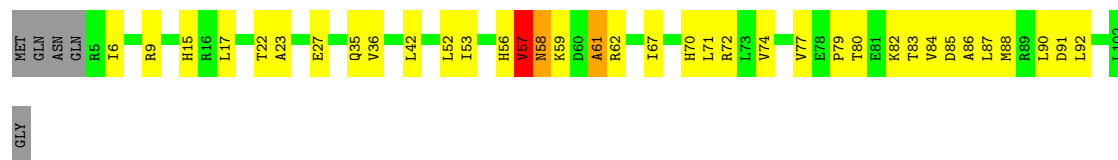
- Molecule 43: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S10

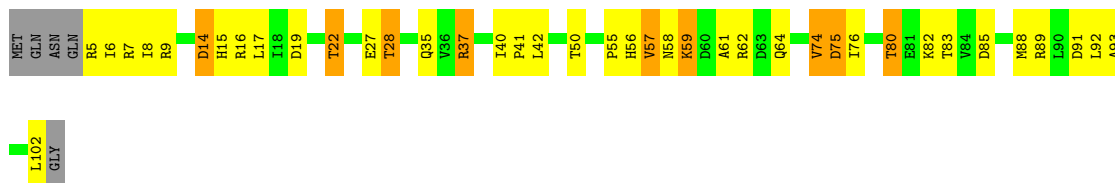


- Molecule 43: 30S ribosomal protein S10

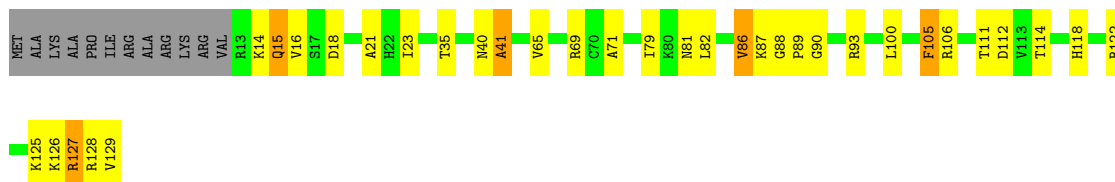


- Molecule 43: 30S ribosomal protein S10

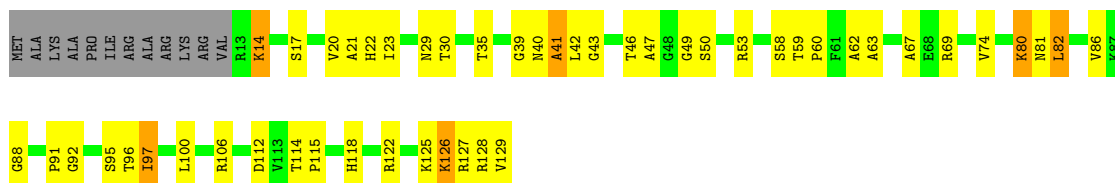




- Molecule 44: 30S ribosomal protein S11



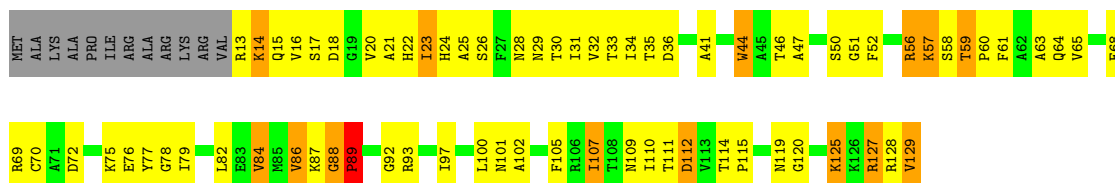
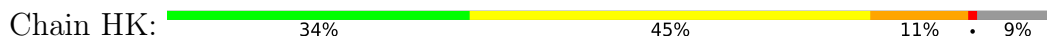
- Molecule 44: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S11

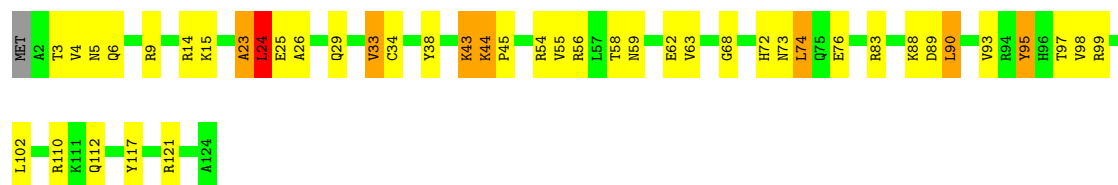


- Molecule 44: 30S ribosomal protein S11



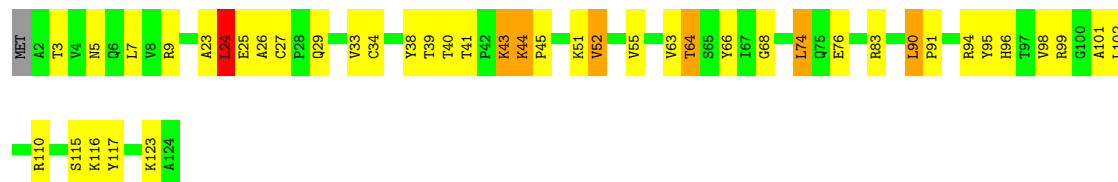
- Molecule 45: 30S ribosomal protein S12





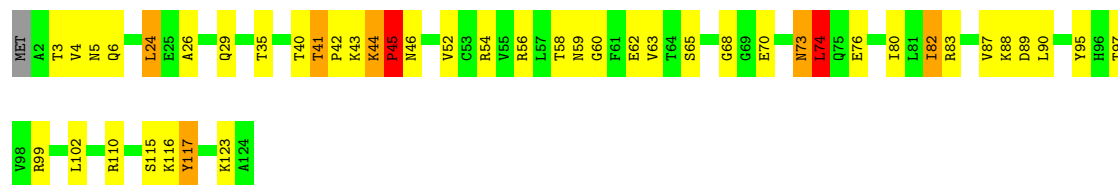
- Molecule 45: 30S ribosomal protein S12

Chain DL: 65% 29% 5% ..



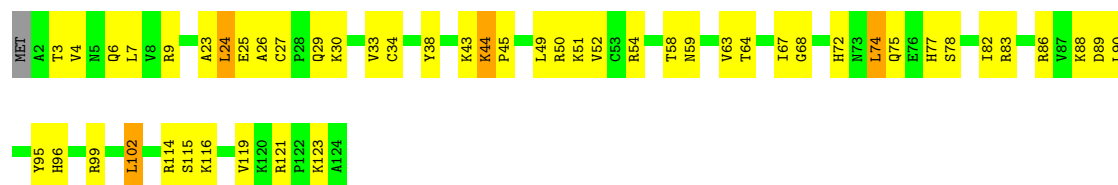
- Molecule 45: 30S ribosomal protein S12

Chain FL: 63% 30% 5% ..



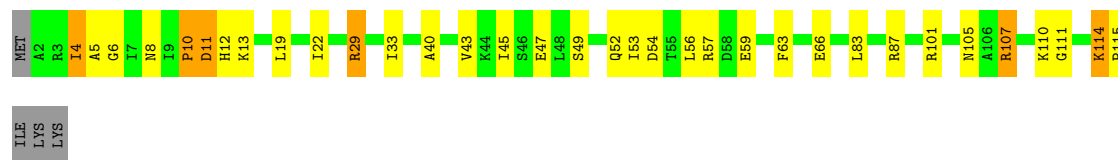
- Molecule 45: 30S ribosomal protein S12

Chain HL: 59% 37% 5% ..



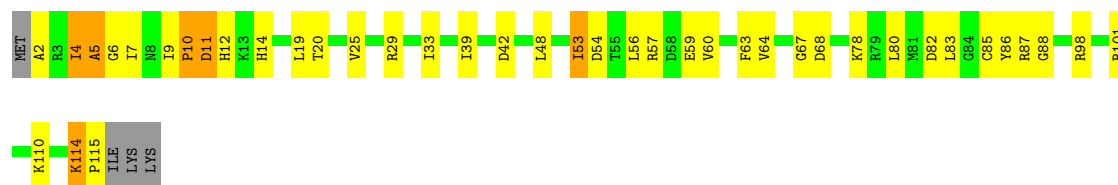
- Molecule 46: 30S ribosomal protein S13

Chain BM: 68% 24% 5% .

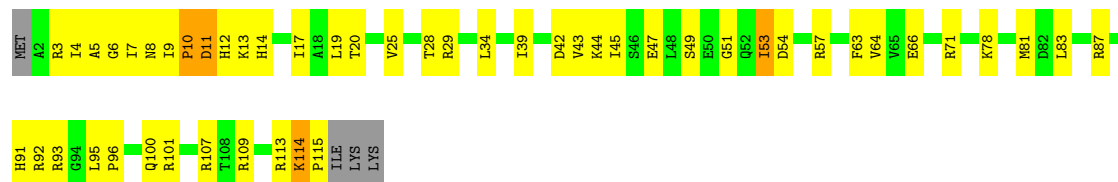


- Molecule 46: 30S ribosomal protein S13

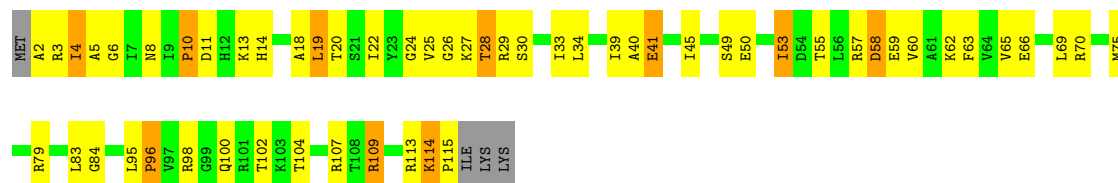
Chain DM: 62% 30% 5% .



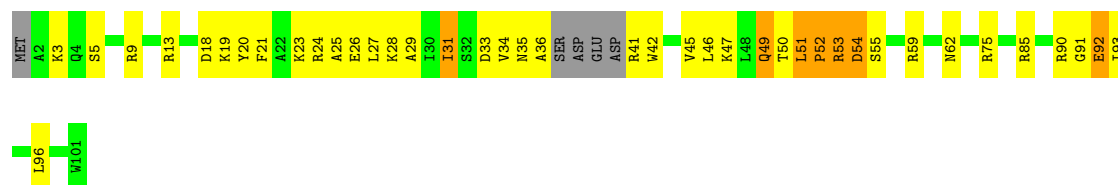
- Molecule 46: 30S ribosomal protein S13



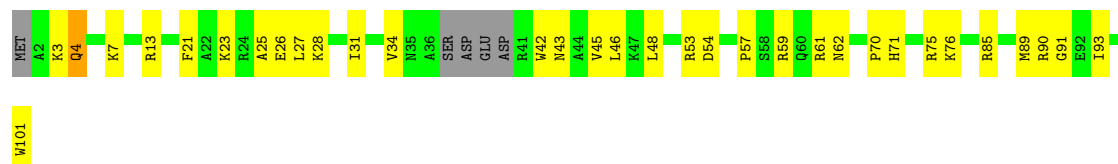
- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14

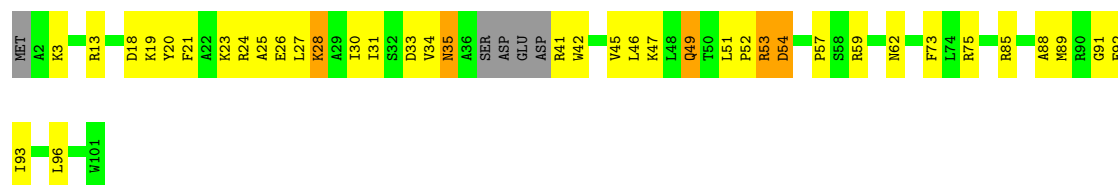


- Molecule 47: 30S ribosomal protein S14



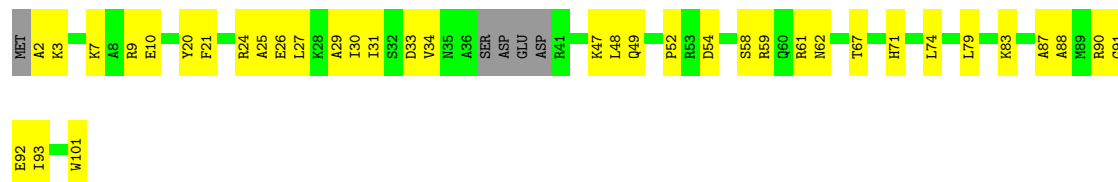
- Molecule 47: 30S ribosomal protein S14





- Molecule 47: 30S ribosomal protein S14

Chain HN: 58% 37% 5%



- Molecule 48: 30S ribosomal protein S15

Chain BO: 78% 18% ..



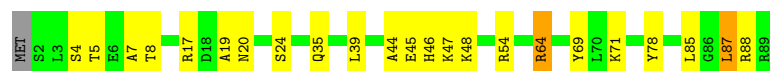
- Molecule 48: 30S ribosomal protein S15

Chain DO: 74% 24% ..



- Molecule 48: 30S ribosomal protein S15

Chain FO: 73% 24% ..



- Molecule 48: 30S ribosomal protein S15

Chain HO: 75% 22% ..



- Molecule 49: 30S ribosomal protein S16

Chain BP: 70% 29% .



- Molecule 49: 30S ribosomal protein S16

Chain DP: 65% 30% 5%



- Molecule 49: 30S ribosomal protein S16

Chain FP: 63% 33% 5%



- Molecule 49: 30S ribosomal protein S16

Chain HP: 70% 30% 5%



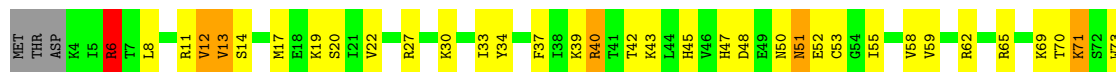
- Molecule 50: 30S ribosomal protein S17

Chain BQ: 64% 29% 5%



- Molecule 50: 30S ribosomal protein S17

Chain DQ: 50% 38% 6% 5%



- Molecule 50: 30S ribosomal protein S17

Chain FQ: 61% 32% 5%



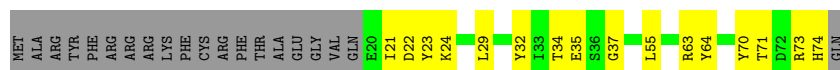
- Molecule 50: 30S ribosomal protein S17

Chain HQ:  52% 32% 11% 5%



- Molecule 51: 30S ribosomal protein S18

Chain BR:  52% 21% 27%



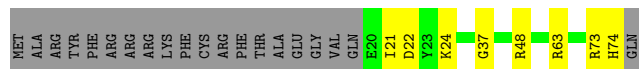
- Molecule 51: 30S ribosomal protein S18

Chain DR:  53% 19% 27%



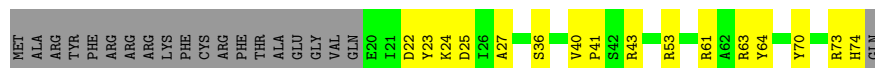
- Molecule 51: 30S ribosomal protein S18

Chain FR:  63% 11% 27%



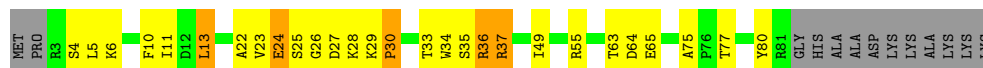
- Molecule 51: 30S ribosomal protein S18

Chain HR:  52% 21% 27%



- Molecule 52: 30S ribosomal protein S19

Chain BS:  55% 25% 5% 14%



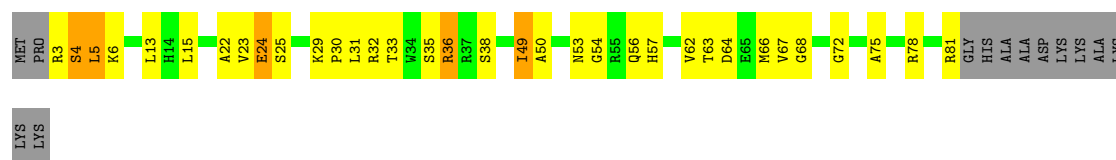
- Molecule 52: 30S ribosomal protein S19

Chain DS:  65% 21% 14%

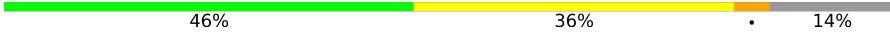


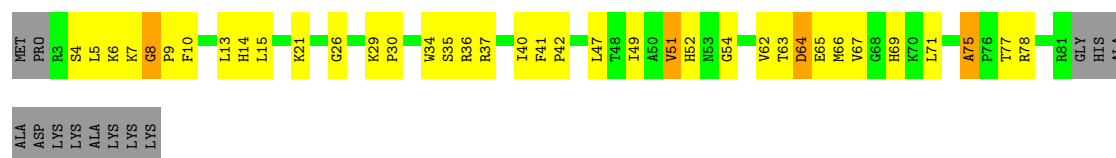
- Molecule 52: 30S ribosomal protein S19

Chain FS: 



- Molecule 52: 30S ribosomal protein S19

Chain HS: 



- Molecule 53: 30S ribosomal protein S20

Chain BT: 



- Molecule 53: 30S ribosomal protein S20

Chain DT: 



- Molecule 53: 30S ribosomal protein S20

Chain FT: 

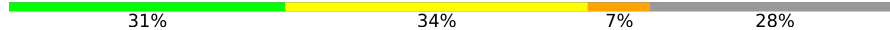


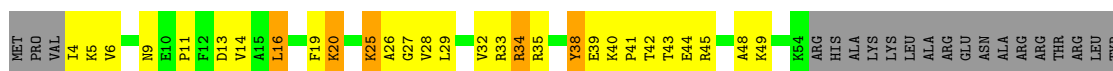
- Molecule 53: 30S ribosomal protein S20

Chain HT: 

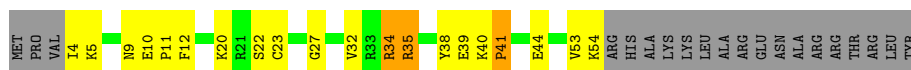


- Molecule 54: 30S ribosomal protein S21

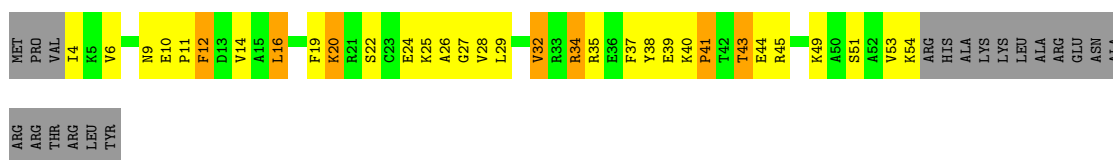
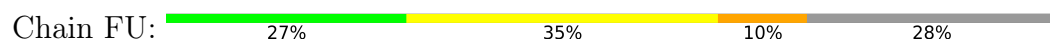
Chain BU: 



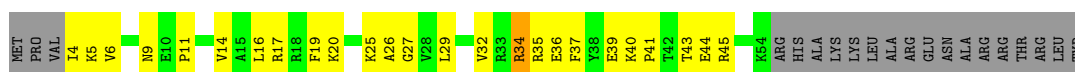
- Molecule 54: 30S ribosomal protein S21



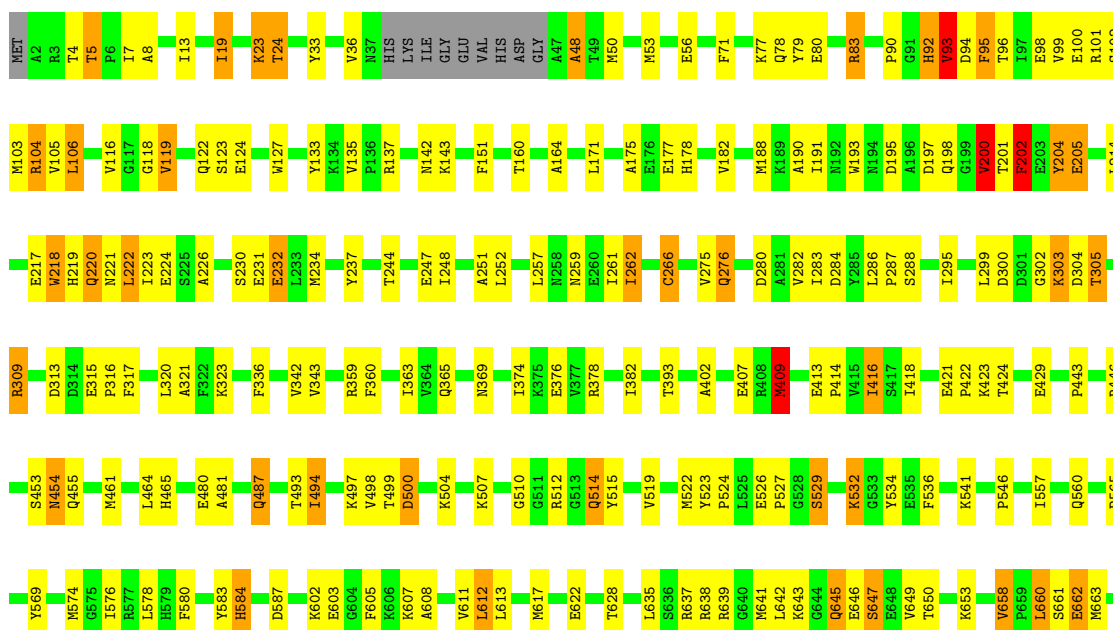
- Molecule 54: 30S ribosomal protein S21



- Molecule 54: 30S ribosomal protein S21



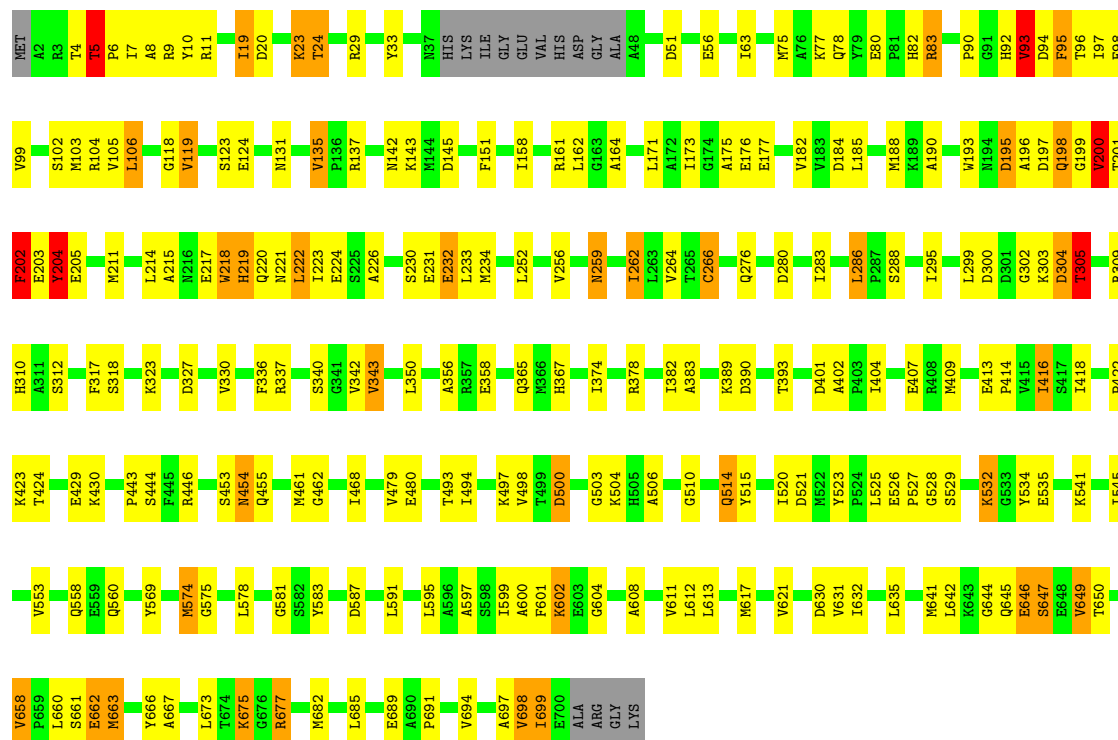
- Molecule 55: Elongation factor G





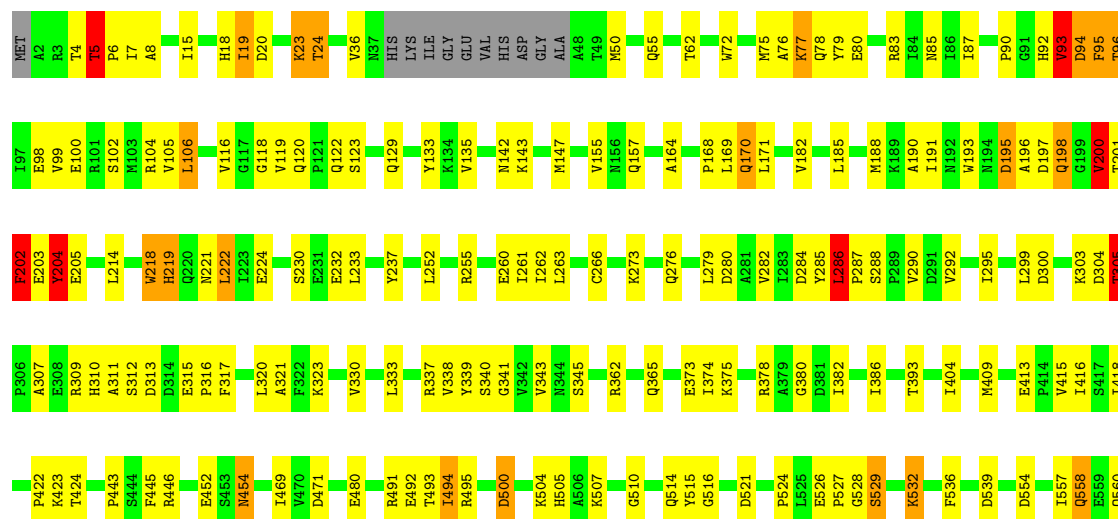
• Molecule 55: Elongation factor G

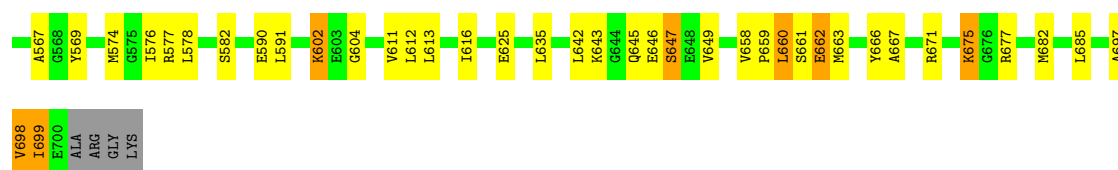
Chain DV: 64% 28% 5% ..



• Molecule 55: Elongation factor G

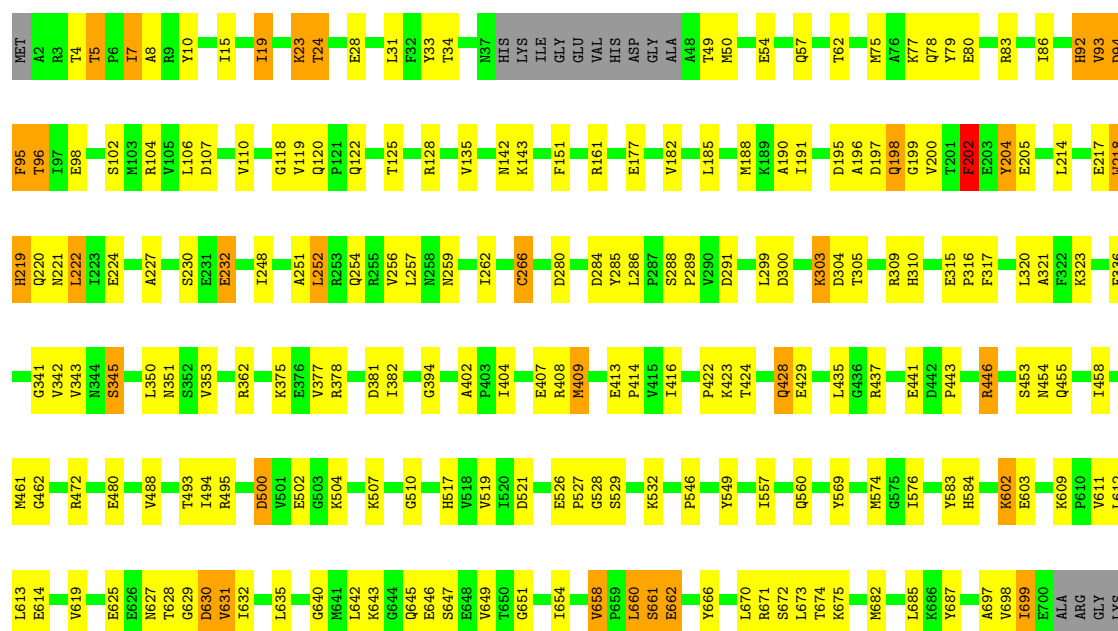
Chain FV: 66% 27% ..





• Molecule 55: Elongation factor G

Chain HV: 68% 25% 5%



• Molecule 56: Viomycin

Chain BW: 17% 67% 17%



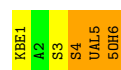
• Molecule 56: Viomycin

Chain DW: 17% 67% 17%



• Molecule 56: Viomycin

Chain FW: 17% 33% 50%



• Molecule 56: Viomycin



KBE1
A2
S3
S4
UAL5
50H6

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	361.60Å 361.77Å 433.20Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (70.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.272	Depositor
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.160	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	592086	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4952e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, DPP, ZN, KBE, 5OH, MG, UAL

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	AB	0.37	0/2828	0.55	0/4410
1	CB	0.30	0/2828	0.52	0/4410
1	EB	0.35	0/2828	0.56	0/4410
1	GB	0.40	0/2828	0.57	0/4410
2	AC	0.71	0/2121	1.10	8/2852 (0.3%)
2	CC	0.60	0/2121	1.00	3/2852 (0.1%)
2	EC	0.69	0/2121	1.04	6/2852 (0.2%)
2	GC	0.59	0/2121	1.00	4/2852 (0.1%)
3	AA	0.44	0/68626	0.60	5/107056 (0.0%)
3	CA	0.34	0/68626	0.55	3/107056 (0.0%)
3	EA	0.41	0/68626	0.60	5/107056 (0.0%)
3	GA	0.35	0/68626	0.59	5/107056 (0.0%)
4	AD	0.74	0/1586	1.12	7/2134 (0.3%)
4	CD	0.66	0/1586	1.06	8/2134 (0.4%)
4	ED	0.71	0/1586	0.99	4/2134 (0.2%)
4	GD	0.62	0/1586	1.01	6/2134 (0.3%)
5	AE	0.69	0/1571	1.02	4/2113 (0.2%)
5	CE	0.54	0/1571	0.95	2/2113 (0.1%)
5	EE	0.69	0/1571	0.99	3/2113 (0.1%)
5	GE	0.72	1/1571 (0.1%)	1.04	4/2113 (0.2%)
6	AF	0.60	0/1434	0.99	5/1926 (0.3%)
6	CF	0.59	0/1434	1.07	2/1926 (0.1%)
6	EF	0.62	0/1434	1.05	3/1926 (0.2%)
6	GF	0.82	1/1434 (0.1%)	1.12	4/1926 (0.2%)
7	AG	0.69	0/1343	0.99	1/1816 (0.1%)
7	CG	0.61	0/1343	0.99	2/1816 (0.1%)
7	EG	0.66	1/1343 (0.1%)	1.03	4/1816 (0.2%)
7	GG	0.64	0/1343	0.96	1/1816 (0.1%)
8	AH	0.68	0/389	1.05	1/523 (0.2%)
8	CH	0.82	0/389	1.07	0/523
8	EH	0.61	0/389	1.09	1/523 (0.2%)
8	GH	0.68	0/389	0.99	0/523

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	AI	0.83	0/1046	1.23	13/1410 (0.9%)
9	CI	0.81	0/1046	1.19	15/1410 (1.1%)
9	EI	0.73	0/1046	1.12	7/1410 (0.5%)
9	GI	1.02	1/1046 (0.1%)	1.25	14/1410 (1.0%)
10	AJ	0.81	1/1152 (0.1%)	1.07	3/1551 (0.2%)
10	CJ	0.64	0/1152	1.00	4/1551 (0.3%)
10	EJ	0.80	1/1152 (0.1%)	1.08	5/1551 (0.3%)
10	GJ	0.61	0/1152	1.00	2/1551 (0.1%)
11	AK	0.83	0/947	1.02	1/1268 (0.1%)
11	CK	0.72	0/947	1.07	1/1268 (0.1%)
11	EK	0.72	1/947 (0.1%)	1.03	2/1268 (0.2%)
11	GK	0.66	0/947	1.05	2/1268 (0.2%)
12	AL	0.74	0/1054	1.01	0/1403
12	CL	0.57	0/1054	0.98	1/1403 (0.1%)
12	EL	0.74	0/1054	1.03	1/1403 (0.1%)
12	GL	0.71	0/1054	1.06	4/1403 (0.3%)
13	AM	0.79	0/1093	1.05	3/1460 (0.2%)
13	CM	0.62	0/1093	0.97	6/1460 (0.4%)
13	EM	0.71	0/1093	1.03	3/1460 (0.2%)
13	GM	0.59	0/1093	1.01	2/1460 (0.1%)
14	AN	0.68	0/973	0.91	0/1301
14	CN	0.57	0/973	0.89	0/1301
14	EN	0.64	0/973	0.94	2/1301 (0.2%)
14	GN	0.57	0/973	0.90	0/1301
15	AO	0.59	0/902	0.98	1/1209 (0.1%)
15	CO	0.49	0/902	0.97	0/1209
15	EO	0.57	0/902	1.03	0/1209
15	GO	0.67	0/902	1.19	3/1209 (0.2%)
16	AP	0.67	0/929	1.03	2/1242 (0.2%)
16	CP	0.62	0/929	1.07	3/1242 (0.2%)
16	EP	0.69	0/929	1.10	3/1242 (0.2%)
16	GP	0.64	0/929	1.08	3/1242 (0.2%)
17	AQ	0.79	0/960	0.96	1/1278 (0.1%)
17	CQ	0.63	0/960	0.95	0/1278
17	EQ	0.74	0/960	0.93	0/1278
17	GQ	0.60	0/960	0.98	1/1278 (0.1%)
18	AR	0.71	0/829	1.04	3/1107 (0.3%)
18	CR	0.60	0/829	0.98	3/1107 (0.3%)
18	ER	0.71	0/829	1.04	3/1107 (0.3%)
18	GR	0.74	0/829	1.03	4/1107 (0.4%)
19	AS	0.76	1/864 (0.1%)	0.99	2/1156 (0.2%)
19	CS	0.64	0/864	0.90	0/1156
19	ES	0.76	0/864	1.00	1/1156 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	GS	0.61	0/864	0.97	1/1156 (0.1%)
20	AT	0.73	0/744	1.11	3/994 (0.3%)
20	CT	0.65	0/744	1.02	2/994 (0.2%)
20	ET	0.79	0/744	1.12	3/994 (0.3%)
20	GT	0.71	0/744	1.03	1/994 (0.1%)
21	AU	0.69	0/787	1.08	0/1051
21	CU	0.55	0/787	1.01	2/1051 (0.2%)
21	EU	0.61	0/787	1.13	7/1051 (0.7%)
21	GU	0.74	0/787	1.09	2/1051 (0.2%)
22	AV	0.61	0/766	0.92	3/1025 (0.3%)
22	CV	0.53	0/766	0.86	0/1025
22	EV	0.63	0/766	0.91	1/1025 (0.1%)
22	GV	0.73	0/766	1.08	2/1025 (0.2%)
23	AW	0.95	2/603 (0.3%)	1.30	5/797 (0.6%)
23	CW	0.79	1/603 (0.2%)	1.22	6/797 (0.8%)
23	EW	0.94	1/603 (0.2%)	1.30	5/797 (0.6%)
23	GW	0.79	0/603	1.21	5/797 (0.6%)
24	AX	0.66	0/635	1.00	1/848 (0.1%)
24	CX	0.54	0/635	0.91	2/848 (0.2%)
24	EX	0.67	0/635	0.95	0/848
24	GX	0.55	0/635	0.92	1/848 (0.1%)
25	AY	0.55	0/510	0.98	0/677
25	CY	0.58	0/510	1.01	1/677 (0.1%)
25	EY	0.61	0/510	1.04	1/677 (0.1%)
25	GY	0.67	0/510	1.06	1/677 (0.1%)
26	AZ	0.74	0/453	1.08	0/605
26	CZ	0.69	0/453	1.09	2/605 (0.3%)
26	EZ	0.72	0/453	0.98	2/605 (0.3%)
26	GZ	0.78	0/453	1.17	2/605 (0.3%)
27	A0	0.69	0/450	0.91	0/599
27	C0	0.57	0/450	0.90	0/599
27	E0	0.67	0/450	0.89	0/599
27	G0	0.57	0/450	0.88	0/599
28	A1	0.68	0/416	1.01	2/554 (0.4%)
28	C1	0.64	0/416	0.99	0/554
28	E1	0.60	0/416	1.05	3/554 (0.5%)
28	G1	0.65	0/416	1.03	0/554
29	A2	0.72	0/380	1.00	0/498
29	C2	0.62	0/380	1.10	3/498 (0.6%)
29	E2	0.65	0/380	0.90	0/498
29	G2	0.56	0/380	0.90	0/498
30	A3	0.71	0/513	0.99	1/676 (0.1%)
30	C3	0.53	0/513	0.91	1/676 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	E3	0.71	0/513	1.03	2/676 (0.3%)
30	G3	0.62	0/513	0.96	1/676 (0.1%)
31	A4	0.86	1/303 (0.3%)	1.19	1/397 (0.3%)
31	C4	0.72	0/303	1.07	0/397
31	E4	0.83	0/303	1.10	0/397
31	G4	0.67	0/303	1.09	0/397
32	A5	0.90	1/1131 (0.1%)	2.04	51/1524 (3.3%)
32	C5	0.85	0/1131	2.06	54/1524 (3.5%)
32	E5	0.83	0/1115	2.07	56/1502 (3.7%)
33	A6	0.78	0/227	0.98	1/304 (0.3%)
34	BB	0.61	0/1735	0.98	4/2338 (0.2%)
34	DB	0.65	0/1735	0.99	5/2338 (0.2%)
34	FB	0.63	0/1735	1.07	5/2338 (0.2%)
34	HB	0.74	0/1735	1.00	5/2338 (0.2%)
35	BA	0.36	0/36834	0.57	1/57462 (0.0%)
35	DA	0.33	0/36834	0.55	0/57462
35	FA	0.34	0/36834	0.57	0/57462
35	HA	0.39	0/36834	0.57	0/57462
36	BC	0.58	0/1651	0.96	6/2225 (0.3%)
36	DC	0.55	0/1651	0.92	1/2225 (0.0%)
36	FC	0.63	0/1651	0.97	1/2225 (0.0%)
36	HC	0.73	0/1651	1.04	7/2225 (0.3%)
37	BD	0.66	0/1665	1.08	6/2227 (0.3%)
37	DD	0.63	0/1665	1.02	6/2227 (0.3%)
37	FD	0.64	0/1665	0.95	2/2227 (0.1%)
37	HD	0.67	0/1665	1.04	5/2227 (0.2%)
38	BE	0.66	0/1118	1.07	4/1504 (0.3%)
38	DE	0.58	0/1118	1.00	2/1504 (0.1%)
38	FE	0.61	0/1118	0.98	1/1504 (0.1%)
38	HE	0.62	0/1118	0.94	1/1504 (0.1%)
39	BF	0.64	0/851	0.92	0/1150
39	DF	0.70	0/835	1.09	2/1128 (0.2%)
39	FF	0.64	1/835 (0.1%)	1.04	8/1128 (0.7%)
39	HF	0.79	1/835 (0.1%)	1.14	4/1128 (0.4%)
40	BG	0.65	0/1195	0.93	0/1602
40	DG	0.65	1/1195 (0.1%)	1.05	3/1602 (0.2%)
40	FG	0.59	0/1195	1.01	2/1602 (0.1%)
40	HG	0.79	1/1195 (0.1%)	1.13	3/1602 (0.2%)
41	BH	0.62	0/989	0.95	2/1326 (0.2%)
41	DH	0.57	0/989	0.95	1/1326 (0.1%)
41	FH	0.57	0/989	0.92	1/1326 (0.1%)
41	HH	0.72	0/989	1.09	2/1326 (0.2%)
42	BI	0.70	0/1034	1.07	2/1375 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	DI	0.68	0/1034	1.01	3/1375 (0.2%)
42	FI	0.69	0/1034	1.02	3/1375 (0.2%)
42	HI	0.75	0/1034	1.00	2/1375 (0.1%)
43	BJ	0.73	0/796	1.05	1/1077 (0.1%)
43	DJ	0.76	0/796	0.96	0/1077
43	FJ	0.69	0/796	0.99	0/1077
43	HJ	0.87	1/796 (0.1%)	1.12	3/1077 (0.3%)
44	BK	0.66	0/893	1.07	2/1205 (0.2%)
44	DK	0.68	0/893	1.03	3/1205 (0.2%)
44	FK	0.68	0/893	1.08	1/1205 (0.1%)
44	HK	0.92	0/893	1.27	12/1205 (1.0%)
45	BL	0.69	0/969	1.08	4/1300 (0.3%)
45	DL	0.62	0/969	1.03	3/1300 (0.2%)
45	FL	0.61	0/969	1.10	3/1300 (0.2%)
45	HL	0.65	0/969	1.06	1/1300 (0.1%)
46	BM	0.62	0/892	1.06	0/1193
46	DM	0.70	0/892	1.05	2/1193 (0.2%)
46	FM	0.57	0/892	1.01	3/1193 (0.3%)
46	HM	0.97	0/892	1.23	6/1193 (0.5%)
47	BN	0.65	0/785	1.02	4/1043 (0.4%)
47	DN	0.58	0/785	0.97	1/1043 (0.1%)
47	FN	0.64	0/785	1.03	2/1043 (0.2%)
47	HN	0.70	0/785	1.08	2/1043 (0.2%)
48	BO	0.59	0/722	0.97	2/964 (0.2%)
48	DO	0.56	0/722	1.01	0/964
48	FO	0.56	0/722	0.88	1/964 (0.1%)
48	HO	0.68	0/722	1.03	0/964
49	BP	0.65	0/659	1.01	1/884 (0.1%)
49	DP	0.56	0/659	0.96	0/884
49	FP	0.63	0/659	0.98	2/884 (0.2%)
49	HP	0.59	0/659	0.96	3/884 (0.3%)
50	BQ	0.61	0/657	1.00	0/881
50	DQ	0.59	0/657	0.99	0/881
50	FQ	0.57	0/657	0.91	0/881
50	HQ	0.66	0/657	1.03	0/881
51	BR	0.55	0/462	0.86	0/621
51	DR	0.70	1/462 (0.2%)	1.02	1/621 (0.2%)
51	FR	0.59	0/462	0.87	0/621
51	HR	0.73	0/462	1.11	0/621
52	BS	0.59	0/652	1.14	4/877 (0.5%)
52	DS	0.62	0/652	1.03	0/877
52	FS	0.58	0/652	0.95	2/877 (0.2%)
52	HS	0.97	0/652	1.30	9/877 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
53	BT	0.60	0/671	0.88	0/888
53	DT	0.65	0/671	0.99	1/888 (0.1%)
53	FT	0.53	0/671	1.02	4/888 (0.5%)
53	HT	0.56	0/671	1.00	2/888 (0.2%)
54	BU	0.82	0/430	1.12	2/570 (0.4%)
54	DU	0.93	1/430 (0.2%)	1.12	0/570
54	FU	0.87	1/430 (0.2%)	1.24	2/570 (0.4%)
54	HU	0.85	0/430	0.96	0/570
55	BV	0.58	0/5444	0.94	7/7367 (0.1%)
55	DV	0.56	0/5439	0.94	9/7360 (0.1%)
55	FV	0.59	0/5439	0.93	9/7360 (0.1%)
55	HV	0.62	0/5439	0.97	9/7360 (0.1%)
56	BW	3.15	1/11 (9.1%)	1.47	0/13
56	DW	3.31	1/11 (9.1%)	1.60	0/13
56	FW	3.34	1/11 (9.1%)	1.80	0/13
56	HW	3.51	1/11 (9.1%)	1.65	0/13
All	All	0.49	26/636829 (0.0%)	0.74	685/948879 (0.1%)

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	AC	0	1
2	GC	0	1
4	AD	0	1
4	CD	0	2
4	ED	0	1
4	GD	0	1
10	AJ	0	1
10	GJ	0	1
11	AK	0	1
32	A5	0	1
39	BF	0	1
39	FF	0	1
42	DI	0	1
45	BL	0	1
45	DL	0	1
45	HL	0	1
53	DT	0	1
55	BV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DV	0	1
55	FV	0	1
55	HV	0	1
All	All	0	22

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	HW	3	SER	C-N	10.99	1.48	1.33
56	DW	3	SER	C-N	10.13	1.47	1.33
56	FW	3	SER	C-N	10.12	1.47	1.33
56	BW	3	SER	C-N	9.26	1.46	1.33
23	AW	35	ILE	CA-CB	7.23	1.62	1.54

The worst 5 of 685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C5	122	GLN	N-CA-C	15.21	121.25	108.78
4	AD	151	THR	CA-C-N	-14.34	103.99	119.19
4	AD	151	THR	C-N-CA	-14.34	103.99	119.19
32	A5	131	THR	N-CA-C	-13.37	96.71	111.28
32	E5	72	LEU	CA-C-N	12.97	140.15	120.17

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	A5	130	PRO	Peptide
2	AC	233	GLY	Peptide
4	AD	9	VAL	Peptide
10	AJ	110	PRO	Peptide
11	AK	71	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2529	0	1281	20	0
1	CB	2529	0	1281	30	0
1	EB	2529	0	1281	32	0
1	GB	2529	0	1281	59	0
2	AC	2082	0	2157	53	0
2	CC	2082	0	2157	70	0
2	EC	2082	0	2157	67	0
2	GC	2082	0	2157	73	0
3	AA	61274	0	30819	794	0
3	CA	61274	0	30819	837	0
3	EA	61274	0	30819	744	0
3	GA	61274	0	30817	1246	2
4	AD	1565	0	1616	57	0
4	CD	1565	0	1616	53	0
4	ED	1565	0	1616	52	0
4	GD	1565	0	1616	52	0
5	AE	1552	0	1619	40	0
5	CE	1552	0	1619	44	0
5	EE	1552	0	1619	35	0
5	GE	1552	0	1619	72	0
6	AF	1410	0	1447	43	0
6	CF	1410	0	1447	40	0
6	EF	1410	0	1447	51	0
6	GF	1410	0	1447	62	0
7	AG	1323	0	1374	42	0
7	CG	1323	0	1374	52	0
7	EG	1323	0	1374	46	0
7	GG	1323	0	1374	56	0
8	AH	384	0	405	15	0
8	CH	384	0	405	21	0
8	EH	384	0	405	11	0
8	GH	384	0	405	8	0
9	AI	1032	0	1088	58	0
9	CI	1032	0	1088	47	0
9	EI	1032	0	1088	48	0
9	GI	1032	0	1088	63	0
10	AJ	1129	0	1162	60	0
10	CJ	1129	0	1162	59	0
10	EJ	1129	0	1162	53	0
10	GJ	1129	0	1162	56	0
11	AK	938	0	1012	43	0
11	CK	938	0	1012	38	0
11	EK	938	0	1012	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	GK	938	0	1012	28	0
12	AL	1045	0	1117	41	0
12	CL	1045	0	1116	35	0
12	EL	1045	0	1117	37	0
12	GL	1045	0	1117	53	0
13	AM	1074	0	1157	29	0
13	CM	1074	0	1157	35	0
13	EM	1074	0	1157	29	0
13	GM	1074	0	1157	27	0
14	AN	960	0	1000	30	0
14	CN	960	0	1000	34	0
14	EN	960	0	1000	26	0
14	GN	960	0	1000	26	0
15	AO	892	0	923	20	0
15	CO	892	0	923	27	0
15	EO	892	0	923	19	0
15	GO	892	0	923	33	0
16	AP	917	0	965	47	0
16	CP	917	0	965	42	0
16	EP	917	0	965	45	0
16	GP	917	0	965	39	0
17	AQ	947	0	1022	57	0
17	CQ	947	0	1022	53	0
17	EQ	947	0	1022	46	0
17	GQ	947	0	1022	60	0
18	AR	816	0	839	35	0
18	CR	816	0	839	38	0
18	ER	816	0	839	36	0
18	GR	816	0	839	47	0
19	AS	857	0	922	30	0
19	CS	857	0	922	19	0
19	ES	857	0	922	20	0
19	GS	857	0	922	32	0
20	AT	738	0	807	38	0
20	CT	738	0	807	30	0
20	ET	738	0	807	33	0
20	GT	738	0	807	32	0
21	AU	779	0	834	30	0
21	CU	779	0	834	13	0
21	EU	779	0	834	23	0
21	GU	779	0	834	30	0
22	AV	753	0	780	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	753	0	780	20	0
22	EV	753	0	780	12	0
22	GV	753	0	780	14	0
23	AW	596	0	610	80	0
23	CW	596	0	610	63	0
23	EW	596	0	610	77	0
23	GW	596	0	610	61	0
24	AX	625	0	655	17	0
24	CX	625	0	655	14	0
24	EX	625	0	655	23	0
24	GX	625	0	655	19	0
25	AY	509	0	543	16	0
25	CY	509	0	543	10	0
25	EY	509	0	543	18	0
25	GY	509	0	543	11	0
26	AZ	449	0	491	18	0
26	CZ	449	0	491	22	0
26	EZ	449	0	491	10	0
26	GZ	449	0	491	28	0
27	A0	444	0	461	20	0
27	C0	444	0	461	17	0
27	E0	444	0	461	13	0
27	G0	444	0	461	8	0
28	A1	409	0	440	15	0
28	C1	409	0	440	11	0
28	E1	409	0	440	15	0
28	G1	409	0	440	16	0
29	A2	377	0	418	8	0
29	C2	377	0	418	11	0
29	E2	377	0	418	9	0
29	G2	377	0	418	18	0
30	A3	504	0	574	11	0
30	C3	504	0	574	7	0
30	E3	504	0	574	15	0
30	G3	504	0	574	27	0
31	A4	302	0	340	18	0
31	C4	302	0	340	13	0
31	E4	302	0	340	9	0
31	G4	302	0	340	10	0
32	A5	1117	0	1155	133	0
32	C5	1117	0	1155	148	0
32	E5	1101	0	1140	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A6	227	0	237	7	0
34	BB	1704	0	1732	56	0
34	DB	1704	0	1732	66	0
34	FB	1704	0	1732	80	0
34	HB	1704	0	1732	59	0
35	BA	32895	0	16553	337	0
35	DA	32895	0	16553	476	0
35	FA	32895	0	16553	402	1
35	HA	32895	0	16552	579	0
36	BC	1624	0	1696	34	0
36	DC	1624	0	1696	43	0
36	FC	1624	0	1696	44	0
36	HC	1624	0	1696	34	0
37	BD	1643	0	1707	73	0
37	DD	1643	0	1707	65	0
37	FD	1643	0	1707	66	0
37	HD	1643	0	1707	77	0
38	BE	1105	0	1148	45	0
38	DE	1105	0	1148	36	0
38	FE	1105	0	1148	37	0
38	HE	1105	0	1148	37	0
39	BF	832	0	824	24	0
39	DF	817	0	808	38	0
39	FF	817	0	808	24	0
39	HF	817	0	808	37	0
40	BG	1181	0	1238	23	0
40	DG	1181	0	1238	31	0
40	FG	1181	0	1238	21	0
40	HG	1181	0	1238	51	0
41	BH	979	0	1031	31	0
41	DH	979	0	1031	27	0
41	FH	979	0	1031	33	0
41	HH	979	0	1031	34	0
42	BI	1022	0	1070	47	0
42	DI	1022	0	1070	40	0
42	FI	1022	0	1070	48	0
42	HI	1022	0	1070	39	0
43	BJ	786	0	828	23	0
43	DJ	786	0	828	29	0
43	FJ	786	0	828	19	1
43	HJ	786	0	828	29	0
44	BK	877	0	887	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DK	877	0	887	39	0
44	FK	877	0	887	41	0
44	HK	877	0	887	60	0
45	BL	955	0	1016	40	0
45	DL	955	0	1016	39	0
45	FL	955	0	1016	37	0
45	HL	955	0	1016	46	0
46	BM	883	0	941	22	0
46	DM	883	0	941	34	0
46	FM	883	0	941	34	0
46	HM	883	0	941	44	0
47	BN	774	0	824	27	0
47	DN	774	0	824	35	0
47	FN	774	0	824	28	0
47	HN	774	0	824	28	0
48	BO	714	0	734	9	0
48	DO	714	0	734	15	0
48	FO	714	0	734	12	0
48	HO	714	0	734	18	0
49	BP	649	0	666	13	0
49	DP	649	0	666	17	0
49	FP	649	0	666	18	0
49	HP	649	0	666	13	0
50	BQ	648	0	691	12	0
50	DQ	648	0	691	34	0
50	FQ	648	0	691	23	0
50	HQ	648	0	691	27	0
51	BR	455	0	478	11	0
51	DR	455	0	478	10	0
51	FR	455	0	478	4	0
51	HR	455	0	478	25	0
52	BS	637	0	665	20	0
52	DS	637	0	665	13	0
52	FS	637	0	665	28	0
52	HS	637	0	665	34	0
53	BT	665	0	714	15	0
53	DT	665	0	714	25	0
53	FT	665	0	714	16	0
53	HT	665	0	714	15	0
54	BU	425	0	449	32	0
54	DU	425	0	449	18	0
54	FU	425	0	449	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	HU	425	0	449	28	0
55	BV	5345	0	5311	124	0
55	DV	5340	0	5306	137	0
55	FV	5340	0	5306	114	0
55	HV	5340	0	5307	121	0
56	BW	48	0	41	5	0
56	DW	48	0	41	5	0
56	FW	48	0	41	3	0
56	HW	48	0	40	6	0
57	A4	1	0	0	0	0
57	AA	136	0	0	0	0
57	AB	4	0	0	0	0
57	AC	1	0	0	0	0
57	AE	1	0	0	0	0
57	BA	40	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BU	1	0	0	0	0
57	BV	1	0	0	0	0
57	C4	1	0	0	0	0
57	CA	136	0	0	0	0
57	CB	4	0	0	0	0
57	CE	1	0	0	0	0
57	CN	1	0	0	0	0
57	DA	43	0	0	0	0
57	DV	1	0	0	0	0
57	EA	137	0	0	0	0
57	EB	4	0	0	0	0
57	ED	1	0	0	0	0
57	EE	1	0	0	0	0
57	FA	39	0	0	0	0
57	FE	1	0	0	0	0
57	FN	2	0	0	0	0
57	FU	1	0	0	0	0
57	FV	1	0	0	0	0
57	GA	136	0	0	0	0
57	GB	4	0	0	0	0
57	GC	2	0	0	0	0
57	GL	1	0	0	0	0
57	HA	41	0	0	0	0
57	HE	1	0	0	0	0
57	HK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	HV	1	0	0	0	0
58	A4	1	0	0	0	0
58	C4	1	0	0	0	0
58	E4	1	0	0	0	0
58	G4	1	0	0	0	0
59	BV	32	0	14	1	0
59	DV	32	0	14	1	0
59	FV	32	0	14	2	0
59	HV	32	0	14	1	0
60	A0	2	0	0	0	0
60	A2	1	0	0	0	0
60	A3	1	0	0	0	0
60	A4	1	0	0	0	0
60	AA	614	0	0	102	0
60	AB	18	0	0	1	0
60	AC	6	0	0	1	0
60	AD	4	0	0	0	0
60	AE	1	0	0	0	0
60	AF	1	0	0	0	0
60	AJ	1	0	0	0	0
60	AL	5	0	0	1	0
60	AN	2	0	0	0	0
60	AP	1	0	0	0	0
60	AQ	2	0	0	0	0
60	AS	1	0	0	0	0
60	BA	202	0	0	31	0
60	BL	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	2	0	0	0	0
60	BV	1	0	0	1	0
60	C0	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	607	0	0	84	0
60	CB	21	0	0	2	0
60	CC	8	0	0	0	0
60	CD	3	0	0	0	0
60	CE	1	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	5	0	0	0	0
60	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	CQ	1	0	0	1	0
60	CS	2	0	0	1	0
60	CT	2	0	0	1	0
60	CU	1	0	0	0	0
60	DA	186	0	0	27	0
60	DC	2	0	0	0	0
60	DD	1	0	0	0	0
60	DE	1	0	0	0	0
60	DG	1	0	0	0	0
60	DK	1	0	0	0	0
60	DL	2	0	0	0	0
60	DN	8	0	0	3	0
60	DQ	1	0	0	0	0
60	DT	4	0	0	1	0
60	DU	1	0	0	0	0
60	DV	1	0	0	0	0
60	E0	1	0	0	0	0
60	E2	1	0	0	0	0
60	E3	2	0	0	0	0
60	E4	2	0	0	0	0
60	EA	610	0	0	105	0
60	EB	18	0	0	3	0
60	EC	9	0	0	1	0
60	ED	3	0	0	0	0
60	EE	2	0	0	1	0
60	EL	4	0	0	0	0
60	EN	3	0	0	0	0
60	ER	1	0	0	0	0
60	ET	2	0	0	0	0
60	EV	2	0	0	0	0
60	FA	197	0	0	24	0
60	FC	1	0	0	0	0
60	FE	2	0	0	0	0
60	FN	3	0	0	0	0
60	FT	4	0	0	0	0
60	FU	1	0	0	0	0
60	FV	1	0	0	0	0
60	G2	2	0	0	0	0
60	G3	1	0	0	0	0
60	G4	1	0	0	0	0
60	GA	606	0	0	137	0
60	GB	19	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	GC	10	0	0	0	0
60	GD	3	0	0	0	0
60	GE	2	0	0	1	0
60	GJ	1	0	0	0	0
60	GL	4	0	0	1	0
60	GN	4	0	0	0	0
60	GQ	1	0	0	0	0
60	GR	2	0	0	1	0
60	GS	2	0	0	0	0
60	GU	1	0	0	0	0
60	GV	1	0	0	0	0
60	HA	193	0	0	31	0
60	HD	3	0	0	2	0
60	HE	3	0	0	0	0
60	HN	7	0	0	3	0
60	HQ	1	0	0	0	0
60	HT	1	0	0	0	0
60	HV	1	0	0	0	0
All	All	592086	0	404164	11482	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 11482 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)
32:C5:24:SER:CB	32:C5:116:GLU:HG2	1.46	1.44
32:C5:24:SER:O	32:C5:116:GLU:HB3	1.41	1.16
32:C5:24:SER:HB2	32:C5:116:GLU:CG	1.76	1.14
32:E5:24:SER:HB2	32:E5:116:GLU:HG2	1.27	1.14
3:AA:912:C:OP1	13:AM:8:LYS:NZ	1.79	1.12

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FA:1029:U:O3'	3:GA:1508:A:N6[1_565]	2.04	0.16
43:FJ:85:ASP:OD1	3:GA:1722:A:O2'[1_565]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	1	4
2	CC	269/273 (98%)	211 (78%)	42 (16%)	16 (6%)	1	4
2	EC	269/273 (98%)	212 (79%)	44 (16%)	13 (5%)	2	7
2	GC	269/273 (98%)	210 (78%)	42 (16%)	17 (6%)	1	3
4	AD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	2
4	CD	207/209 (99%)	166 (80%)	27 (13%)	14 (7%)	1	2
4	ED	207/209 (99%)	165 (80%)	29 (14%)	13 (6%)	1	3
4	GD	207/209 (99%)	161 (78%)	32 (16%)	14 (7%)	1	2
5	AE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	1	6
5	CE	199/201 (99%)	159 (80%)	27 (14%)	13 (6%)	1	3
5	EE	199/201 (99%)	164 (82%)	24 (12%)	11 (6%)	1	4
5	GE	199/201 (99%)	159 (80%)	30 (15%)	10 (5%)	1	6
6	AF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	5	19
6	CF	175/179 (98%)	145 (83%)	25 (14%)	5 (3%)	3	15
6	EF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	1	6
6	GF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	1	6
7	AG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	0	1
7	CG	174/177 (98%)	131 (75%)	28 (16%)	15 (9%)	0	1
7	EG	174/177 (98%)	125 (72%)	35 (20%)	14 (8%)	1	2
7	GG	174/177 (98%)	126 (72%)	30 (17%)	18 (10%)	0	1
8	AH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0	1
8	CH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	0	1
8	EH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	0	1
8	GH	48/50 (96%)	30 (62%)	15 (31%)	3 (6%)	1	3
9	AI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CI	139/142 (98%)	95 (68%)	38 (27%)	6 (4%)	2	8
9	EI	139/142 (98%)	97 (70%)	38 (27%)	4 (3%)	3	15
9	GI	139/142 (98%)	95 (68%)	34 (24%)	10 (7%)	1	2
10	AJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	3
10	CJ	140/142 (99%)	112 (80%)	20 (14%)	8 (6%)	1	4
10	EJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	1	3
10	GJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	1	4
11	AK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	0	1
11	CK	120/123 (98%)	93 (78%)	21 (18%)	6 (5%)	1	6
11	EK	120/123 (98%)	92 (77%)	21 (18%)	7 (6%)	1	4
11	GK	120/123 (98%)	92 (77%)	20 (17%)	8 (7%)	1	3
12	AL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3	12
12	CL	141/144 (98%)	103 (73%)	33 (23%)	5 (4%)	3	12
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	1	6
12	GL	141/144 (98%)	103 (73%)	32 (23%)	6 (4%)	2	8
13	AM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	0	2
13	CM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	1	4
13	EM	134/136 (98%)	106 (79%)	18 (13%)	10 (8%)	1	2
13	GM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	1	4
14	AN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	16	44
14	CN	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	16	44
14	EN	118/127 (93%)	100 (85%)	17 (14%)	1 (1%)	16	44
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	16	44
15	AO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	14	41
15	CO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	3	12
15	EO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	14	41
15	GO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	3	12
16	AP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	2
16	CP	112/115 (97%)	87 (78%)	16 (14%)	9 (8%)	1	2
16	EP	112/115 (97%)	84 (75%)	16 (14%)	12 (11%)	0	1
16	GP	112/115 (97%)	85 (76%)	19 (17%)	8 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	CQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	EQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	12
17	GQ	115/118 (98%)	99 (86%)	14 (12%)	2 (2%)	7	26
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	14
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	14
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	14
18	GR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	1	6
19	AS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	7
19	CS	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	2	11
19	ES	108/110 (98%)	92 (85%)	10 (9%)	6 (6%)	1	4
19	GS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	1	4
20	AT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	1
20	CT	91/100 (91%)	55 (60%)	25 (28%)	11 (12%)	0	1
20	ET	91/100 (91%)	56 (62%)	26 (29%)	9 (10%)	0	1
20	GT	91/100 (91%)	58 (64%)	23 (25%)	10 (11%)	0	1
21	AU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	1
21	CU	100/104 (96%)	75 (75%)	17 (17%)	8 (8%)	1	2
21	EU	100/104 (96%)	74 (74%)	15 (15%)	11 (11%)	0	1
21	GU	100/104 (96%)	76 (76%)	14 (14%)	10 (10%)	0	1
22	AV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
22	CV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	11	36
22	EV	92/94 (98%)	80 (87%)	12 (13%)	0	100	100
22	GV	92/94 (98%)	78 (85%)	13 (14%)	1 (1%)	11	36
23	AW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	0
23	CW	77/85 (91%)	41 (53%)	17 (22%)	19 (25%)	0	0
23	EW	77/85 (91%)	41 (53%)	21 (27%)	15 (20%)	0	0
23	GW	77/85 (91%)	40 (52%)	21 (27%)	16 (21%)	0	0
24	AX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	2	9
24	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	4	16
24	EX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	2	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	GX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	2	9
25	AY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	3
25	CY	61/63 (97%)	42 (69%)	15 (25%)	4 (7%)	1	3
25	EY	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	3
25	GY	61/63 (97%)	39 (64%)	20 (33%)	2 (3%)	3	13
26	AZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	2	11
26	CZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	2	11
26	EZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	2	11
26	GZ	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	2	11
27	A0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	2
27	C0	54/57 (95%)	45 (83%)	3 (6%)	6 (11%)	0	1
27	E0	54/57 (95%)	44 (82%)	6 (11%)	4 (7%)	1	2
27	G0	54/57 (95%)	46 (85%)	4 (7%)	4 (7%)	1	2
28	A1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	3
28	C1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	2	9
28	E1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	2	9
28	G1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	3
29	A2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
29	C2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	19
29	E2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
29	G2	44/46 (96%)	40 (91%)	3 (7%)	1 (2%)	5	19
30	A3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	13
30	C3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	13
30	E3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	13
30	G3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	13
31	A4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	1
31	C4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	1
31	E4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	1
31	G4	36/38 (95%)	30 (83%)	2 (6%)	4 (11%)	0	1
32	A5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	0
32	C5	146/165 (88%)	78 (53%)	45 (31%)	23 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	E5	143/165 (87%)	79 (55%)	41 (29%)	23 (16%)	0	0
33	A6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	2	11
34	BB	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	3
34	DB	216/241 (90%)	157 (73%)	47 (22%)	12 (6%)	1	4
34	FB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	1	4
34	HB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	1	4
36	BC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	4	17
36	DC	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	4	17
36	FC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	3	15
36	HC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	3	15
37	BD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	1	5
37	DD	203/206 (98%)	162 (80%)	29 (14%)	12 (6%)	1	4
37	FD	203/206 (98%)	163 (80%)	29 (14%)	11 (5%)	1	5
37	HD	203/206 (98%)	165 (81%)	26 (13%)	12 (6%)	1	4
38	BE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	2	7
38	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	3	12
38	FE	148/167 (89%)	122 (82%)	20 (14%)	6 (4%)	2	9
38	HE	148/167 (89%)	121 (82%)	20 (14%)	7 (5%)	2	7
39	BF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	1	4
39	DF	98/135 (73%)	80 (82%)	13 (13%)	5 (5%)	1	6
39	FF	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	4
39	HF	98/135 (73%)	76 (78%)	18 (18%)	4 (4%)	2	9
40	BG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	18	48
40	DG	149/179 (83%)	125 (84%)	22 (15%)	2 (1%)	9	32
40	FG	149/179 (83%)	127 (85%)	21 (14%)	1 (1%)	18	48
40	HG	149/179 (83%)	127 (85%)	20 (13%)	2 (1%)	9	32
41	BH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	16	44
41	DH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	7	27
41	FH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	7	27
41	HH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	7	27
42	BI	125/130 (96%)	105 (84%)	14 (11%)	6 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DI	125/130 (96%)	102 (82%)	22 (18%)	1 (1%)	16	44
42	FI	125/130 (96%)	106 (85%)	13 (10%)	6 (5%)	2	7
42	HI	125/130 (96%)	103 (82%)	19 (15%)	3 (2%)	4	18
43	BJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	2
43	DJ	96/103 (93%)	71 (74%)	19 (20%)	6 (6%)	1	3
43	FJ	96/103 (93%)	69 (72%)	21 (22%)	6 (6%)	1	3
43	HJ	96/103 (93%)	68 (71%)	19 (20%)	9 (9%)	0	1
44	BK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	1	5
44	DK	115/129 (89%)	92 (80%)	19 (16%)	4 (4%)	3	12
44	FK	115/129 (89%)	96 (84%)	13 (11%)	6 (5%)	1	5
44	HK	115/129 (89%)	91 (79%)	15 (13%)	9 (8%)	1	2
45	BL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	3	13
45	DL	121/124 (98%)	98 (81%)	20 (16%)	3 (2%)	4	17
45	FL	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	1	4
45	HL	121/124 (98%)	101 (84%)	15 (12%)	5 (4%)	2	9
46	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	1	5
46	DM	112/118 (95%)	96 (86%)	11 (10%)	5 (4%)	2	8
46	FM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	1	5
46	HM	112/118 (95%)	92 (82%)	12 (11%)	8 (7%)	1	2
47	BN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	3
47	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	5	20
47	FN	92/101 (91%)	71 (77%)	17 (18%)	4 (4%)	2	8
47	HN	92/101 (91%)	70 (76%)	18 (20%)	4 (4%)	2	8
48	BO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	19
48	DO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	FO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	HO	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	3	12
49	BP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	2	10
49	DP	80/82 (98%)	60 (75%)	15 (19%)	5 (6%)	1	3
49	FP	80/82 (98%)	62 (78%)	15 (19%)	3 (4%)	2	10
49	HP	80/82 (98%)	56 (70%)	21 (26%)	3 (4%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	1	6
50	DQ	78/84 (93%)	58 (74%)	14 (18%)	6 (8%)	1	2
50	FQ	78/84 (93%)	58 (74%)	17 (22%)	3 (4%)	2	10
50	HQ	78/84 (93%)	58 (74%)	13 (17%)	7 (9%)	0	1
51	BR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
51	DR	53/75 (71%)	46 (87%)	7 (13%)	0	100	100
51	FR	53/75 (71%)	48 (91%)	5 (9%)	0	100	100
51	HR	53/75 (71%)	49 (92%)	4 (8%)	0	100	100
52	BS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	9	32
52	DS	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
52	FS	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	4	17
52	HS	77/92 (84%)	66 (86%)	9 (12%)	2 (3%)	4	17
53	BT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	4	18
53	DT	83/87 (95%)	74 (89%)	6 (7%)	3 (4%)	2	11
53	FT	83/87 (95%)	75 (90%)	6 (7%)	2 (2%)	4	18
53	HT	83/87 (95%)	73 (88%)	8 (10%)	2 (2%)	4	18
54	BU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	1	4
54	DU	49/71 (69%)	25 (51%)	20 (41%)	4 (8%)	0	2
54	FU	49/71 (69%)	24 (49%)	21 (43%)	4 (8%)	0	2
54	HU	49/71 (69%)	29 (59%)	18 (37%)	2 (4%)	2	9
55	BV	686/704 (97%)	559 (82%)	92 (13%)	35 (5%)	1	6
55	DV	685/704 (97%)	559 (82%)	93 (14%)	33 (5%)	2	7
55	FV	685/704 (97%)	564 (82%)	89 (13%)	32 (5%)	2	7
55	HV	685/704 (97%)	562 (82%)	88 (13%)	35 (5%)	1	6
56	BW	2/6 (33%)	0	0	2 (100%)	0	0
56	DW	2/6 (33%)	0	1 (50%)	1 (50%)	0	0
56	FW	2/6 (33%)	2 (100%)	0	0	100	100
56	HW	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	25302/27000 (94%)	20075 (79%)	3885 (15%)	1342 (5%)	1	5

5 of 1342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	70	LYS
2	AC	104	LEU
2	AC	121	ALA
2	AC	140	VAL
4	AD	43	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	216/218 (99%)	199 (92%)	17 (8%)	11	34
2	CC	216/218 (99%)	200 (93%)	16 (7%)	13	38
2	EC	216/218 (99%)	193 (89%)	23 (11%)	6	22
2	GC	216/218 (99%)	203 (94%)	13 (6%)	17	47
4	AD	164/164 (100%)	143 (87%)	21 (13%)	4	14
4	CD	164/164 (100%)	146 (89%)	18 (11%)	6	20
4	ED	164/164 (100%)	146 (89%)	18 (11%)	6	20
4	GD	164/164 (100%)	149 (91%)	15 (9%)	9	28
5	AE	165/165 (100%)	146 (88%)	19 (12%)	5	18
5	CE	165/165 (100%)	153 (93%)	12 (7%)	13	38
5	EE	165/165 (100%)	148 (90%)	17 (10%)	7	23
5	GE	165/165 (100%)	149 (90%)	16 (10%)	8	25
6	AF	148/150 (99%)	135 (91%)	13 (9%)	9	29
6	CF	148/150 (99%)	138 (93%)	10 (7%)	14	42
6	EF	148/150 (99%)	131 (88%)	17 (12%)	5	18
6	GF	148/150 (99%)	145 (98%)	3 (2%)	48	78
7	AG	137/138 (99%)	122 (89%)	15 (11%)	6	20
7	CG	137/138 (99%)	125 (91%)	12 (9%)	9	29
7	EG	137/138 (99%)	119 (87%)	18 (13%)	4	13
7	GG	137/138 (99%)	126 (92%)	11 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	40/40 (100%)	38 (95%)	2 (5%)	22	53
8	CH	40/40 (100%)	39 (98%)	1 (2%)	42	74
8	EH	40/40 (100%)	36 (90%)	4 (10%)	7	24
8	GH	40/40 (100%)	38 (95%)	2 (5%)	22	53
9	AI	109/110 (99%)	106 (97%)	3 (3%)	38	72
9	CI	109/110 (99%)	105 (96%)	4 (4%)	30	64
9	EI	109/110 (99%)	105 (96%)	4 (4%)	30	64
9	GI	109/110 (99%)	106 (97%)	3 (3%)	38	72
10	AJ	116/116 (100%)	97 (84%)	19 (16%)	2	8
10	CJ	116/116 (100%)	100 (86%)	16 (14%)	3	12
10	EJ	116/116 (100%)	93 (80%)	23 (20%)	1	5
10	GJ	116/116 (100%)	102 (88%)	14 (12%)	5	16
11	AK	103/104 (99%)	88 (85%)	15 (15%)	3	10
11	CK	103/104 (99%)	87 (84%)	16 (16%)	2	9
11	EK	103/104 (99%)	87 (84%)	16 (16%)	2	9
11	GK	103/104 (99%)	89 (86%)	14 (14%)	3	12
12	AL	102/103 (99%)	90 (88%)	12 (12%)	5	17
12	CL	102/103 (99%)	92 (90%)	10 (10%)	7	25
12	EL	102/103 (99%)	90 (88%)	12 (12%)	5	17
12	GL	102/103 (99%)	95 (93%)	7 (7%)	14	41
13	AM	109/109 (100%)	93 (85%)	16 (15%)	3	10
13	CM	109/109 (100%)	93 (85%)	16 (15%)	3	10
13	EM	109/109 (100%)	96 (88%)	13 (12%)	5	16
13	GM	109/109 (100%)	99 (91%)	10 (9%)	8	27
14	AN	100/103 (97%)	90 (90%)	10 (10%)	7	24
14	CN	100/103 (97%)	94 (94%)	6 (6%)	17	47
14	EN	100/103 (97%)	94 (94%)	6 (6%)	17	47
14	GN	100/103 (97%)	92 (92%)	8 (8%)	11	34
15	AO	86/87 (99%)	78 (91%)	8 (9%)	8	27
15	CO	86/87 (99%)	79 (92%)	7 (8%)	11	33
15	EO	86/87 (99%)	77 (90%)	9 (10%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	GO	86/87 (99%)	79 (92%)	7 (8%)	11	33
16	AP	99/100 (99%)	86 (87%)	13 (13%)	4	13
16	CP	99/100 (99%)	86 (87%)	13 (13%)	4	13
16	EP	99/100 (99%)	86 (87%)	13 (13%)	4	13
16	GP	99/100 (99%)	87 (88%)	12 (12%)	5	16
17	AQ	89/90 (99%)	80 (90%)	9 (10%)	7	24
17	CQ	89/90 (99%)	84 (94%)	5 (6%)	19	50
17	EQ	89/90 (99%)	82 (92%)	7 (8%)	11	34
17	GQ	89/90 (99%)	82 (92%)	7 (8%)	11	34
18	AR	84/84 (100%)	74 (88%)	10 (12%)	5	16
18	CR	84/84 (100%)	75 (89%)	9 (11%)	6	22
18	ER	84/84 (100%)	72 (86%)	12 (14%)	3	11
18	GR	84/84 (100%)	73 (87%)	11 (13%)	4	13
19	AS	93/93 (100%)	83 (89%)	10 (11%)	6	21
19	CS	93/93 (100%)	81 (87%)	12 (13%)	4	13
19	ES	93/93 (100%)	82 (88%)	11 (12%)	5	17
19	GS	93/93 (100%)	88 (95%)	5 (5%)	20	51
20	AT	80/84 (95%)	75 (94%)	5 (6%)	16	45
20	CT	80/84 (95%)	75 (94%)	5 (6%)	16	45
20	ET	80/84 (95%)	72 (90%)	8 (10%)	7	24
20	GT	80/84 (95%)	77 (96%)	3 (4%)	29	64
21	AU	83/85 (98%)	75 (90%)	8 (10%)	8	26
21	CU	83/85 (98%)	79 (95%)	4 (5%)	23	55
21	EU	83/85 (98%)	78 (94%)	5 (6%)	17	47
21	GU	83/85 (98%)	79 (95%)	4 (5%)	23	55
22	AV	78/78 (100%)	73 (94%)	5 (6%)	16	44
22	CV	78/78 (100%)	72 (92%)	6 (8%)	12	35
22	EV	78/78 (100%)	74 (95%)	4 (5%)	21	53
22	GV	78/78 (100%)	74 (95%)	4 (5%)	21	53
23	AW	59/63 (94%)	50 (85%)	9 (15%)	3	9
23	CW	59/63 (94%)	53 (90%)	6 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	EW	59/63 (94%)	50 (85%)	9 (15%)	3	9
23	GW	59/63 (94%)	55 (93%)	4 (7%)	14	42
24	AX	67/68 (98%)	59 (88%)	8 (12%)	5	16
24	CX	67/68 (98%)	60 (90%)	7 (10%)	7	23
24	EX	67/68 (98%)	55 (82%)	12 (18%)	2	6
24	GX	67/68 (98%)	60 (90%)	7 (10%)	7	23
25	AY	55/55 (100%)	51 (93%)	4 (7%)	13	38
25	CY	55/55 (100%)	49 (89%)	6 (11%)	6	20
25	EY	55/55 (100%)	48 (87%)	7 (13%)	4	14
25	GY	55/55 (100%)	50 (91%)	5 (9%)	9	28
26	AZ	48/49 (98%)	38 (79%)	10 (21%)	1	4
26	CZ	48/49 (98%)	39 (81%)	9 (19%)	1	5
26	EZ	48/49 (98%)	42 (88%)	6 (12%)	4	15
26	GZ	48/49 (98%)	43 (90%)	5 (10%)	7	23
27	A0	47/48 (98%)	46 (98%)	1 (2%)	47	77
27	C0	47/48 (98%)	46 (98%)	1 (2%)	47	77
27	E0	47/48 (98%)	45 (96%)	2 (4%)	26	60
27	G0	47/48 (98%)	45 (96%)	2 (4%)	26	60
28	A1	45/49 (92%)	42 (93%)	3 (7%)	15	43
28	C1	45/49 (92%)	43 (96%)	2 (4%)	25	59
28	E1	45/49 (92%)	42 (93%)	3 (7%)	15	43
28	G1	45/49 (92%)	44 (98%)	1 (2%)	45	77
29	A2	38/38 (100%)	35 (92%)	3 (8%)	11	34
29	C2	38/38 (100%)	34 (90%)	4 (10%)	6	22
29	E2	38/38 (100%)	35 (92%)	3 (8%)	11	34
29	G2	38/38 (100%)	34 (90%)	4 (10%)	6	22
30	A3	51/52 (98%)	45 (88%)	6 (12%)	5	17
30	C3	51/52 (98%)	48 (94%)	3 (6%)	18	48
30	E3	51/52 (98%)	47 (92%)	4 (8%)	11	35
30	G3	51/52 (98%)	47 (92%)	4 (8%)	11	35
31	A4	34/34 (100%)	29 (85%)	5 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	C4	34/34 (100%)	29 (85%)	5 (15%)	3	10
31	E4	34/34 (100%)	31 (91%)	3 (9%)	9	29
31	G4	34/34 (100%)	31 (91%)	3 (9%)	9	29
32	A5	112/123 (91%)	93 (83%)	19 (17%)	2	7
32	C5	112/123 (91%)	97 (87%)	15 (13%)	4	12
32	E5	111/123 (90%)	95 (86%)	16 (14%)	3	11
33	A6	26/85 (31%)	21 (81%)	5 (19%)	1	5
34	BB	180/199 (90%)	165 (92%)	15 (8%)	10	32
34	DB	180/199 (90%)	166 (92%)	14 (8%)	11	35
34	FB	180/199 (90%)	167 (93%)	13 (7%)	13	39
34	HB	180/199 (90%)	167 (93%)	13 (7%)	13	39
36	BC	170/190 (90%)	153 (90%)	17 (10%)	7	24
36	DC	170/190 (90%)	158 (93%)	12 (7%)	13	40
36	FC	170/190 (90%)	155 (91%)	15 (9%)	9	29
36	HC	170/190 (90%)	159 (94%)	11 (6%)	15	44
37	BD	172/173 (99%)	164 (95%)	8 (5%)	23	56
37	DD	172/173 (99%)	163 (95%)	9 (5%)	21	52
37	FD	172/173 (99%)	164 (95%)	8 (5%)	23	56
37	HD	172/173 (99%)	166 (96%)	6 (4%)	32	66
38	BE	113/126 (90%)	104 (92%)	9 (8%)	11	34
38	DE	113/126 (90%)	106 (94%)	7 (6%)	16	46
38	FE	113/126 (90%)	103 (91%)	10 (9%)	9	29
38	HE	113/126 (90%)	104 (92%)	9 (8%)	11	34
39	BF	89/116 (77%)	80 (90%)	9 (10%)	7	24
39	DF	87/116 (75%)	84 (97%)	3 (3%)	32	66
39	FF	87/116 (75%)	79 (91%)	8 (9%)	8	27
39	HF	87/116 (75%)	83 (95%)	4 (5%)	24	57
40	BG	124/147 (84%)	114 (92%)	10 (8%)	11	33
40	DG	124/147 (84%)	121 (98%)	3 (2%)	43	75
40	FG	124/147 (84%)	120 (97%)	4 (3%)	34	68
40	HG	124/147 (84%)	122 (98%)	2 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BH	104/105 (99%)	95 (91%)	9 (9%)	9	30
41	DH	104/105 (99%)	97 (93%)	7 (7%)	15	43
41	FH	104/105 (99%)	99 (95%)	5 (5%)	23	55
41	HH	104/105 (99%)	94 (90%)	10 (10%)	8	26
42	BI	105/107 (98%)	93 (89%)	12 (11%)	5	18
42	DI	105/107 (98%)	100 (95%)	5 (5%)	23	55
42	FI	105/107 (98%)	96 (91%)	9 (9%)	10	30
42	HI	105/107 (98%)	99 (94%)	6 (6%)	18	49
43	BJ	86/90 (96%)	83 (96%)	3 (4%)	32	66
43	DJ	86/90 (96%)	80 (93%)	6 (7%)	14	40
43	FJ	86/90 (96%)	81 (94%)	5 (6%)	18	49
43	HJ	86/90 (96%)	81 (94%)	5 (6%)	18	49
44	BK	90/99 (91%)	85 (94%)	5 (6%)	19	50
44	DK	90/99 (91%)	88 (98%)	2 (2%)	45	77
44	FK	90/99 (91%)	81 (90%)	9 (10%)	7	24
44	HK	90/99 (91%)	83 (92%)	7 (8%)	11	35
45	BL	103/104 (99%)	95 (92%)	8 (8%)	11	35
45	DL	103/104 (99%)	96 (93%)	7 (7%)	14	42
45	FL	103/104 (99%)	95 (92%)	8 (8%)	11	35
45	HL	103/104 (99%)	98 (95%)	5 (5%)	22	54
46	BM	92/96 (96%)	86 (94%)	6 (6%)	15	44
46	DM	92/96 (96%)	89 (97%)	3 (3%)	33	67
46	FM	92/96 (96%)	88 (96%)	4 (4%)	26	60
46	HM	92/96 (96%)	87 (95%)	5 (5%)	20	51
47	BN	79/84 (94%)	74 (94%)	5 (6%)	16	45
47	DN	79/84 (94%)	77 (98%)	2 (2%)	42	74
47	FN	79/84 (94%)	76 (96%)	3 (4%)	29	64
47	HN	79/84 (94%)	79 (100%)	0	100	100
48	BO	76/77 (99%)	72 (95%)	4 (5%)	20	52
48	DO	76/77 (99%)	73 (96%)	3 (4%)	28	63
48	FO	76/77 (99%)	70 (92%)	6 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	HO	76/77 (99%)	73 (96%)	3 (4%)	28	63
49	BP	65/65 (100%)	61 (94%)	4 (6%)	16	46
49	DP	65/65 (100%)	62 (95%)	3 (5%)	24	57
49	FP	65/65 (100%)	62 (95%)	3 (5%)	24	57
49	HP	65/65 (100%)	63 (97%)	2 (3%)	35	69
50	BQ	74/78 (95%)	66 (89%)	8 (11%)	6	21
50	DQ	74/78 (95%)	71 (96%)	3 (4%)	27	61
50	FQ	74/78 (95%)	70 (95%)	4 (5%)	20	51
50	HQ	74/78 (95%)	69 (93%)	5 (7%)	14	42
51	BR	48/65 (74%)	46 (96%)	2 (4%)	26	60
51	DR	48/65 (74%)	46 (96%)	2 (4%)	26	60
51	FR	48/65 (74%)	47 (98%)	1 (2%)	47	77
51	HR	48/65 (74%)	48 (100%)	0	100	100
52	BS	70/79 (89%)	64 (91%)	6 (9%)	10	30
52	DS	70/79 (89%)	68 (97%)	2 (3%)	37	71
52	FS	70/79 (89%)	67 (96%)	3 (4%)	26	60
52	HS	70/79 (89%)	68 (97%)	2 (3%)	37	71
53	BT	65/66 (98%)	58 (89%)	7 (11%)	6	21
53	DT	65/66 (98%)	59 (91%)	6 (9%)	8	27
53	FT	65/66 (98%)	59 (91%)	6 (9%)	8	27
53	HT	65/66 (98%)	55 (85%)	10 (15%)	2	9
54	BU	44/61 (72%)	37 (84%)	7 (16%)	2	8
54	DU	44/61 (72%)	41 (93%)	3 (7%)	14	42
54	FU	44/61 (72%)	39 (89%)	5 (11%)	5	18
54	HU	44/61 (72%)	43 (98%)	1 (2%)	44	76
55	BV	568/578 (98%)	510 (90%)	58 (10%)	7	23
55	DV	568/578 (98%)	514 (90%)	54 (10%)	8	26
55	FV	568/578 (98%)	519 (91%)	49 (9%)	10	30
55	HV	568/578 (98%)	525 (92%)	43 (8%)	12	36
56	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	FW	2/2 (100%)	1 (50%)	1 (50%)	0 0
56	HW	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	21011/21990 (96%)	19244 (92%)	1767 (8%)	10 31

5 of 1767 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	DV	685	LEU
19	ES	45	VAL
55	HV	560	GLN
26	GZ	7	THR
4	ED	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
2	EC	24	HIS
38	FE	12	GLN
55	HV	579	HIS
43	HJ	56	HIS
6	EF	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	117/120 (97%)	17 (14%)	0
1	CB	117/120 (97%)	19 (16%)	0
1	EB	117/120 (97%)	18 (15%)	0
1	GB	117/120 (97%)	20 (17%)	0
3	AA	2850/2904 (98%)	457 (16%)	40 (1%)
3	CA	2850/2904 (98%)	457 (16%)	39 (1%)
3	EA	2850/2904 (98%)	452 (15%)	36 (1%)
3	GA	2850/2904 (98%)	459 (16%)	38 (1%)
35	BA	1532/1542 (99%)	265 (17%)	17 (1%)
35	DA	1532/1542 (99%)	264 (17%)	14 (0%)
35	FA	1532/1542 (99%)	263 (17%)	16 (1%)
35	HA	1532/1542 (99%)	268 (17%)	15 (0%)
All	All	17996/18264 (98%)	2959 (16%)	215 (1%)

5 of 2959 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	3	C
1	AB	15	A
1	AB	16	G
1	AB	21	G
1	AB	30	C

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	EA	503	A
3	EA	2423	U
3	GA	2902	C
3	EA	784	G
3	EA	1378	A

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

16 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	$\# Z > 2$
56	5OH	DW	6	56	7,12,13	1.82	2 (28%)	4,16,18	1.91	3 (75%)
56	KBE	BW	1	56	8,8,9	1.23	2 (25%)	6,8,10	1.30	1 (16%)
56	DPP	DW	2	56	4,5,6	0.89	0	1,5,7	0.82	0
56	UAL	DW	5	56	6,8,9	2.50	3 (50%)	4,9,11	4.33	2 (50%)
56	UAL	HW	5	56	6,8,9	3.19	3 (50%)	4,9,11	4.61	3 (75%)
56	KBE	DW	1	56	8,8,9	0.98	0	6,8,10	1.47	2 (33%)
56	DPP	BW	2	56	4,5,6	1.00	0	1,5,7	0.46	0
56	KBE	FW	1	56	8,8,9	0.96	0	6,8,10	1.09	0
56	KBE	HW	1	56	8,8,9	0.94	0	6,8,10	1.24	1 (16%)
56	DPP	HW	2	56	4,5,6	0.99	0	1,5,7	0.35	0
56	5OH	FW	6	56	7,12,13	2.07	2 (28%)	4,16,18	1.75	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	UAL	FW	5	56	6,8,9	2.47	3 (50%)	4,9,11	5.15	1 (25%)
56	5OH	HW	6	56	7,12,13	1.77	2 (28%)	4,16,18	1.42	1 (25%)
56	UAL	BW	5	56	6,8,9	2.51	3 (50%)	4,9,11	4.46	1 (25%)
56	5OH	BW	6	56	7,12,13	1.81	2 (28%)	4,16,18	2.49	2 (50%)
56	DPP	FW	2	56	4,5,6	1.23	0	1,5,7	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5OH	DW	6	56	-	1/2/18/20	0/1/1/1
56	KBE	BW	1	56	-	7/7/7/8	-
56	DPP	DW	2	56	-	0/2/4/6	-
56	UAL	DW	5	56	-	1/3/7/9	-
56	UAL	HW	5	56	-	1/3/7/9	-
56	KBE	DW	1	56	-	3/7/7/8	-
56	DPP	BW	2	56	-	0/2/4/6	-
56	KBE	FW	1	56	-	3/7/7/8	-
56	KBE	HW	1	56	-	4/7/7/8	-
56	DPP	HW	2	56	-	0/2/4/6	-
56	5OH	FW	6	56	-	0/2/18/20	0/1/1/1
56	UAL	FW	5	56	-	0/3/7/9	-
56	5OH	HW	6	56	-	1/2/18/20	0/1/1/1
56	UAL	BW	5	56	-	0/3/7/9	-
56	5OH	BW	6	56	-	0/2/18/20	0/1/1/1
56	DPP	FW	2	56	-	0/2/4/6	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	HW	5	UAL	C1-N1	4.85	1.47	1.40
56	HW	5	UAL	CB-N1	4.44	1.47	1.35
56	FW	5	UAL	CB-N1	4.16	1.46	1.35
56	HW	5	UAL	C-CA	4.15	1.52	1.45
56	BW	5	UAL	CB-N1	4.15	1.46	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	FW	5	UAL	O-C-CA	-10.13	112.69	125.39
56	BW	5	UAL	O-C-CA	-8.81	114.35	125.39
56	HW	5	UAL	O-C-CA	-8.73	114.45	125.39
56	DW	5	UAL	O-C-CA	-8.24	115.06	125.39
56	BW	6	5OH	O-C-CA	-3.70	115.26	124.77

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	1	KBE	O-C-CA-CB
56	BW	1	KBE	C-CA-CB-N
56	BW	1	KBE	C-CA-CB-CG
56	BW	1	KBE	N-CB-CG-CD
56	BW	1	KBE	CA-CB-CG-CD

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DW	6	5OH	1	0
56	BW	1	KBE	2	0
56	DW	5	UAL	2	0
56	DW	1	KBE	2	0
56	FW	1	KBE	1	0
56	HW	1	KBE	3	0
56	HW	2	DPP	1	0
56	FW	6	5OH	1	0
56	FW	5	UAL	1	0
56	HW	6	5OH	2	0
56	BW	5	UAL	2	0
56	BW	6	5OH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 756 ligands modelled in this entry, 752 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
59	GCP	BV	801	57	32,34,34	1.85	9 (28%)	49,54,54	1.95	13 (26%)
59	GCP	DV	801	57	32,34,34	1.76	8 (25%)	49,54,54	1.94	13 (26%)
59	GCP	FV	801	57	32,34,34	1.74	7 (21%)	49,54,54	1.99	14 (28%)
59	GCP	HV	801	57	32,34,34	1.71	7 (21%)	49,54,54	1.91	18 (36%)

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
59	GCP	BV	801	57	-	2/19/38/38	0/3/3/3
59	GCP	DV	801	57	-	1/19/38/38	0/3/3/3
59	GCP	FV	801	57	-	3/19/38/38	0/3/3/3
59	GCP	HV	801	57	-	3/19/38/38	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	HV	801	GCP	C2-N2	4.90	1.45	1.34
59	FV	801	GCP	C2-N2	4.69	1.45	1.34
59	DV	801	GCP	C2-N2	4.52	1.44	1.34
59	BV	801	GCP	C2-N2	4.51	1.44	1.34
59	FV	801	GCP	C2'-C3'	-4.18	1.42	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BV	801	GCP	PB-O3A-PA	-5.82	113.39	132.37
59	FV	801	GCP	C2-N3-C4	5.69	122.10	112.30
59	FV	801	GCP	C5-C4-N3	-5.55	119.56	128.39
59	DV	801	GCP	PB-O3A-PA	-5.22	115.35	132.37
59	HV	801	GCP	C2-N3-C4	5.20	121.25	112.30

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BV	801	GCP	PB-C3B-PG-O3G
59	FV	801	GCP	PB-C3B-PG-O1G
59	FV	801	GCP	PB-C3B-PG-O2G
59	FV	801	GCP	PB-C3B-PG-O3G
59	HV	801	GCP	PB-C3B-PG-O1G

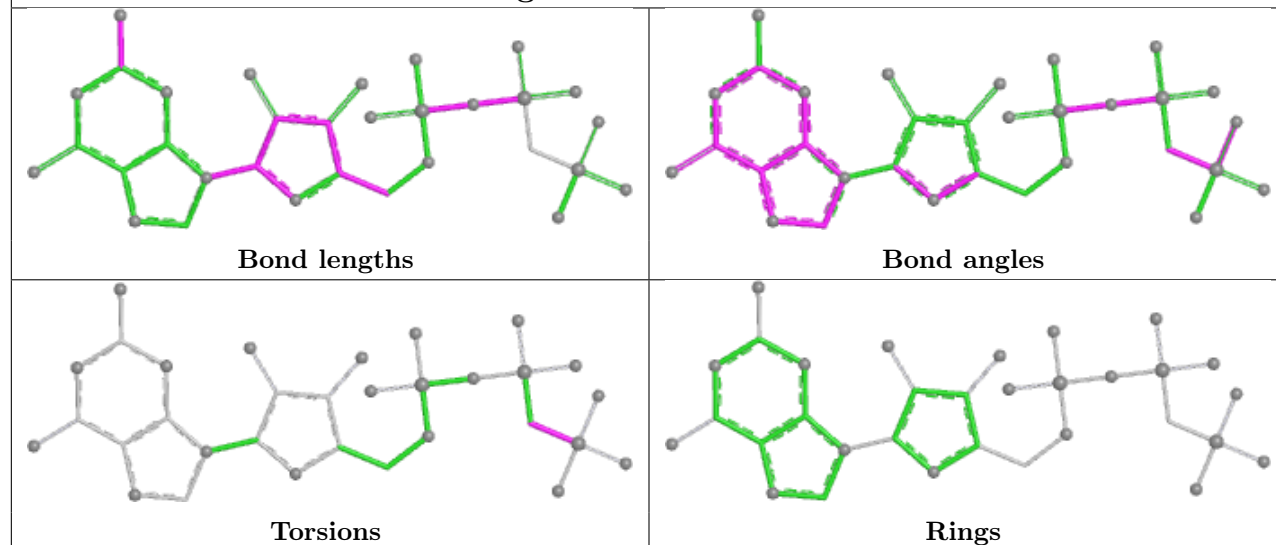
There are no ring outliers.

4 monomers are involved in 5 short contacts:

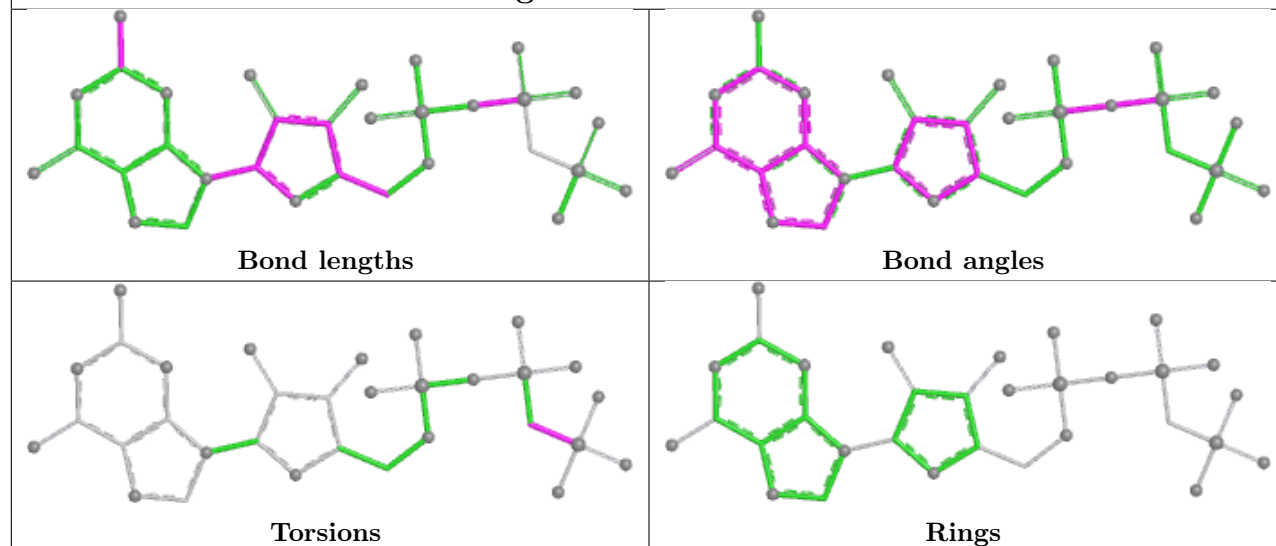
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	BV	801	GCP	1	0
59	DV	801	GCP	1	0
59	FV	801	GCP	2	0
59	HV	801	GCP	1	0

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

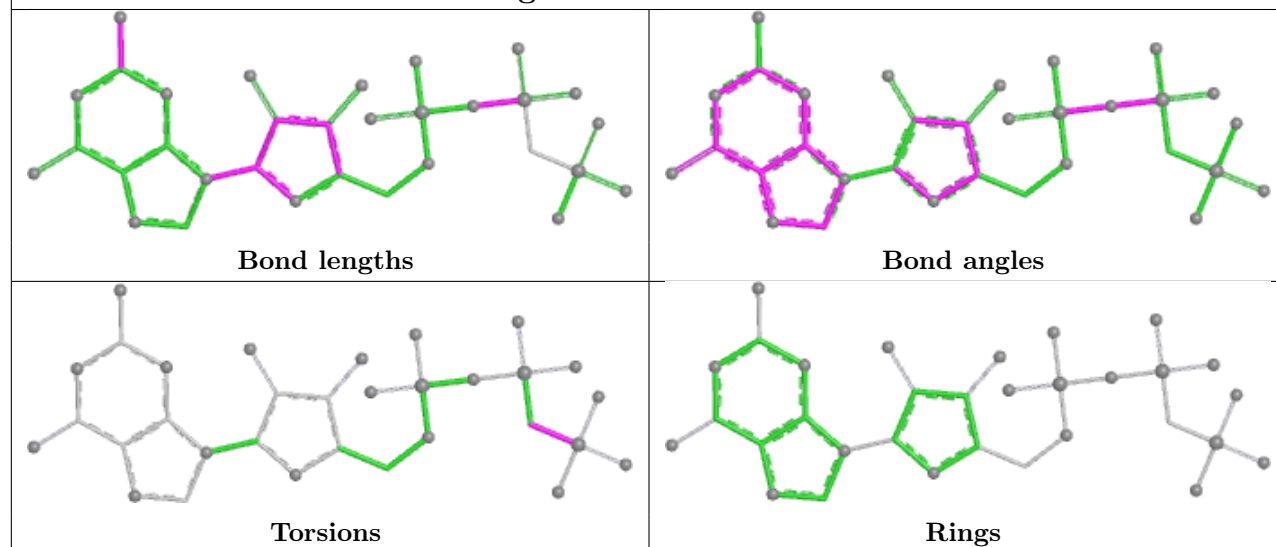
Ligand GCP BV 801

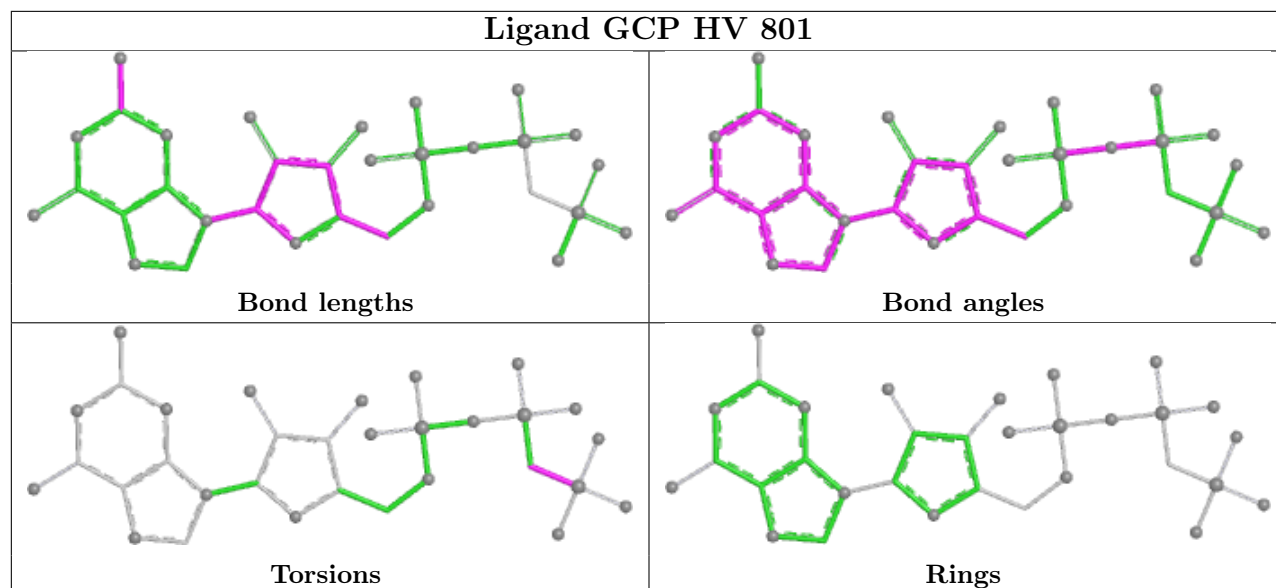


Ligand GCP DV 801



Ligand GCP FV 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.