



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:36 am BST

PDB ID : 6BOH
Title : Antibiotic blasticidin S and E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-11-20
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

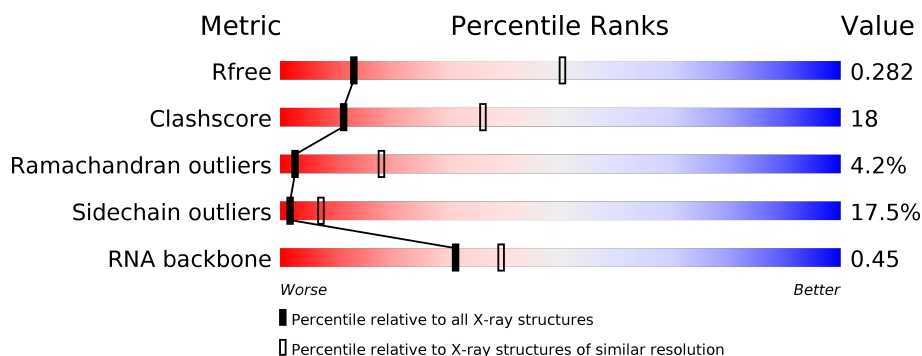
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



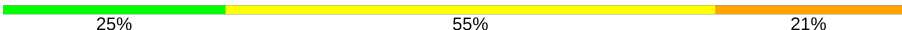

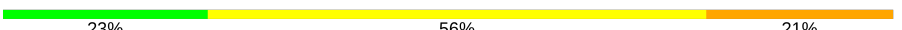
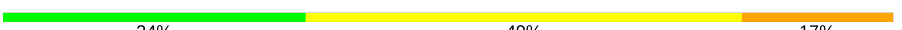





















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	1507	34% 50% 15%
1	FB	1507	35% 50% 14% .
2	B	2880	34% 45% 19% .
2	GB	2880	37% 43% 18% .
3	C	120	40% 50% 10%
3	HB	120	40% 51% 8% .



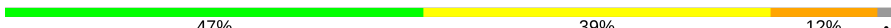

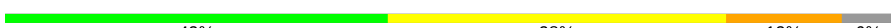
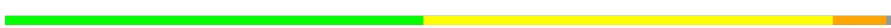



















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Mol	Chain	Length	Quality of chain
4	D	77	
4	IA	77	
4	IB	77	
4	NC	77	
5	E	275	
5	JB	275	
6	F	206	
6	KB	206	
7	G	205	
7	LB	205	
8	H	182	
8	MB	182	
9	I	180	
9	NB	180	
10	J	148	
10	OB	148	
11	K	140	
11	PB	140	
12	L	122	
12	QB	122	
13	M	150	
13	RB	150	
14	N	141	
14	SB	141	
15	O	118	




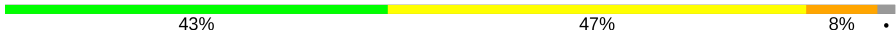





















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Mol	Chain	Length	Quality of chain
15	TB	118	
16	P	112	
16	UB	112	
17	Q	146	
17	VB	146	
18	R	118	
18	WB	118	
19	S	101	
19	XB	101	
20	T	113	
20	YB	113	
21	U	96	
21	ZB	96	
22	AC	110	
22	V	110	
23	BC	206	
23	W	206	
24	CC	85	
24	X	85	
25	DC	98	
25	Y	98	
26	EC	72	
26	Z	72	
27	AA	60	
27	FC	60	

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Mol	Chain	Length	Quality of chain
28	BA	71	
28	GC	71	
29	CA	60	
29	HC	60	
30	DA	54	
30	IC	54	
31	EA	49	
31	JC	49	
32	FA	65	
32	KC	65	
33	GA	37	
33	LC	37	
34	HA	27	
34	MC	27	
35	JA	365	
35	KA	365	
35	OC	365	
35	PC	365	
36	LA	256	
36	QC	256	
37	MA	239	
37	RC	239	
38	NA	209	
38	SC	209	
39	OA	162	

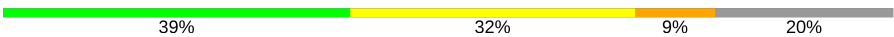
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Mol	Chain	Length	Quality of chain
39	TC	162	
40	PA	101	
40	UC	101	
41	QA	156	
41	VC	156	
42	RA	138	
42	WC	138	
43	SA	128	
43	XC	128	
44	TA	105	
44	YC	105	
45	UA	129	
45	ZC	129	
46	AD	132	
46	VA	132	
47	BD	126	
47	WA	126	
48	CD	61	
48	XA	61	
49	DD	89	
49	YA	89	
50	ED	88	
50	ZA	88	
51	AB	105	
51	FD	105	

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Mol	Chain	Length	Quality of chain
52	BB	88	
52	GD	88	
53	CB	93	
53	HD	93	
54	DB	106	
54	ID	106	
55	EB	27	
55	JD	27	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 298186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	FB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	GB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	154A	C	UNK	conflict	GB 46197919
GB	154A	C	UNK	conflict	GB 46197919

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	HB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	IB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	NC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	JB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	KB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	LB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	MB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	NB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	OB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	PB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	QB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	RB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	SB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	TB	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
16	UB	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	VB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	WB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	XB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	YB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	ZB	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	AC	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	BC	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	CC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	11	ARG	LYS	conflict	UNP Q72HR3

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	DC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	EC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	FC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	GC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	HC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	IC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	EA	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	JC	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	FA	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	KC	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	GA	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	LC	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	MC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	110	Total 850	C 525	N 157	O 164	S 4	0	0	0
35	KA	55	Total 455	C 281	N 83	O 89	S 2	0	0	0
35	OC	110	Total 850	C 525	N 157	O 164	S 4	0	0	0
35	PC	55	Total 455	C 281	N 83	O 89	S 2	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	?	-	ASP	deletion	UNP B7MKB3
JA	?	-	ARG	deletion	UNP B7MKB3
JA	?	-	SER	deletion	UNP B7MKB3
JA	358	LEU	-	expression tag	UNP B7MKB3
JA	359	GLU	-	expression tag	UNP B7MKB3
JA	360	HIS	-	expression tag	UNP B7MKB3
JA	361	HIS	-	expression tag	UNP B7MKB3
JA	362	HIS	-	expression tag	UNP B7MKB3
JA	363	HIS	-	expression tag	UNP B7MKB3
JA	364	HIS	-	expression tag	UNP B7MKB3
JA	365	HIS	-	expression tag	UNP B7MKB3
KA	?	-	ASP	deletion	UNP B7MKB3
KA	?	-	ARG	deletion	UNP B7MKB3
KA	?	-	SER	deletion	UNP B7MKB3
KA	361	LEU	-	expression tag	UNP B7MKB3
KA	362	GLU	-	expression tag	UNP B7MKB3
KA	363	HIS	-	expression tag	UNP B7MKB3
KA	364	HIS	-	expression tag	UNP B7MKB3
KA	365	HIS	-	expression tag	UNP B7MKB3
KA	366	HIS	-	expression tag	UNP B7MKB3
KA	367	HIS	-	expression tag	UNP B7MKB3
KA	368	HIS	-	expression tag	UNP B7MKB3
OC	?	-	ASP	deletion	UNP B7MKB3
OC	?	-	ARG	deletion	UNP B7MKB3
OC	?	-	SER	deletion	UNP B7MKB3
OC	358	LEU	-	expression tag	UNP B7MKB3
OC	359	GLU	-	expression tag	UNP B7MKB3
OC	360	HIS	-	expression tag	UNP B7MKB3
OC	361	HIS	-	expression tag	UNP B7MKB3
OC	362	HIS	-	expression tag	UNP B7MKB3
OC	363	HIS	-	expression tag	UNP B7MKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
OC	364	HIS	-	expression tag	UNP B7MKB3
OC	365	HIS	-	expression tag	UNP B7MKB3
PC	?	-	ASP	deletion	UNP B7MKB3
PC	?	-	ARG	deletion	UNP B7MKB3
PC	?	-	SER	deletion	UNP B7MKB3
PC	361	LEU	-	expression tag	UNP B7MKB3
PC	362	GLU	-	expression tag	UNP B7MKB3
PC	363	HIS	-	expression tag	UNP B7MKB3
PC	364	HIS	-	expression tag	UNP B7MKB3
PC	365	HIS	-	expression tag	UNP B7MKB3
PC	366	HIS	-	expression tag	UNP B7MKB3
PC	367	HIS	-	expression tag	UNP B7MKB3
PC	368	HIS	-	expression tag	UNP B7MKB3

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	LA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
36	QC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	MA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
37	RC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 38 is a protein called 50S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	NA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	SC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	OA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	TC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	PA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	UC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	QA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	VC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	WC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	SA	127	Total	C	N	O		0	0	0
			1011	639	198	174				
43	XC	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	TA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	YC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	UA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	ZC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	VA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	AD	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	WA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	BD	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	XA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	CD	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	YA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	DD	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	ZA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	ED	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	AB	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	FD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	GD	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	HD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	ID	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	EB	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	JD	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	MC	3	Total	Mg	0	0
			3	3		
56	NC	10	Total	Mg	0	0
			10	10		
56	QA	1	Total	Mg	0	0
			1	1		
56	K	4	Total	Mg	0	0
			4	4		
56	JC	1	Total	Mg	0	0
			1	1		
56	LB	4	Total	Mg	0	0
			4	4		
56	B	433	Total	Mg	0	0
			433	433		
56	YA	3	Total	Mg	0	0
			3	3		
56	RC	2	Total	Mg	0	0
			2	2		
56	UA	1	Total	Mg	0	0
			1	1		
56	AC	1	Total	Mg	0	0
			1	1		
56	HA	3	Total	Mg	0	0
			3	3		
56	ZC	1	Total	Mg	0	0
			1	1		
56	OA	4	Total	Mg	0	0
			4	4		
56	PA	3	Total	Mg	0	0
			3	3		
56	SC	4	Total	Mg	0	0
			4	4		
56	DC	1	Total	Mg	0	0
			1	1		
56	S	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	1	Total 1	Mg 1	0	0
56	BB	1	Total 1	Mg 1	0	0
56	J	1	Total 1	Mg 1	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	CC	1	Total 1	Mg 1	0	0
56	E	6	Total 6	Mg 6	0	0
56	VC	1	Total 1	Mg 1	0	0
56	IA	9	Total 9	Mg 9	0	0
56	V	2	Total 2	Mg 2	0	0
56	FB	194	Total 194	Mg 194	0	0
56	IB	2	Total 2	Mg 2	0	0
56	AA	1	Total 1	Mg 1	0	0
56	IC	1	Total 1	Mg 1	0	0
56	SB	2	Total 2	Mg 2	0	0
56	GB	402	Total 402	Mg 402	0	0
56	R	1	Total 1	Mg 1	0	0
56	HB	20	Total 20	Mg 20	0	0
56	VB	3	Total 3	Mg 3	0	0
56	AB	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	M	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FA	1	Total 1	Mg 1	0	0
56	GC	1	Total 1	Mg 1	0	0
56	PB	2	Total 2	Mg 2	0	0
56	D	5	Total 5	Mg 5	0	0
56	DD	1	Total 1	Mg 1	0	0
56	MA	6	Total 6	Mg 6	0	0
56	NA	2	Total 2	Mg 2	0	0
56	UC	3	Total 3	Mg 3	0	0
56	XB	2	Total 2	Mg 2	0	0
56	JA	1	Total 1	Mg 1	0	0
56	TB	1	Total 1	Mg 1	0	0
56	VA	2	Total 2	Mg 2	0	0
56	A	183	Total 183	Mg 183	0	0
56	Z	1	Total 1	Mg 1	0	0
56	KC	1	Total 1	Mg 1	0	0
56	SA	1	Total 1	Mg 1	0	0
56	U	1	Total 1	Mg 1	0	0
56	QB	2	Total 2	Mg 2	0	0
56	L	3	Total 3	Mg 3	0	0
56	EA	1	Total 1	Mg 1	0	0
56	LA	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	OC	1	Total 1	Mg 1	0	0
56	PC	1	Total 1	Mg 1	0	0
56	G	2	Total 2	Mg 2	0	0
56	ED	1	Total 1	Mg 1	0	0
56	Q	1	Total 1	Mg 1	0	0
56	NB	1	Total 1	Mg 1	0	0
56	UB	4	Total 4	Mg 4	0	0
56	WC	1	Total 1	Mg 1	0	0
56	H	2	Total 2	Mg 2	0	0
56	JB	5	Total 5	Mg 5	0	0
56	TC	3	Total 3	Mg 3	0	0
56	C	22	Total 22	Mg 22	0	0
56	QC	3	Total 3	Mg 3	0	0
56	KB	2	Total 2	Mg 2	0	0
56	CB	1	Total 1	Mg 1	0	0
56	BD	1	Total 1	Mg 1	0	0
56	T	2	Total 2	Mg 2	0	0
56	HD	1	Total 1	Mg 1	0	0
56	AD	4	Total 4	Mg 4	0	0
56	O	2	Total 2	Mg 2	0	0
56	Y	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	OB	1	Total Mg 1 1	0	0
56	F	4	Total Mg 4 4	0	0
56	RB	3	Total Mg 3 3	0	0

- # BLS

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	B	1	Total 30	C 17	N 8	O 5	0	0
57	GB	1	Total 30	C 17	N 8	O 5	0	0

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 58 | BA | 1 | Total Zn
1 1 | 0 | 0 |
| 58 | CA | 1 | Total Zn
1 1 | 0 | 0 |
| 58 | AC | 1 | Total Zn
1 1 | 0 | 0 |
| 58 | V | 1 | Total Zn
1 1 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

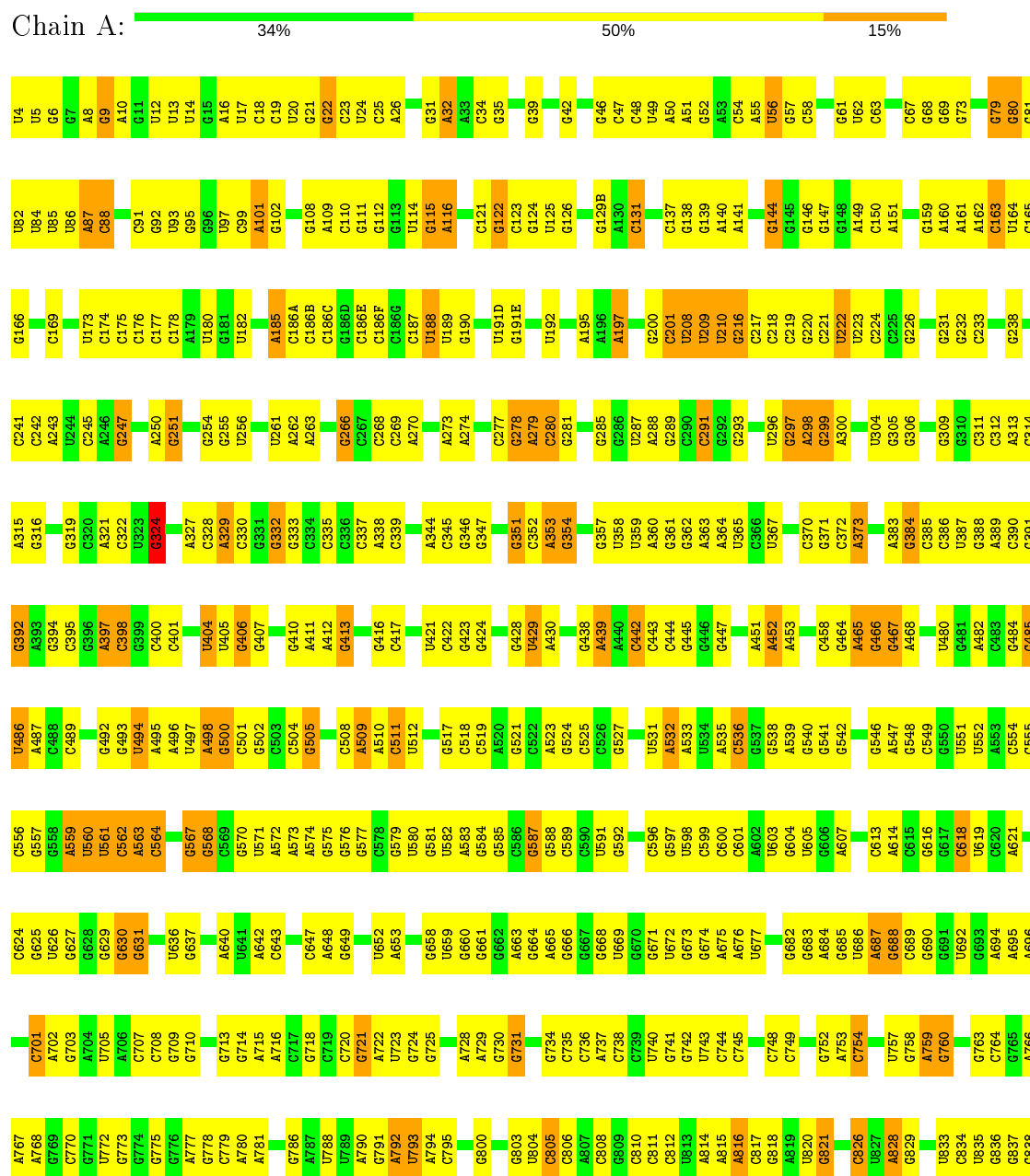
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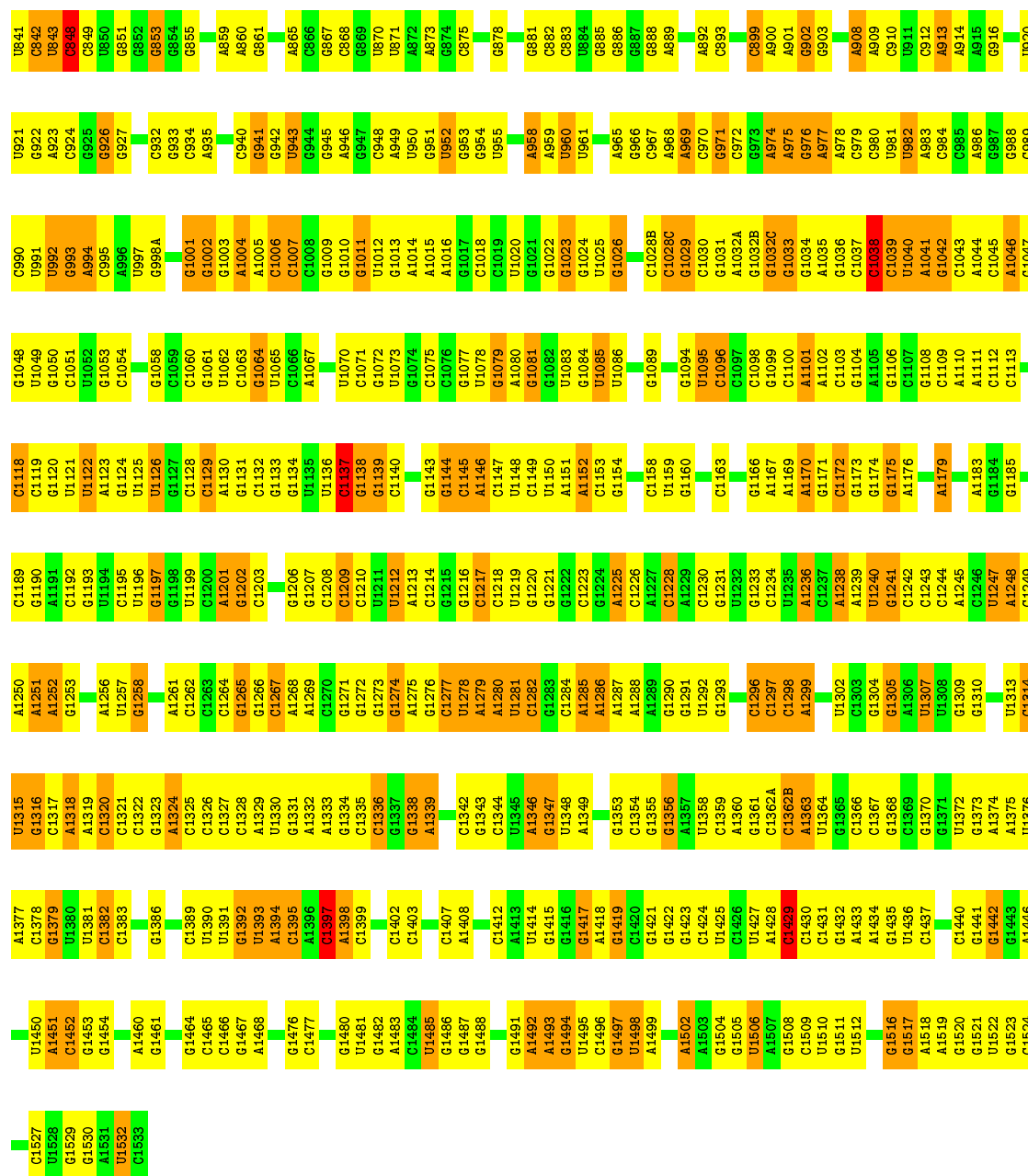
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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58	IC	1	Total 1	Zn 1	0	0
58	DA	1	Total 1	Zn 1	0	0
58	GC	1	Total 1	Zn 1	0	0
58	HC	1	Total 1	Zn 1	0	0
58	LC	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

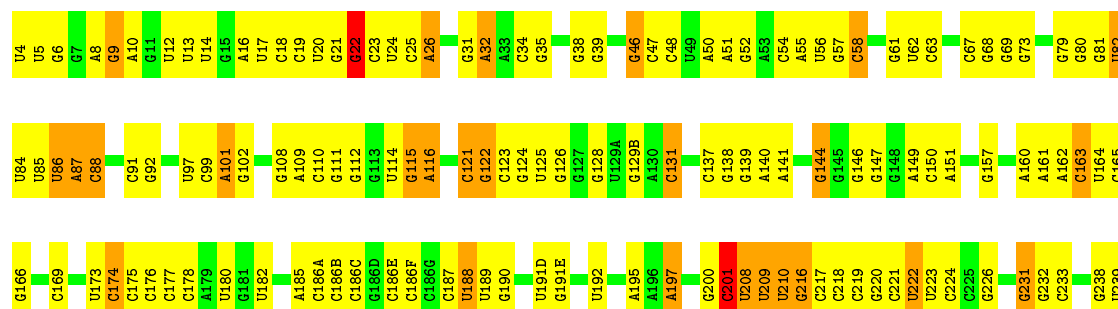
• Molecule 1: 16S ribosomal RNA



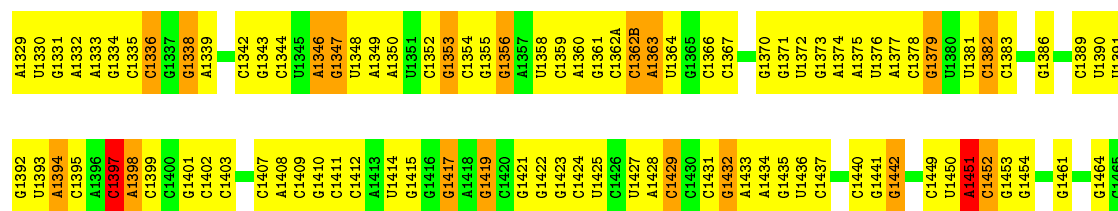


• Molecule 1: 16S ribosomal RNA

Chain FB: 35% 50% 14%

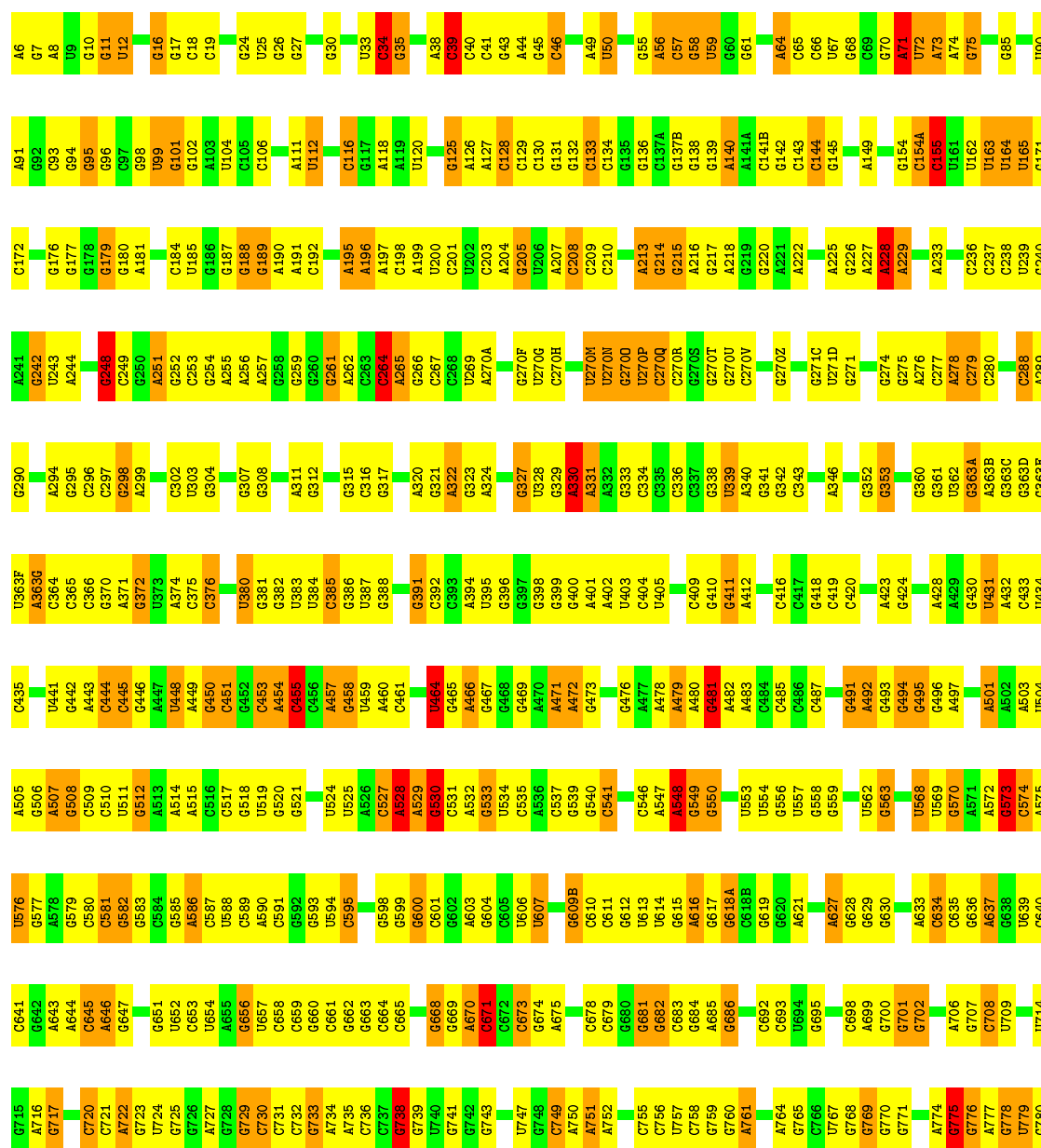


G1266	C1267	A1268	A1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	A1279	A1280	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	A1306	G1307	G1308	G1309	G1310	U1313	C1314	U1315	G1316	C1317	A1318	C1319	C1320	C1321	C1322	G1323	G1324	A1325	A1326	A1327	A1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	G1348	A1349	C1350	C1351	C1352	A1353	G1354	G1357	A1360	G1361	G1362	G1363	A1364	G1365	C1366	U1367	A1370	G1371	A1372	A1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	C1401	U1404	U1405	A1406	G1407	G1410	A1411	A1412	G1413	G1416	G1417	A1418	G1419	U1421	C1422	G1423	G1424	G1428	U1429	A1430	A1431	G1439	U1440	C1442	C1443	C1444	G1445	G1446	G1447	A1451	A1452	C1453	G1458	G1459	G1464	A1465	G1466	G1467	A1468	U1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	U1512	G1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	U1531	A1532	U1533	U1534	A1535	A1536	A1537	G1538	A1539	G1540	G1541	G1542	G1546	A1547	G1548	G1549	G1550	G1551	U1552	A1553	C1554	C1555	A1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	A1602	U1603	G1604	U1605	G1606	A1607	C1613	A1614	G1615	G1616	G1617	G1618	G1619	U1620	A1621	C1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	G1683	A1684	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743	A1744	A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A1791	A1792	A1793	A1794	A1795	A1796	A1797	A1798	A1799	A1800	A1801	A1802	A1803	A1804	A1805	A1806	A1807	A1808	A1809	A1810	A1811	A1812	A1813	A1814	A1815	A1816	A1817	A1818	A1819	A1820	A1821	A1822	A1823	A1824	A1825	A1826	A1827	A1828	A1829	A1830	A1831	A1832	A1833	A1834	A1835	A1836	A1837	A1838	A1839	A1840	A1841	A1842	A1843	A1844	A1845	A1846	A1847	A1848	A1849	A1850	A1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2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• Molecule 2: 23S ribosomal RNA

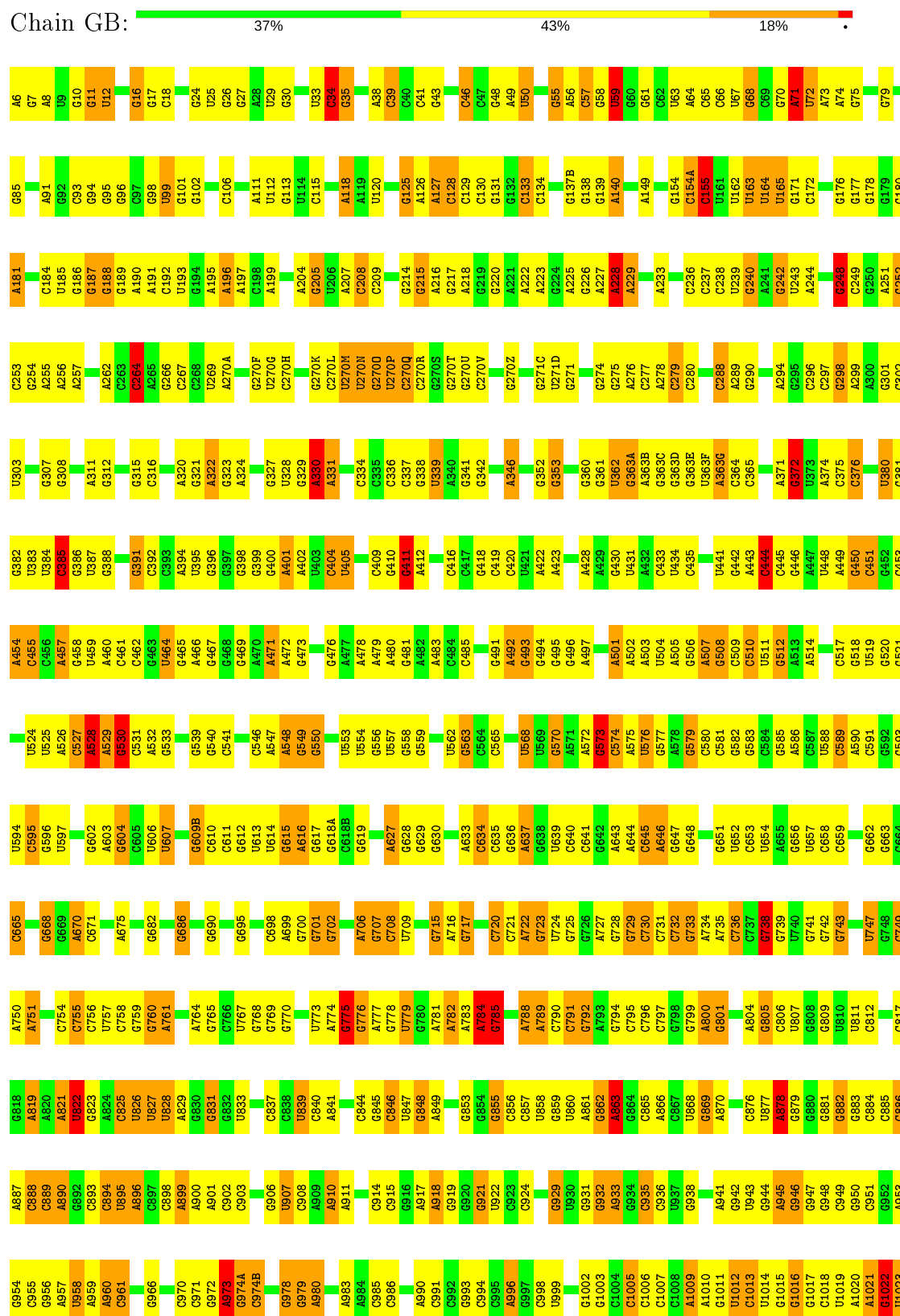
Chain B:  34%  45%  19% •





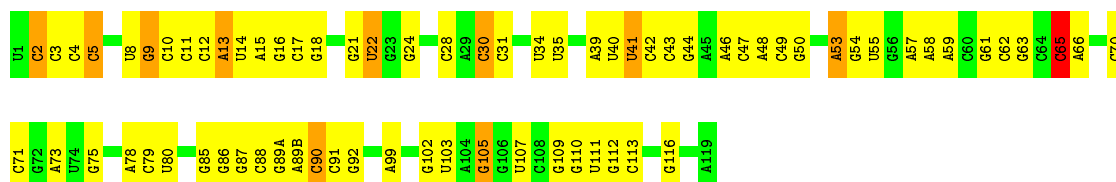


• Molecule 2: 23S ribosomal RNA

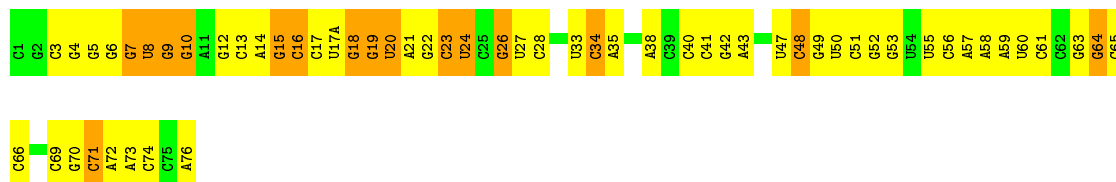


WORLDWIDE
PDB
PROTEIN DATA BANK

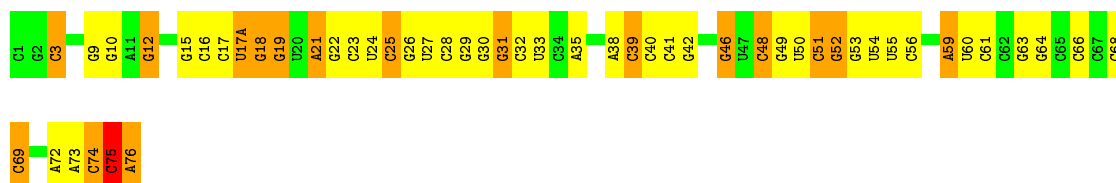




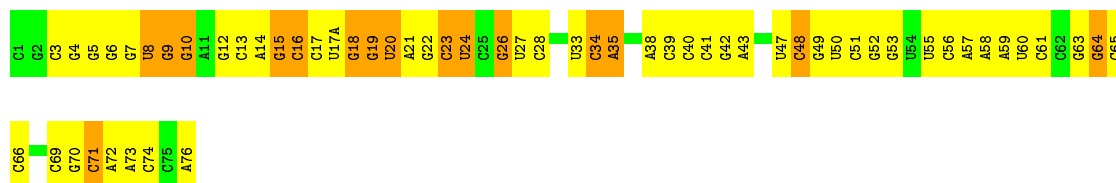
- Molecule 4: tRNA



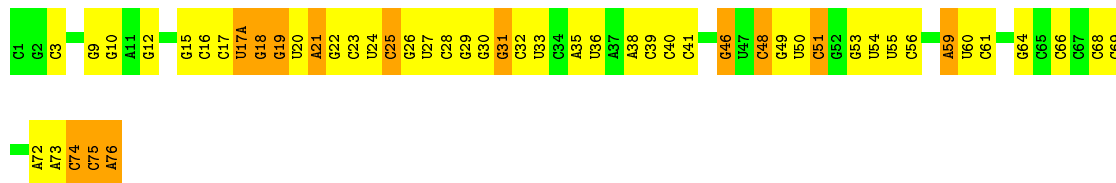
- Molecule 4: tRNA



- Molecule 4: tRNA

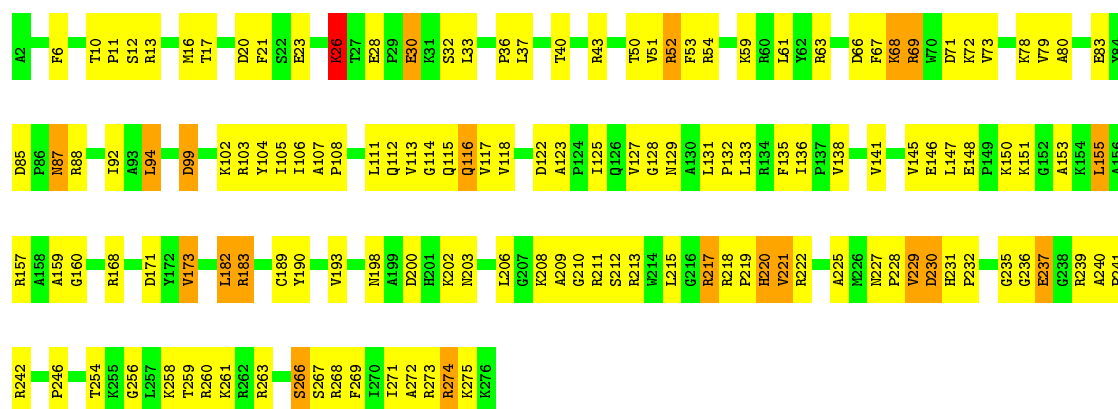


- Molecule 4: tRNA



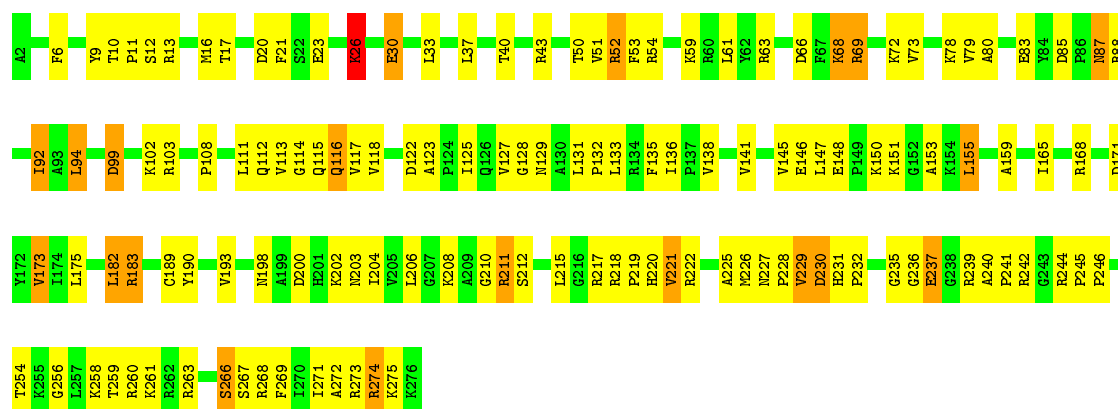
- Molecule 5: 50S ribosomal protein L2





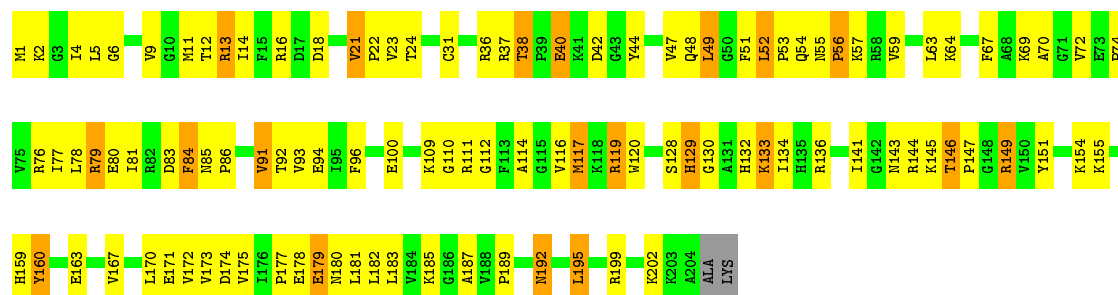
• Molecule 5: 50S ribosomal protein L2

Chain JB: 51% 41% 7%



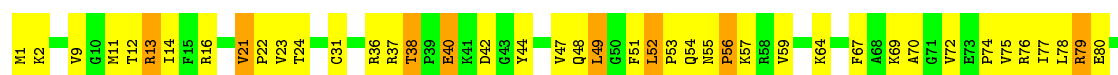
• Molecule 6: 50S ribosomal protein L3

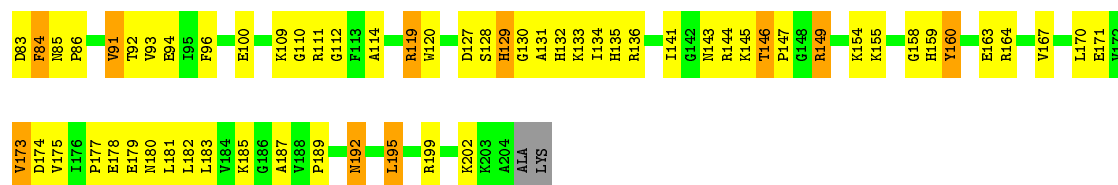
Chain F: 47% 42% 10%



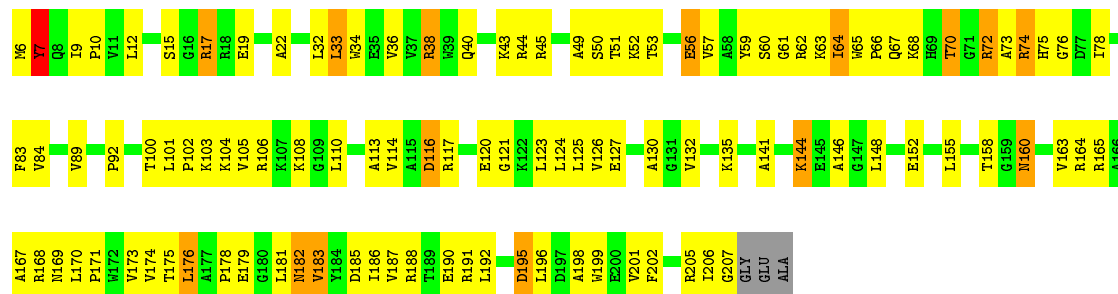
• Molecule 6: 50S ribosomal protein L3

Chain KB: 49% 41% 9%

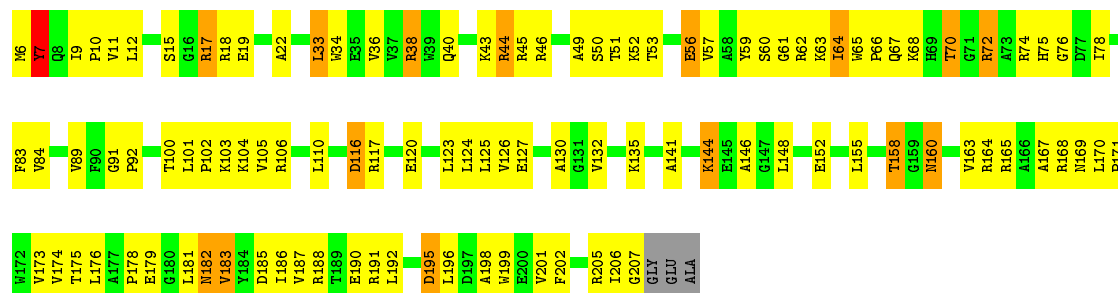




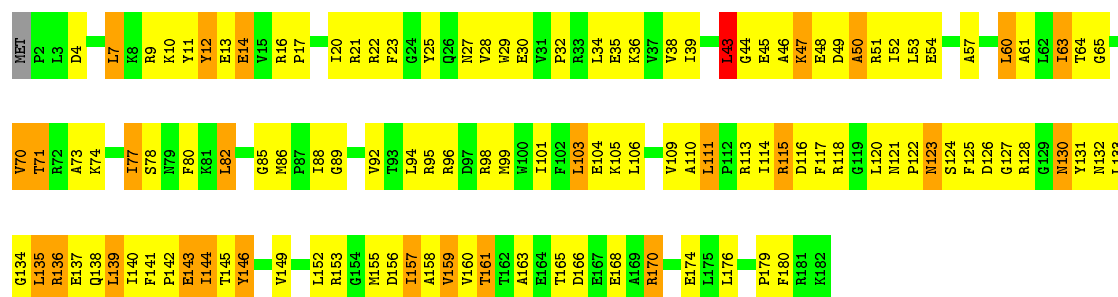
• Molecule 7: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L4

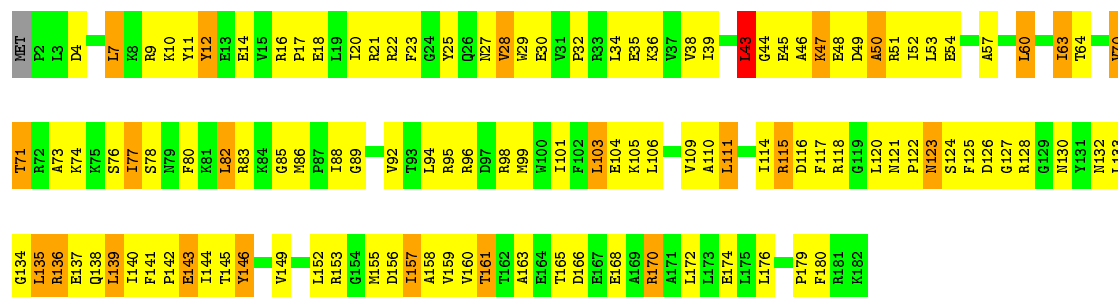


• Molecule 8: 50S ribosomal protein L5

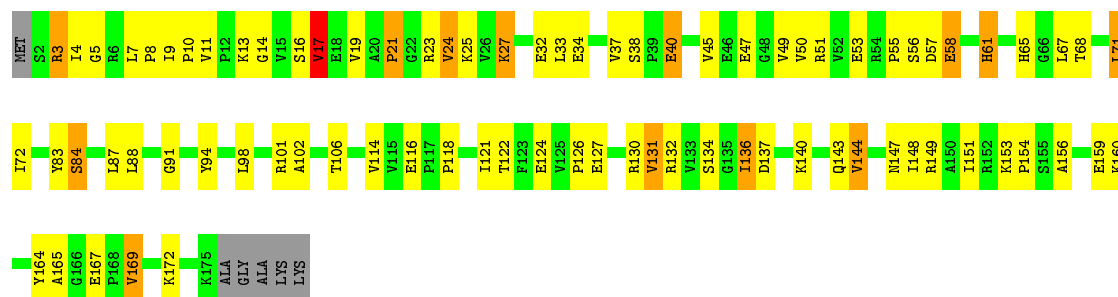


• Molecule 8: 50S ribosomal protein L5

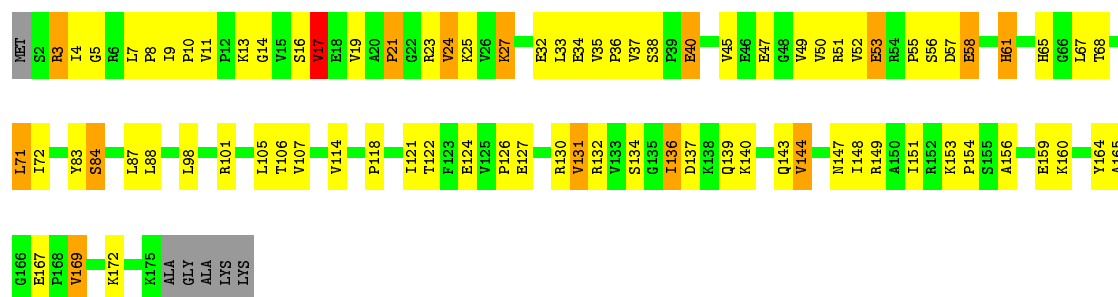




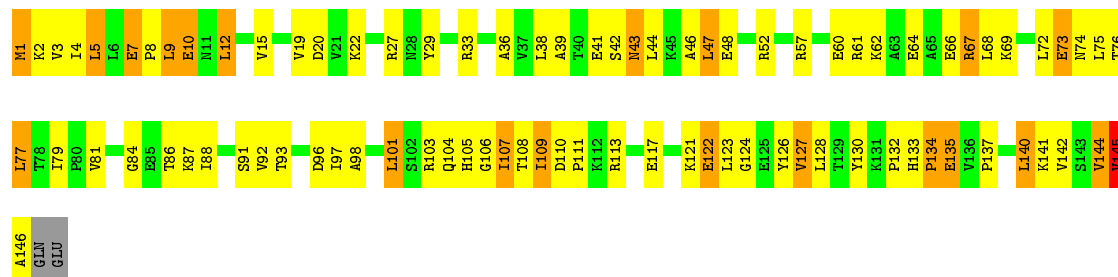
• Molecule 9: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L6

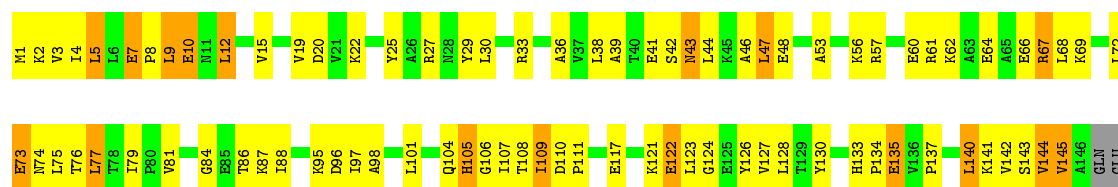


• Molecule 10: 50S ribosomal protein L9



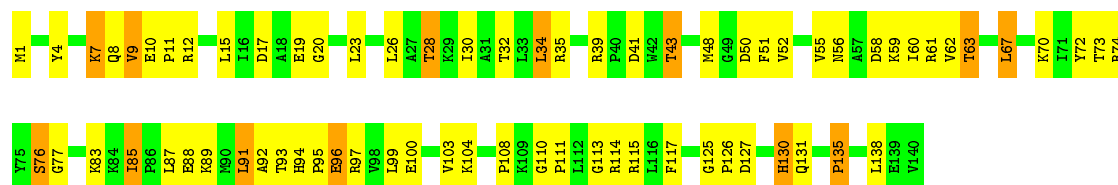
• Molecule 10: 50S ribosomal protein L9

Chain OB: 



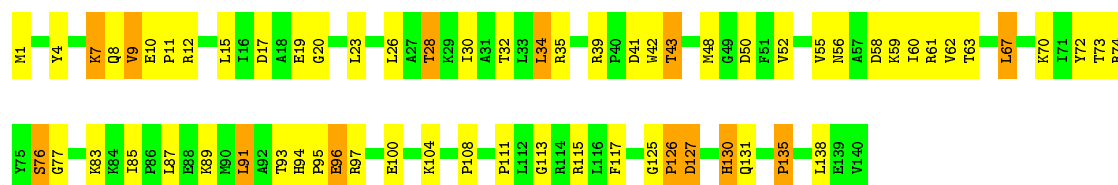
- Molecule 11: 50S ribosomal protein L13

Chain K: 



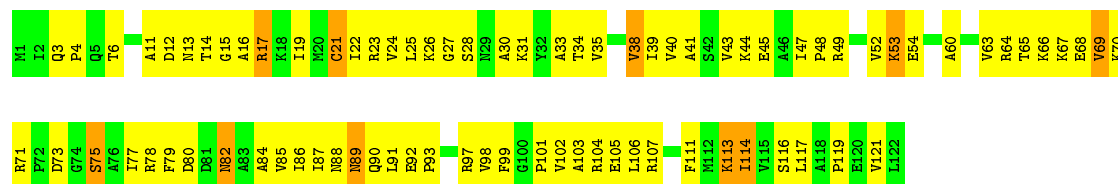
- Molecule 11: 50S ribosomal protein L13

Chain PB: 




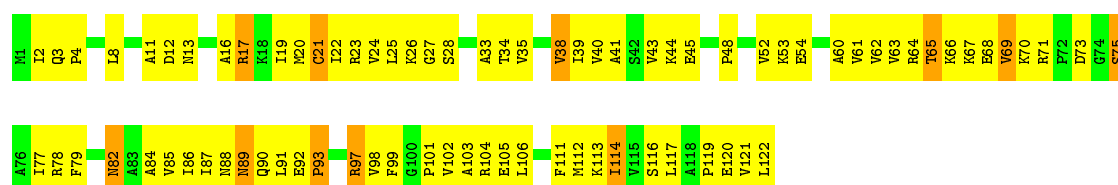
- Molecule 12: 50S ribosomal protein L14

Chain L: 

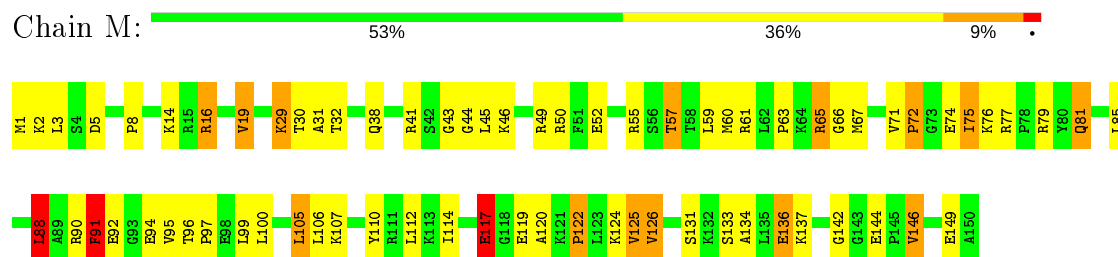


- Molecule 12: 50S ribosomal protein L14

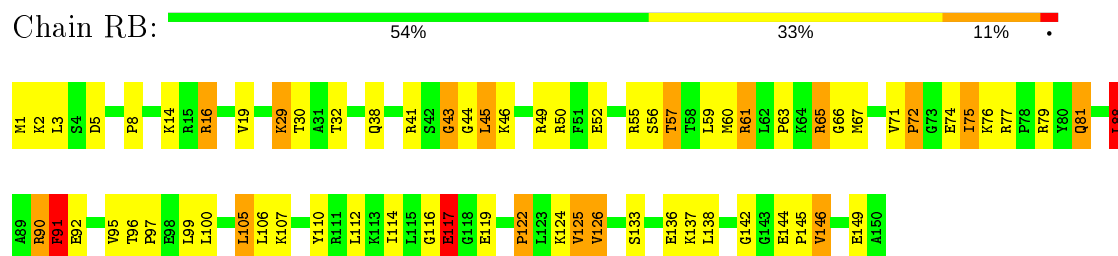
Chain QB: 



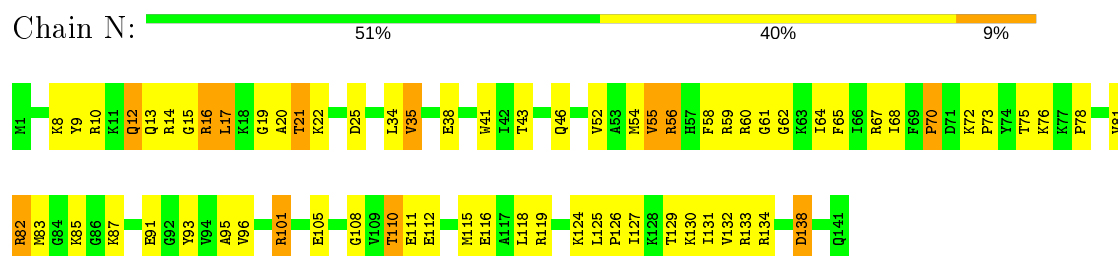
- Molecule 13: 50S ribosomal protein L15



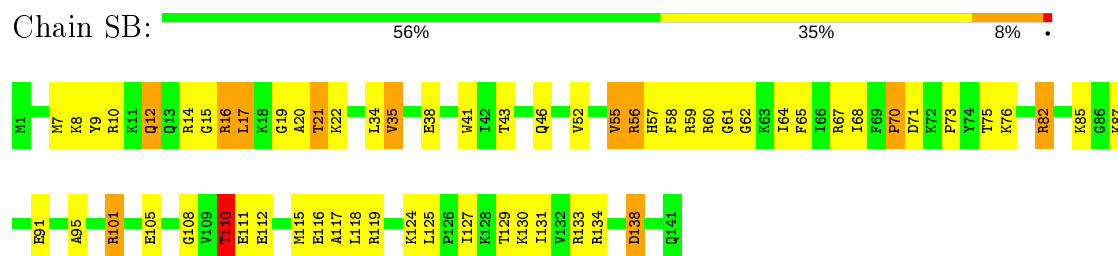
- Molecule 13: 50S ribosomal protein L15



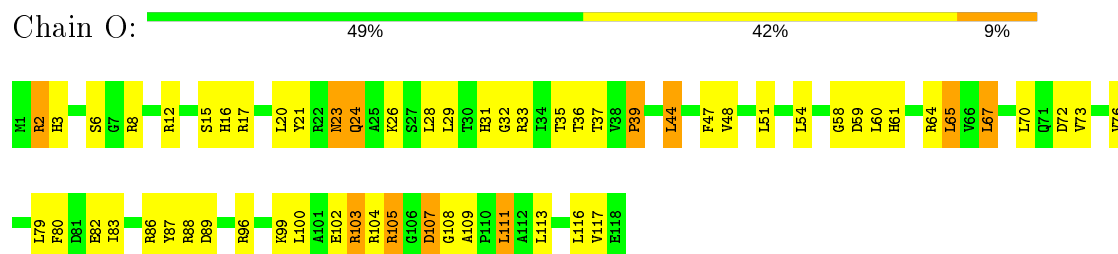
- Molecule 14: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L16

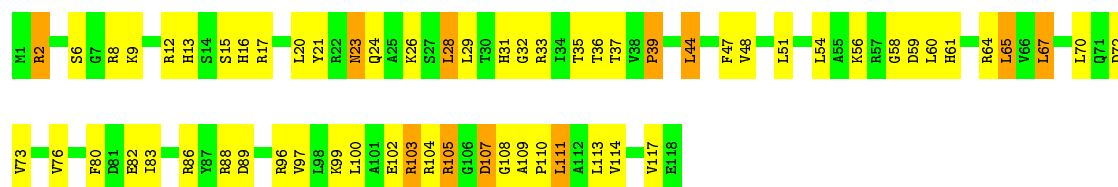


- Molecule 15: 50S ribosomal protein L17



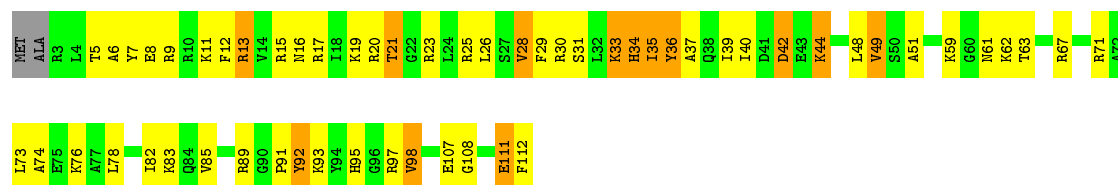
- Molecule 15: 50S ribosomal protein L17

Chain TB: 



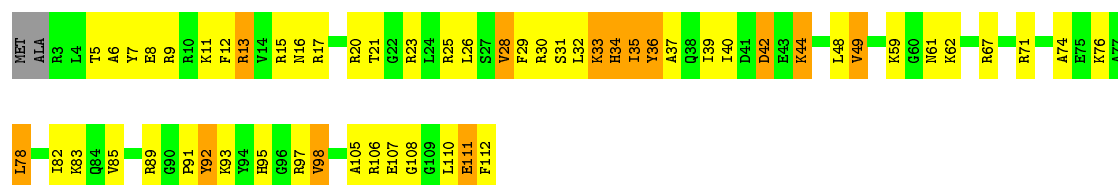
- Molecule 16: 50S ribosomal protein L18

Chain P: 



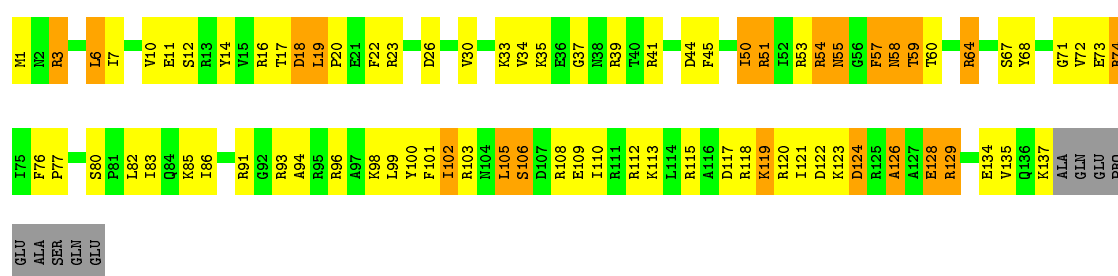
- Molecule 16: 50S ribosomal protein L18

Chain UB: 



- Molecule 17: 50S ribosomal protein L19

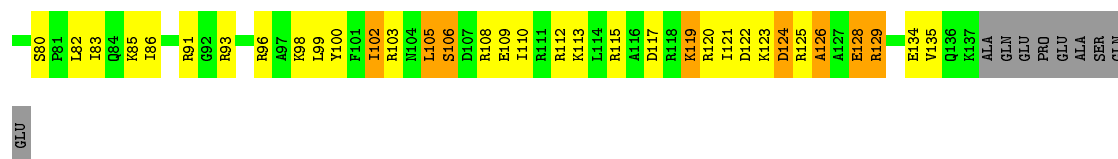
Chain Q: 



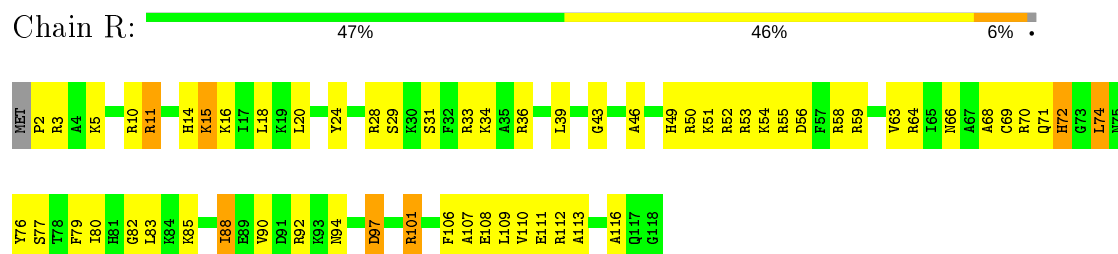
- Molecule 17: 50S ribosomal protein L19

Chain VB: 

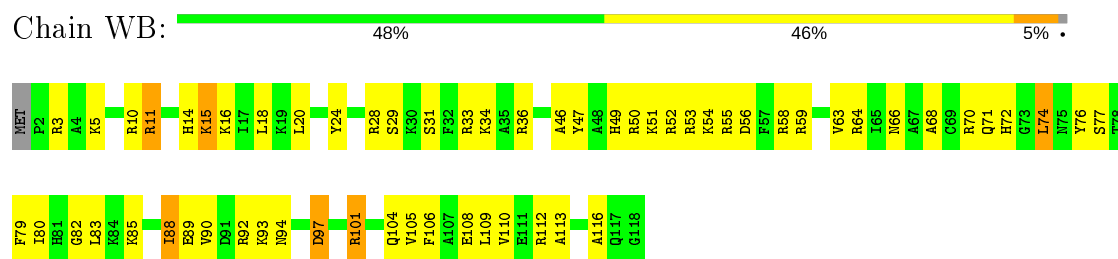




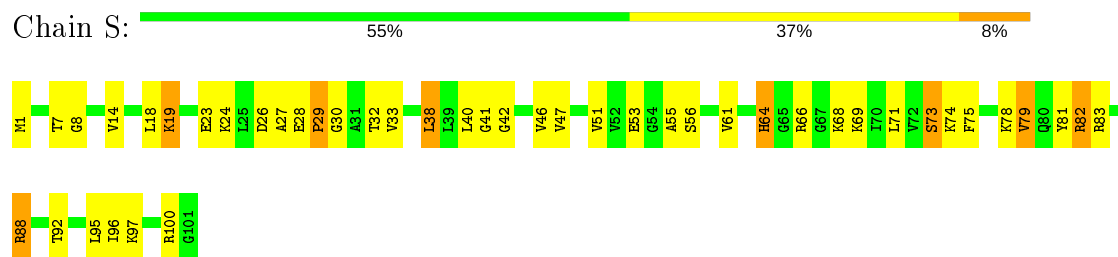
- Molecule 18: 50S ribosomal protein L20



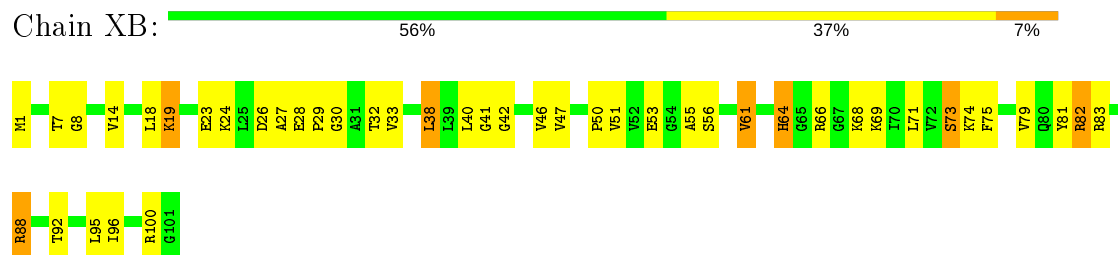
- Molecule 18: 50S ribosomal protein L20



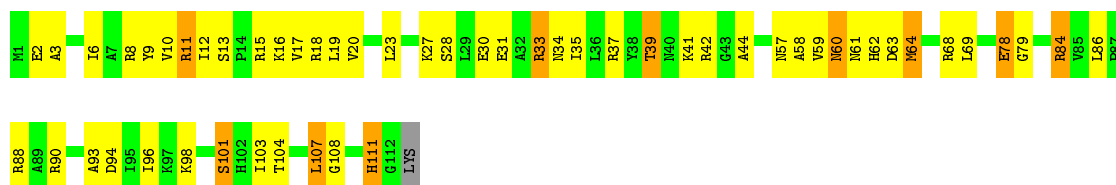
- Molecule 19: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L21

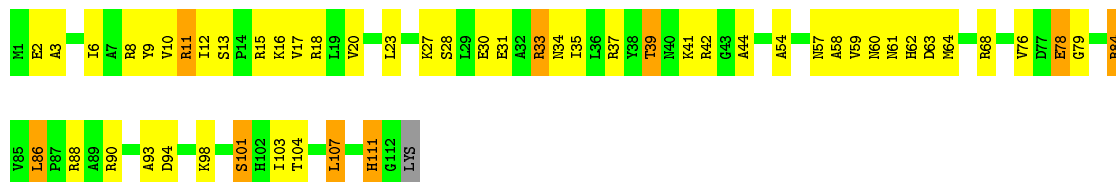


- Molecule 20: 50S ribosomal protein L22



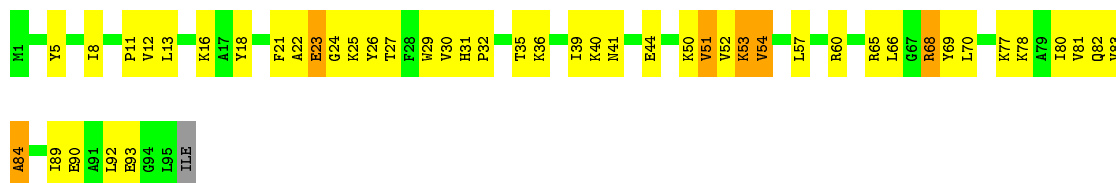
- Molecule 20: 50S ribosomal protein L22

Chain YB: 53% 38% 8% .



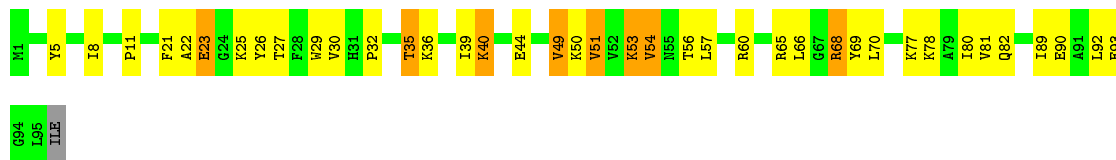
- Molecule 21: 50S ribosomal protein L23

Chain U: 50% 43% 6% .



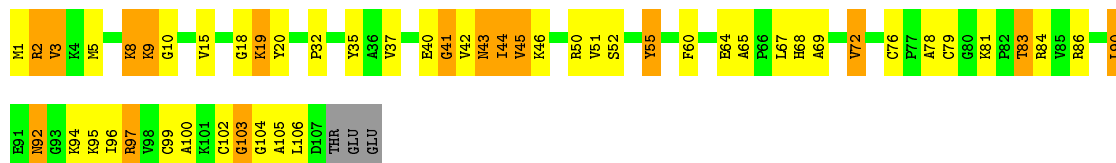
- Molecule 21: 50S ribosomal protein L23

Chain ZB: 58% 32% 8% .



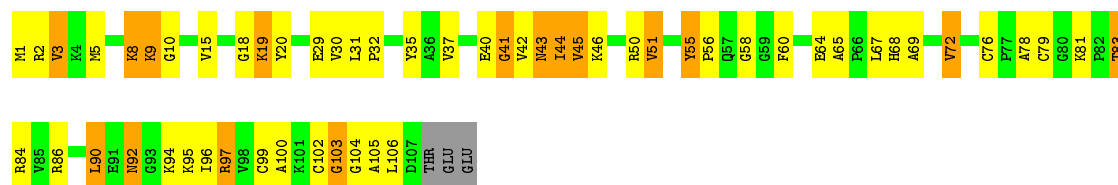
- Molecule 22: 50S ribosomal protein L24

Chain V: 50% 33% 15% .



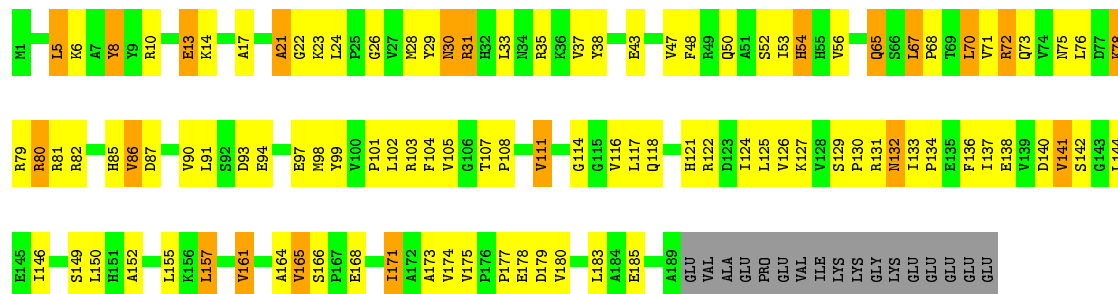
- Molecule 22: 50S ribosomal protein L24

Chain AC: 46% 36% 15% .



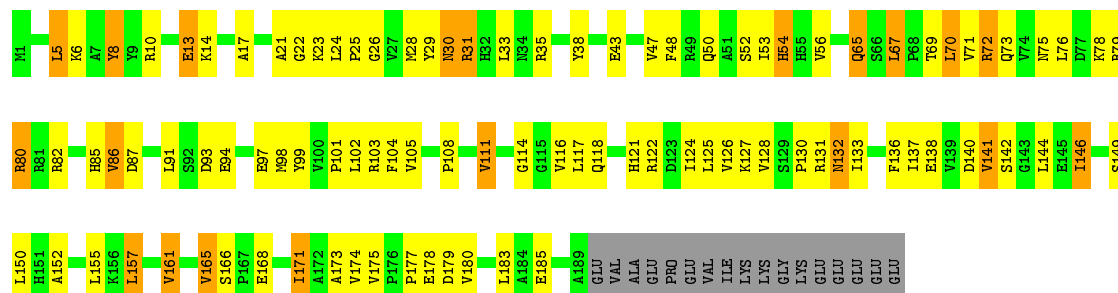
- Molecule 23: 50S ribosomal protein L25

Chain W: 41% 40% 10% 8%



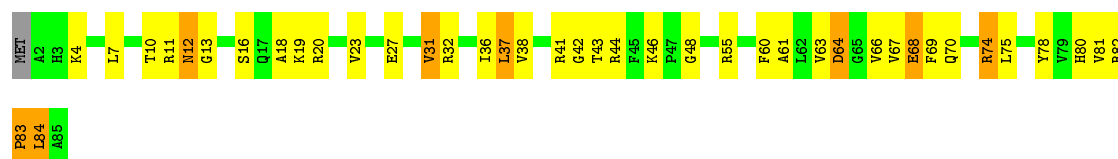
- Molecule 23: 50S ribosomal protein L25

Chain BC: 44% 38% 10% 8%



- Molecule 24: 50S ribosomal protein L27

Chain X: 51% 39% 9%



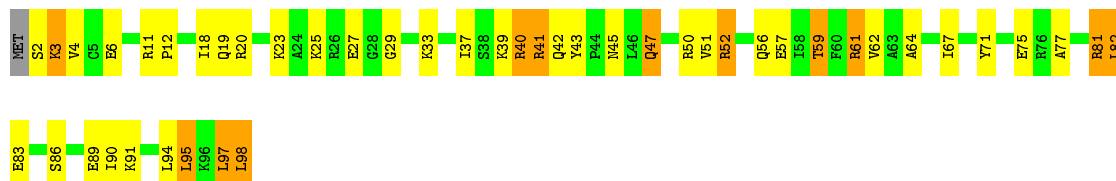
- Molecule 24: 50S ribosomal protein L27

Chain CC: 51% 41% 7%

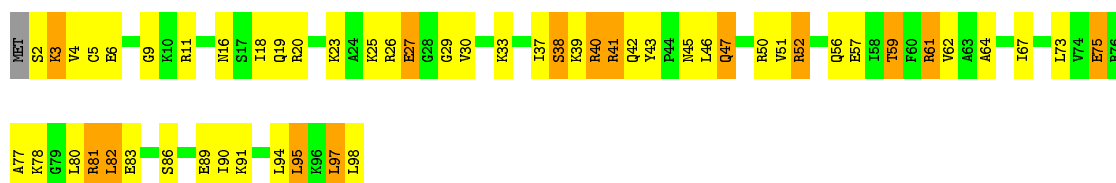


A85

- Molecule 25: 50S ribosomal protein L28

Chain Y:  52% 35% 12%

- Molecule 25: 50S ribosomal protein L28

Chain DC:  44% 41% 14%

- Molecule 26: 50S ribosomal protein L29

Chain Z:  51% 35% 11%

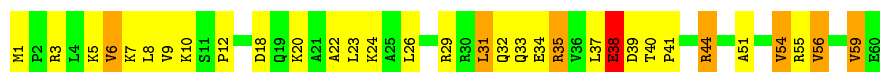
- Molecule 26: 50S ribosomal protein L29

Chain EC:  53% 33% 11%

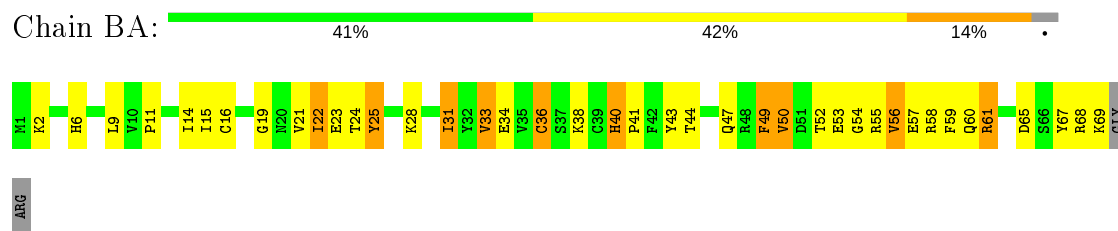
- Molecule 27: 50S ribosomal protein L30

Chain AA:  43% 42% 13%

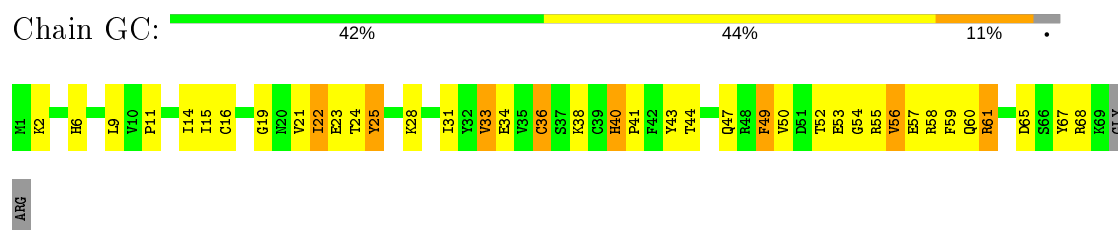
- Molecule 27: 50S ribosomal protein L30

Chain FC:  47% 40% 12%

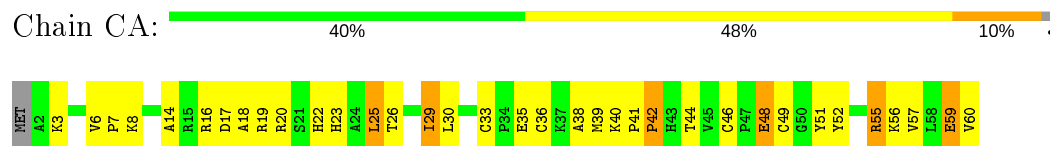
• Molecule 28: 50S ribosomal protein L31



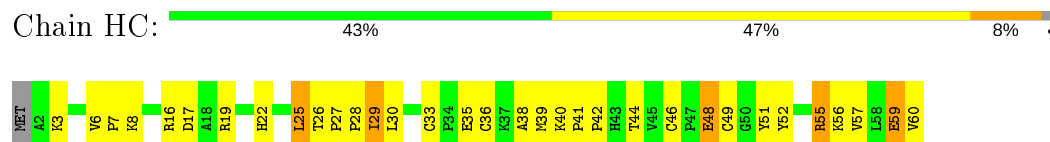
• Molecule 28: 50S ribosomal protein L31



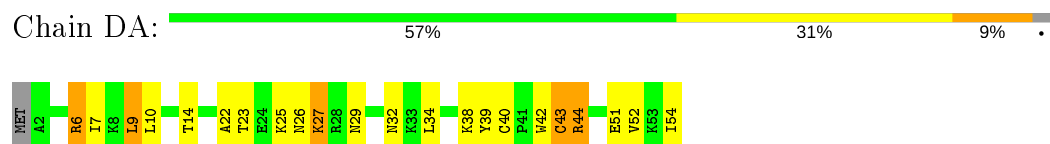
• Molecule 29: 50S ribosomal protein L32



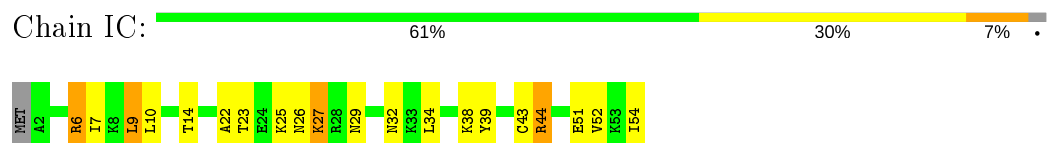
• Molecule 29: 50S ribosomal protein L32



• Molecule 30: 50S ribosomal protein L33

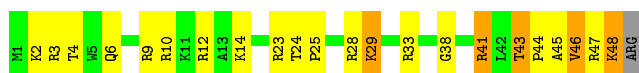


• Molecule 30: 50S ribosomal protein L33



• Molecule 31: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



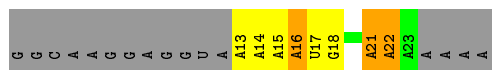
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36

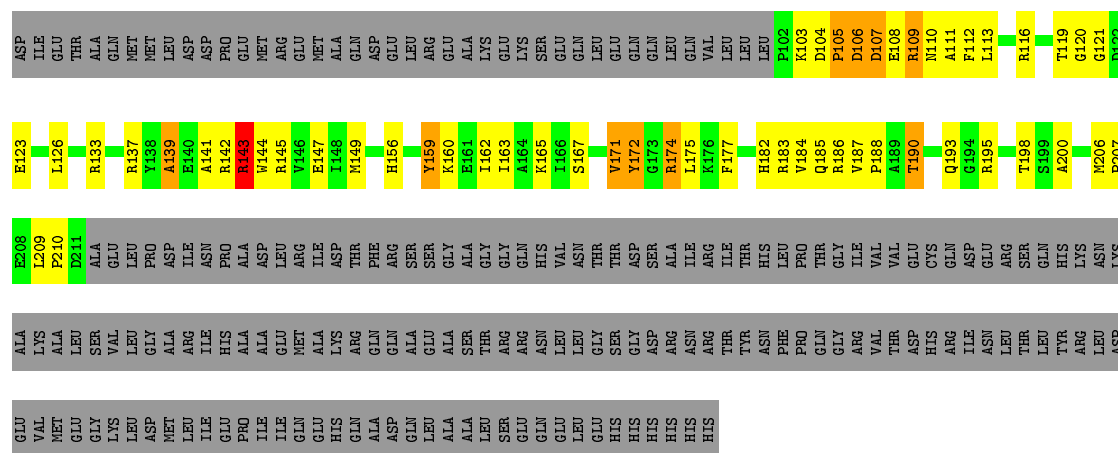


- Molecule 34: mRNA



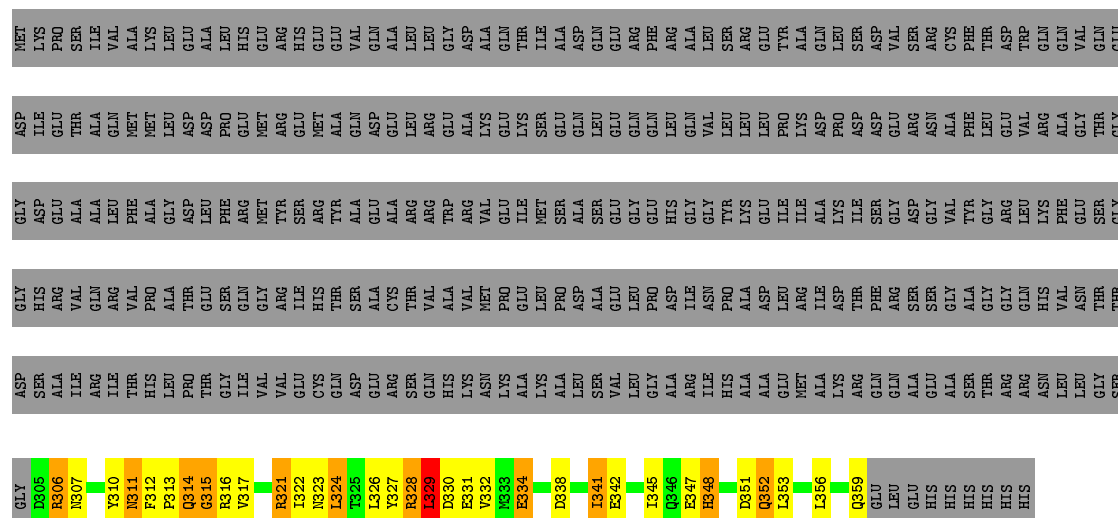
- Molecule 34: mRNA





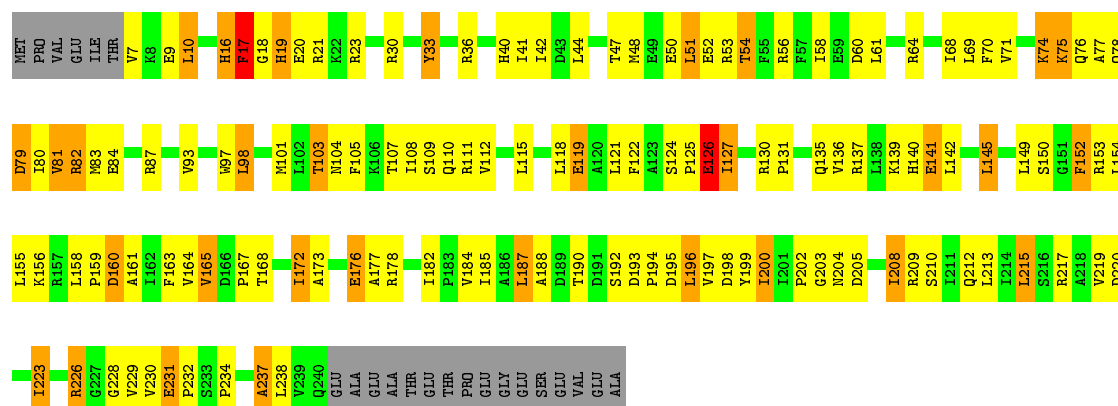
• Molecule 35: Peptide chain release factor 1

Chain PC: 6% 6% . 85%



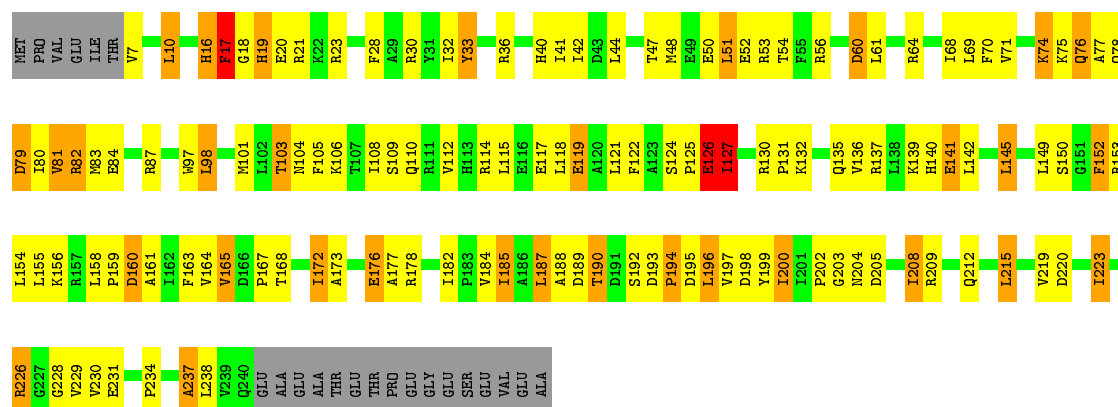
• Molecule 36: 30S ribosomal protein S2

Chain LA: 38% 40% 12% . 9%



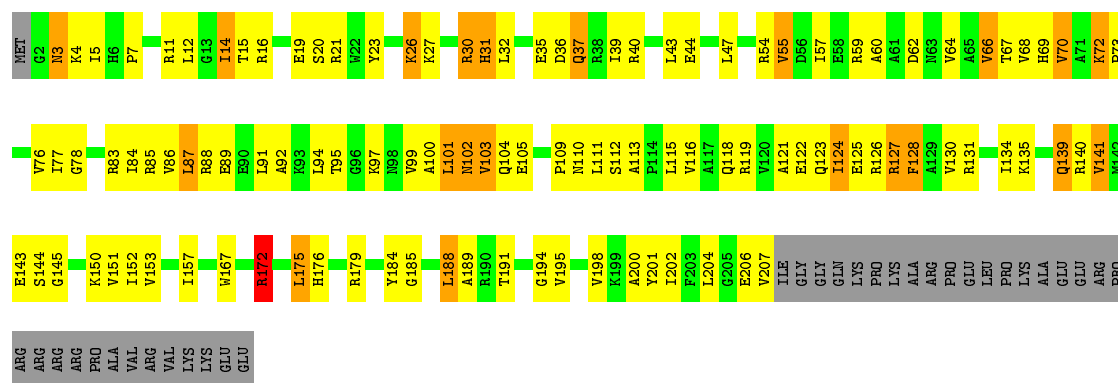
• Molecule 36: 30S ribosomal protein S2

Chain QC: 



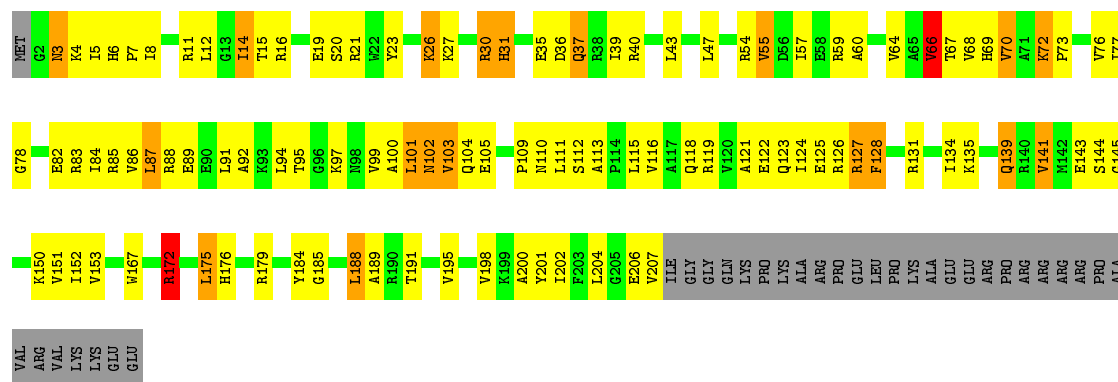
- Molecule 37: 30S ribosomal protein S3

Chain MA: 



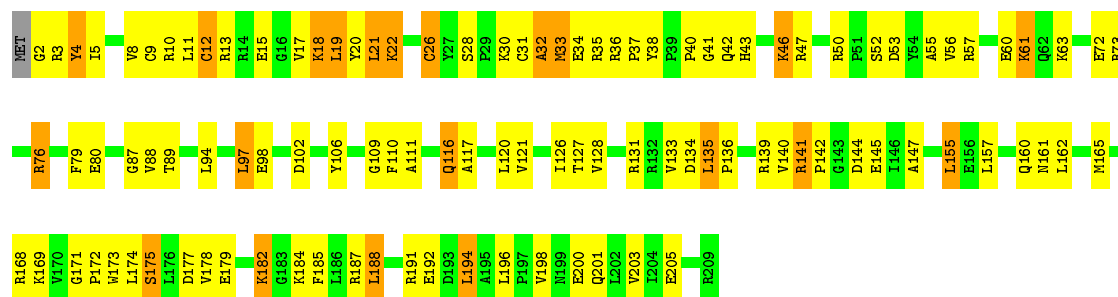
- Molecule 37: 30S ribosomal protein S3

Chain RC: 

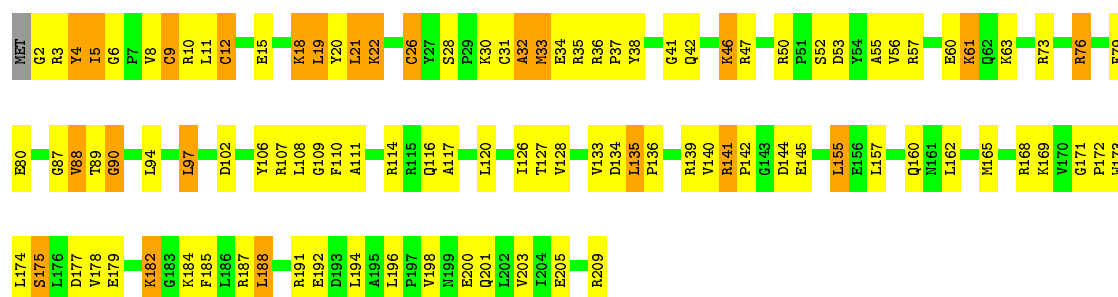


- Molecule 38: 50S ribosomal protein S4

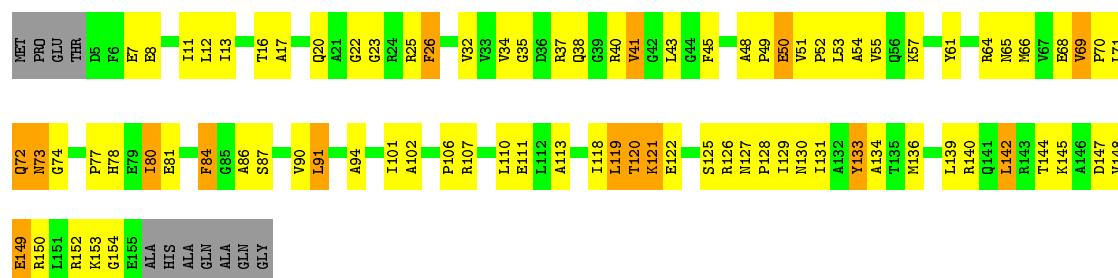
Chain NA: 



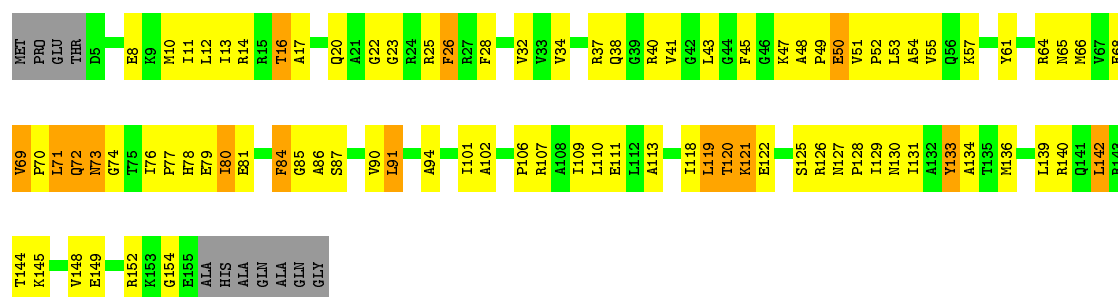
- Molecule 38: 50S ribosomal protein S4



- Molecule 39: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S5



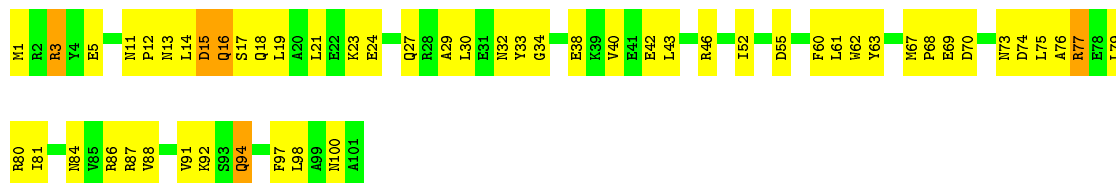
- Molecule 40: 30S ribosomal protein S6

Chain PA:  51% 44% 5%



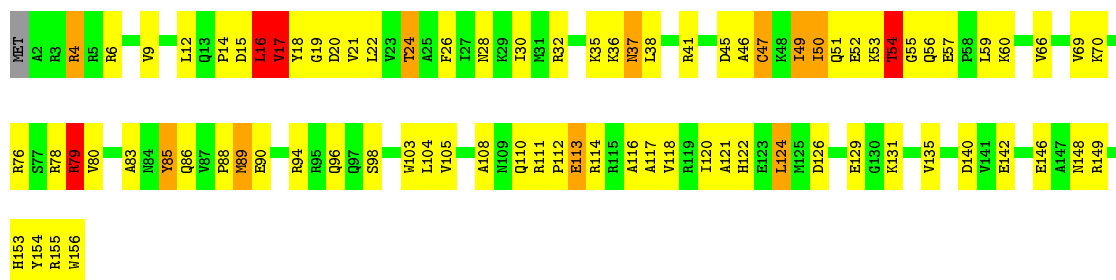
- Molecule 40: 30S ribosomal protein S6

Chain UC:  47% 49% 5%



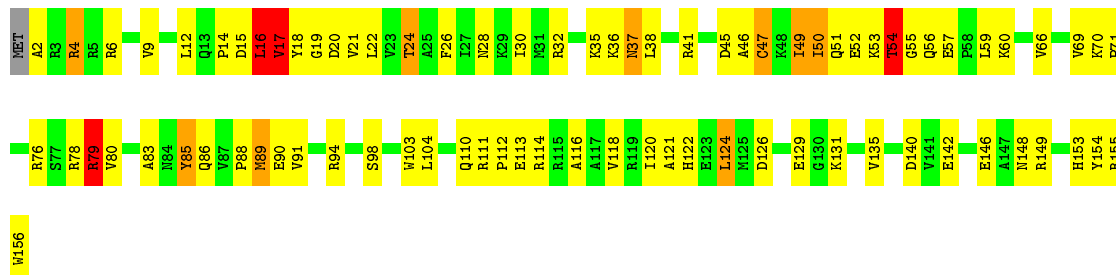
- Molecule 41: 30S ribosomal protein S7

Chain QA:  47% 44% 6% ••



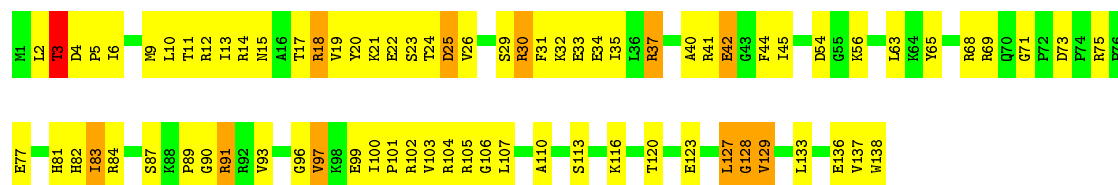
- Molecule 41: 30S ribosomal protein S7

Chain VC:  47% 44% 6% ••



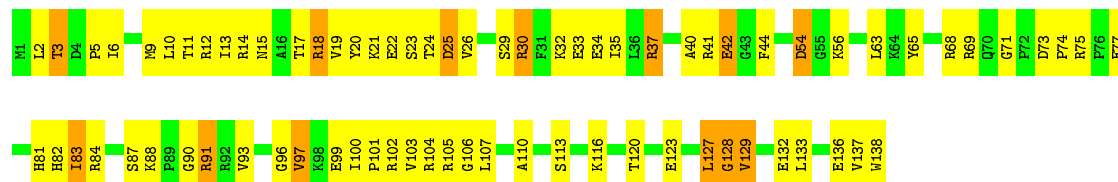
- Molecule 42: 30S ribosomal protein S8

Chain RA:  44% 47% 8% •



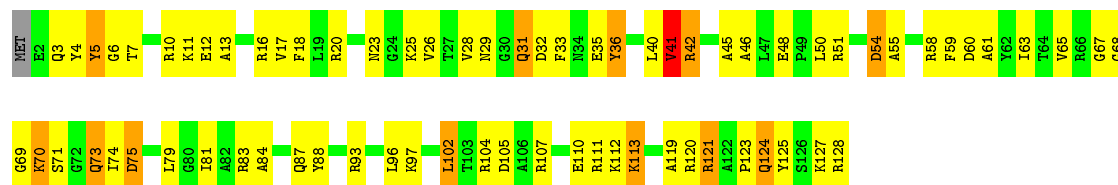
- Molecule 42: 30S ribosomal protein S8

Chain WC: 45% 46% 9%



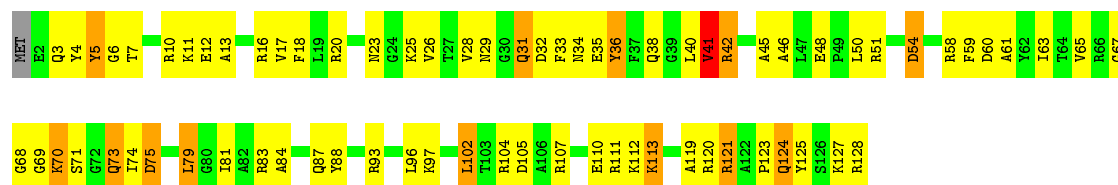
- Molecule 43: 30S ribosomal protein S9

Chain SA: 43% 46% 9% ..



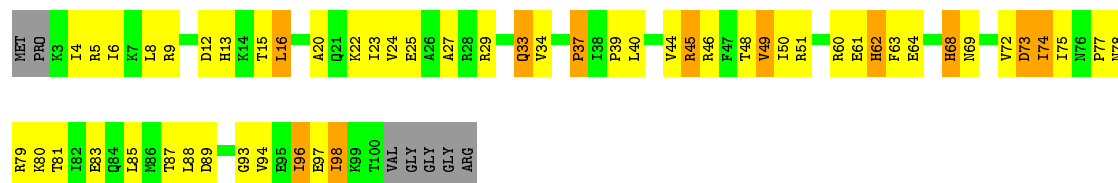
- Molecule 43: 30S ribosomal protein S9

Chain XC: 42% 46% 10% ..



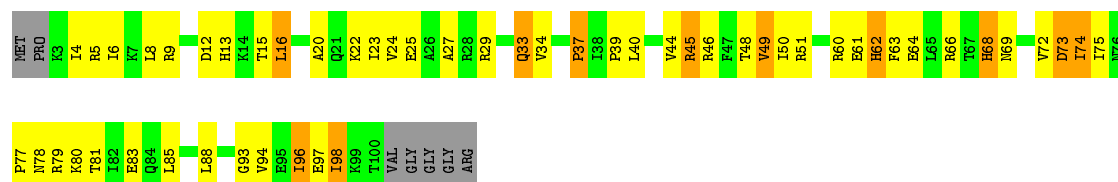
- Molecule 44: 30S ribosomal protein S10

Chain TA: 42% 41% 10% 7%



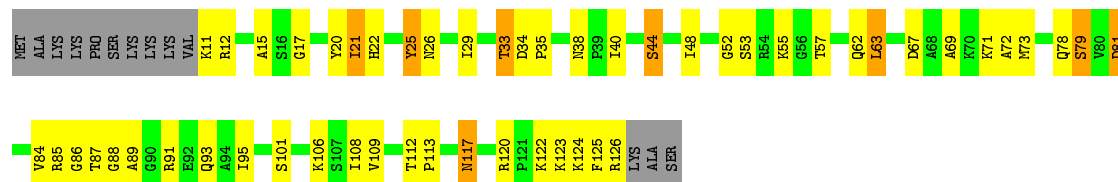
- Molecule 44: 30S ribosomal protein S10

Chain YC: 43% 40% 10% 7%



• Molecule 45: 30S ribosomal protein S11

Chain UA: 49% 35% 6% 10%



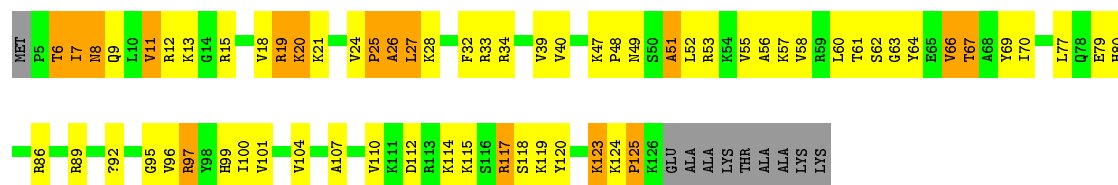
• Molecule 45: 30S ribosomal protein S11

Chain ZC: 47% 39% 5% 10%



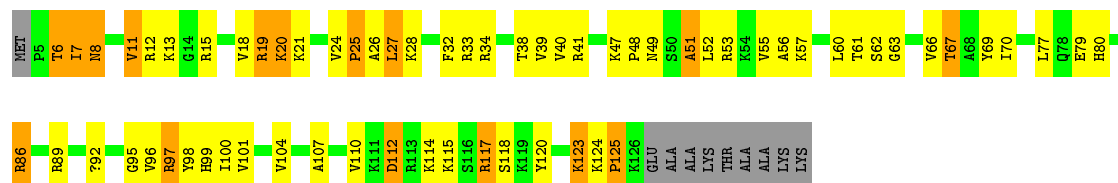
• Molecule 46: 30S ribosomal protein S12

Chain VA: 42% 38% 12% 8%



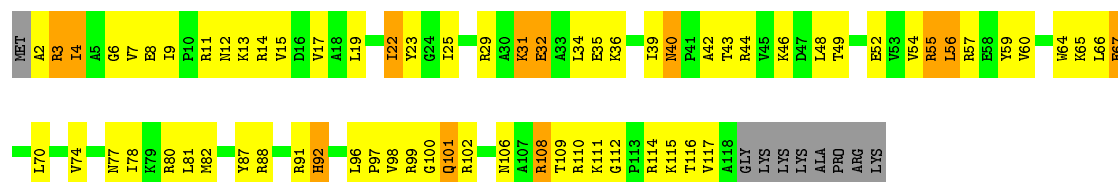
• Molecule 46: 30S ribosomal protein S12

Chain AD: 43% 37% 12% 8%



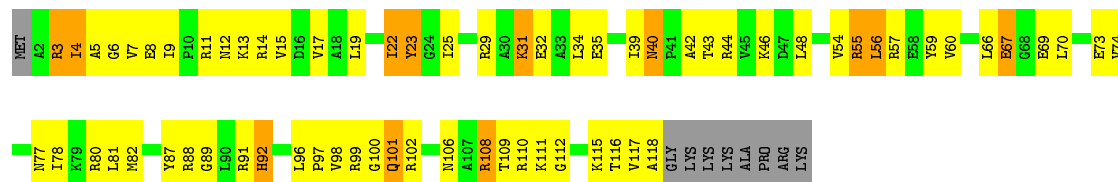
• Molecule 47: 30S ribosomal protein S13

Chain WA: 37% 46% 10% 7%



- Molecule 47: 30S ribosomal protein S13

Chain BD:



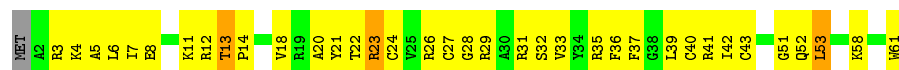
- Molecule 48: 30S ribosomal protein S14 type Z

Chain XA:



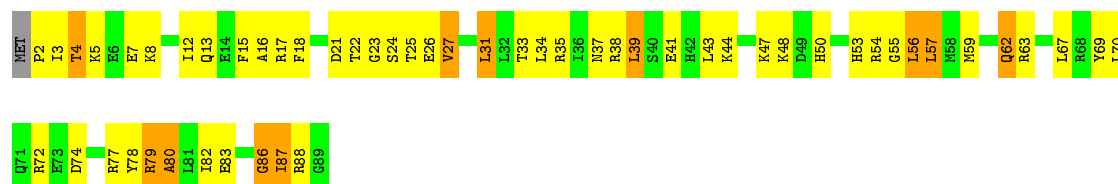
- Molecule 48: 30S ribosomal protein S14 type Z

Chain CD:



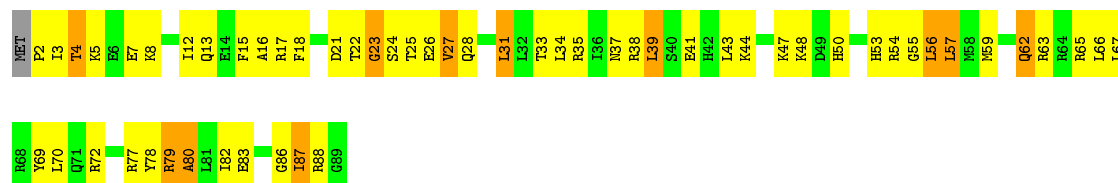
- Molecule 49: 30S ribosomal protein S15

Chain YA:

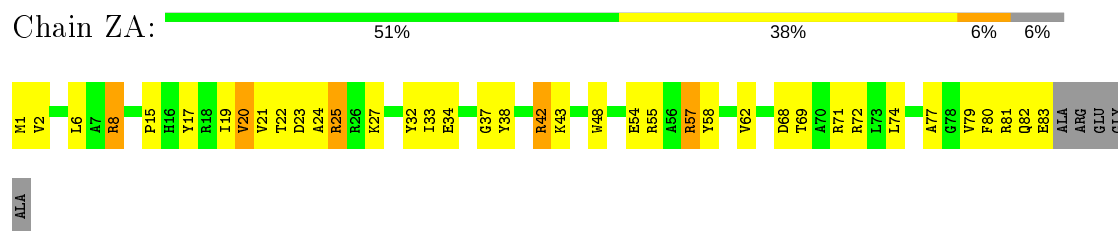


- Molecule 49: 30S ribosomal protein S15

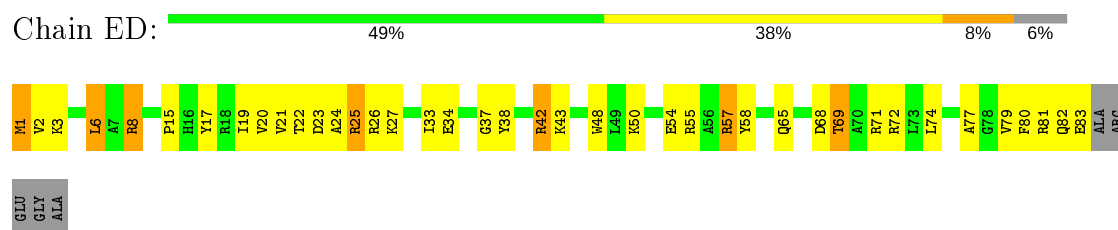
Chain DD:



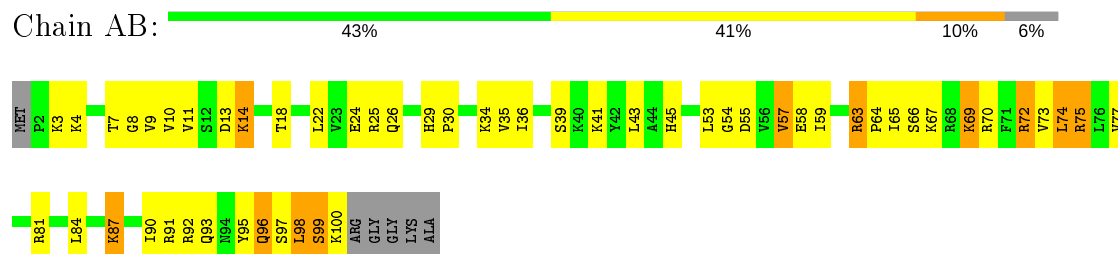
- Molecule 50: 30S ribosomal protein S16



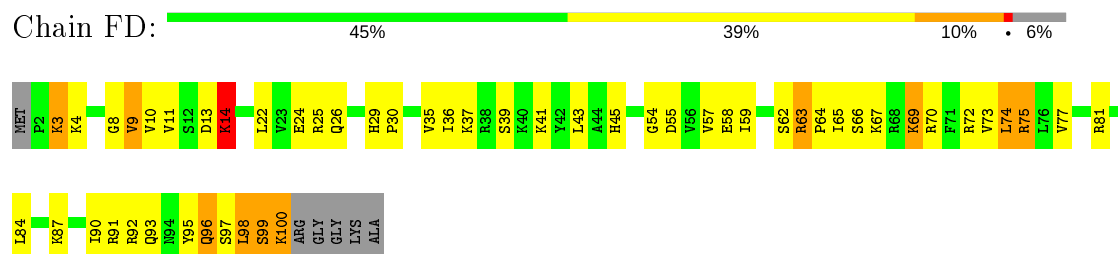
- Molecule 50: 30S ribosomal protein S16



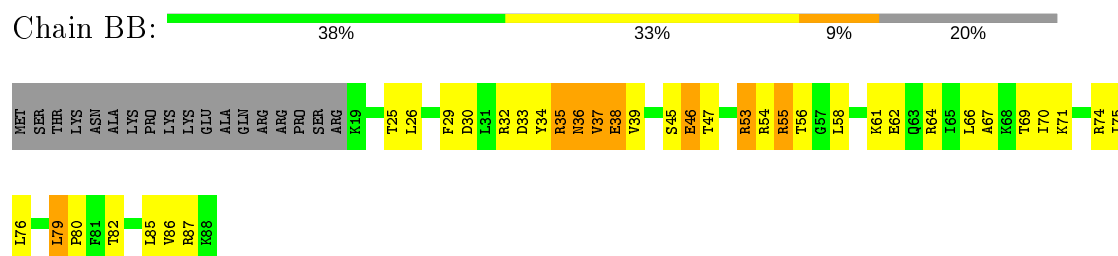
- Molecule 51: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S17



- Molecule 52: 30S ribosomal protein S18

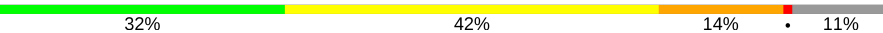


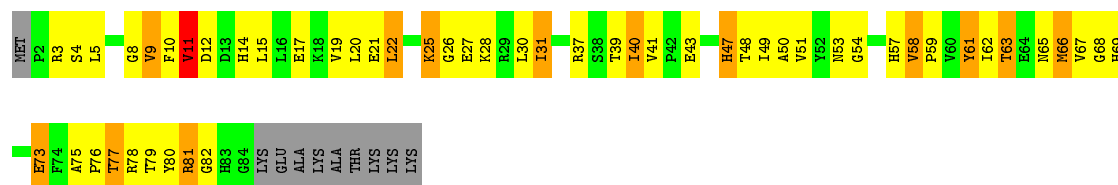
- Molecule 52: 30S ribosomal protein S18

Chain GD: 



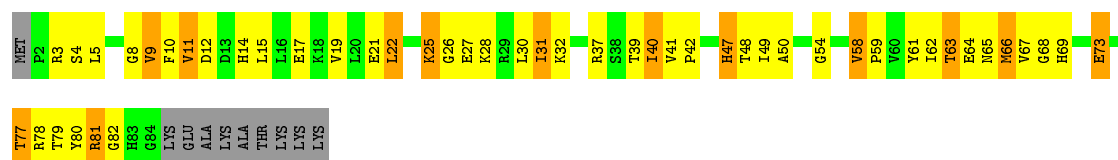
- Molecule 53: 30S ribosomal protein S19

Chain CB: 



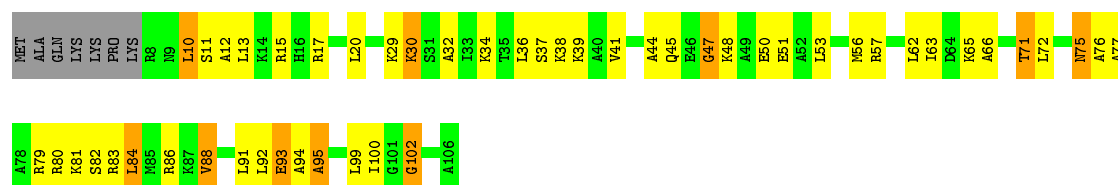
- Molecule 53: 30S ribosomal protein S19

Chain HD: 



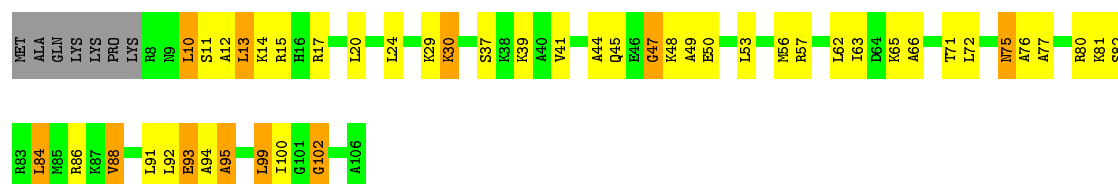
- Molecule 54: 30S ribosomal protein S20

Chain DB: 



- Molecule 54: 30S ribosomal protein S20

Chain ID: 



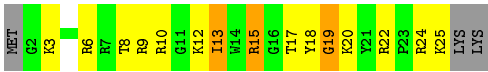
- Molecule 55: 30S ribosomal protein Thx

Chain EB: 30% 48% 11% 11%



● Molecule 55: 30S ribosomal protein Thx

Chain JD: 33% 44% 11% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.86 Å 450.69 Å 615.88 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 69.13 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 100.0 (69.13-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.41 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.243 , 0.282	Depositor DCC
R_{free} test set	7928 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298186	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, 2MU, 0TD, MG, BLS, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/35961 (0.0%)	1.09	67/56125 (0.1%)
1	FB	0.59	1/35961 (0.0%)	1.09	73/56125 (0.1%)
2	B	0.94	58/69214 (0.1%)	1.41	808/108048 (0.7%)
2	GB	0.83	32/69214 (0.0%)	1.33	620/108048 (0.6%)
3	C	0.56	0/2881	1.05	3/4494 (0.1%)
3	HB	0.51	0/2881	1.02	2/4494 (0.0%)
4	D	0.40	0/1744	0.90	0/2719
4	IA	0.60	0/1744	1.06	4/2719 (0.1%)
4	IB	0.37	0/1744	0.90	0/2719
4	NC	0.50	0/1744	1.00	0/2719
5	E	0.80	4/2195 (0.2%)	0.80	1/2955 (0.0%)
5	JB	0.63	2/2195 (0.1%)	0.73	1/2955 (0.0%)
6	F	0.52	0/1596	0.69	1/2153 (0.0%)
6	KB	0.57	0/1596	0.70	1/2153 (0.0%)
7	G	0.61	0/1621	0.69	0/2194
7	LB	0.51	0/1621	0.65	0/2194
8	H	0.36	0/1496	0.57	0/2013
8	MB	0.33	0/1496	0.57	0/2013
9	I	0.43	0/1356	0.59	0/1834
9	NB	0.34	0/1356	0.55	0/1834
10	J	0.46	0/1152	0.62	0/1559
10	OB	0.42	0/1152	0.61	0/1559
11	K	0.49	0/1148	0.62	0/1547
11	PB	0.44	0/1148	0.59	0/1547
12	L	0.59	0/942	0.66	0/1268
12	QB	0.65	0/942	0.68	0/1268
13	M	0.54	0/1162	0.69	0/1544
13	RB	0.47	0/1162	0.65	0/1544
14	N	0.51	0/1142	0.62	0/1525
14	SB	0.49	0/1142	0.60	0/1525
15	O	0.51	0/982	0.63	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	TB	0.53	0/982	0.64	0/1312
16	P	0.42	0/887	0.56	0/1180
16	UB	0.40	0/887	0.56	0/1180
17	Q	0.48	0/1157	0.57	0/1544
17	VB	0.54	0/1157	0.59	0/1544
18	R	0.55	0/982	0.60	0/1306
18	WB	0.49	0/982	0.60	0/1306
19	S	0.49	0/790	0.65	0/1057
19	XB	0.44	0/790	0.61	0/1057
20	T	0.65	0/901	0.69	0/1209
20	YB	0.60	0/901	0.68	0/1209
21	U	0.71	0/764	0.68	0/1025
21	ZB	0.60	0/764	0.61	0/1025
22	AC	0.50	0/827	0.61	0/1103
22	V	0.58	0/827	0.64	0/1103
23	BC	0.40	0/1527	0.58	0/2073
23	W	0.44	0/1527	0.60	0/2073
24	CC	0.50	0/671	0.62	0/892
24	X	0.52	0/671	0.63	0/892
25	DC	0.57	0/768	0.69	0/1021
25	Y	0.63	0/768	0.68	0/1021
26	EC	0.50	0/594	0.64	0/785
26	Z	0.61	0/594	0.71	0/785
27	AA	0.50	0/482	0.63	0/646
27	FC	0.44	0/482	0.59	0/646
28	BA	0.39	0/565	0.53	0/761
28	GC	0.35	0/565	0.52	0/761
29	CA	0.54	0/474	0.66	0/640
29	HC	0.54	0/474	0.64	0/640
30	DA	0.34	0/460	0.51	0/613
30	IC	0.33	0/460	0.51	0/613
31	EA	0.77	0/426	0.76	0/561
31	JC	0.65	0/426	0.72	0/561
32	FA	0.60	0/525	0.64	0/691
32	KC	0.53	0/525	0.62	0/691
33	GA	0.41	0/310	0.58	0/407
33	LC	0.45	0/310	0.60	0/407
34	HA	0.72	0/247	0.92	0/382
34	MC	0.72	0/247	0.91	0/382
35	JA	0.37	0/867	0.51	0/1165
35	KA	0.39	0/461	0.56	0/622
35	OC	0.34	0/867	0.51	0/1165
35	PC	0.36	0/461	0.56	0/622

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	LA	0.39	0/1935	0.57	0/2609
36	QC	0.35	0/1935	0.55	0/2609
37	MA	0.37	0/1636	0.54	0/2205
37	RC	0.36	0/1636	0.54	0/2205
38	NA	0.47	1/1733 (0.1%)	0.59	1/2318 (0.0%)
38	SC	0.53	1/1733 (0.1%)	0.62	1/2318 (0.0%)
39	OA	0.45	0/1171	0.62	0/1576
39	TC	0.44	0/1171	0.61	0/1576
40	PA	0.51	0/856	0.62	0/1154
40	UC	0.43	0/856	0.60	0/1154
41	QA	0.36	0/1276	0.51	0/1709
41	VC	0.34	0/1276	0.50	0/1709
42	RA	0.37	0/1136	0.57	0/1527
42	WC	0.38	0/1136	0.56	0/1527
43	SA	0.34	0/1029	0.54	0/1378
43	XC	0.32	0/1029	0.53	1/1378 (0.1%)
44	TA	0.36	0/807	0.56	0/1085
44	YC	0.34	0/807	0.57	0/1085
45	UA	0.48	0/879	0.64	0/1187
45	ZC	0.41	0/879	0.59	0/1187
46	AD	0.52	0/963	0.62	0/1287
46	VA	0.50	0/963	0.61	0/1287
47	BD	0.33	0/943	0.51	0/1265
47	WA	0.36	0/943	0.52	0/1265
48	CD	0.35	0/501	0.48	0/664
48	XA	0.37	0/501	0.52	0/664
49	DD	0.42	0/745	0.55	0/992
49	YA	0.49	0/745	0.58	0/992
50	ED	0.40	0/716	0.59	0/963
50	ZA	0.34	0/716	0.56	0/963
51	AB	0.47	0/836	0.57	0/1117
51	FD	0.48	0/836	0.58	0/1117
52	BB	0.46	0/579	0.54	0/768
52	GD	0.41	0/579	0.52	0/768
53	CB	0.32	0/680	0.50	0/915
53	HD	0.30	0/680	0.51	0/915
54	DB	0.36	0/764	0.53	0/1006
54	ID	0.40	0/764	0.54	0/1006
55	EB	0.31	0/212	0.48	0/277
55	JD	0.31	0/212	0.46	0/277
All	All	0.71	100/320836 (0.0%)	1.12	1584/479388 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	U	0	1

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	237	GLU	CG-CD	10.38	1.67	1.51
5	E	237	GLU	CB-CG	8.22	1.67	1.52
38	SC	12	CYS	CB-SG	8.17	1.96	1.82
38	NA	12	CYS	CB-SG	7.71	1.95	1.82
2	GB	1780	A	N9-C4	-7.60	1.33	1.37

The worst 5 of 1584 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	298	G	N1-C6-O6	16.25	129.65	119.90
2	B	2593	U	N3-C4-C5	-15.20	105.48	114.60
2	B	2593	U	C6-N1-C2	-14.08	112.55	121.00
2	GB	2593	U	N3-C4-C5	-13.88	106.27	114.60
2	B	2032	G	C4-C5-N7	13.65	116.26	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	U	84	ALA	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	A	32394	0	16367	824	0
1	FB	32394	0	16367	817	0
2	B	62031	0	31273	1297	0
2	GB	62031	0	31275	1270	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2576	0	1305	62	0
3	HB	2576	0	1305	63	0
4	D	1642	0	841	47	0
4	IA	1642	0	841	44	0
4	IB	1642	0	841	46	0
4	NC	1642	0	841	41	0
5	E	2145	0	2234	111	0
5	JB	2145	0	2234	105	0
6	F	1563	0	1629	90	0
6	KB	1563	0	1629	88	0
7	G	1586	0	1632	110	0
7	LB	1586	0	1632	105	0
8	H	1471	0	1526	90	0
8	MB	1471	0	1526	86	1
9	I	1330	0	1407	63	0
9	NB	1330	0	1407	58	0
10	J	1137	0	1225	56	0
10	OB	1137	0	1225	55	0
11	K	1121	0	1195	57	0
11	PB	1121	0	1195	54	0
12	L	932	0	994	75	0
12	QB	932	0	994	72	0
13	M	1145	0	1228	56	0
13	RB	1145	0	1228	47	0
14	N	1121	0	1179	64	0
14	SB	1121	0	1179	59	0
15	O	968	0	1033	33	0
15	TB	968	0	1033	38	0
16	P	877	0	938	48	0
16	UB	877	0	938	48	0
17	Q	1143	0	1211	81	0
17	VB	1143	0	1211	67	0
18	R	964	0	1022	61	0
18	WB	964	0	1022	55	0
19	S	779	0	852	28	0
19	XB	779	0	852	25	0
20	T	890	0	951	37	0
20	YB	890	0	951	40	0
21	U	750	0	814	40	0
21	ZB	750	0	814	37	0
22	AC	814	0	907	40	0
22	V	814	0	907	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BC	1495	0	1521	80	0
23	W	1495	0	1521	90	0
24	CC	662	0	688	40	0
24	X	662	0	688	38	0
25	DC	761	0	837	52	0
25	Y	761	0	837	46	0
26	EC	592	0	654	32	0
26	Z	592	0	654	33	0
27	AA	477	0	529	27	0
27	FC	477	0	529	25	0
28	BA	552	0	537	31	0
28	GC	552	0	537	30	0
29	CA	460	0	481	32	0
29	HC	460	0	482	30	0
30	DA	453	0	477	15	0
30	IC	453	0	477	13	0
31	EA	418	0	467	24	0
31	JC	418	0	467	30	0
32	FA	517	0	582	31	0
32	KC	517	0	582	28	0
33	GA	307	0	337	11	0
33	LC	307	0	337	9	0
34	HA	220	0	108	10	0
34	MC	220	0	108	10	0
35	JA	850	0	816	38	0
35	KA	455	0	444	24	0
35	OC	850	0	816	38	0
35	PC	455	0	444	26	0
36	LA	1900	0	1951	101	0
36	QC	1900	0	1951	96	0
37	MA	1612	0	1677	91	0
37	RC	1612	0	1677	80	0
38	NA	1703	0	1767	94	0
38	SC	1703	0	1767	91	0
39	OA	1155	0	1213	64	0
39	TC	1155	0	1213	75	0
40	PA	843	0	857	35	0
40	UC	843	0	857	37	0
41	QA	1257	0	1296	62	0
41	VC	1257	0	1296	61	0
42	RA	1116	0	1177	61	0
42	WC	1116	0	1177	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	SA	1011	0	1043	61	0
43	XC	1011	0	1043	59	0
44	TA	794	0	840	37	0
44	YC	794	0	840	38	0
45	UA	864	0	881	39	0
45	ZC	864	0	881	45	0
46	AD	958	0	1047	54	0
46	VA	958	0	1047	55	0
47	BD	933	0	992	62	0
47	WA	933	0	992	64	0
48	CD	492	0	533	37	0
48	XA	492	0	533	39	0
49	DD	734	0	771	41	0
49	YA	734	0	771	37	0
50	ED	700	0	720	33	0
50	ZA	700	0	720	28	0
51	AB	823	0	893	40	0
51	FD	823	0	893	40	0
52	BB	574	0	644	32	0
52	GD	574	0	644	31	0
53	CB	665	0	686	43	0
53	HD	665	0	686	43	0
54	DB	762	0	859	43	0
54	ID	762	0	859	41	0
55	EB	208	0	221	16	0
55	JD	208	0	221	16	0
56	A	183	0	0	0	0
56	AA	1	0	0	0	0
56	AB	2	0	0	0	0
56	AC	1	0	0	0	0
56	AD	4	0	0	0	0
56	B	433	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
56	C	22	0	0	0	0
56	CA	1	0	0	0	0
56	CB	1	0	0	0	0
56	CC	1	0	0	0	0
56	D	5	0	0	0	0
56	DC	1	0	0	0	0
56	DD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	E	6	0	0	0	0
56	EA	1	0	0	0	0
56	ED	1	0	0	0	0
56	F	4	0	0	0	0
56	FA	1	0	0	0	0
56	FB	194	0	0	0	0
56	G	2	0	0	0	0
56	GB	402	0	0	0	0
56	GC	1	0	0	0	0
56	H	2	0	0	0	0
56	HA	3	0	0	0	0
56	HB	20	0	0	0	0
56	HD	1	0	0	0	0
56	IA	9	0	0	0	0
56	IB	2	0	0	0	0
56	IC	1	0	0	0	0
56	J	1	0	0	0	0
56	JA	1	0	0	0	0
56	JB	5	0	0	0	0
56	JC	1	0	0	0	0
56	K	4	0	0	0	0
56	KB	2	0	0	0	0
56	KC	1	0	0	0	0
56	L	3	0	0	0	0
56	LA	1	0	0	0	0
56	LB	4	0	0	0	0
56	M	3	0	0	0	0
56	MA	6	0	0	0	0
56	MC	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	NC	10	0	0	0	0
56	O	2	0	0	0	0
56	OA	4	0	0	0	0
56	OB	1	0	0	0	0
56	OC	1	0	0	0	0
56	PA	3	0	0	0	0
56	PB	2	0	0	0	0
56	PC	1	0	0	0	0
56	Q	1	0	0	0	0
56	QA	1	0	0	0	0
56	QB	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QC	3	0	0	0	0
56	R	1	0	0	0	0
56	RB	3	0	0	0	0
56	RC	2	0	0	0	0
56	S	1	0	0	0	0
56	SA	1	0	0	0	0
56	SB	2	0	0	0	0
56	SC	4	0	0	0	0
56	T	2	0	0	0	0
56	TB	1	0	0	0	0
56	TC	3	0	0	0	0
56	U	1	0	0	0	0
56	UA	1	0	0	0	0
56	UB	4	0	0	0	0
56	UC	3	0	0	0	0
56	V	2	0	0	0	0
56	VA	2	0	0	0	0
56	VB	3	0	0	0	0
56	VC	1	0	0	0	0
56	WC	1	0	0	0	0
56	XB	2	0	0	0	0
56	Y	3	0	0	0	0
56	YA	3	0	0	0	0
56	Z	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	B	30	0	24	4	0
57	GB	30	0	24	7	0
58	AC	1	0	0	0	0
58	BA	1	0	0	0	0
58	CA	1	0	0	0	0
58	DA	1	0	0	0	0
58	GA	1	0	0	0	0
58	GC	1	0	0	0	0
58	HC	1	0	0	0	0
58	IC	1	0	0	0	0
58	LC	1	0	0	0	0
58	V	1	0	0	0	0
All	All	298186	0	202351	8489	1

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

The worst 5 of 8489 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)
38:SC:18:LYS:NZ	38:SC:26:CYS:SG	2.02	1.33
38:SC:18:LYS:NZ	38:SC:31:CYS:SG	2.07	1.27
38:NA:18:LYS:NZ	38:NA:26:CYS:SG	2.09	1.26
3:C:90:C:OP2	14:N:16:ARG:NH1	1.77	1.18
1:FB:9:G:OP2	39:TC:121:LYS:NZ	1.76	1.16

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GB:1412:A:O2'	8:MB:9:ARG:NH1[1_655]	1.99	0.21

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	
5	E	273/275 (99%)	243 (89%)	24 (9%)	6 (2%)	6	29
5	JB	273/275 (99%)	245 (90%)	22 (8%)	6 (2%)	6	29
6	F	202/206 (98%)	166 (82%)	28 (14%)	8 (4%)	3	18
6	KB	202/206 (98%)	167 (83%)	29 (14%)	6 (3%)	4	23
7	G	200/205 (98%)	173 (86%)	24 (12%)	3 (2%)	10	36
7	LB	200/205 (98%)	172 (86%)	25 (12%)	3 (2%)	10	36
8	H	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2	16
8	MB	179/182 (98%)	134 (75%)	37 (21%)	8 (4%)	2	16
9	I	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3	21
9	NB	172/180 (96%)	134 (78%)	32 (19%)	6 (4%)	3	21
10	J	144/148 (97%)	111 (77%)	23 (16%)	10 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	OB	144/148 (97%)	111 (77%)	24 (17%)	9 (6%)	1	9
11	K	138/140 (99%)	115 (83%)	17 (12%)	6 (4%)	2	17
11	PB	138/140 (99%)	118 (86%)	15 (11%)	5 (4%)	3	21
12	L	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	51
12	QB	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	5	26
13	M	148/150 (99%)	126 (85%)	12 (8%)	10 (7%)	1	8
13	RB	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1	8
14	N	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	11	37
14	SB	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6	29
15	O	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	2	17
15	TB	116/118 (98%)	97 (84%)	13 (11%)	6 (5%)	2	13
16	P	108/112 (96%)	82 (76%)	23 (21%)	3 (3%)	5	24
16	UB	108/112 (96%)	83 (77%)	22 (20%)	3 (3%)	5	24
17	Q	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	4	23
17	VB	135/146 (92%)	117 (87%)	15 (11%)	3 (2%)	6	29
18	R	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
18	WB	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	49
19	S	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	3	18
19	XB	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	4	23
20	T	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	8	32
20	YB	110/113 (97%)	98 (89%)	12 (11%)	0	100	100
21	U	93/96 (97%)	83 (89%)	8 (9%)	2 (2%)	6	29
21	ZB	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	6	29
22	AC	105/110 (96%)	83 (79%)	16 (15%)	6 (6%)	1	12
22	V	105/110 (96%)	83 (79%)	14 (13%)	8 (8%)	1	6
23	BC	187/206 (91%)	137 (73%)	43 (23%)	7 (4%)	3	20
23	W	187/206 (91%)	139 (74%)	41 (22%)	7 (4%)	3	20
24	CC	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	2	14
24	X	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	3	20
25	DC	95/98 (97%)	87 (92%)	7 (7%)	1 (1%)	14	44
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	EC	68/72 (94%)	61 (90%)	4 (6%)	3 (4%)	2	16
26	Z	68/72 (94%)	59 (87%)	6 (9%)	3 (4%)	2	16
27	AA	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3	21
27	FC	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	21
28	BA	67/71 (94%)	43 (64%)	16 (24%)	8 (12%)	0	3
28	GC	67/71 (94%)	44 (66%)	15 (22%)	8 (12%)	0	3
29	CA	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	8	32
29	HC	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
30	DA	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	7	30
30	IC	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	7	30
31	EA	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	JC	46/49 (94%)	38 (83%)	8 (17%)	0	100	100
32	FA	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
32	KC	62/65 (95%)	53 (86%)	9 (14%)	0	100	100
33	GA	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	5
33	LC	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	5
35	JA	108/365 (30%)	84 (78%)	18 (17%)	6 (6%)	2	12
35	KA	53/365 (14%)	31 (58%)	13 (24%)	9 (17%)	0	0
35	OC	108/365 (30%)	83 (77%)	19 (18%)	6 (6%)	2	12
35	PC	53/365 (14%)	31 (58%)	14 (26%)	8 (15%)	0	0
36	LA	232/256 (91%)	176 (76%)	40 (17%)	16 (7%)	1	8
36	QC	232/256 (91%)	174 (75%)	41 (18%)	17 (7%)	1	7
37	MA	204/239 (85%)	166 (81%)	28 (14%)	10 (5%)	2	14
37	RC	204/239 (85%)	167 (82%)	25 (12%)	12 (6%)	1	11
38	NA	206/209 (99%)	162 (79%)	35 (17%)	9 (4%)	2	16
38	SC	206/209 (99%)	158 (77%)	39 (19%)	9 (4%)	2	16
39	OA	149/162 (92%)	126 (85%)	19 (13%)	4 (3%)	5	26
39	TC	149/162 (92%)	124 (83%)	20 (13%)	5 (3%)	3	21
40	PA	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	3	18
40	UC	99/101 (98%)	82 (83%)	13 (13%)	4 (4%)	3	18
41	QA	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	VC	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	2	13
42	RA	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	3	20
42	WC	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	3	20
43	SA	125/128 (98%)	91 (73%)	28 (22%)	6 (5%)	2	15
43	XC	125/128 (98%)	93 (74%)	25 (20%)	7 (6%)	2	12
44	TA	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	0	4
44	YC	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	0	4
45	UA	114/129 (88%)	87 (76%)	23 (20%)	4 (4%)	3	21
45	ZC	114/129 (88%)	87 (76%)	24 (21%)	3 (3%)	5	26
46	AD	119/132 (90%)	91 (76%)	20 (17%)	8 (7%)	1	8
46	VA	119/132 (90%)	89 (75%)	22 (18%)	8 (7%)	1	8
47	BD	115/126 (91%)	90 (78%)	18 (16%)	7 (6%)	1	10
47	WA	115/126 (91%)	91 (79%)	18 (16%)	6 (5%)	2	13
48	CD	58/61 (95%)	45 (78%)	12 (21%)	1 (2%)	9	34
48	XA	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9	34
49	DD	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	21
49	YA	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	15
50	ED	81/88 (92%)	72 (89%)	8 (10%)	1 (1%)	13	41
50	ZA	81/88 (92%)	71 (88%)	9 (11%)	1 (1%)	13	41
51	AB	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	3	18
51	FD	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	13
52	BB	68/88 (77%)	63 (93%)	4 (6%)	1 (2%)	10	36
52	GD	68/88 (77%)	61 (90%)	5 (7%)	2 (3%)	4	24
53	CB	81/93 (87%)	58 (72%)	16 (20%)	7 (9%)	1	5
53	HD	81/93 (87%)	58 (72%)	17 (21%)	6 (7%)	1	7
54	DB	97/106 (92%)	79 (81%)	11 (11%)	7 (7%)	1	7
54	ID	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	10
55	EB	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	1	4
55	JD	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	1	4
All	All	11806/13576 (87%)	9599 (81%)	1713 (14%)	494 (4%)	3	18

5 of 494 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	122	ASP
7	G	130	ALA
8	H	12	TYR
8	H	43	LEU
8	H	47	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	177 (82%)	40 (18%)	1	5
5	JB	217/217 (100%)	176 (81%)	41 (19%)	1	4
6	F	165/166 (99%)	139 (84%)	26 (16%)	2	10
6	KB	165/166 (99%)	139 (84%)	26 (16%)	2	10
7	G	161/162 (99%)	136 (84%)	25 (16%)	2	11
7	LB	161/162 (99%)	134 (83%)	27 (17%)	2	8
8	H	154/156 (99%)	121 (79%)	33 (21%)	1	3
8	MB	154/156 (99%)	121 (79%)	33 (21%)	1	3
9	I	144/148 (97%)	123 (85%)	21 (15%)	3	12
9	NB	144/148 (97%)	122 (85%)	22 (15%)	2	11
10	J	122/124 (98%)	95 (78%)	27 (22%)	1	2
10	OB	122/124 (98%)	94 (77%)	28 (23%)	1	2
11	K	119/119 (100%)	99 (83%)	20 (17%)	2	8
11	PB	119/119 (100%)	98 (82%)	21 (18%)	2	6
12	L	100/100 (100%)	88 (88%)	12 (12%)	5	19
12	QB	100/100 (100%)	87 (87%)	13 (13%)	4	16
13	M	116/116 (100%)	86 (74%)	30 (26%)	0	2
13	RB	116/116 (100%)	86 (74%)	30 (26%)	0	2
14	N	111/111 (100%)	94 (85%)	17 (15%)	2	11
14	SB	111/111 (100%)	94 (85%)	17 (15%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	101/101 (100%)	83 (82%)	18 (18%)	2	6
15	TB	101/101 (100%)	84 (83%)	17 (17%)	2	8
16	P	87/88 (99%)	72 (83%)	15 (17%)	2	8
16	UB	87/88 (99%)	73 (84%)	14 (16%)	2	10
17	Q	121/128 (94%)	97 (80%)	24 (20%)	1	4
17	VB	121/128 (94%)	96 (79%)	25 (21%)	1	3
18	R	93/94 (99%)	82 (88%)	11 (12%)	5	19
18	WB	93/94 (99%)	82 (88%)	11 (12%)	5	19
19	S	82/82 (100%)	64 (78%)	18 (22%)	1	3
19	XB	82/82 (100%)	64 (78%)	18 (22%)	1	3
20	T	91/92 (99%)	78 (86%)	13 (14%)	3	13
20	YB	91/92 (99%)	79 (87%)	12 (13%)	4	15
21	U	77/78 (99%)	70 (91%)	7 (9%)	9	32
21	ZB	77/78 (99%)	68 (88%)	9 (12%)	5	20
22	AC	87/91 (96%)	71 (82%)	16 (18%)	1	5
22	V	87/91 (96%)	71 (82%)	16 (18%)	1	5
23	BC	163/179 (91%)	133 (82%)	30 (18%)	1	5
23	W	163/179 (91%)	133 (82%)	30 (18%)	1	5
24	CC	66/67 (98%)	54 (82%)	12 (18%)	1	6
24	X	66/67 (98%)	53 (80%)	13 (20%)	1	4
25	DC	81/83 (98%)	64 (79%)	17 (21%)	1	3
25	Y	81/83 (98%)	67 (83%)	14 (17%)	2	7
26	EC	66/67 (98%)	60 (91%)	6 (9%)	9	32
26	Z	66/67 (98%)	59 (89%)	7 (11%)	6	24
27	AA	52/52 (100%)	38 (73%)	14 (27%)	0	1
27	FC	52/52 (100%)	37 (71%)	15 (29%)	0	1
28	BA	59/63 (94%)	44 (75%)	15 (25%)	0	2
28	GC	59/63 (94%)	44 (75%)	15 (25%)	0	2
29	CA	51/52 (98%)	43 (84%)	8 (16%)	2	10
29	HC	51/52 (98%)	43 (84%)	8 (16%)	2	10
30	DA	51/52 (98%)	41 (80%)	10 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	IC	51/52 (98%)	41 (80%)	10 (20%)	1	4
31	EA	41/42 (98%)	33 (80%)	8 (20%)	1	4
31	JC	41/42 (98%)	33 (80%)	8 (20%)	1	4
32	FA	54/55 (98%)	50 (93%)	4 (7%)	13	42
32	KC	54/55 (98%)	49 (91%)	5 (9%)	9	31
33	GA	34/34 (100%)	33 (97%)	1 (3%)	42	69
33	LC	34/34 (100%)	33 (97%)	1 (3%)	42	69
35	JA	85/305 (28%)	68 (80%)	17 (20%)	1	3
35	KA	50/305 (16%)	38 (76%)	12 (24%)	0	2
35	OC	85/305 (28%)	68 (80%)	17 (20%)	1	3
35	PC	50/305 (16%)	38 (76%)	12 (24%)	0	2
36	LA	202/220 (92%)	156 (77%)	46 (23%)	1	2
36	QC	202/220 (92%)	154 (76%)	48 (24%)	0	2
37	MA	160/188 (85%)	137 (86%)	23 (14%)	3	13
37	RC	160/188 (85%)	138 (86%)	22 (14%)	3	14
38	NA	180/181 (99%)	155 (86%)	25 (14%)	3	13
38	SC	180/181 (99%)	155 (86%)	25 (14%)	3	13
39	OA	116/123 (94%)	93 (80%)	23 (20%)	1	4
39	TC	116/123 (94%)	94 (81%)	22 (19%)	1	4
40	PA	90/90 (100%)	79 (88%)	11 (12%)	5	18
40	UC	90/90 (100%)	78 (87%)	12 (13%)	4	15
41	QA	126/127 (99%)	105 (83%)	21 (17%)	2	8
41	VC	126/127 (99%)	105 (83%)	21 (17%)	2	8
42	RA	119/119 (100%)	105 (88%)	14 (12%)	5	19
42	WC	119/119 (100%)	106 (89%)	13 (11%)	6	23
43	SA	98/99 (99%)	79 (81%)	19 (19%)	1	4
43	XC	98/99 (99%)	79 (81%)	19 (19%)	1	4
44	TA	88/92 (96%)	72 (82%)	16 (18%)	1	6
44	YC	88/92 (96%)	71 (81%)	17 (19%)	1	4
45	UA	88/99 (89%)	77 (88%)	11 (12%)	4	17
45	ZC	88/99 (89%)	77 (88%)	11 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	AD	102/108 (94%)	84 (82%)	18 (18%)	2	6
46	VA	102/108 (94%)	84 (82%)	18 (18%)	2	6
47	BD	94/101 (93%)	74 (79%)	20 (21%)	1	3
47	WA	94/101 (93%)	74 (79%)	20 (21%)	1	3
48	CD	49/50 (98%)	42 (86%)	7 (14%)	3	13
48	XA	49/50 (98%)	42 (86%)	7 (14%)	3	13
49	DD	79/80 (99%)	62 (78%)	17 (22%)	1	3
49	YA	79/80 (99%)	62 (78%)	17 (22%)	1	3
50	ED	72/74 (97%)	60 (83%)	12 (17%)	2	8
50	ZA	72/74 (97%)	61 (85%)	11 (15%)	2	11
51	AB	94/97 (97%)	77 (82%)	17 (18%)	1	6
51	FD	94/97 (97%)	76 (81%)	18 (19%)	1	4
52	BB	61/77 (79%)	49 (80%)	12 (20%)	1	4
52	GD	61/77 (79%)	50 (82%)	11 (18%)	1	6
53	CB	72/80 (90%)	57 (79%)	15 (21%)	1	3
53	HD	72/80 (90%)	58 (81%)	14 (19%)	1	4
54	DB	76/82 (93%)	66 (87%)	10 (13%)	4	15
54	ID	76/82 (93%)	66 (87%)	10 (13%)	4	15
55	EB	19/22 (86%)	15 (79%)	4 (21%)	1	3
55	JD	19/22 (86%)	15 (79%)	4 (21%)	1	3
All	All	9972/11276 (88%)	8229 (82%)	1743 (18%)	2	7

5 of 1743 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	YA	39	LEU
8	MB	82	LEU
45	ZC	95	ILE
51	AB	11	VAL
5	JB	150	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
45	UA	22	HIS
12	QB	82	ASN
45	ZC	22	HIS
47	WA	101	GLN
10	OB	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	347 (23%)	12 (0%)
1	FB	1502/1507 (99%)	343 (22%)	12 (0%)
2	B	2876/2880 (99%)	658 (22%)	22 (0%)
2	GB	2876/2880 (99%)	658 (22%)	22 (0%)
3	C	119/120 (99%)	19 (15%)	0
3	HB	119/120 (99%)	20 (16%)	0
34	HA	9/27 (33%)	3 (33%)	0
34	MC	9/27 (33%)	3 (33%)	0
4	D	76/77 (98%)	27 (35%)	0
4	IA	76/77 (98%)	20 (26%)	0
4	IB	76/77 (98%)	26 (34%)	0
4	NC	76/77 (98%)	19 (25%)	0
All	All	9316/9376 (99%)	2143 (23%)	68 (0%)

5 of 2143 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	U
1	A	22	G
1	A	26	A
1	A	31	G

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2405	G
1	FB	560	U
2	GB	2110	G
2	B	2439	A
1	FB	81	G

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

64 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
4	5MU	IB	54	4	15,22,23	1.67	3 (20%)	16,32,35	1.80	1 (6%)
1	5MC	FB	1400	1	15,22,23	1.43	2 (13%)	19,32,35	1.16	2 (10%)
2	5MC	B	1942	2	15,22,23	1.53	2 (13%)	19,32,35	1.30	3 (15%)
4	4SU	IB	8	4	14,21,22	2.77	4 (28%)	15,30,33	2.02	3 (20%)
1	5MC	FB	967	1	15,22,23	1.40	2 (13%)	19,32,35	1.19	1 (5%)
4	PSU	IA	55	4	17,21,22	1.44	3 (17%)	20,30,33	3.27	6 (30%)
4	4SU	NC	8	4	14,21,22	2.91	4 (28%)	15,30,33	2.10	2 (13%)
2	PSU	GB	1911	2	17,21,22	1.46	3 (17%)	20,30,33	3.09	6 (30%)
1	UR3	FB	1498	1	14,22,23	1.64	1 (7%)	15,32,35	0.71	0
1	7MG	FB	527	1	22,26,27	2.28	7 (31%)	28,39,42	1.91	7 (25%)
1	5MC	A	1400	1	15,22,23	1.45	2 (13%)	19,32,35	1.27	3 (15%)
2	OMG	GB	2251	2	18,26,27	1.70	2 (11%)	20,38,41	1.78	6 (30%)
1	MA6	A	1518	1	19,26,27	1.66	3 (15%)	18,38,41	1.40	3 (16%)
2	4OC	B	1920	56,2	15,22,24	0.91	1 (6%)	17,31,35	2.19	4 (23%)
2	2MU	GB	2552	2	14,22,24	2.35	3 (21%)	14,31,36	1.20	1 (7%)
2	5MU	GB	1915	2	15,22,23	1.68	3 (20%)	16,32,35	1.87	2 (12%)
1	2MG	FB	1207	1	19,26,27	2.43	3 (15%)	21,38,41	1.80	7 (33%)
4	5MU	D	54	4	15,22,23	1.69	3 (20%)	16,32,35	1.79	1 (6%)
1	PSU	FB	516	1	17,21,22	1.73	4 (23%)	20,30,33	3.80	6 (30%)
2	5MC	B	1962	2	15,22,23	1.69	3 (20%)	19,32,35	1.73	3 (15%)
2	2MU	B	2552	2	14,22,24	2.55	4 (28%)	14,31,36	1.45	2 (14%)
2	5MU	B	1915	2	15,22,23	1.64	3 (20%)	16,32,35	1.82	2 (12%)
2	PSU	GB	2605	2	17,21,22	1.47	3 (17%)	20,30,33	2.89	6 (30%)
4	PSU	IB	55	4	17,21,22	1.54	4 (23%)	20,30,33	3.39	6 (30%)
46	0TD	AD	92	46	4,9,10	1.43	1 (25%)	3,11,13	3.36	2 (66%)
2	4OC	GB	1920	2	15,22,24	0.85	1 (6%)	17,31,35	2.02	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	FB	966	1	20,27,28	2.07	3 (15%)	22,40,43	1.57	6 (27%)
2	PSU	GB	1917	2	17,21,22	1.61	3 (17%)	20,30,33	3.38	6 (30%)
1	5MC	A	1407	1	15,22,23	1.43	2 (13%)	19,32,35	1.29	3 (15%)
1	MA6	FB	1519	1	19,26,27	1.77	3 (15%)	18,38,41	1.42	2 (11%)
2	OMG	B	2251	2	18,26,27	1.78	2 (11%)	20,38,41	1.88	6 (30%)
1	MA6	FB	1518	1	19,26,27	1.56	3 (15%)	18,38,41	1.47	2 (11%)
1	5MC	FB	1404	1	15,22,23	1.55	2 (13%)	19,32,35	1.50	3 (15%)
2	2MA	GB	2503	2	17,25,26	1.45	2 (11%)	19,37,40	1.57	3 (15%)
2	5MC	GB	1962	2	15,22,23	1.47	2 (13%)	19,32,35	1.42	3 (15%)
4	5MC	D	32	4	15,22,23	1.43	2 (13%)	19,32,35	1.32	3 (15%)
1	2MG	A	1207	1	19,26,27	2.48	2 (10%)	21,38,41	1.91	7 (33%)
2	PSU	B	1917	2	17,21,22	1.55	4 (23%)	20,30,33	3.24	5 (25%)
1	7MG	A	527	1	22,26,27	2.16	7 (31%)	28,39,42	1.88	7 (25%)
4	5MU	NC	54	4	15,22,23	1.73	3 (20%)	16,32,35	1.92	1 (6%)
1	5MC	A	1404	1	15,22,23	1.59	3 (20%)	19,32,35	1.70	3 (15%)
1	PSU	A	516	1	17,21,22	1.61	4 (23%)	20,30,33	3.70	5 (25%)
46	0TD	VA	92	46	4,9,10	1.57	1 (25%)	3,11,13	3.52	2 (66%)
1	5MC	A	967	1	15,22,23	1.41	2 (13%)	19,32,35	1.21	2 (10%)
1	4OC	A	1402	1	16,23,24	0.94	1 (6%)	17,32,35	2.46	2 (11%)
2	PSU	B	2605	2	17,21,22	1.32	3 (17%)	20,30,33	3.35	6 (30%)
1	5MC	FB	1407	1	15,22,23	1.40	2 (13%)	19,32,35	1.16	2 (10%)
2	5MU	B	1939	2	15,22,23	1.56	3 (20%)	16,32,35	1.76	2 (12%)
4	PSU	NC	55	4	17,21,22	1.53	4 (23%)	20,30,33	3.32	6 (30%)
1	UR3	A	1498	1	14,22,23	1.66	1 (7%)	15,32,35	0.76	0
1	M2G	A	966	1	20,27,28	2.15	3 (15%)	22,40,43	1.59	6 (27%)
4	5MC	IA	32	4	15,22,23	1.44	2 (13%)	19,32,35	1.36	2 (10%)
2	2MA	B	2503	2	17,25,26	1.61	4 (23%)	19,37,40	1.57	3 (15%)
2	5MU	GB	1939	2	15,22,23	1.72	3 (20%)	16,32,35	1.81	2 (12%)
4	PSU	D	55	4	17,21,22	1.56	4 (23%)	20,30,33	3.31	6 (30%)
4	5MU	IA	54	4	15,22,23	1.75	3 (20%)	16,32,35	1.90	1 (6%)
4	4SU	IA	8	4	14,21,22	3.07	5 (35%)	15,30,33	2.03	2 (13%)
1	MA6	A	1519	1	19,26,27	1.43	3 (15%)	18,38,41	1.37	1 (5%)
4	4SU	D	8	4	14,21,22	2.89	4 (28%)	15,30,33	1.85	2 (13%)
2	5MC	GB	1942	2	15,22,23	1.30	2 (13%)	19,32,35	1.27	1 (5%)
1	4OC	FB	1402	1	16,23,24	0.89	1 (6%)	17,32,35	2.71	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	B	1911	2	17,21,22	1.26	3 (17%)	20,30,33	3.38	6 (30%)
4	5MC	NC	32	4	15,22,23	1.41	2 (13%)	19,32,35	1.39	4 (21%)
4	5MC	IB	32	4	15,22,23	1.37	2 (13%)	19,32,35	1.24	2 (10%)

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
4	5MU	IB	54	4	-	0/5/25/26	0/2/2/2
1	5MC	FB	1400	1	-	0/5/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/5/25/26	0/2/2/2
4	4SU	IB	8	4	-	1/5/25/26	0/2/2/2
1	5MC	FB	967	1	-	0/5/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
4	4SU	NC	8	4	-	1/5/25/26	0/2/2/2
2	PSU	GB	1911	2	-	0/7/25/26	0/2/2/2
1	UR3	FB	1498	1	-	2/5/25/26	0/2/2/2
1	7MG	FB	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1400	1	-	0/5/25/26	0/2/2/2
2	OMG	GB	2251	2	-	3/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	3/7/29/30	0/3/3/3
2	4OC	B	1920	56,2	-	1/7/27/30	0/2/2/2
2	2MU	GB	2552	2	-	1/7/27/28	0/2/2/2
2	5MU	GB	1915	2	-	0/5/25/26	0/2/2/2
1	2MG	FB	1207	1	-	0/5/27/28	0/3/3/3
4	5MU	D	54	4	-	0/5/25/26	0/2/2/2
1	PSU	FB	516	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	4/5/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/7/27/28	0/2/2/2
2	5MU	B	1915	2	-	0/5/25/26	0/2/2/2
2	PSU	GB	2605	2	-	0/7/25/26	0/2/2/2
4	PSU	IB	55	4	-	1/7/25/26	0/2/2/2
46	0TD	AD	92	46	-	2/3/12/14	-
2	4OC	GB	1920	2	-	1/7/27/30	0/2/2/2
1	M2G	FB	966	1	-	4/7/29/30	0/3/3/3
2	PSU	GB	1917	2	-	1/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	MA6	FB	1519	1	-	4/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	B	2251	2	-	3/5/27/28	0/3/3/3
1	MA6	FB	1518	1	-	3/7/29/30	0/3/3/3
1	5MC	FB	1404	1	-	0/5/25/26	0/2/2/2
2	2MA	GB	2503	2	-	2/3/25/26	0/3/3/3
2	5MC	GB	1962	2	-	4/5/25/26	0/2/2/2
4	5MC	D	32	4	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
4	5MU	NC	54	4	-	0/5/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
46	0TD	VA	92	46	-	3/3/12/14	-
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
1	5MC	FB	1407	1	-	0/5/25/26	0/2/2/2
2	5MU	B	1939	2	-	1/5/25/26	0/2/2/2
4	PSU	NC	55	4	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/5/25/26	0/2/2/2
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
4	5MC	IA	32	4	-	0/5/25/26	0/2/2/2
2	2MA	B	2503	2	-	2/3/25/26	0/3/3/3
2	5MU	GB	1939	2	-	0/5/25/26	0/2/2/2
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
4	5MU	IA	54	4	-	0/5/25/26	0/2/2/2
4	4SU	IA	8	4	-	1/5/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
4	4SU	D	8	4	-	1/5/25/26	0/2/2/2
2	5MC	GB	1942	2	-	0/5/25/26	0/2/2/2
1	4OC	FB	1402	1	-	4/9/29/30	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
4	5MC	NC	32	4	-	0/5/25/26	0/2/2/2
4	5MC	IB	32	4	-	0/5/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	8.19	1.41	1.34
1	FB	1207	2MG	C2-N2	7.80	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FB	527	7MG	O6-C6	7.44	1.43	1.24
1	A	527	7MG	O6-C6	7.21	1.42	1.24
4	IA	8	4SU	C5-C4	7.19	1.46	1.38

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FB	516	PSU	N1-C2-N3	-13.04	118.06	128.43
1	A	516	PSU	N1-C2-N3	-12.78	118.27	128.43
4	IB	55	PSU	N1-C2-N3	-11.03	119.66	128.43
2	B	1917	PSU	N1-C2-N3	-10.93	119.74	128.43
2	GB	1917	PSU	N1-C2-N3	-10.91	119.75	128.43

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	IB	8	4SU	C4'-C5'-O5'-P
4	NC	8	4SU	C2'-C1'-N1-C6
1	FB	1498	UR3	O4'-C4'-C5'-O5'
1	FB	1498	UR3	C3'-C4'-C5'-O5'
2	GB	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

43 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	IB	8	4SU	2	0
1	FB	967	5MC	4	0
4	IA	55	PSU	1	0
1	FB	1498	UR3	3	0
1	FB	527	7MG	1	0
2	GB	2251	OMG	3	0
1	A	1518	MA6	1	0
2	B	1920	4OC	4	0
2	GB	1915	5MU	1	0
1	FB	1207	2MG	3	0
2	B	1962	5MC	1	0
2	B	2552	2MU	1	0
2	B	1915	5MU	1	0
46	AD	92	0TD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	GB	1920	4OC	1	0
1	FB	966	M2G	1	0
2	GB	1917	PSU	2	0
1	A	1407	5MC	1	0
1	FB	1519	MA6	1	0
2	B	2251	OMG	3	0
1	FB	1518	MA6	1	0
2	GB	2503	2MA	3	0
2	GB	1962	5MC	1	0
1	A	1207	2MG	3	0
1	A	527	7MG	1	0
4	NC	54	5MU	4	0
46	VA	92	0TD	1	0
1	A	967	5MC	4	0
1	A	1402	4OC	1	0
1	FB	1407	5MC	1	0
2	B	1939	5MU	1	0
4	NC	55	PSU	1	0
1	A	1498	UR3	2	0
1	A	966	M2G	2	0
4	IA	32	5MC	3	0
2	B	2503	2MA	3	0
2	GB	1939	5MU	2	0
4	IA	54	5MU	4	0
1	A	1519	MA6	1	0
4	D	8	4SU	3	0
2	GB	1942	5MC	1	0
1	FB	1402	4OC	2	0
4	NC	32	5MC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1440 ligands modelled in this entry, 1438 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	BLS	B	9001	-	25,31,31	3.37	9 (36%)	23,43,43	2.82	8 (34%)
57	BLS	GB	9001	-	25,31,31	3.35	9 (36%)	23,43,43	2.42	7 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	BLS	B	9001	-	-	7/17/38/38	0/2/2/2
57	BLS	GB	9001	-	-	7/17/38/38	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	9001	BLS	C14-N12	8.87	1.54	1.35
57	GB	9001	BLS	C14-N12	8.44	1.53	1.35
57	GB	9001	BLS	C7-N6	7.66	1.50	1.34
57	B	9001	BLS	C7-N6	6.79	1.48	1.34
57	B	9001	BLS	O5'-C5'	6.44	1.51	1.44

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	9001	BLS	C1'-C2'-C3'	-8.94	110.80	122.52
57	GB	9001	BLS	C1'-C2'-C3'	-7.21	113.08	122.52
57	B	9001	BLS	C10-C11-N12	5.48	120.97	112.15
57	GB	9001	BLS	C10-C11-N12	5.44	120.91	112.15
57	B	9001	BLS	C2-N3-C4	3.95	120.34	116.34

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	GB	9001	BLS	C11-C10-C9-C8
57	GB	9001	BLS	C11-C10-C9-N9
57	GB	9001	BLS	C10-C11-N12-C13

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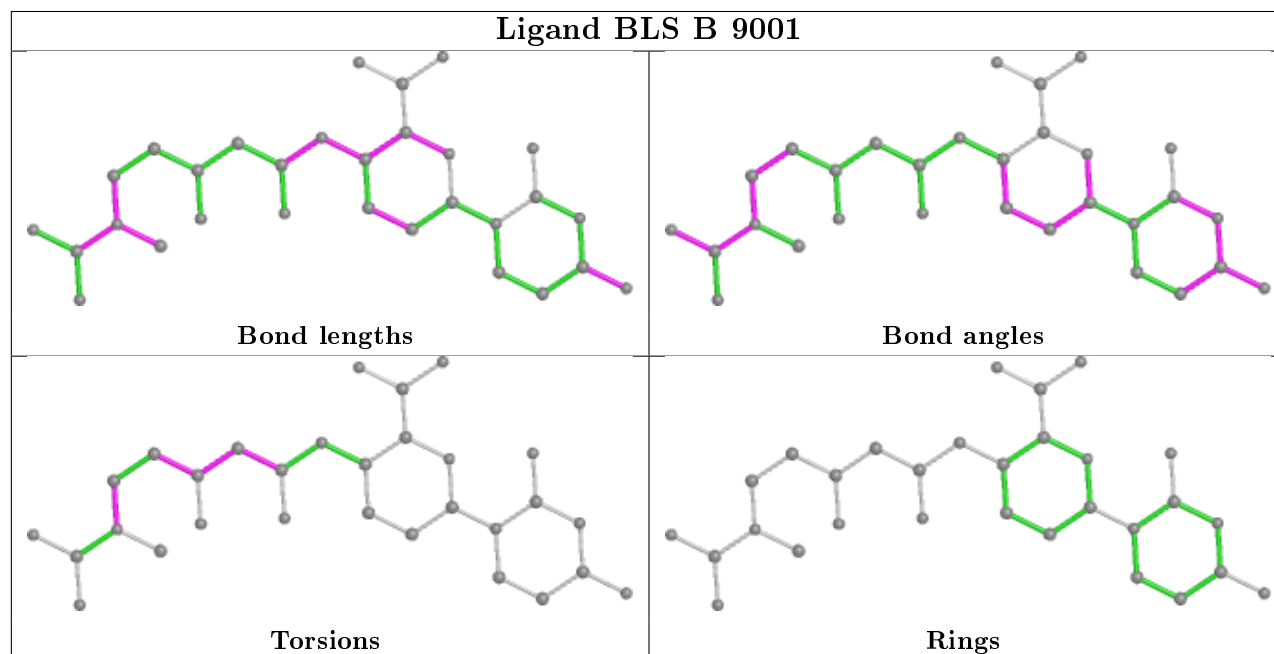
Mol	Chain	Res	Type	Atoms
57	GB	9001	BLS	C10-C11-N12-C14
57	B	9001	BLS	C11-C10-C9-C8

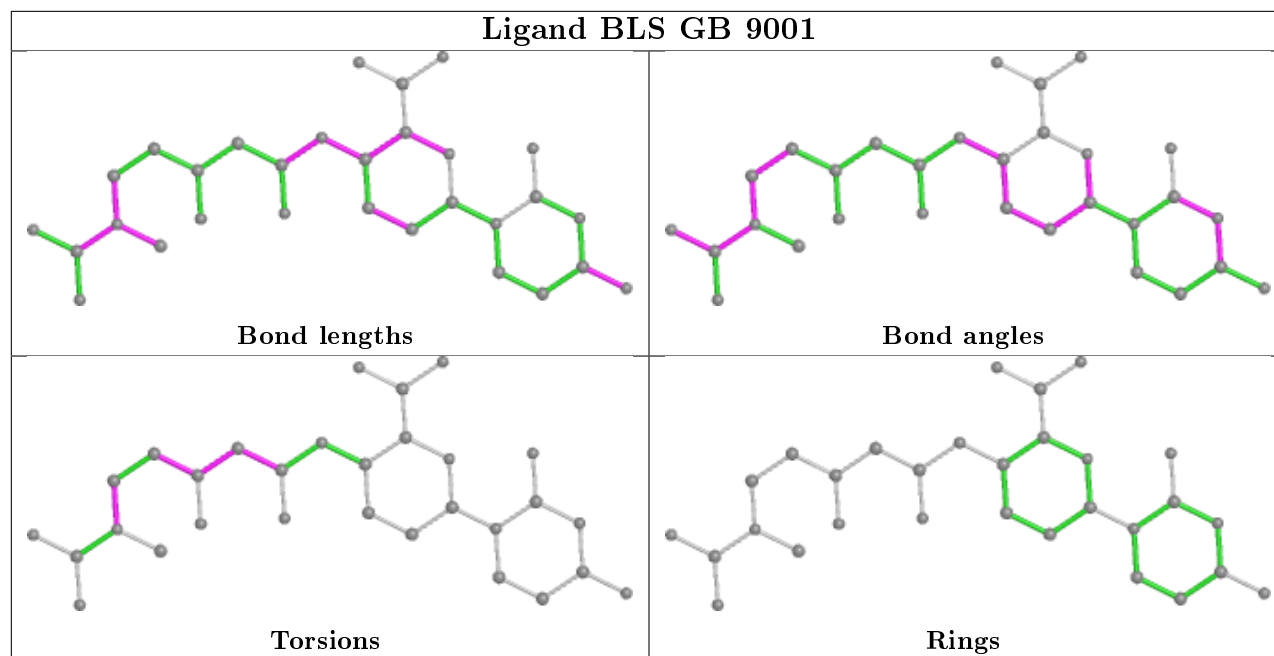
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	9001	BLS	4	0
57	GB	9001	BLS	7	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

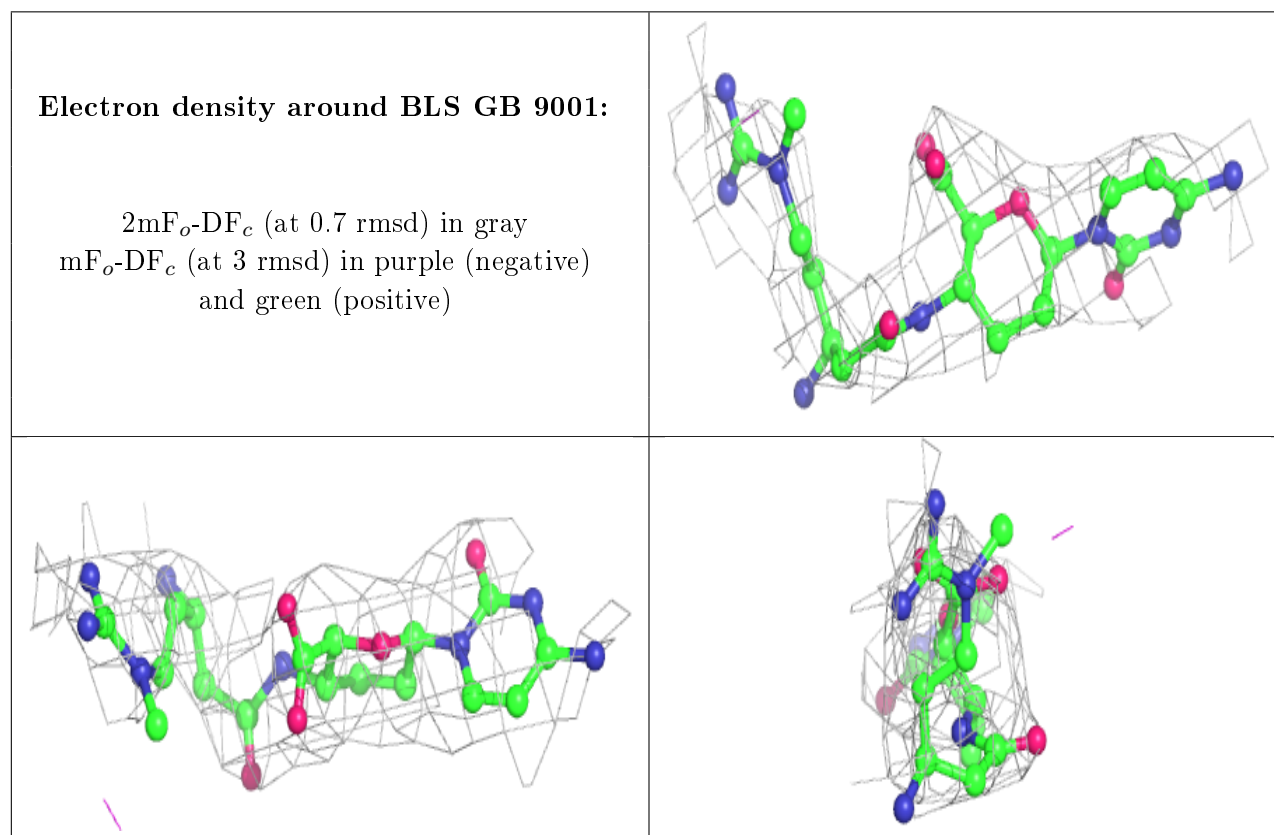
6.3 Carbohydrates ⓘ

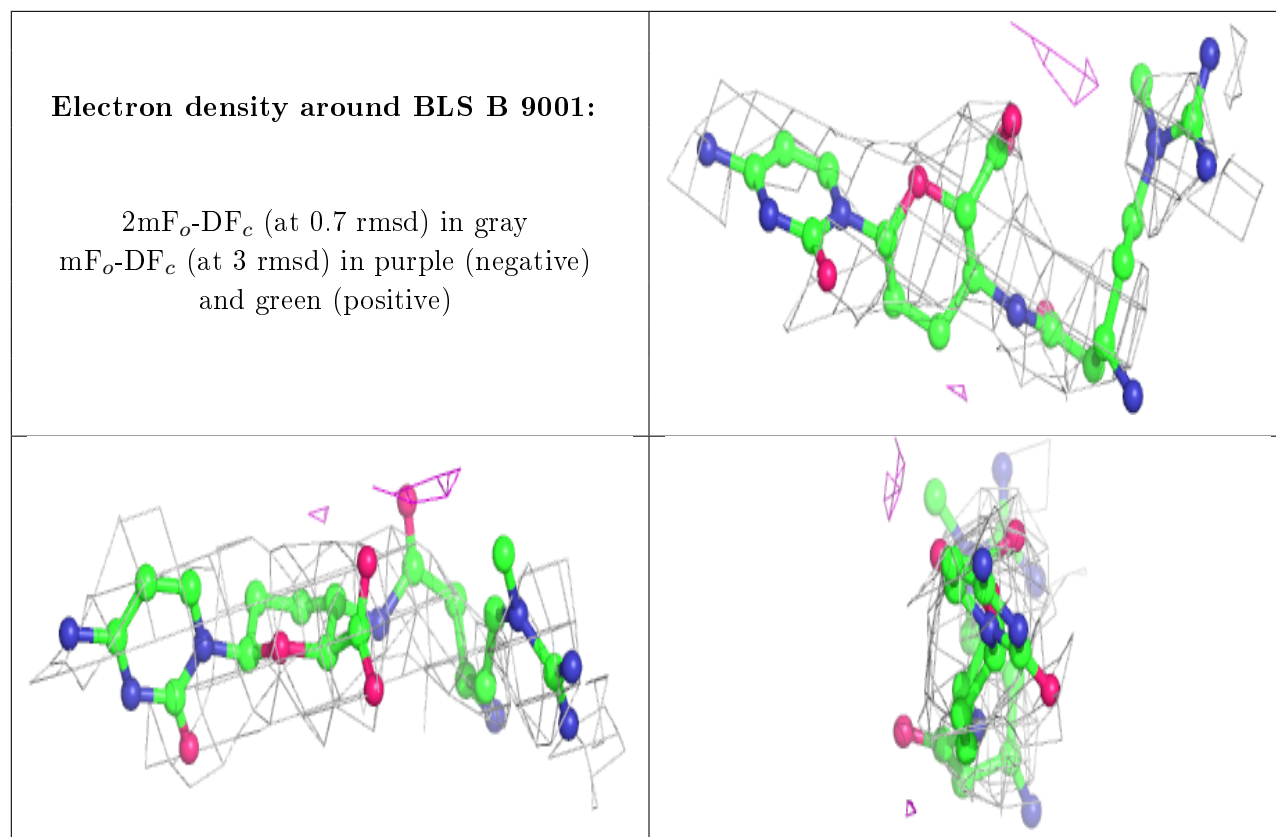
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.