



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:03 pm BST

PDB ID : 6B4V
Title : Antibiotic blasticidin S and E. coli release factor 1 bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-09-27
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

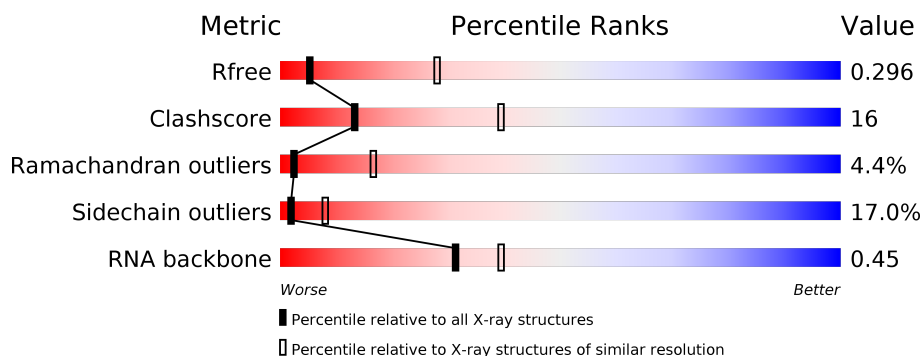
1 Overall quality at a glance

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.



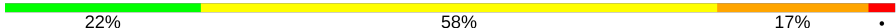
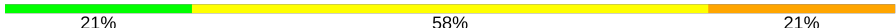
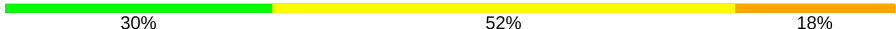
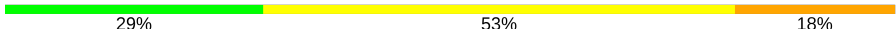






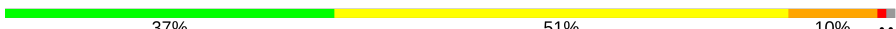
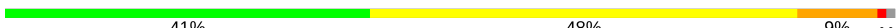







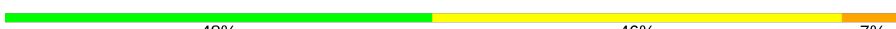





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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	<div> <div>38%</div> <div>48%</div> <div>13%</div> </div>
1	EB	1507	<div> <div>38%</div> <div>49%</div> <div>12%</div> <div>.</div> </div>
2	B	2880	<div> <div>40%</div> <div>41%</div> <div>16%</div> <div>.</div> </div>
2	FB	2880	<div> <div>43%</div> <div>41%</div> <div>14%</div> <div>.</div> </div>
3	C	120	<div> <div>45%</div> <div>42%</div> <div>13%</div> </div>
3	GB	120	<div> <div>42%</div> <div>46%</div> <div>13%</div> </div>


























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






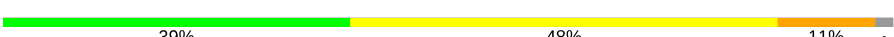




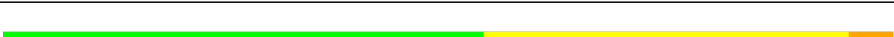


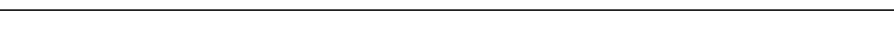

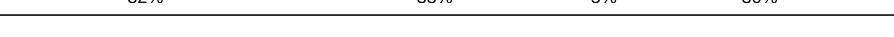
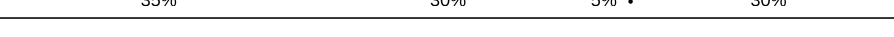





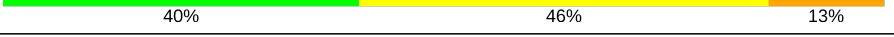


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Mol	Chain	Length	Quality of chain
15	SB	118	
16	P	112	
16	TB	112	
17	Q	146	
17	UB	146	
18	R	118	
18	VB	118	
19	S	101	
19	WB	101	
20	T	113	
20	XB	113	
21	U	96	
21	YB	96	
22	V	110	
22	ZB	110	
23	AC	206	
23	W	206	
24	BC	85	
24	X	85	
25	CC	98	
25	Y	98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



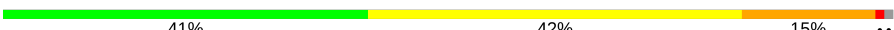
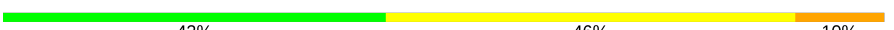
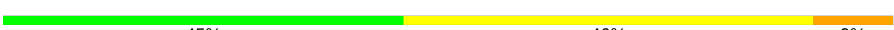
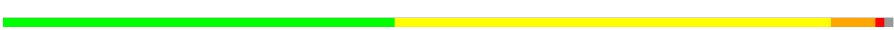


















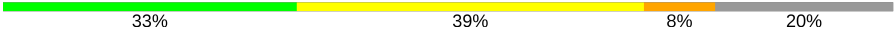
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Mol	Chain	Length	Quality of chain
28	BA	71	
28	FC	71	
29	CA	60	
29	GC	60	
30	DA	54	
30	HC	54	
31	EA	49	
31	IC	49	
32	FA	65	
32	JC	65	
33	GA	37	
33	KC	37	
34	HA	23	
34	LC	23	
35	JA	368	
35	NC	368	
36	KA	256	
36	OC	256	
37	LA	239	
37	PC	239	
38	MA	209	
38	QC	209	
39	NA	162	
39	RC	162	
40	OA	101	

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

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Mol	Chain	Length	Quality of chain
53	BB	93	
53	FD	93	
54	CB	106	
54	GD	106	
55	DB	27	
55	HD	27	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 299841 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	EB	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	FB	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
FB	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	GB	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	HB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	MC	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	IB	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	JB	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	KB	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	LB	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	MB	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	NB	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	OB	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	PB	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	QB	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	RB	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	SB	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	TB	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	UB	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	VB	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	WB	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	XB	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	YB	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	ZB	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	AC	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	BC	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
BC	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	CC	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	DC	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	EC	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	FC	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	GC	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	HC	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	IC	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	JC	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	KC	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	LC	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	258	Total 2005	C 1227	N 380	O 390	S 8	0	0	0
35	NC	258	Total 2005	C 1227	N 380	O 390	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	361	LEU	-	expression tag	UNP A7ZKY5
JA	362	GLU	-	expression tag	UNP A7ZKY5
JA	363	HIS	-	expression tag	UNP A7ZKY5
JA	364	HIS	-	expression tag	UNP A7ZKY5
JA	365	HIS	-	expression tag	UNP A7ZKY5
JA	366	HIS	-	expression tag	UNP A7ZKY5
JA	367	HIS	-	expression tag	UNP A7ZKY5
JA	368	HIS	-	expression tag	UNP A7ZKY5
NC	361	LEU	-	expression tag	UNP A7ZKY5
NC	362	GLU	-	expression tag	UNP A7ZKY5
NC	363	HIS	-	expression tag	UNP A7ZKY5
NC	364	HIS	-	expression tag	UNP A7ZKY5
NC	365	HIS	-	expression tag	UNP A7ZKY5
NC	366	HIS	-	expression tag	UNP A7ZKY5
NC	367	HIS	-	expression tag	UNP A7ZKY5
NC	368	HIS	-	expression tag	UNP A7ZKY5

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

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

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

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
38	QC	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	NA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
39	RC	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	OA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
40	SC	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	PA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
41	TC	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	QA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
42	UC	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	RA	127	Total	C	N	O		0	0	0
			1011	639	198	174				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	VC	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	SA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
44	WC	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	TA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
45	XC	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	UA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
46	YC	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	VA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
47	ZC	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	WA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
48	AD	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	XA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
49	BD	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	YA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
50	CD	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	ZA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
51	DD	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	AB	70	Total	C	N	O	0	0	0
			574	367	112	95			
52	ED	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	BB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
53	FD	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	CB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
54	GD	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	DB	24	Total	C	N	O	0	0	0
			208	128	50	30			
55	HD	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	XC	1	Total	Mg	0	0
			1	1		
56	MC	5	Total	Mg	0	0
			5	5		
56	NC	5	Total	Mg	0	0
			5	5		
56	QA	2	Total	Mg	0	0
			2	2		
56	BA	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	VB	1	Total	Mg	0	0
			1	1		
56	B	562	Total	Mg	0	0
			562	562		
56	KA	1	Total	Mg	0	0
			1	1		
56	RC	3	Total	Mg	0	0
			3	3		
56	UA	4	Total	Mg	0	0
			4	4		
56	W	2	Total	Mg	0	0
			2	2		
56	HA	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	EB	206	Total 206	Mg 206	0	0
56	X	1	Total 1	Mg 1	0	0
56	WB	1	Total 1	Mg 1	0	0
56	SC	1	Total 1	Mg 1	0	0
56	DC	1	Total 1	Mg 1	0	0
56	S	2	Total 2	Mg 2	0	0
56	MB	2	Total 2	Mg 2	0	0
56	CA	1	Total 1	Mg 1	0	0
56	J	2	Total 2	Mg 2	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	LC	1	Total 1	Mg 1	0	0
56	TA	3	Total 3	Mg 3	0	0
56	E	1	Total 1	Mg 1	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	VC	1	Total 1	Mg 1	0	0
56	IA	6	Total 6	Mg 6	0	0
56	V	2	Total 2	Mg 2	0	0
56	FB	475	Total 475	Mg 475	0	0
56	IB	4	Total 4	Mg 4	0	0
56	A	214	Total 214	Mg 214	0	0
56	SB	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	GB	15	Total 15	Mg 15	0	0
56	HB	9	Total 9	Mg 9	0	0
56	AB	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	M	5	Total 5	Mg 5	0	0
56	BD	1	Total 1	Mg 1	0	0
56	AA	2	Total 2	Mg 2	0	0
56	PB	1	Total 1	Mg 1	0	0
56	D	5	Total 5	Mg 5	0	0
56	YC	5	Total 5	Mg 5	0	0
56	MA	2	Total 2	Mg 2	0	0
56	NA	2	Total 2	Mg 2	0	0
56	UC	2	Total 2	Mg 2	0	0
56	I	3	Total 3	Mg 3	0	0
56	JA	6	Total 6	Mg 6	0	0
56	XA	6	Total 6	Mg 6	0	0
56	TB	1	Total 1	Mg 1	0	0
56	CC	7	Total 7	Mg 7	0	0
56	Z	4	Total 4	Mg 4	0	0
56	SA	3	Total 3	Mg 3	0	0
56	DA	2	Total 2	Mg 2	0	0

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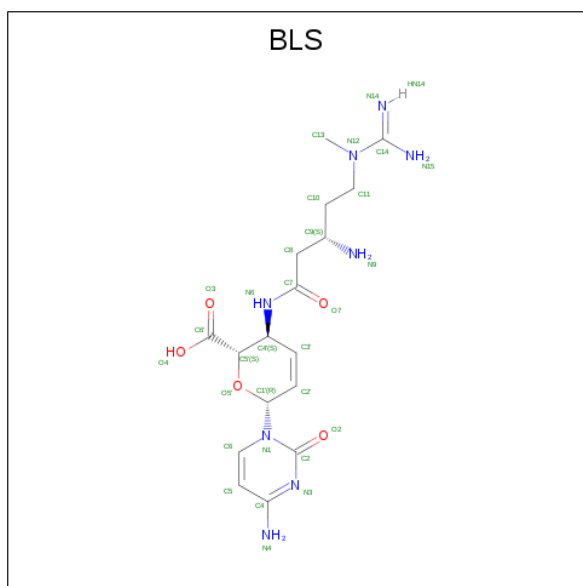
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	U	2	Total 2	Mg 2	0	0
56	L	2	Total 2	Mg 2	0	0
56	EA	1	Total 1	Mg 1	0	0
56	LA	2	Total 2	Mg 2	0	0
56	OC	5	Total 5	Mg 5	0	0
56	PC	1	Total 1	Mg 1	0	0
56	G	2	Total 2	Mg 2	0	0
56	Q	2	Total 2	Mg 2	0	0
56	NB	3	Total 3	Mg 3	0	0
56	UB	3	Total 3	Mg 3	0	0
56	WC	1	Total 1	Mg 1	0	0
56	H	1	Total 1	Mg 1	0	0
56	JB	2	Total 2	Mg 2	0	0
56	TC	1	Total 1	Mg 1	0	0
56	C	21	Total 21	Mg 21	0	0
56	QC	4	Total 4	Mg 4	0	0
56	KB	4	Total 4	Mg 4	0	0
56	CB	1	Total 1	Mg 1	0	0
56	CD	1	Total 1	Mg 1	0	0
56	EC	1	Total 1	Mg 1	0	0
56	T	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AD	2	Total	Mg	0	0
			2	2		
56	O	2	Total	Mg	0	0
			2	2		
56	FC	1	Total	Mg	0	0
			1	1		
56	Y	1	Total	Mg	0	0
			1	1		
56	OB	3	Total	Mg	0	0
			3	3		
56	F	2	Total	Mg	0	0
			2	2		
56	RB	1	Total	Mg	0	0
			1	1		

- Molecule 57 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).



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

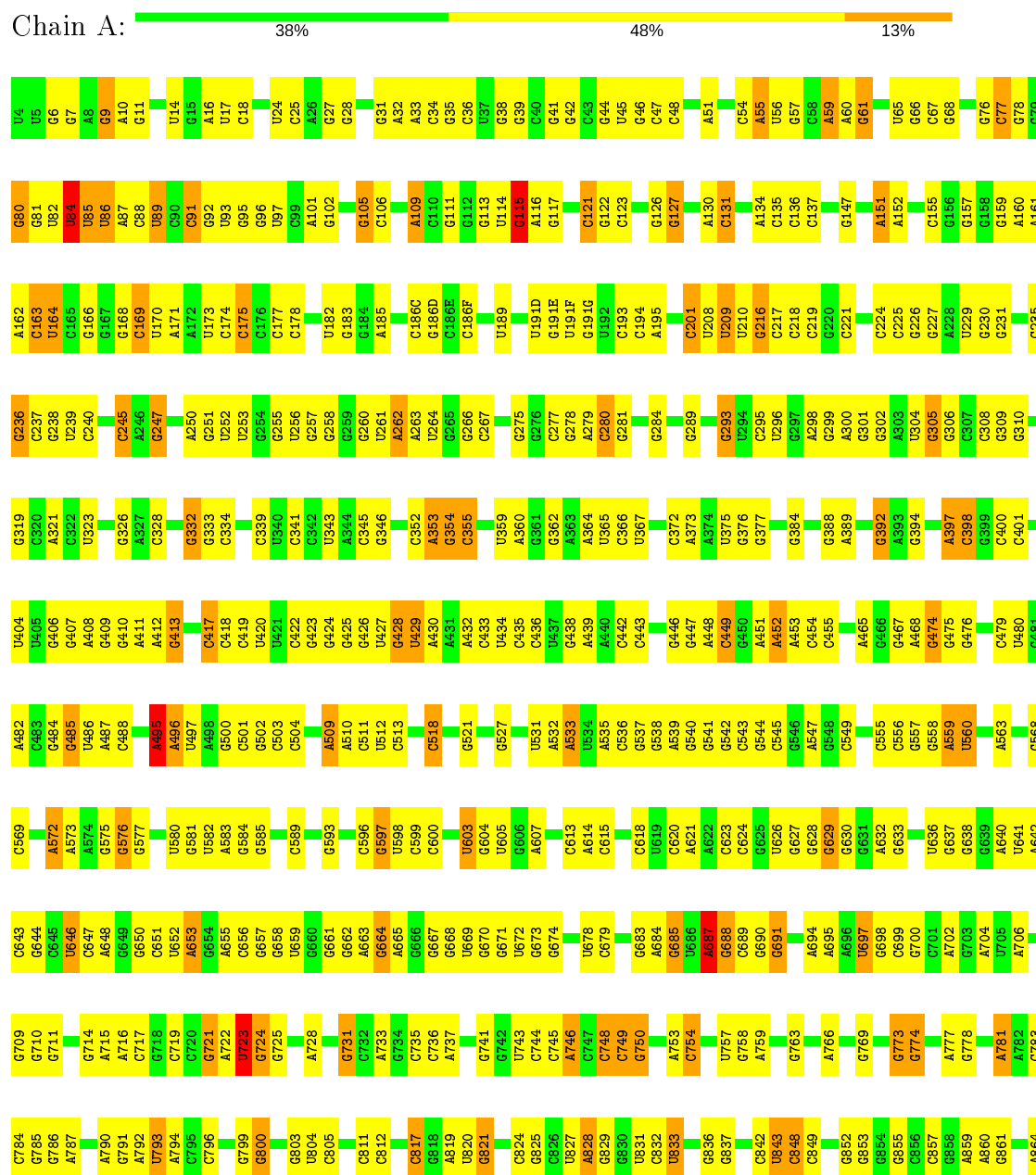
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

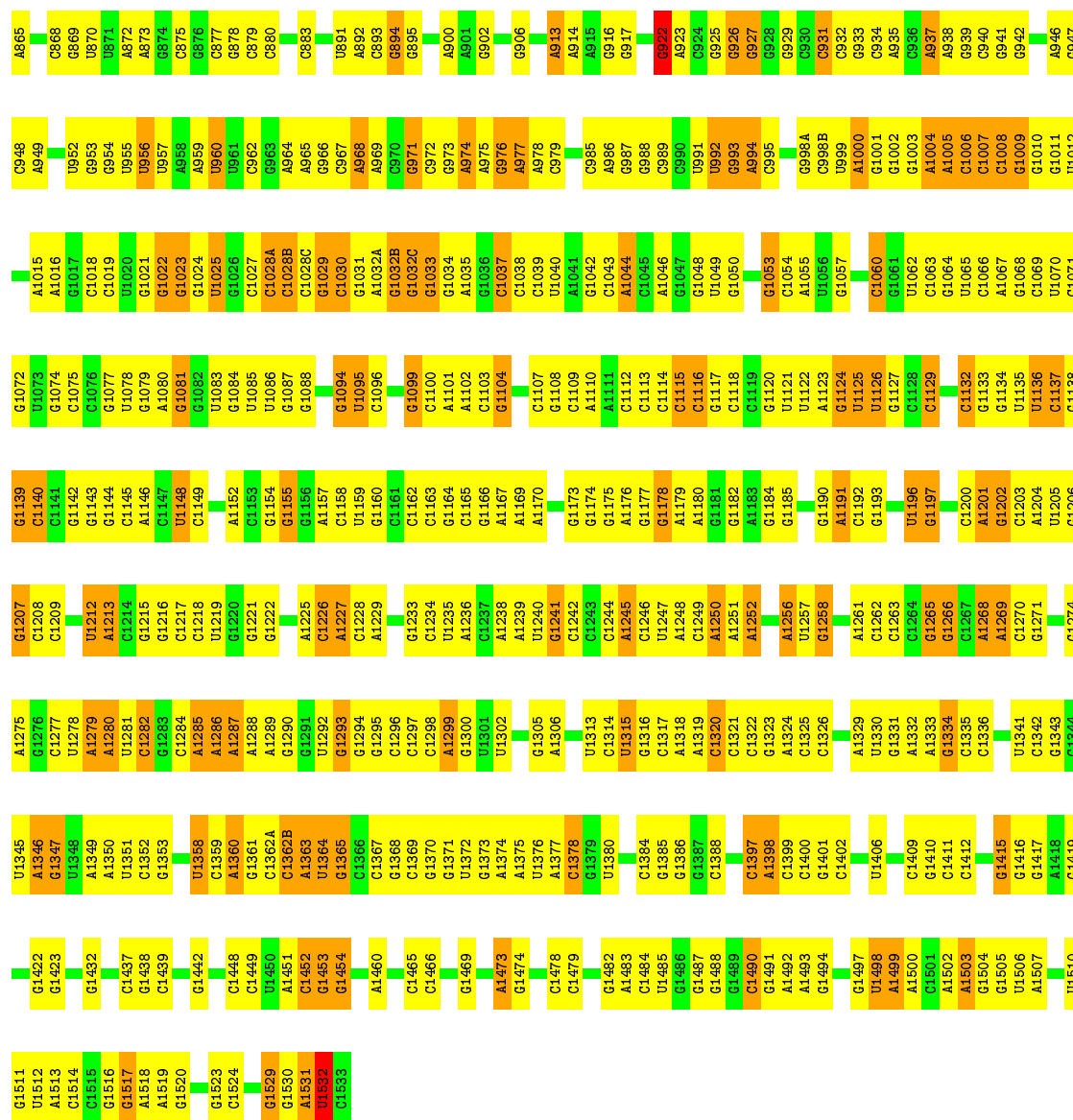
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	1	Total	Zn	0	0
			1	1		
58	CA	1	Total	Zn	0	0
			1	1		
58	V	1	Total	Zn	0	0
			1	1		
58	GA	1	Total	Zn	0	0
			1	1		
58	KC	1	Total	Zn	0	0
			1	1		
58	DA	1	Total	Zn	0	0
			1	1		
58	GC	1	Total	Zn	0	0
			1	1		
58	HC	1	Total	Zn	0	0
			1	1		
58	ZB	1	Total	Zn	0	0
			1	1		
58	FC	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

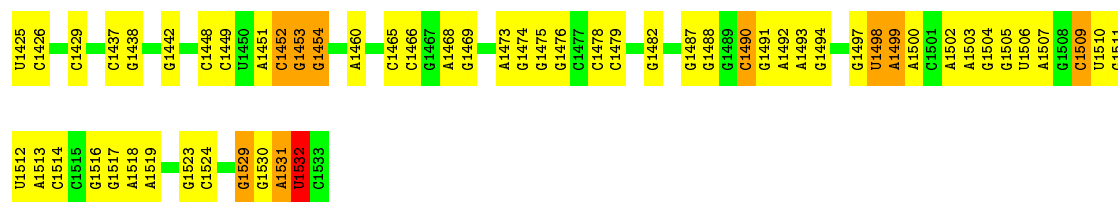
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



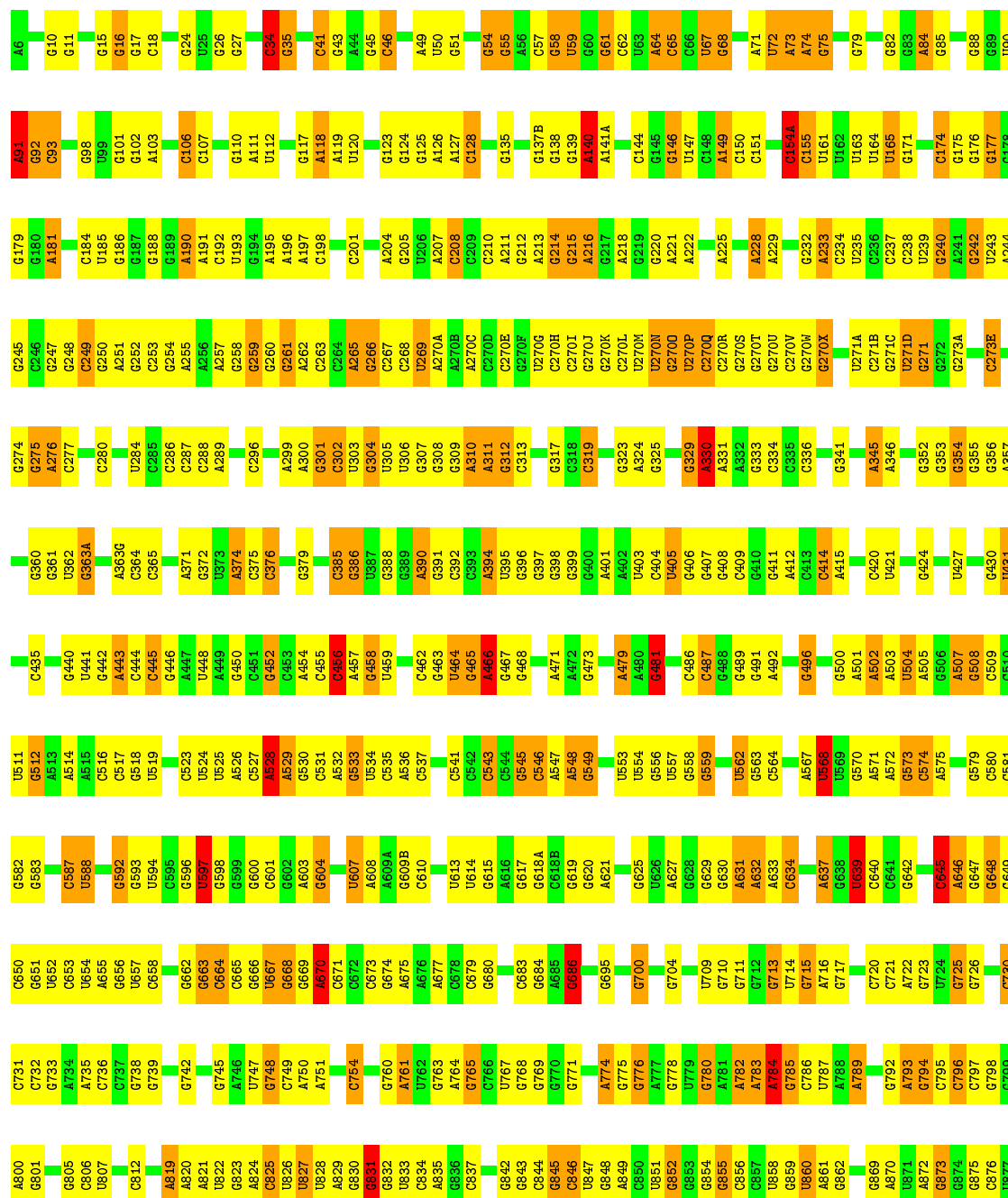


G1353	A1287	G1215	U1148	G1081	G1022	A958	U870	A780	G703	G631	U561	C483	G407	A325
C1358	A1288	G1216	C1149	G1082	G1023	A959	U871	A781	A704	A632	C562	G484	A408	G326
G1359	A1289	C1217		U1083	U1024	U960	A872		A705	G633	G563	G485	G409	A327
A1360	G1290	C1218	A1152	U1084	U1025	U961	A873	G785	A706	U961	C564	U486	G410	C328
G1361	U1291	G1154	C1153	U1085	G1026	C962	G874			U636		A487	A411	G332
C1362A	G1292	G1220	G1155	U1086	C1027	C963	C875	A790	G709	G637	G568	C488	A412	G333
C1362B	G1293	G1221	G1156	G1087	C1028A	A964	G876	C791	G710	G638	C569		G413	C334
A1363	G1294		G1157	G1088	C1028B	A965	C877	A792		G639		A495		
G1295	C1295	A1225	A1158	U1094	C1028C	G966	C878	A793	G714	U580	A572	A496	C417	C341
U1364	C1296	C1226	C1159	G1095	G1029	A967	C879	A794	G715	G581	A573	U497	C418	C342
C1365	C1297	C1297	U1159	U1096	C1030	A968	C880	G795	A716	U582	A574	A498	C419	U343
C1366	C1298	C1228	G1160	C1096	G1031	A969		C796		G575	G576	C501	U420	U344
A1298	A1298	A1229	C1161		G1032A	C970	A892		C719	G644	G577	G502	U421	A344
G1300	G1300		C1162	G1099	G1032B	G971	C893	G799	C720	G645		G503	C422	C345
U1301	U1301	G1233	C1163	G1100	G1032C	C972	C894	G800	G721	U646		C504	G423	
G1302	G1302	G1370	A1164	A1101	G1033	G973	G895		A722	G647	U580	G505	G424	C352
G1305	G1305	A1238		A1102	A1034	A974		G803	U723	A648	G581		C425	A353
A1306	U1307	A1239	A1167	C1103	G1035	A975	C899	U804	G724	G649	U582		G426	G354
U1307	A1306	U1240	A1169	G1104	G1036	G976	A900		G725	G650	A583	A509	U427	C355
A1374	U1307	G1241	A1170		C1037	A977	A901	C811		G651	G584	A510	G428	U359
A1375		C1242		G1107	C1038	A978	G902	C812	G730	U652	G585	C511	U429	A360
U1376	G1309			G1108	C1039	C979	A913		C732	C513		C513	A431	G361
A1377				G1109	U1040		A914	C817	A733	G657	G583	U516	A432	G362
		A1245	G1173	A1110	A1041	C985		G818	G734	G658		G517	C433	A363
		C1246	G1175	A1111	G1042	A986	G917	A819	C735	U659		C518	U434	A364
		U1247	A1176	C1112	C1043	G987		U820	G736	G660	C596	C519	C435	U365
A1248	G1177	A1248	G1177	C1113	A1044	G988		G821	A737	G661	U598	C366	C436	U367
C1249	A1178	C1249	A1178	G1114	C1045	C989	G922	C824	G741	G662	C599	G521		
U1249	G1179	C1114	A1179	C1115	A1046	C990	A923	G825	G742	A663	C600		A439	G371
G1241	A1181	G1116	C1116	C1117	G1047	U991	G924		G743	G664	C601		A440	C372
C1242	G1182	G1117	G1117	G1118	U1048	U992	G925	A828	U743	A665	G602	G527	C442	A373
	A1256	C1118	C1118	C1119	G1049	G993	G926		C744	G666	A603		C443	U374
	U1257	G1184	G1184	G1120	G1050	A994	G927	U831	C745	U673	A608	A535	G444	U375
G1258	G1258	U1186	G1186	U1121		C995	G928	C832	A746	G674	A609	G536	G445	U376
		G1187	G1187	U1122	G1051		G929	U833	C747		G610	G537	G446	G376
	A1261	A1123	A1123	U1124	U1052	G998A	C930	U833	C748	G671	A607	U534	G447	G377
C1262	C1262	G1124	G1124	U1125	U1053	C998B	C931		C749	U672	A608		A448	
C1263	G1264	U1125	U1125	U1126	G1054	U999	G933	G836	G750	G673	A609	A535	C449	A382
G1265	C1265	G1127	G1127	G1127	U1055	A1000	C934	G837	A753	G674	G610	G536	A451	A383
C1266	G1267	G1128	G1128	G1129	C1056	G1001	A935		C754			G537	A452	G384
G1267		U1061	U1061	C1129	U1057	G1002	C936	C842		U678		G538	A453	G388
A1268	A1268	G1062	U1062	G1129	U1063	G1003	A937	C848	U757	C679	C613	A539	A454	A389
C1269	C1269	C1063	C1063	C1132	C1064	A1004	A938	C849	G758	G683	A614	G540	C454	
C1270	C1270	U1065	U1065	G1133	U1066	C1005	A939	U850	A759	A694	C615	G541	C455	C390
G1271	G1271	G1134	G1134	G1133	C1067	C1006	C940	G851		G685	G616	G542	C456	G391
		U1135	U1135	G1134	U1068	C1007	G941	G852	G763	U686	G617	C543		G392
		A1201	A1201	U1135	A1067	G1008	G942	G853		A687	C618	G544	A465	A393
G1274	G1274	G1068	G1068	G1136	G1009	G1010		G854	G763	U686	U619	C545	G466	G394
A1275	A1275	C1137	C1137	C1137	G1010	G1011	A946	G855	A767	G688	C620	C546	G467	C395
G1276	G1276	U1070	U1070	G1138	U1012	G1011	G947		A768	C689	A621	A547	A468	G396
C1277	C1277	U1071	U1071	G1139	G1013	U1012	C948	A859	G769	G690	G622	G548	G474	A397
U1278	U1278	G1072	G1072	C1140	A1014	U1013	A949	A860	C770	G691	C623	C549	G475	C398
A1279	A1279	U1073	U1073	G1141	A1015	G1009		G861			C624		G476	G399
G1280	G1280	G1074	G1074	G1142	U1016	G1009	U952		G773	U697	G625	C555	C400	C401
C1281	C1281			G1143	G1017	G1017	G953	A864	G774	G698	U626	C556	A478	
U1282	U1282	G1077	G1077	C1144	C1018	G1018	G954	A865		C699	G627	G557	C479	U404
G1283	G1283	U1078	U1078	G1145	U1019	C1018	G955		A777	G700	G628	G558	U480	U405
C1284	C1284	U1079	U1079	C1146	U1020	U1020	U956	C868	G778	C701	G629	A559	G481	
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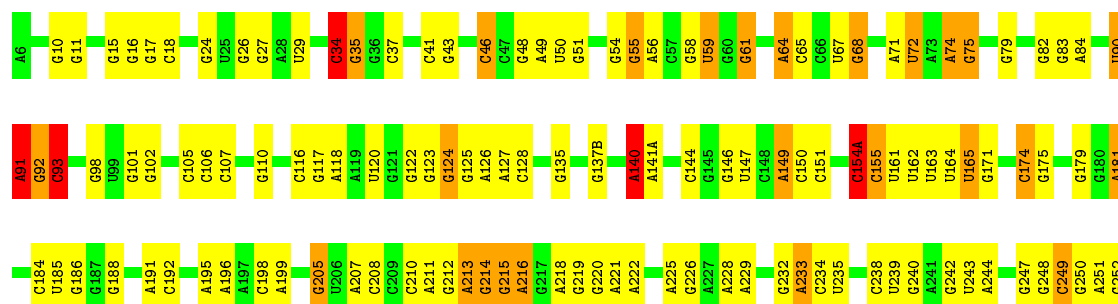


• Molecule 2: 23S ribosomal RNA

Chain B: 40% 41% 16%

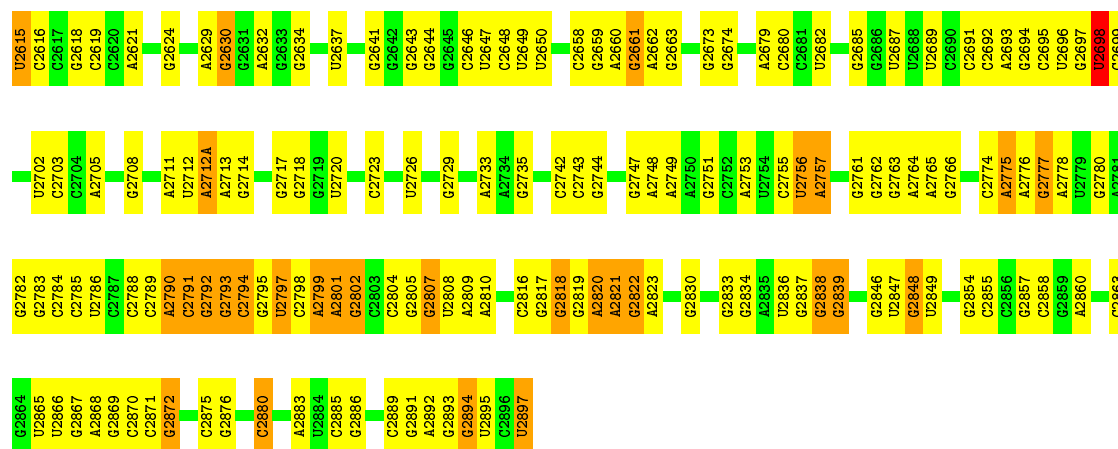


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	G1826	G1750	G1651	G1566	G1488	G1417	G1344	U1264		A1103	G1041	G887
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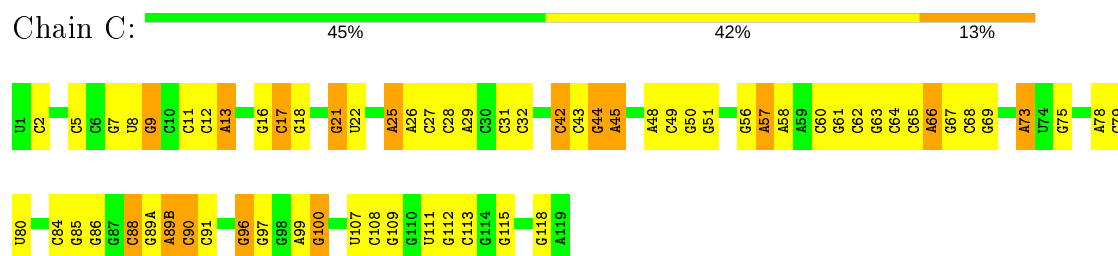




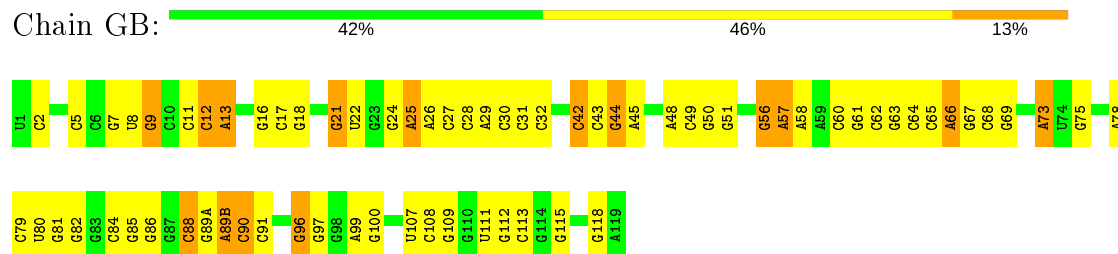
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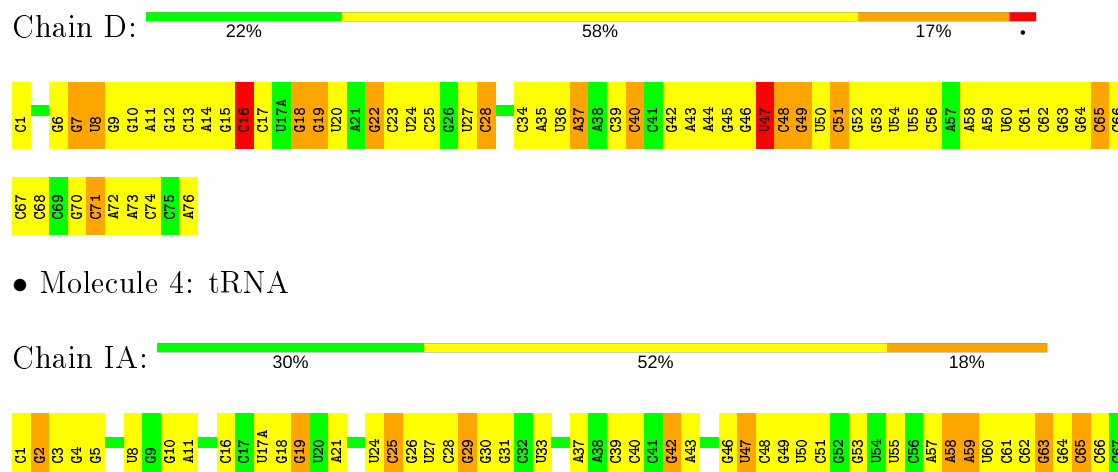
• Molecule 3: 5S ribosomal RNA



• Molecule 3: 5S ribosomal RNA



• Molecule 4: tRNA

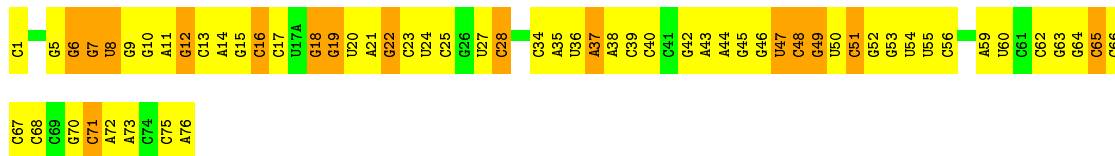


• Molecule 4: tRNA



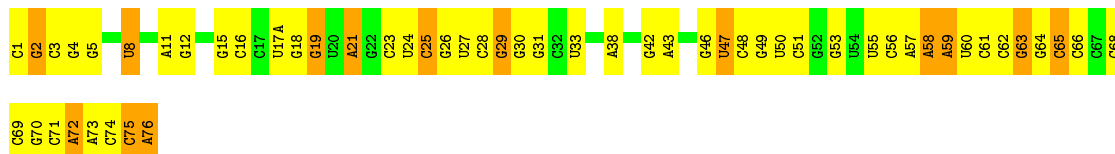
• Molecule 4: tRNA

Chain HB: 21% 58% 21%



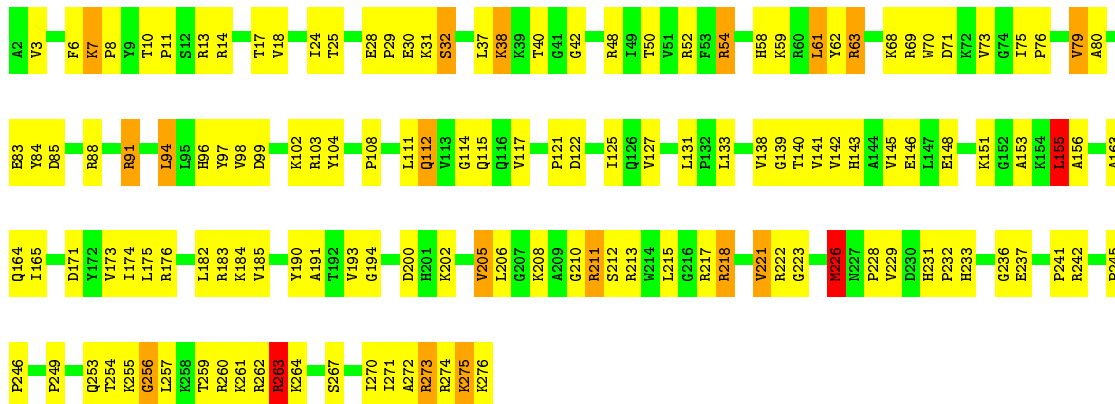
• Molecule 4: tRNA

Chain MC: 29% 53% 18%



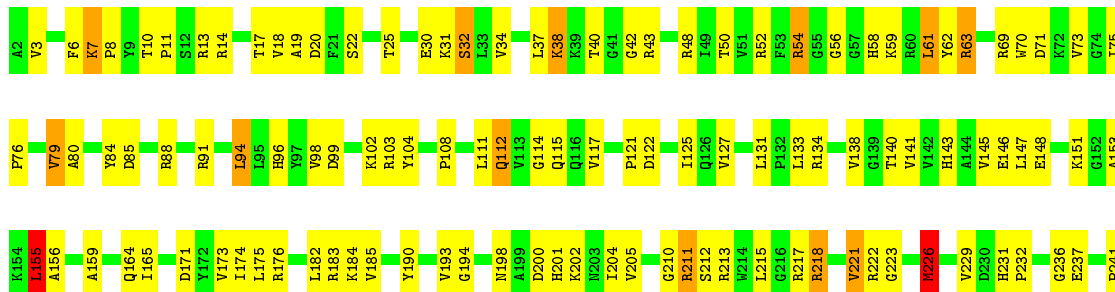
• Molecule 5: 50S ribosomal protein L2

Chain E: 49% 44% 6%



• Molecule 5: 50S ribosomal protein L2

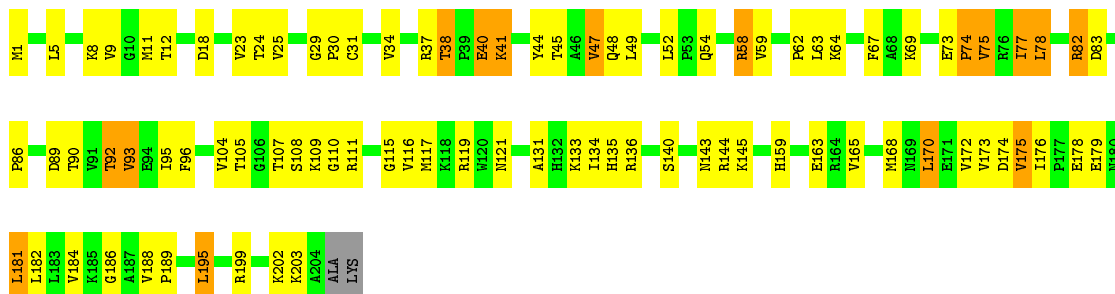
Chain IB: 51% 43% 6%





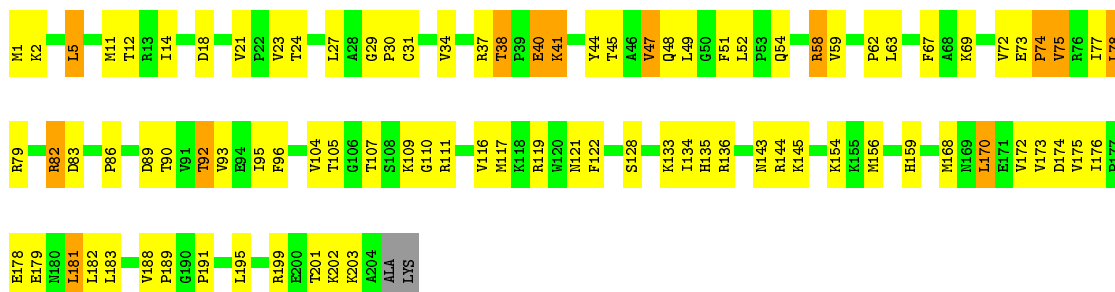
- Molecule 6: 50S ribosomal protein L3

Chain F: 56% 35% 8% .



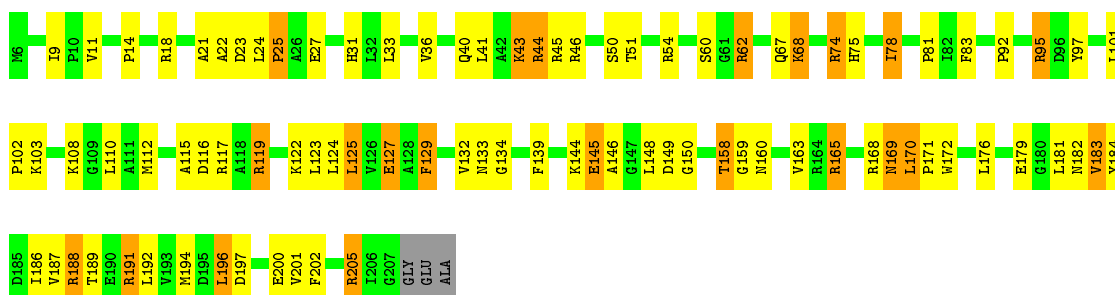
- Molecule 6: 50S ribosomal protein L3

Chain JB: 55% 38% 6% .



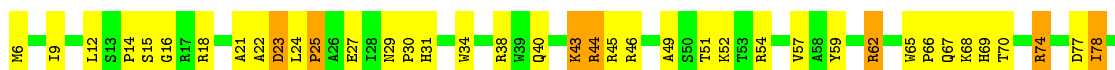
- Molecule 7: 50S ribosomal protein L4

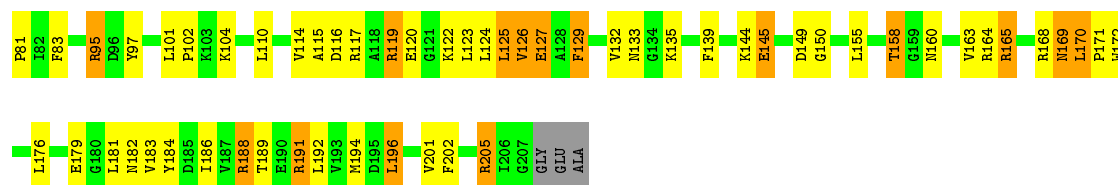
Chain G: 55% 33% 11% .



- Molecule 7: 50S ribosomal protein L4

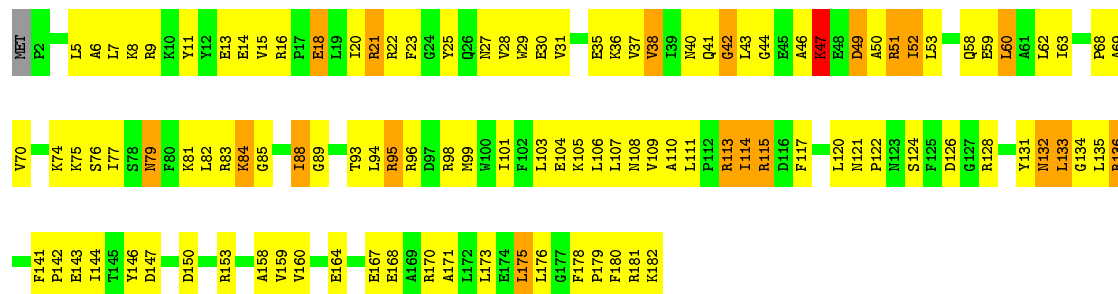
Chain KB: 52% 36% 11% .





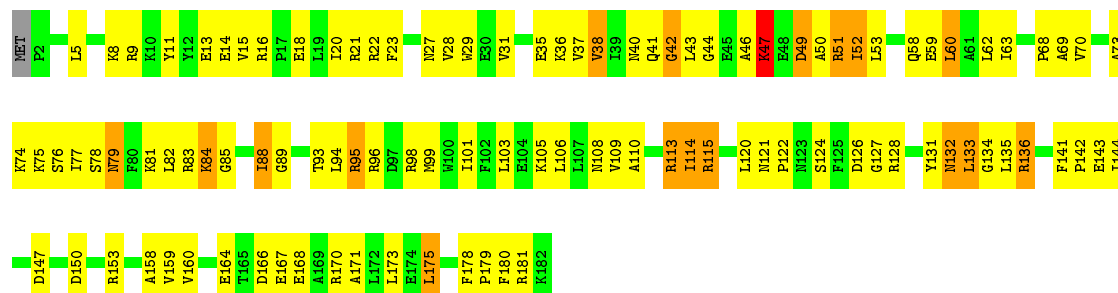
• Molecule 8: 50S ribosomal protein L5

Chain H: 37% 51% 10% ..



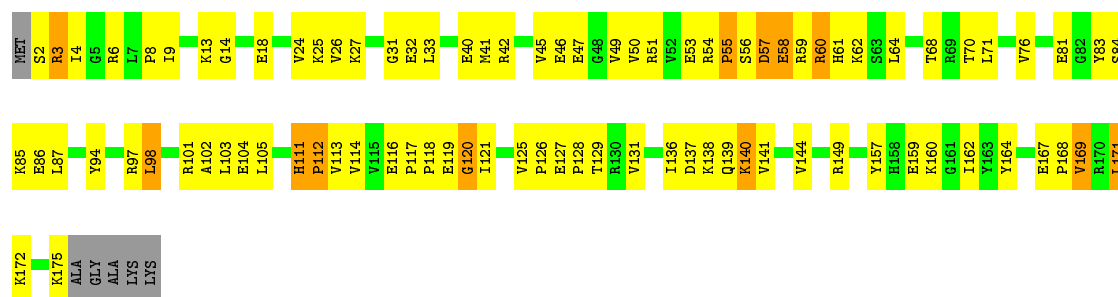
• Molecule 8: 50S ribosomal protein L5

Chain LB: 41% 48% 9% ..



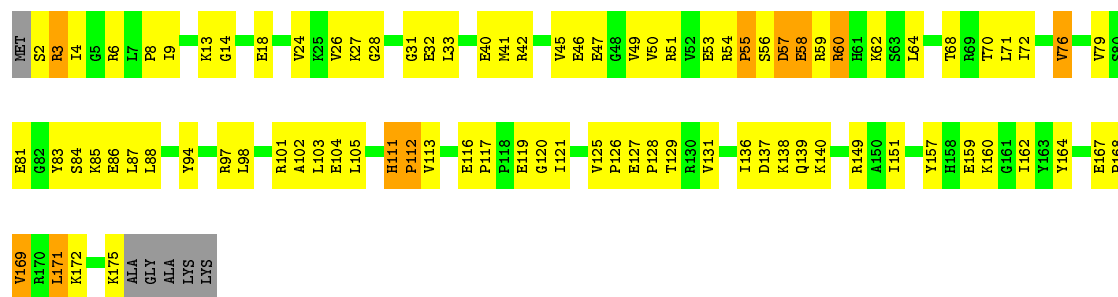
• Molecule 9: 50S ribosomal protein L6

Chain I: 47% 43% 7% .



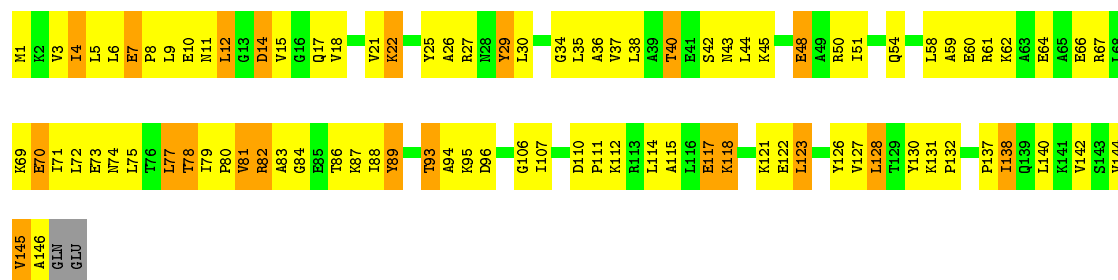
• Molecule 9: 50S ribosomal protein L6

Chain MB: 48% 43% 6% .



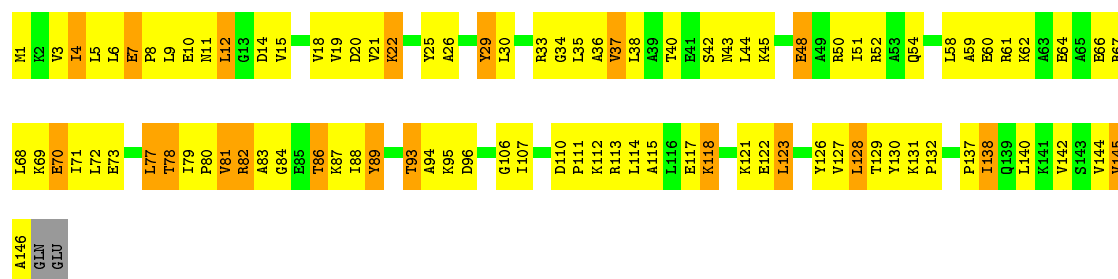
- Molecule 10: 50S ribosomal protein L9

Chain J: 36% 48% 14%



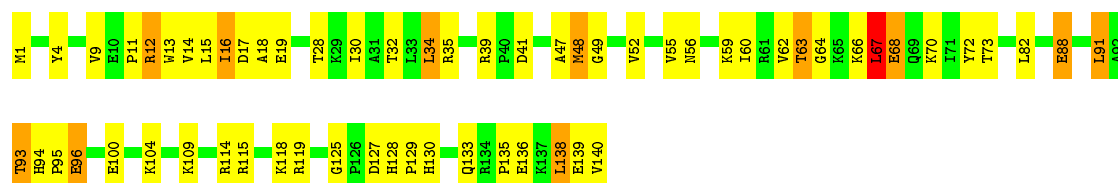
- Molecule 10: 50S ribosomal protein L9

Chain NB: 34% 51% 14%



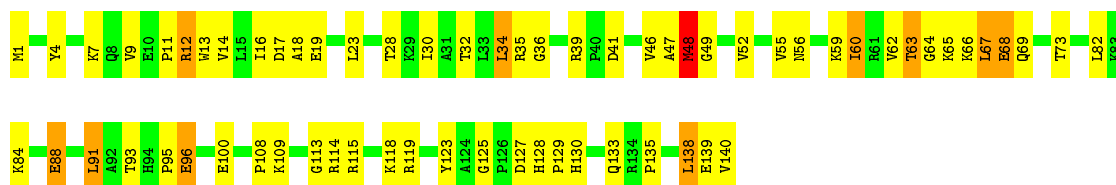
- Molecule 11: 50S ribosomal protein L13

Chain K: 56% 35% 8%

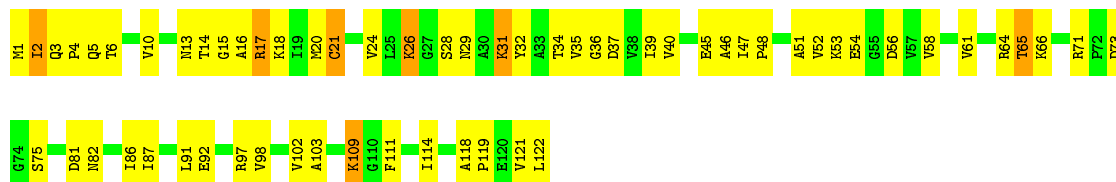


- Molecule 11: 50S ribosomal protein L13

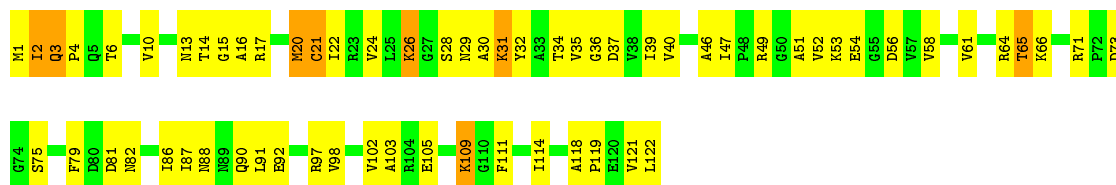
Chain OB: 54% 39% 7%



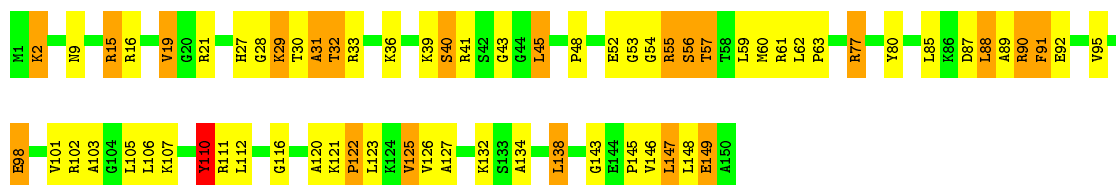
- Molecule 12: 50S ribosomal protein L14



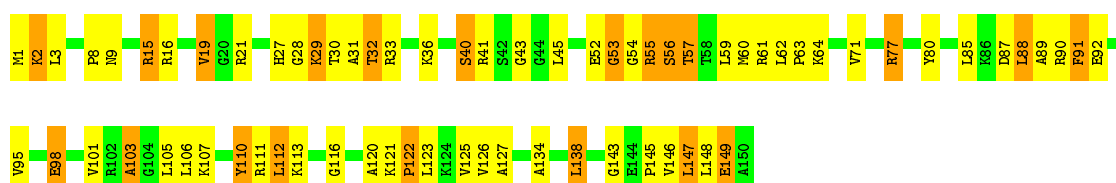
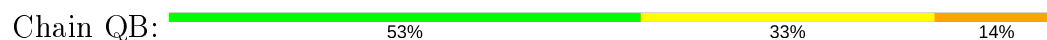
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15

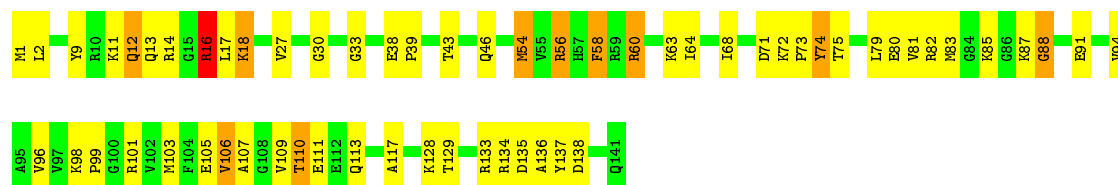


- Molecule 13: 50S ribosomal protein L15



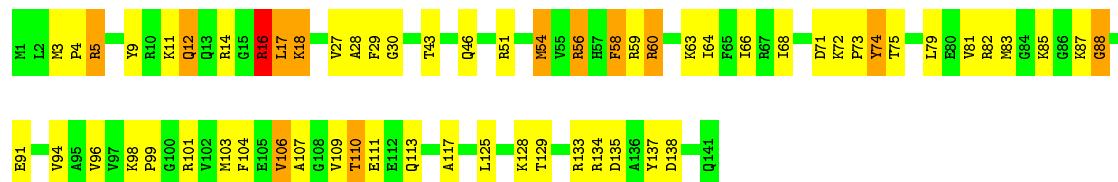
- Molecule 14: 50S ribosomal protein L16





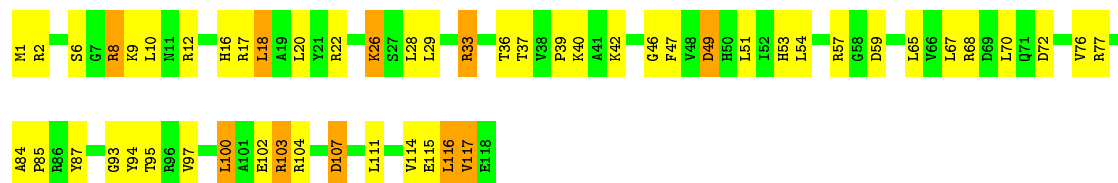
• Molecule 14: 50S ribosomal protein L16

Chain RB: 57% 34% 9%



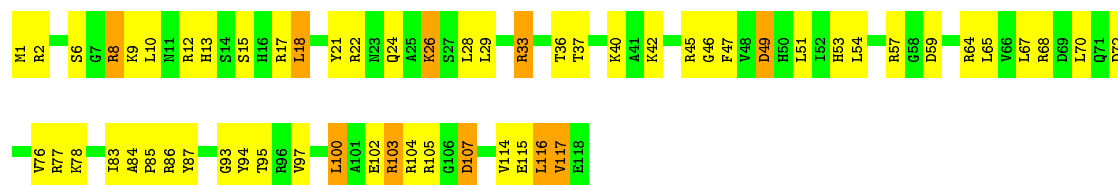
• Molecule 15: 50S ribosomal protein L17

Chain O: 55% 36% 8%



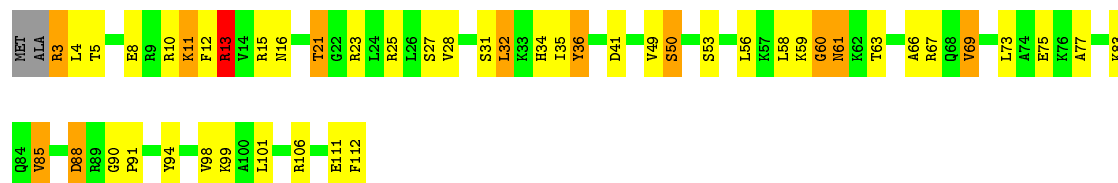
• Molecule 15: 50S ribosomal protein L17

Chain SB: 50% 42% 8%



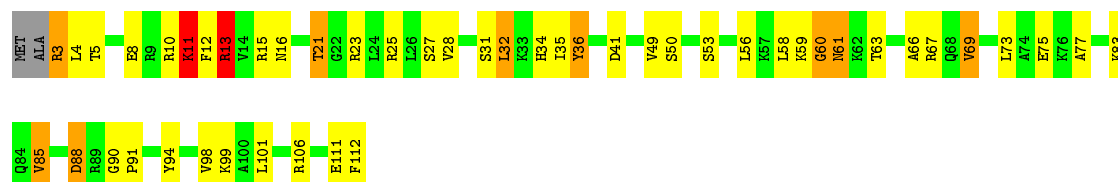
• Molecule 16: 50S ribosomal protein L18

Chain P: 55% 32% 10%



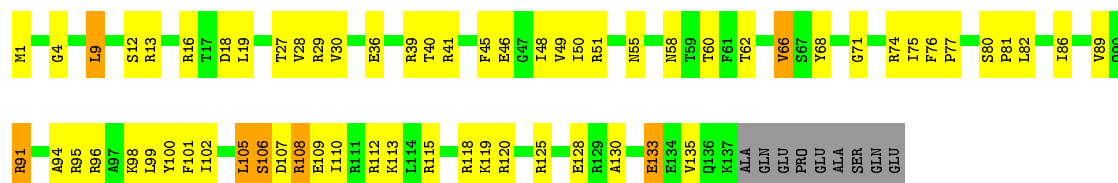
• Molecule 16: 50S ribosomal protein L18

Chain TB: 55% 33% 8%



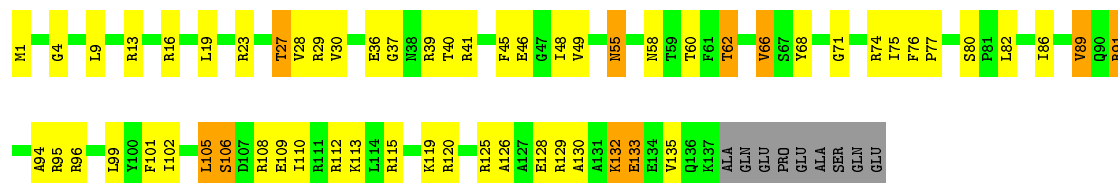
- Molecule 17: 50S ribosomal protein L19

Chain Q: 50% 39% 5% 6%



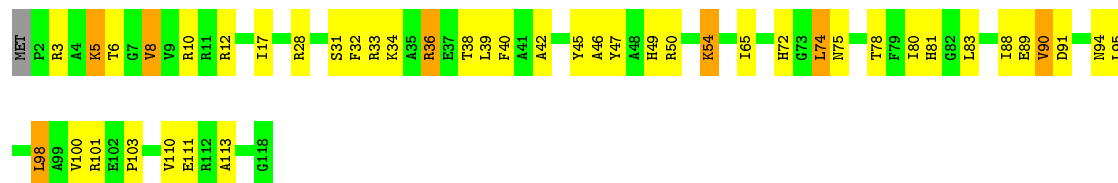
- Molecule 17: 50S ribosomal protein L19

Chain UB: 53% 34% 7% 6%



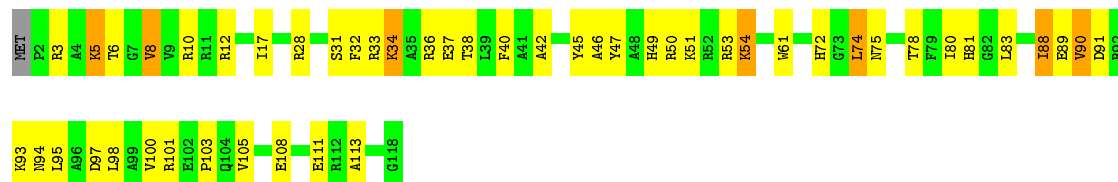
- Molecule 18: 50S ribosomal protein L20

Chain R: 62% 31% 6%



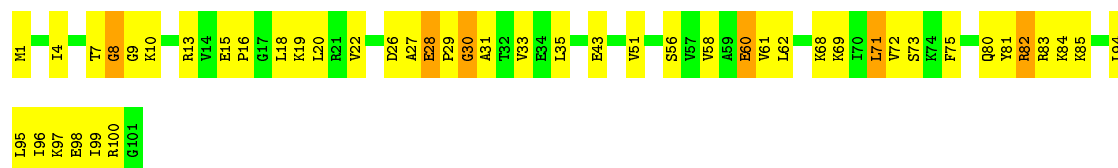
- Molecule 18: 50S ribosomal protein L20

Chain VB: 58% 36% 6%

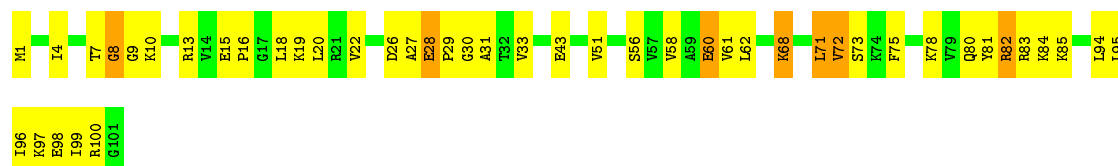


- Molecule 19: 50S ribosomal protein L21

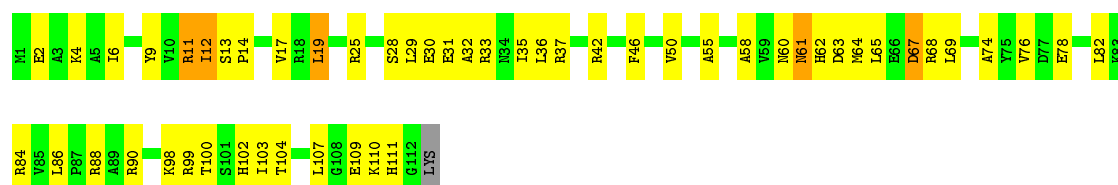
Chain S: 53% 41% 6%



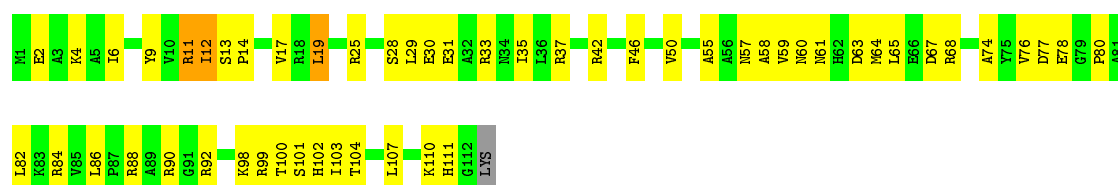
- Molecule 19: 50S ribosomal protein L21



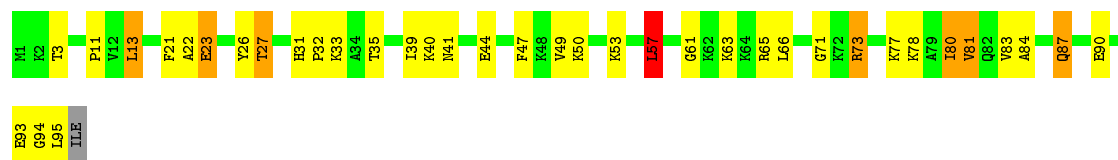
- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22



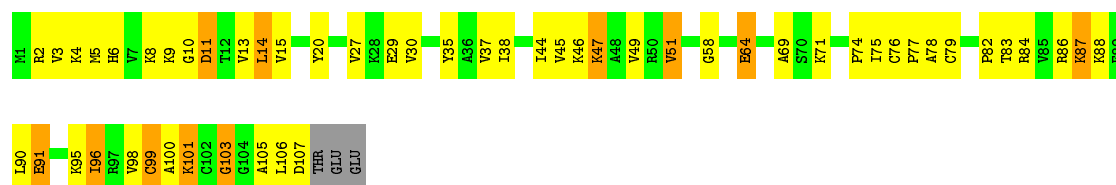
- Molecule 21: 50S ribosomal protein L23



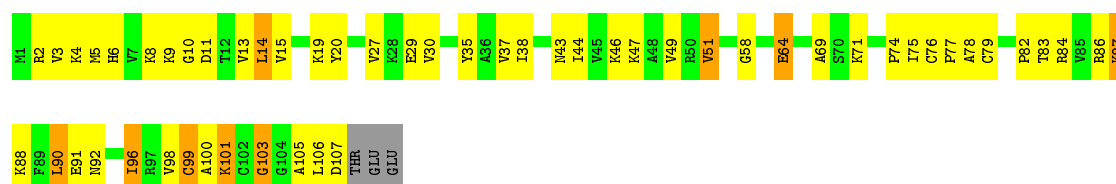
- Molecule 21: 50S ribosomal protein L23



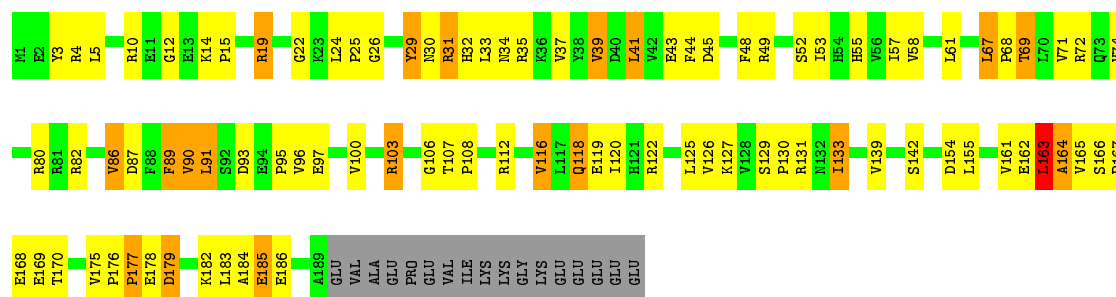
- Molecule 22: 50S ribosomal protein L24



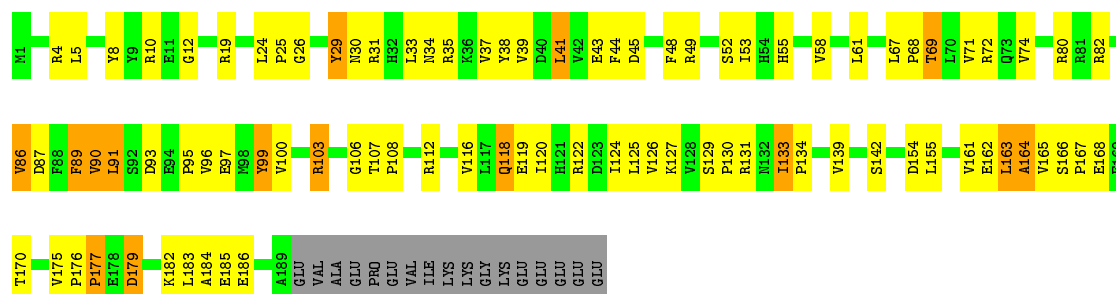
- Molecule 22: 50S ribosomal protein L24



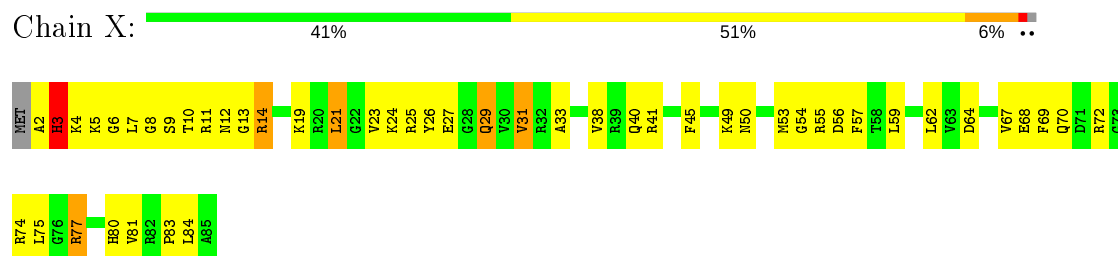
- Molecule 23: 50S ribosomal protein L25



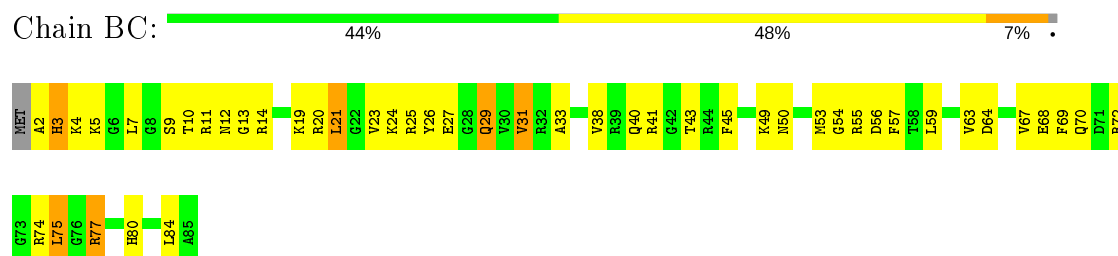
- Molecule 23: 50S ribosomal protein L25



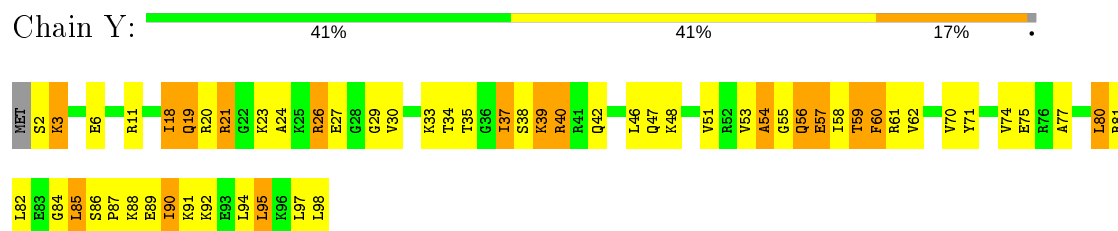
- Molecule 24: 50S ribosomal protein L27



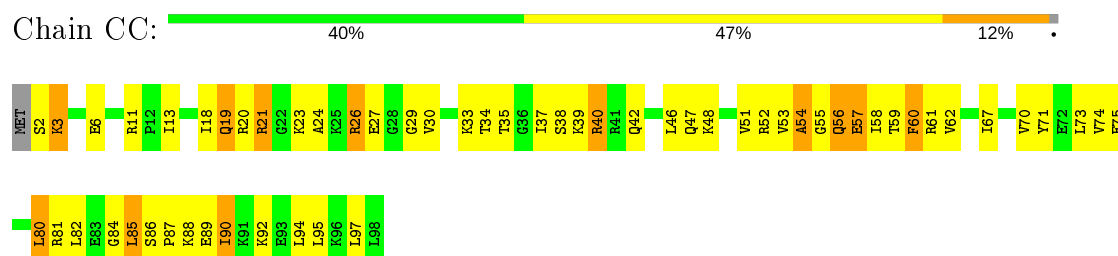
- Molecule 24: 50S ribosomal protein L27



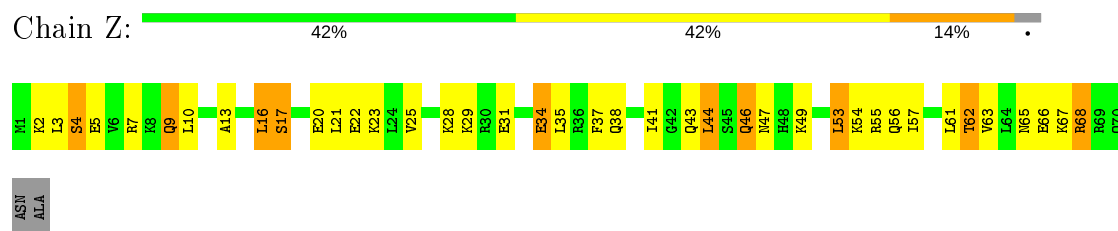
- Molecule 25: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L28

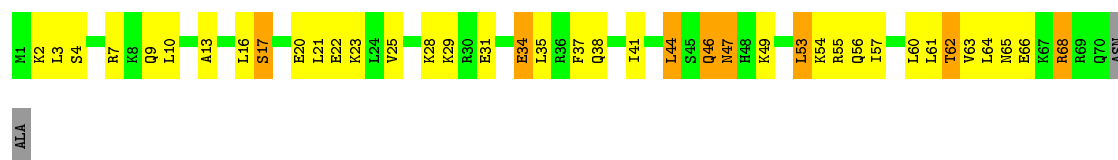


- Molecule 26: 50S ribosomal protein L29



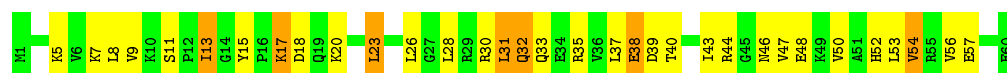
- Molecule 26: 50S ribosomal protein L29

Chain DC: 



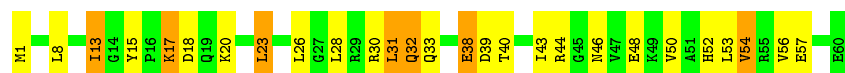
- Molecule 27: 50S ribosomal protein L30

Chain AA: 



- Molecule 27: 50S ribosomal protein L30

Chain EC: 



- Molecule 28: 50S ribosomal protein L31

Chain BA: 



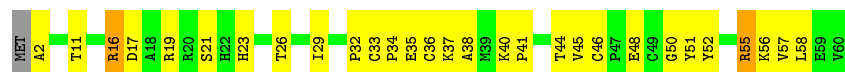
- Molecule 28: 50S ribosomal protein L31

Chain FC: 



- Molecule 29: 50S ribosomal protein L32

Chain CA: 



- Molecule 29: 50S ribosomal protein L32

Chain GC: 



- Molecule 30: 50S ribosomal protein L33

Chain DA:  39% 48% 11% .



- Molecule 30: 50S ribosomal protein L33

Chain HC:  39% 48% 11% .



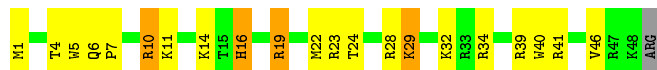
- Molecule 31: 50S ribosomal protein L34

Chain EA:  55% 35% 8% .



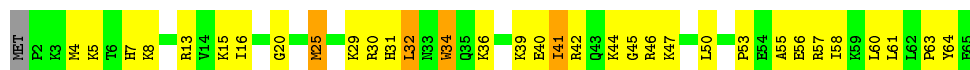
- Molecule 31: 50S ribosomal protein L34

Chain IC:  55% 35% 8% .



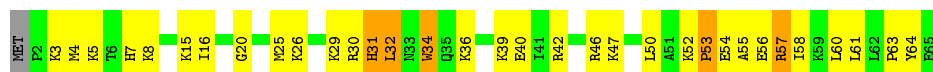
- Molecule 32: 50S ribosomal protein L35

Chain FA:  48% 45% 6% .



- Molecule 32: 50S ribosomal protein L35

Chain JC:  48% 43% 8% .



- Molecule 33: 50S ribosomal protein L36

Chain GA:  54% 41% 5% .




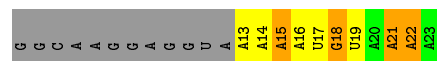
- Molecule 33: 50S ribosomal protein L36

Chain KC: 




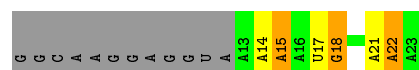
• Molecule 34: mRNA

Chain HA: 



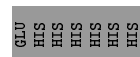
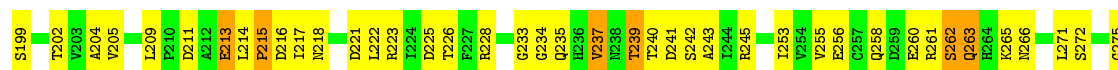
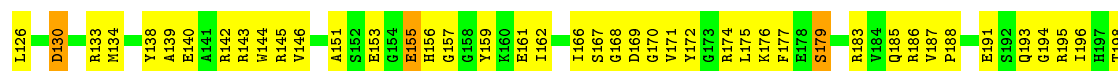
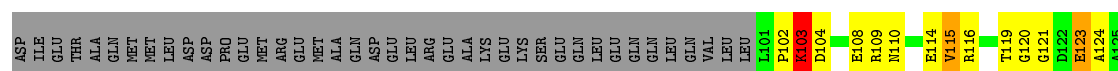
• Molecule 34: mRNA

Chain LC: 



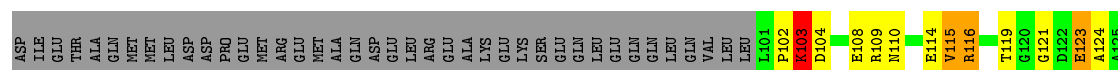
• Molecule 35: Peptide chain release factor 1

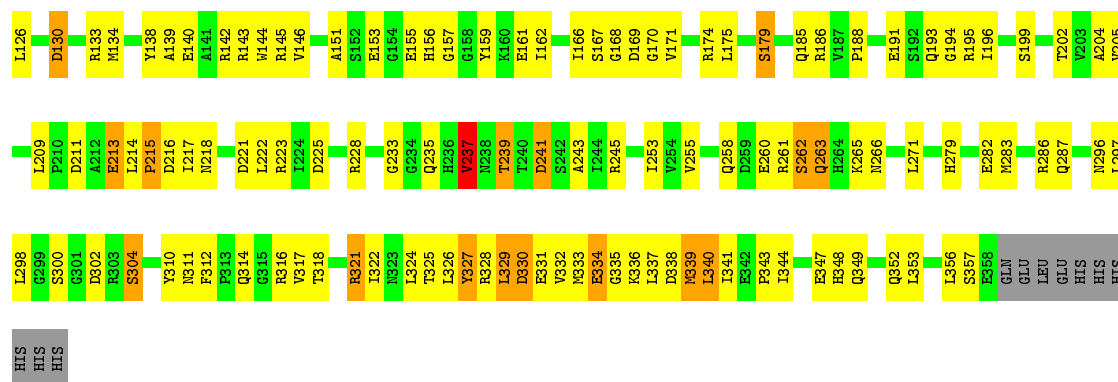
Chain JA: 



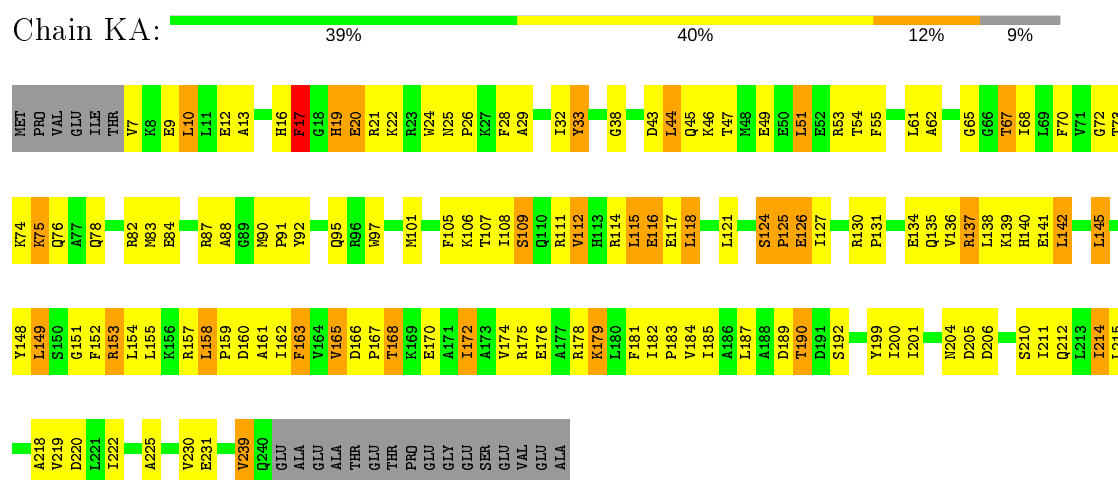
• Molecule 35: Peptide chain release factor 1

Chain NC: 

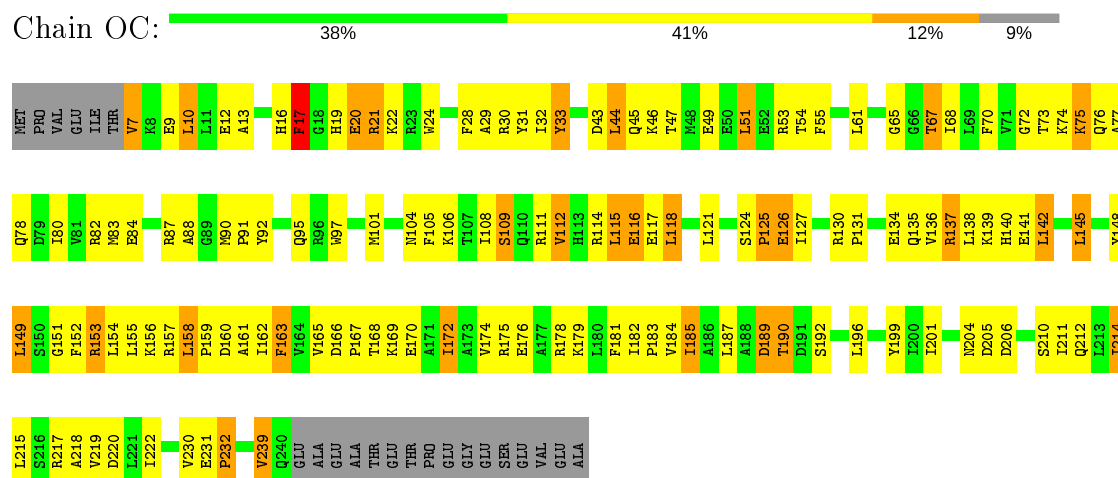




• Molecule 36: 30S ribosomal protein S2

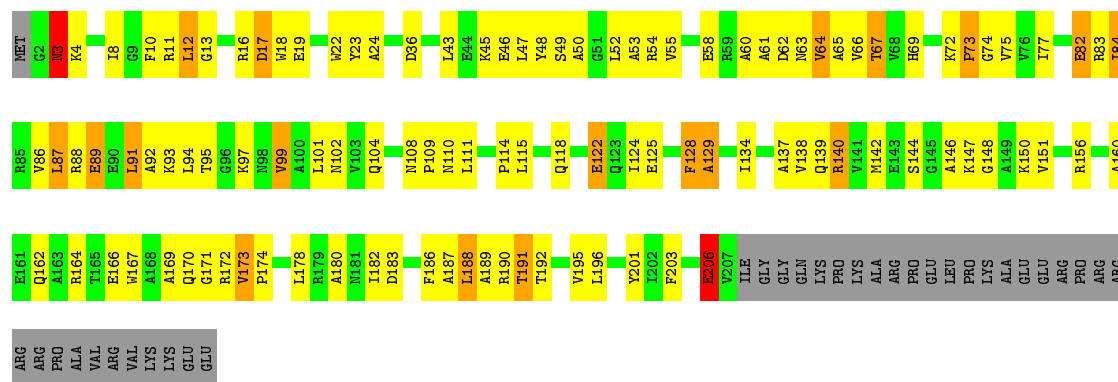


• Molecule 36: 30S ribosomal protein S2

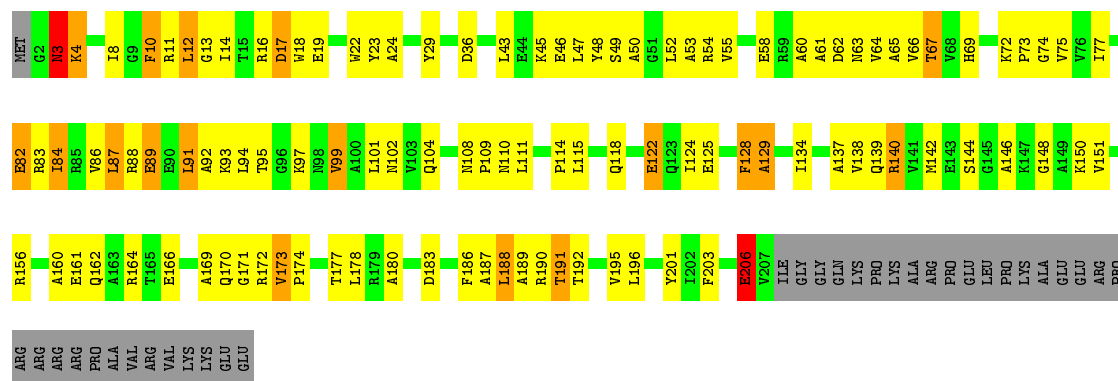


• Molecule 37: 30S ribosomal protein S3

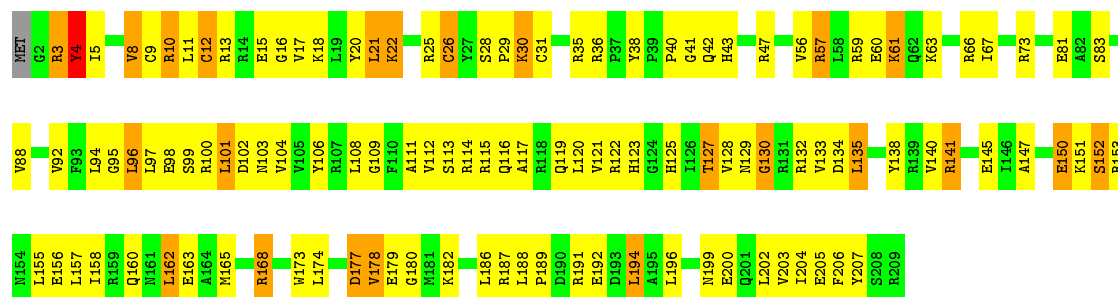




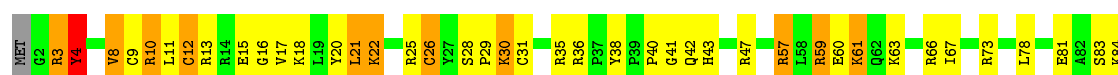
• Molecule 37: 30S ribosomal protein S3

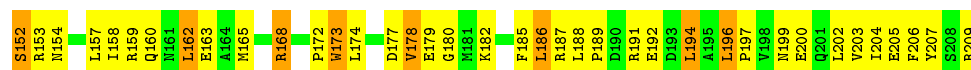


• Molecule 38: 30S ribosomal protein S4

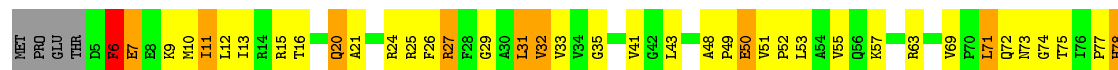


• Molecule 38: 30S ribosomal protein S4

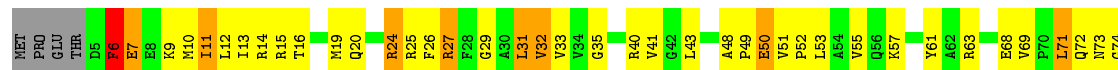




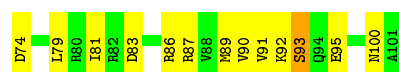
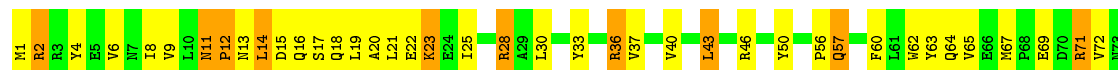
- Molecule 39: 30S ribosomal protein S5



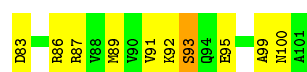
- Molecule 39: 30S ribosomal protein S5



- Molecule 40: 30S ribosomal protein S6

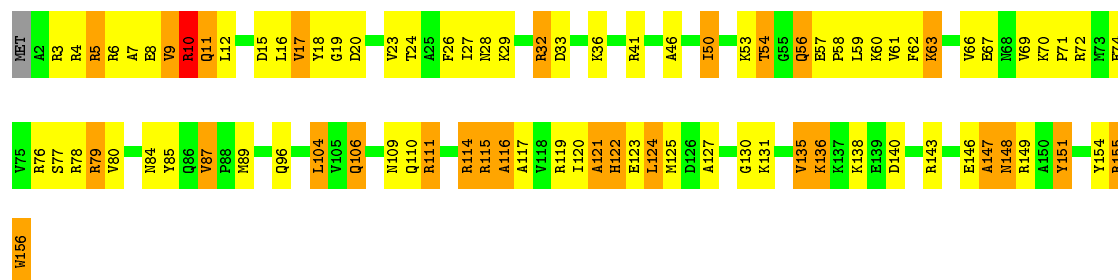


- Molecule 40: 30S ribosomal protein S6



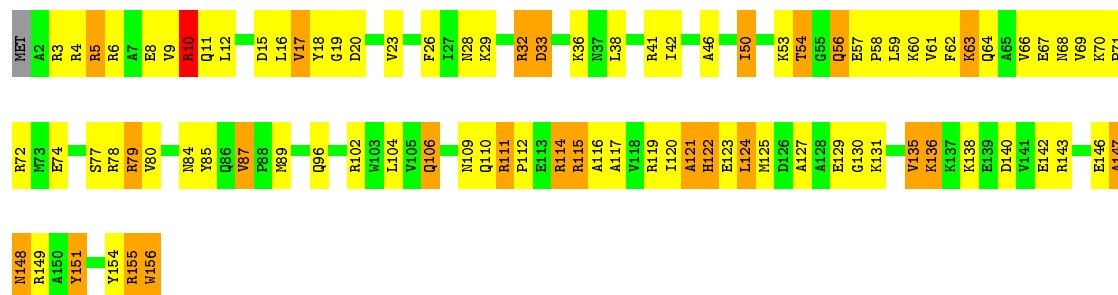
- Molecule 41: 30S ribosomal protein S7





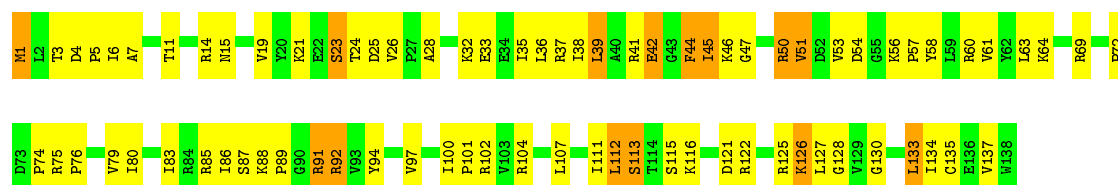
- Molecule 41: 30S ribosomal protein S7

Chain TC: 41% 42% 15% ..



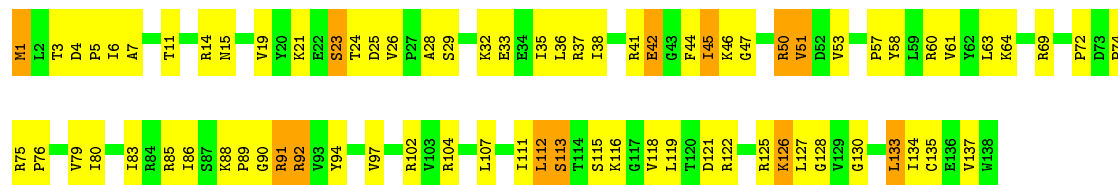
- Molecule 42: 30S ribosomal protein S8

Chain QA: 43% 46% 10%



- Molecule 42: 30S ribosomal protein S8

Chain UC: 45% 46% 9%



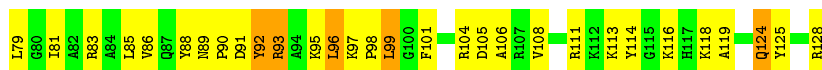
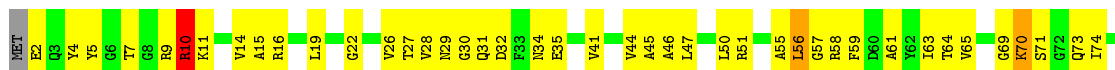
- Molecule 43: 30S ribosomal protein S9

Chain RA: 44% 49% 5% ..

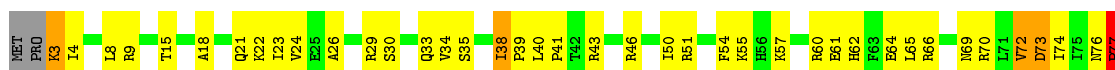




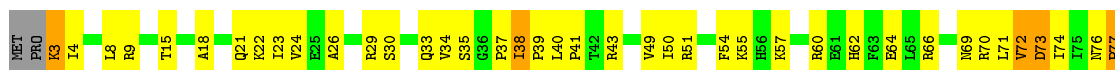
- Molecule 43: 30S ribosomal protein S9



- Molecule 44: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S10

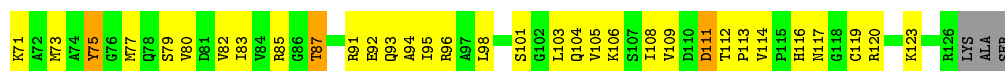


- Molecule 45: 30S ribosomal protein S11



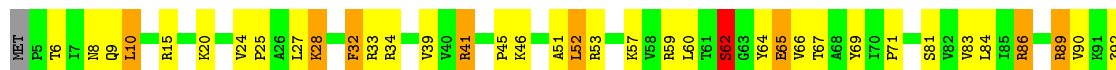
- Molecule 45: 30S ribosomal protein S11





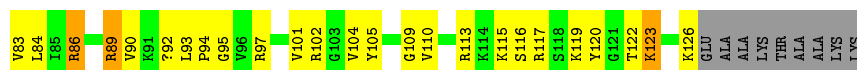
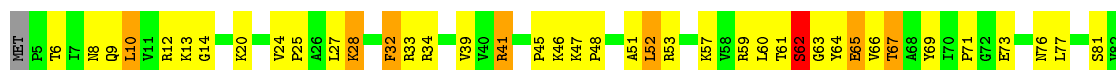
- Molecule 46: 30S ribosomal protein S12

Chain UA: 51% 34% 7% 8%



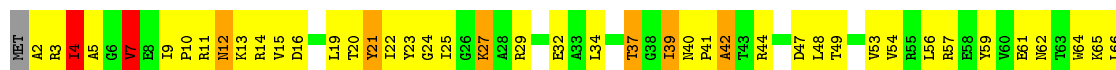
- Molecule 46: 30S ribosomal protein S12

Chain YC: 43% 41% 8% 8%



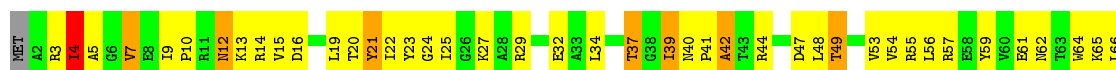
- Molecule 47: 30S ribosomal protein S13

Chain VA: 35% 44% 11% 7%



- Molecule 47: 30S ribosomal protein S13

Chain ZC: 34% 44% 13% 7%



- Molecule 48: 30S ribosomal protein S14 type Z

Chain WA: 43% 46% 10% 1%



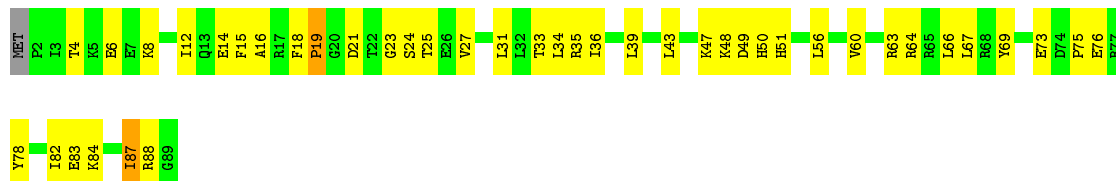
- Molecule 48: 30S ribosomal protein S14 type Z

Chain AD:  46% 46% 7%



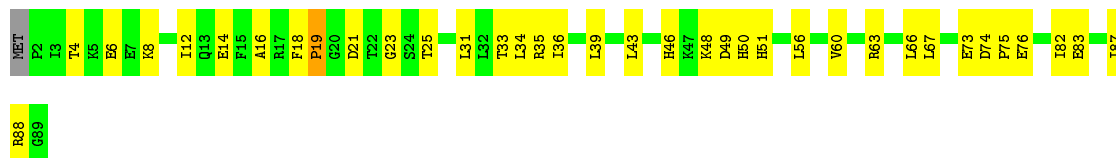
- Molecule 49: 30S ribosomal protein S15

Chain XA:  52% 45%



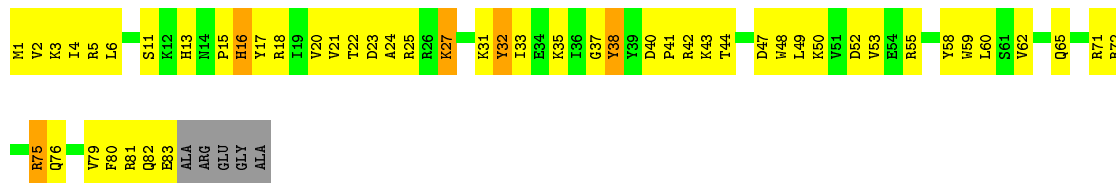
- Molecule 49: 30S ribosomal protein S15

Chain BD:  58% 39%



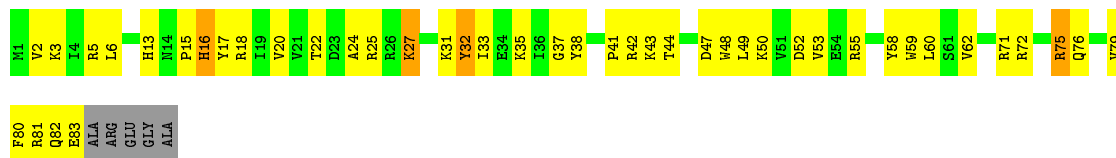
- Molecule 50: 30S ribosomal protein S16

Chain YA:  36% 52% 6% 6%



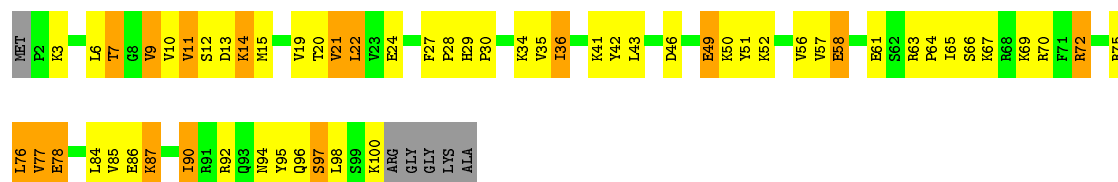
- Molecule 50: 30S ribosomal protein S16

Chain CD:  44% 45% 5% 6%

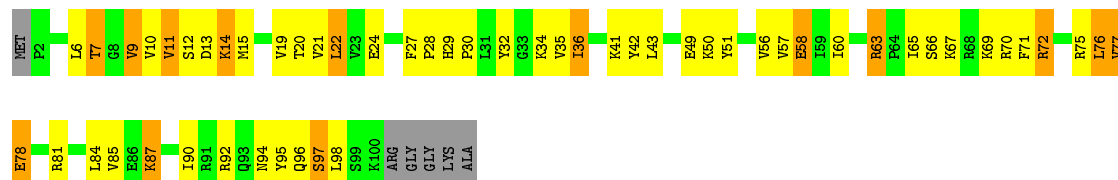


- Molecule 51: 30S ribosomal protein S17

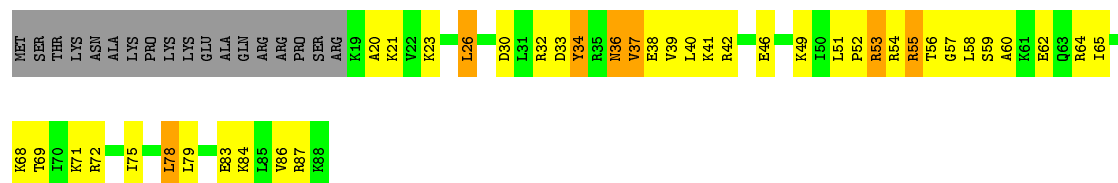
Chain ZA:  39% 40% 15% 6%



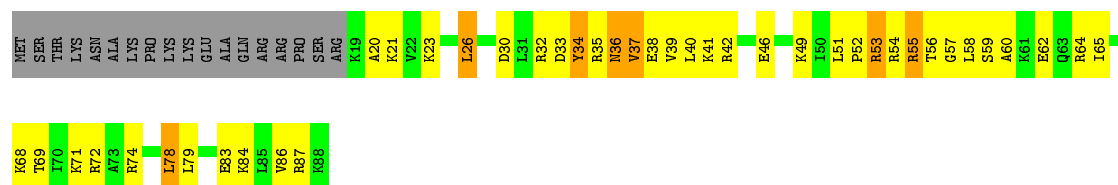
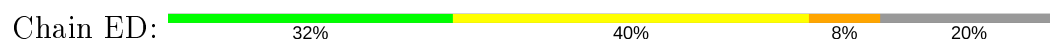
• Molecule 51: 30S ribosomal protein S17



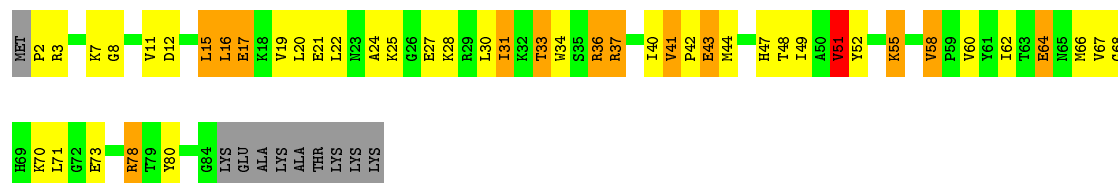
• Molecule 52: 30S ribosomal protein S18



• Molecule 52: 30S ribosomal protein S18

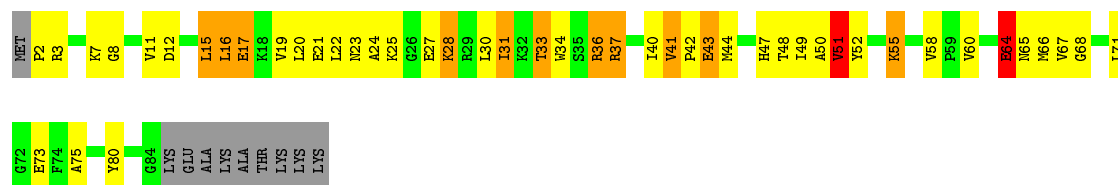


• Molecule 53: 30S ribosomal protein S19



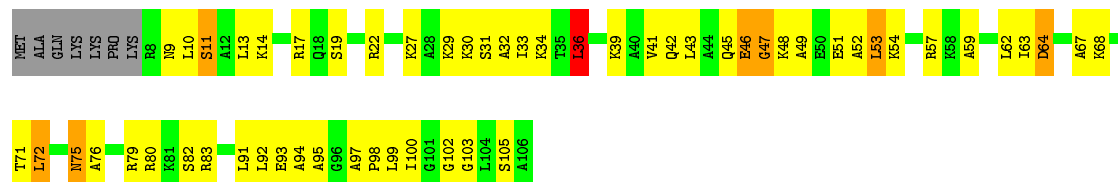
• Molecule 53: 30S ribosomal protein S19





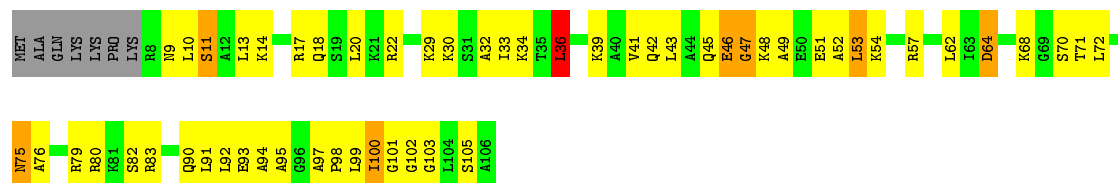
- Molecule 54: 30S ribosomal protein S20

Chain CB: 41% 45% 7% • 7%



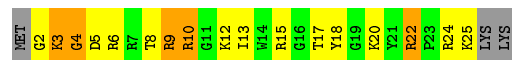
- Molecule 54: 30S ribosomal protein S20

Chain GD: 42% 44% 7% • 7%



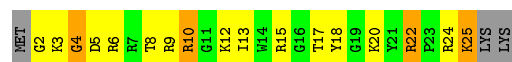
- Molecule 55: 30S ribosomal protein Thx

Chain DB: 26% 44% 19% 11%



- Molecule 55: 30S ribosomal protein Thx

Chain HD: 26% 48% 15% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.85Å 452.54Å 624.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 87.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (87.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.261 , 0.296	Depositor DCC
R_{free} test set	16277 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299841	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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	0.56	0/35961	1.08	64/56125 (0.1%)
1	EB	0.59	0/35961	1.11	67/56125 (0.1%)
2	B	0.90	35/69214 (0.1%)	1.38	667/108048 (0.6%)
2	FB	0.77	20/69214 (0.0%)	1.28	431/108048 (0.4%)
3	C	0.61	0/2881	1.13	3/4494 (0.1%)
3	GB	0.57	0/2881	1.09	1/4494 (0.0%)
4	D	0.43	0/1744	1.04	7/2719 (0.3%)
4	HB	0.43	0/1744	1.04	8/2719 (0.3%)
4	IA	0.53	0/1744	1.04	0/2719
4	MC	0.51	0/1744	1.03	0/2719
5	E	0.71	3/2195 (0.1%)	0.74	2/2955 (0.1%)
5	IB	0.65	2/2195 (0.1%)	0.73	1/2955 (0.0%)
6	F	0.61	1/1596 (0.1%)	0.65	0/2153
6	JB	0.55	2/1596 (0.1%)	0.62	0/2153
7	G	0.63	0/1621	0.66	0/2194
7	KB	0.55	0/1621	0.64	0/2194
8	H	0.36	0/1496	0.58	0/2013
8	LB	0.35	0/1496	0.57	0/2013
9	I	0.49	0/1356	0.58	0/1834
9	MB	0.36	0/1356	0.54	0/1834
10	J	0.44	0/1152	0.62	0/1559
10	NB	0.41	0/1152	0.60	0/1559
11	K	0.54	0/1148	0.64	0/1547
11	OB	0.44	0/1148	0.61	0/1547
12	L	0.65	0/942	0.64	0/1268
12	PB	0.56	0/942	0.64	0/1268
13	M	0.56	0/1162	0.72	0/1544
13	QB	0.51	0/1162	0.69	0/1544
14	N	0.57	0/1142	0.65	0/1525
14	RB	0.51	0/1142	0.63	0/1525
15	O	0.55	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	SB	0.51	0/982	0.65	0/1312
16	P	0.38	0/887	0.56	0/1180
16	TB	0.38	0/887	0.56	0/1180
17	Q	0.52	0/1157	0.62	0/1544
17	UB	0.50	0/1157	0.61	0/1544
18	R	0.63	0/982	0.63	0/1306
18	VB	0.51	0/982	0.60	0/1306
19	S	0.61	0/790	0.66	0/1057
19	WB	0.55	0/790	0.65	0/1057
20	T	0.67	0/901	0.67	0/1209
20	XB	0.58	0/901	0.62	0/1209
21	U	0.64	0/764	0.72	1/1025 (0.1%)
21	YB	0.57	0/764	0.69	1/1025 (0.1%)
22	V	0.57	0/827	0.66	0/1103
22	ZB	0.49	0/827	0.63	0/1103
23	AC	0.44	0/1527	0.55	0/2073
23	W	0.50	0/1527	0.57	0/2073
24	BC	0.51	0/671	0.69	0/892
24	X	0.53	0/671	0.70	0/892
25	CC	0.55	0/768	0.64	0/1021
25	Y	0.58	0/768	0.69	0/1021
26	DC	0.51	0/594	0.59	0/785
26	Z	0.63	0/594	0.64	0/785
27	AA	0.56	0/482	0.61	0/646
27	EC	0.52	0/482	0.60	0/646
28	BA	0.33	0/565	0.51	0/761
28	FC	0.34	0/565	0.50	0/761
29	CA	0.58	0/474	0.64	0/640
29	GC	0.47	0/474	0.61	0/640
30	DA	0.35	0/460	0.52	0/613
30	HC	0.33	0/460	0.51	0/613
31	EA	0.67	0/426	0.80	0/561
31	IC	0.60	0/426	0.71	0/561
32	FA	0.56	0/525	0.60	0/691
32	JC	0.54	0/525	0.60	0/691
33	GA	0.50	0/310	0.57	0/407
33	KC	0.46	0/310	0.54	0/407
34	HA	0.72	0/247	1.07	0/382
34	LC	0.74	0/247	1.04	0/382
35	JA	0.44	0/2037	0.61	0/2746
35	NC	0.41	0/2037	0.61	0/2746
36	KA	0.44	2/1935 (0.1%)	0.55	0/2609
36	OC	0.46	2/1935 (0.1%)	0.56	0/2609

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	LA	0.35	0/1636	0.55	0/2205
37	PC	0.38	0/1636	0.56	0/2205
38	MA	0.40	0/1733	0.57	0/2318
38	QC	0.48	0/1733	0.59	0/2318
39	NA	0.43	0/1171	0.59	0/1576
39	RC	0.48	0/1171	0.62	0/1576
40	OA	0.49	0/856	0.59	0/1154
40	SC	0.46	0/856	0.59	0/1154
41	PA	0.35	0/1276	0.51	0/1709
41	TC	0.33	0/1276	0.50	0/1709
42	QA	0.38	0/1136	0.57	0/1527
42	UC	0.42	0/1136	0.60	0/1527
43	RA	0.32	0/1029	0.57	0/1378
43	VC	0.34	0/1029	0.58	0/1378
44	SA	0.33	0/807	0.54	0/1085
44	WC	0.34	0/807	0.55	0/1085
45	TA	0.44	0/879	0.61	0/1187
45	XC	0.43	0/879	0.62	0/1187
46	UA	0.48	0/963	0.62	0/1287
46	YC	0.50	0/963	0.63	0/1287
47	VA	0.32	0/943	0.58	0/1265
47	ZC	0.34	0/943	0.58	0/1265
48	AD	0.38	0/501	0.53	0/664
48	WA	0.38	0/501	0.52	0/664
49	BD	0.47	0/745	0.55	0/992
49	XA	0.46	0/745	0.56	0/992
50	CD	0.42	0/716	0.56	0/963
50	YA	0.38	0/716	0.53	0/963
51	DD	0.51	0/836	0.57	0/1117
51	ZA	0.46	0/836	0.56	0/1117
52	AB	0.43	0/579	0.55	0/768
52	ED	0.44	0/579	0.54	0/768
53	BB	0.34	0/680	0.57	0/915
53	FD	0.33	0/680	0.56	0/915
54	CB	0.36	0/764	0.56	0/1006
54	GD	0.42	0/764	0.59	0/1006
55	DB	0.35	0/212	0.54	0/277
55	HD	0.32	0/212	0.52	0/277
All	All	0.68	67/322254 (0.0%)	1.11	1253/481306 (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
24	BC	0	1
24	X	0	1
38	MA	0	1
38	QC	0	1
All	All	0	4

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	945	A	N9-C4	12.76	1.45	1.37
2	B	1762	A	N9-C4	11.81	1.45	1.37
2	FB	945	A	N9-C4	11.72	1.44	1.37
2	B	945	A	C5-C6	10.43	1.50	1.41
2	FB	1762	A	N9-C4	10.17	1.44	1.37

The worst 5 of 1253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	945	A	C2-N3-C4	21.30	121.25	110.60
2	FB	945	A	C2-N3-C4	17.33	119.27	110.60
2	B	945	A	C5-C6-N1	16.78	126.09	117.70
2	B	945	A	N1-C6-N6	-15.09	109.55	118.60
2	FB	945	A	C5-C6-N1	15.07	125.23	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	BC	84	LEU	Peptide
38	MA	21	LEU	Peptide
38	QC	21	LEU	Peptide
24	X	84	LEU	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	16368	745	0
1	EB	32394	0	16366	711	0
2	B	62031	0	31274	1148	0
2	FB	62031	0	31274	1141	1
3	C	2576	0	1305	54	0
3	GB	2576	0	1305	60	0
4	D	1642	0	841	45	0
4	HB	1642	0	841	40	0
4	IA	1642	0	841	54	0
4	MC	1642	0	841	49	0
5	E	2145	0	2234	113	0
5	IB	2145	0	2234	105	0
6	F	1563	0	1629	63	0
6	JB	1563	0	1629	63	0
7	G	1586	0	1632	77	0
7	KB	1586	0	1632	79	0
8	H	1471	0	1526	98	0
8	LB	1471	0	1526	87	1
9	I	1330	0	1407	56	0
9	MB	1330	0	1407	58	0
10	J	1137	0	1225	57	0
10	NB	1137	0	1225	59	0
11	K	1121	0	1195	43	0
11	OB	1121	0	1195	46	0
12	L	932	0	994	36	0
12	PB	932	0	994	40	0
13	M	1145	0	1228	58	0
13	QB	1145	0	1228	59	0
14	N	1121	0	1179	53	0
14	RB	1121	0	1179	55	0
15	O	968	0	1033	46	0
15	SB	968	0	1033	45	0
16	P	877	0	938	45	0
16	TB	877	0	938	42	0
17	Q	1143	0	1211	56	0
17	UB	1143	0	1211	53	0
18	R	964	0	1022	34	0
18	VB	964	0	1022	42	0
19	S	779	0	852	26	0
19	WB	779	0	852	31	0
20	T	890	0	951	38	0
20	XB	890	0	951	39	0
21	U	750	0	814	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	YB	750	0	814	24	0
22	V	814	0	906	33	0
22	ZB	814	0	906	36	0
23	AC	1495	0	1521	59	0
23	W	1495	0	1521	74	0
24	BC	662	0	688	39	0
24	X	662	0	688	36	0
25	CC	761	0	837	40	0
25	Y	761	0	837	42	0
26	DC	592	0	654	28	0
26	Z	592	0	654	29	0
27	AA	477	0	529	22	0
27	EC	477	0	529	18	0
28	BA	552	0	537	26	0
28	FC	552	0	537	21	0
29	CA	460	0	480	15	0
29	GC	460	0	480	17	0
30	DA	453	0	476	19	0
30	HC	453	0	476	19	0
31	EA	418	0	467	19	0
31	IC	418	0	467	17	0
32	FA	517	0	582	26	0
32	JC	517	0	582	26	0
33	GA	307	0	335	14	0
33	KC	307	0	335	17	0
34	HA	220	0	108	14	0
34	LC	220	0	108	5	0
35	JA	2005	0	1964	108	0
35	NC	2005	0	1964	95	0
36	KA	1900	0	1951	87	0
36	OC	1900	0	1951	93	0
37	LA	1612	0	1677	74	0
37	PC	1612	0	1677	74	0
38	MA	1703	0	1767	102	0
38	QC	1703	0	1767	105	0
39	NA	1155	0	1213	48	0
39	RC	1155	0	1213	45	0
40	OA	843	0	857	41	0
40	SC	843	0	857	42	0
41	PA	1257	0	1296	84	0
41	TC	1257	0	1296	77	0
42	QA	1116	0	1177	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	UC	1116	0	1177	65	0
43	RA	1011	0	1043	60	0
43	VC	1011	0	1043	61	0
44	SA	794	0	840	44	0
44	WC	794	0	840	43	0
45	TA	864	0	881	51	0
45	XC	864	0	881	50	0
46	UA	958	0	1047	41	0
46	YC	958	0	1047	52	0
47	VA	933	0	992	64	0
47	ZC	933	0	992	63	0
48	AD	492	0	533	32	0
48	WA	492	0	533	37	0
49	BD	734	0	771	26	0
49	XA	734	0	771	30	0
50	CD	700	0	720	40	0
50	YA	700	0	720	48	0
51	DD	823	0	893	46	0
51	ZA	823	0	893	42	0
52	AB	574	0	644	41	0
52	ED	574	0	644	42	0
53	BB	665	0	686	52	0
53	FD	665	0	686	54	0
54	CB	762	0	859	36	0
54	GD	762	0	859	39	0
55	DB	208	0	221	24	0
55	HD	208	0	221	21	0
56	A	214	0	0	0	0
56	AA	2	0	0	0	0
56	AB	2	0	0	0	0
56	AD	2	0	0	0	0
56	B	562	0	0	0	0
56	BA	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
56	C	21	0	0	0	0
56	CA	1	0	0	0	0
56	CB	1	0	0	0	0
56	CC	7	0	0	0	0
56	CD	1	0	0	0	0
56	D	5	0	0	0	0
56	DA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DC	1	0	0	0	0
56	E	1	0	0	0	0
56	EA	1	0	0	0	0
56	EB	206	0	0	0	0
56	EC	1	0	0	0	0
56	F	2	0	0	0	0
56	FB	475	0	0	0	0
56	FC	1	0	0	0	0
56	G	2	0	0	0	0
56	GB	15	0	0	0	0
56	H	1	0	0	0	0
56	HA	3	0	0	0	0
56	HB	9	0	0	0	0
56	I	3	0	0	0	0
56	IA	6	0	0	0	0
56	IB	4	0	0	0	0
56	J	2	0	0	0	0
56	JA	6	0	0	0	0
56	JB	2	0	0	0	0
56	JC	1	0	0	0	0
56	K	4	0	0	0	0
56	KA	1	0	0	0	0
56	KB	4	0	0	0	0
56	L	2	0	0	0	0
56	LA	2	0	0	0	0
56	LC	1	0	0	0	0
56	M	5	0	0	0	0
56	MA	2	0	0	0	0
56	MB	2	0	0	0	0
56	MC	5	0	0	0	0
56	NA	2	0	0	0	0
56	NB	3	0	0	0	0
56	NC	5	0	0	0	0
56	O	2	0	0	0	0
56	OB	3	0	0	0	0
56	OC	5	0	0	0	0
56	PB	1	0	0	0	0
56	PC	1	0	0	0	0
56	Q	2	0	0	0	0
56	QA	2	0	0	0	0
56	QC	4	0	0	0	0
56	RB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RC	3	0	0	0	0
56	S	2	0	0	0	0
56	SA	3	0	0	0	0
56	SB	2	0	0	0	0
56	SC	1	0	0	0	0
56	T	3	0	0	0	0
56	TA	3	0	0	0	0
56	TB	1	0	0	0	0
56	TC	1	0	0	0	0
56	U	2	0	0	0	0
56	UA	4	0	0	0	0
56	UB	3	0	0	0	0
56	UC	2	0	0	0	0
56	V	2	0	0	0	0
56	VB	1	0	0	0	0
56	VC	1	0	0	0	0
56	W	2	0	0	0	0
56	WB	1	0	0	0	0
56	WC	1	0	0	0	0
56	X	1	0	0	0	0
56	XA	6	0	0	0	0
56	XC	1	0	0	0	0
56	Y	1	0	0	0	0
56	YC	5	0	0	0	0
56	Z	4	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
57	B	30	0	24	2	0
57	FB	30	0	24	1	0
58	BA	1	0	0	0	0
58	CA	1	0	0	0	0
58	DA	1	0	0	0	0
58	FC	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	KC	1	0	0	0	0
58	V	1	0	0	0	0
58	ZB	1	0	0	0	0
All	All	299841	0	203748	7838	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 16.

The worst 5 of 7838 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:QC:18:LYS:NZ	38:QC:26:CYS:SG	2.00	1.34
38:MA:9:CYS:SG	38:MA:18:LYS:NZ	2.05	1.30
38:QC:9:CYS:SG	38:QC:18:LYS:NZ	2.03	1.29
2:B:630:G:OP2	32:FA:15:LYS:NZ	1.65	1.29
38:MA:18:LYS:NZ	38:MA:26:CYS:SG	2.04	1.28

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:FB:1412:A:O2'	8:LB:9:ARG:NH1[1_655]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	238 (87%)	27 (10%)	8 (3%)	4	24
5	IB	273/275 (99%)	238 (87%)	27 (10%)	8 (3%)	4	24
6	F	202/206 (98%)	171 (85%)	25 (12%)	6 (3%)	4	23
6	JB	202/206 (98%)	171 (85%)	26 (13%)	5 (2%)	5	26
7	G	200/205 (98%)	173 (86%)	22 (11%)	5 (2%)	5	26
7	KB	200/205 (98%)	170 (85%)	26 (13%)	4 (2%)	7	30
8	H	179/182 (98%)	137 (76%)	29 (16%)	13 (7%)	1	7
8	LB	179/182 (98%)	135 (75%)	31 (17%)	13 (7%)	1	7
9	I	172/180 (96%)	138 (80%)	24 (14%)	10 (6%)	1	11
9	MB	172/180 (96%)	138 (80%)	25 (14%)	9 (5%)	2	13
10	J	144/148 (97%)	108 (75%)	27 (19%)	9 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	NB	144/148 (97%)	108 (75%)	27 (19%)	9 (6%)	1	9
11	K	138/140 (99%)	120 (87%)	12 (9%)	6 (4%)	2	17
11	OB	138/140 (99%)	121 (88%)	11 (8%)	6 (4%)	2	17
12	L	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	4	22
12	PB	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	4	22
13	M	148/150 (99%)	115 (78%)	24 (16%)	9 (6%)	1	10
13	QB	148/150 (99%)	117 (79%)	24 (16%)	7 (5%)	2	15
14	N	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	4	24
14	RB	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	21
15	O	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	9	34
15	SB	116/118 (98%)	101 (87%)	12 (10%)	3 (3%)	5	26
16	P	108/112 (96%)	88 (82%)	17 (16%)	3 (3%)	5	24
16	TB	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	3	20
17	Q	135/146 (92%)	111 (82%)	20 (15%)	4 (3%)	4	23
17	UB	135/146 (92%)	112 (83%)	19 (14%)	4 (3%)	4	23
18	R	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
18	VB	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
19	S	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	14
19	WB	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	3	18
20	T	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
20	XB	110/113 (97%)	100 (91%)	9 (8%)	1 (1%)	17	49
21	U	93/96 (97%)	80 (86%)	10 (11%)	3 (3%)	4	22
21	YB	93/96 (97%)	82 (88%)	8 (9%)	3 (3%)	4	22
22	V	105/110 (96%)	83 (79%)	15 (14%)	7 (7%)	1	8
22	ZB	105/110 (96%)	84 (80%)	16 (15%)	5 (5%)	2	15
23	AC	187/206 (91%)	153 (82%)	26 (14%)	8 (4%)	2	17
23	W	187/206 (91%)	150 (80%)	29 (16%)	8 (4%)	2	17
24	BC	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	14
24	X	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	1	7
25	CC	95/98 (97%)	81 (85%)	10 (10%)	4 (4%)	3	18
25	Y	95/98 (97%)	81 (85%)	10 (10%)	4 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DC	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	10	36
26	Z	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	10	36
27	AA	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	9	34
27	EC	58/60 (97%)	51 (88%)	6 (10%)	1 (2%)	9	34
28	BA	67/71 (94%)	44 (66%)	14 (21%)	9 (13%)	0	1
28	FC	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	3
29	CA	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
29	GC	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
30	DA	51/54 (94%)	35 (69%)	12 (24%)	4 (8%)	1	6
30	HC	51/54 (94%)	35 (69%)	12 (24%)	4 (8%)	1	6
31	EA	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
31	IC	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
32	FA	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	9	34
32	JC	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	22
33	GA	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	KC	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
35	JA	256/368 (70%)	197 (77%)	46 (18%)	13 (5%)	2	14
35	NC	256/368 (70%)	197 (77%)	44 (17%)	15 (6%)	1	11
36	KA	232/256 (91%)	180 (78%)	38 (16%)	14 (6%)	1	10
36	OC	232/256 (91%)	180 (78%)	36 (16%)	16 (7%)	1	8
37	LA	204/239 (85%)	158 (78%)	35 (17%)	11 (5%)	2	13
37	PC	204/239 (85%)	158 (78%)	35 (17%)	11 (5%)	2	13
38	MA	206/209 (99%)	159 (77%)	33 (16%)	14 (7%)	1	8
38	QC	206/209 (99%)	159 (77%)	34 (16%)	13 (6%)	1	9
39	NA	149/162 (92%)	121 (81%)	21 (14%)	7 (5%)	2	15
39	RC	149/162 (92%)	120 (80%)	22 (15%)	7 (5%)	2	15
40	OA	99/101 (98%)	81 (82%)	16 (16%)	2 (2%)	7	30
40	SC	99/101 (98%)	83 (84%)	14 (14%)	2 (2%)	7	30
41	PA	153/156 (98%)	115 (75%)	25 (16%)	13 (8%)	1	5
41	TC	153/156 (98%)	114 (74%)	26 (17%)	13 (8%)	1	5
42	QA	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	22	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	UC	136/138 (99%)	119 (88%)	16 (12%)	1 (1%)	22	55
43	RA	125/128 (98%)	94 (75%)	22 (18%)	9 (7%)	1	7
43	VC	125/128 (98%)	94 (75%)	23 (18%)	8 (6%)	1	9
44	SA	96/105 (91%)	81 (84%)	14 (15%)	1 (1%)	15	46
44	WC	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	15	46
45	TA	114/129 (88%)	91 (80%)	16 (14%)	7 (6%)	1	10
45	XC	114/129 (88%)	91 (80%)	17 (15%)	6 (5%)	2	13
46	UA	119/132 (90%)	97 (82%)	20 (17%)	2 (2%)	9	34
46	YC	119/132 (90%)	96 (81%)	19 (16%)	4 (3%)	3	21
47	VA	115/126 (91%)	82 (71%)	25 (22%)	8 (7%)	1	7
47	ZC	115/126 (91%)	81 (70%)	25 (22%)	9 (8%)	1	6
48	AD	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
48	WA	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	21
49	BD	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	3	21
49	XA	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	15
50	CD	81/88 (92%)	70 (86%)	9 (11%)	2 (2%)	5	26
50	YA	81/88 (92%)	70 (86%)	9 (11%)	2 (2%)	5	26
51	DD	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	4	23
51	ZA	97/105 (92%)	79 (81%)	15 (16%)	3 (3%)	4	23
52	AB	68/88 (77%)	59 (87%)	7 (10%)	2 (3%)	4	24
52	ED	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	4	24
53	BB	81/93 (87%)	56 (69%)	19 (24%)	6 (7%)	1	7
53	FD	81/93 (87%)	58 (72%)	17 (21%)	6 (7%)	1	7
54	CB	97/106 (92%)	74 (76%)	14 (14%)	9 (9%)	0	4
54	GD	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	5
55	DB	22/27 (82%)	15 (68%)	5 (23%)	2 (9%)	1	4
55	HD	22/27 (82%)	15 (68%)	5 (23%)	2 (9%)	1	4
All	All	11996/12852 (93%)	9782 (82%)	1686 (14%)	528 (4%)	2	16

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	47	LYS

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Mol	Chain	Res	Type
8	H	51	ARG
8	H	52	ILE
8	H	84	LYS
8	H	126	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	178 (82%)	39 (18%)	1	6
5	IB	217/217 (100%)	176 (81%)	41 (19%)	1	4
6	F	165/166 (99%)	136 (82%)	29 (18%)	2	6
6	JB	165/166 (99%)	137 (83%)	28 (17%)	2	8
7	G	161/162 (99%)	132 (82%)	29 (18%)	1	6
7	KB	161/162 (99%)	132 (82%)	29 (18%)	1	6
8	H	154/156 (99%)	131 (85%)	23 (15%)	3	12
8	LB	154/156 (99%)	131 (85%)	23 (15%)	3	12
9	I	144/148 (97%)	122 (85%)	22 (15%)	2	11
9	MB	144/148 (97%)	122 (85%)	22 (15%)	2	11
10	J	122/124 (98%)	92 (75%)	30 (25%)	0	2
10	NB	122/124 (98%)	91 (75%)	31 (25%)	0	2
11	K	119/119 (100%)	102 (86%)	17 (14%)	3	13
11	OB	119/119 (100%)	102 (86%)	17 (14%)	3	13
12	L	100/100 (100%)	85 (85%)	15 (15%)	3	12
12	PB	100/100 (100%)	85 (85%)	15 (15%)	3	12
13	M	116/116 (100%)	92 (79%)	24 (21%)	1	3
13	QB	116/116 (100%)	93 (80%)	23 (20%)	1	4
14	N	111/111 (100%)	93 (84%)	18 (16%)	2	9
14	RB	111/111 (100%)	93 (84%)	18 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	101/101 (100%)	86 (85%)	15 (15%)	3	12
15	SB	101/101 (100%)	86 (85%)	15 (15%)	3	12
16	P	87/88 (99%)	73 (84%)	14 (16%)	2	10
16	TB	87/88 (99%)	73 (84%)	14 (16%)	2	10
17	Q	121/128 (94%)	108 (89%)	13 (11%)	6	24
17	UB	121/128 (94%)	106 (88%)	15 (12%)	4	17
18	R	93/94 (99%)	81 (87%)	12 (13%)	4	16
18	VB	93/94 (99%)	83 (89%)	10 (11%)	6	24
19	S	82/82 (100%)	66 (80%)	16 (20%)	1	4
19	WB	82/82 (100%)	65 (79%)	17 (21%)	1	3
20	T	91/92 (99%)	77 (85%)	14 (15%)	2	11
20	XB	91/92 (99%)	76 (84%)	15 (16%)	2	9
21	U	77/78 (99%)	65 (84%)	12 (16%)	2	11
21	YB	77/78 (99%)	66 (86%)	11 (14%)	3	13
22	V	87/91 (96%)	71 (82%)	16 (18%)	1	5
22	ZB	87/91 (96%)	71 (82%)	16 (18%)	1	5
23	AC	163/179 (91%)	137 (84%)	26 (16%)	2	10
23	W	163/179 (91%)	137 (84%)	26 (16%)	2	10
24	BC	66/67 (98%)	57 (86%)	9 (14%)	3	14
24	X	66/67 (98%)	57 (86%)	9 (14%)	3	14
25	CC	81/83 (98%)	61 (75%)	20 (25%)	0	2
25	Y	81/83 (98%)	61 (75%)	20 (25%)	0	2
26	DC	66/67 (98%)	52 (79%)	14 (21%)	1	3
26	Z	66/67 (98%)	52 (79%)	14 (21%)	1	3
27	AA	52/52 (100%)	40 (77%)	12 (23%)	1	2
27	EC	52/52 (100%)	40 (77%)	12 (23%)	1	2
28	BA	59/63 (94%)	50 (85%)	9 (15%)	2	11
28	FC	59/63 (94%)	50 (85%)	9 (15%)	2	11
29	CA	51/52 (98%)	39 (76%)	12 (24%)	1	2
29	GC	51/52 (98%)	39 (76%)	12 (24%)	1	2
30	DA	51/52 (98%)	42 (82%)	9 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	HC	51/52 (98%)	42 (82%)	9 (18%)	2	6
31	EA	41/42 (98%)	30 (73%)	11 (27%)	0	1
31	IC	41/42 (98%)	29 (71%)	12 (29%)	0	1
32	FA	54/55 (98%)	46 (85%)	8 (15%)	3	12
32	JC	54/55 (98%)	47 (87%)	7 (13%)	4	16
33	GA	34/34 (100%)	31 (91%)	3 (9%)	10	33
33	KC	34/34 (100%)	31 (91%)	3 (9%)	10	33
35	JA	209/308 (68%)	176 (84%)	33 (16%)	2	10
35	NC	209/308 (68%)	178 (85%)	31 (15%)	3	12
36	KA	202/220 (92%)	164 (81%)	38 (19%)	1	4
36	OC	202/220 (92%)	164 (81%)	38 (19%)	1	4
37	LA	160/188 (85%)	133 (83%)	27 (17%)	2	8
37	PC	160/188 (85%)	133 (83%)	27 (17%)	2	8
38	MA	180/181 (99%)	146 (81%)	34 (19%)	1	4
38	QC	180/181 (99%)	145 (81%)	35 (19%)	1	4
39	NA	116/123 (94%)	102 (88%)	14 (12%)	5	18
39	RC	116/123 (94%)	102 (88%)	14 (12%)	5	18
40	OA	90/90 (100%)	75 (83%)	15 (17%)	2	8
40	SC	90/90 (100%)	75 (83%)	15 (17%)	2	8
41	PA	126/127 (99%)	100 (79%)	26 (21%)	1	3
41	TC	126/127 (99%)	99 (79%)	27 (21%)	1	3
42	QA	119/119 (100%)	100 (84%)	19 (16%)	2	10
42	UC	119/119 (100%)	101 (85%)	18 (15%)	3	12
43	RA	98/99 (99%)	86 (88%)	12 (12%)	5	18
43	VC	98/99 (99%)	86 (88%)	12 (12%)	5	18
44	SA	88/92 (96%)	79 (90%)	9 (10%)	7	26
44	WC	88/92 (96%)	80 (91%)	8 (9%)	9	32
45	TA	88/99 (89%)	71 (81%)	17 (19%)	1	4
45	XC	88/99 (89%)	71 (81%)	17 (19%)	1	4
46	UA	102/108 (94%)	85 (83%)	17 (17%)	2	8
46	YC	102/108 (94%)	85 (83%)	17 (17%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	VA	94/101 (93%)	71 (76%)	23 (24%)	0	2
47	ZC	94/101 (93%)	72 (77%)	22 (23%)	1	2
48	AD	49/50 (98%)	42 (86%)	7 (14%)	3	13
48	WA	49/50 (98%)	42 (86%)	7 (14%)	3	13
49	BD	79/80 (99%)	71 (90%)	8 (10%)	7	27
49	XA	79/80 (99%)	71 (90%)	8 (10%)	7	27
50	CD	72/74 (97%)	62 (86%)	10 (14%)	3	13
50	YA	72/74 (97%)	61 (85%)	11 (15%)	2	11
51	DD	94/97 (97%)	72 (77%)	22 (23%)	1	2
51	ZA	94/97 (97%)	72 (77%)	22 (23%)	1	2
52	AB	61/77 (79%)	50 (82%)	11 (18%)	1	6
52	ED	61/77 (79%)	50 (82%)	11 (18%)	1	6
53	BB	72/80 (90%)	58 (81%)	14 (19%)	1	4
53	FD	72/80 (90%)	59 (82%)	13 (18%)	1	6
54	CB	76/82 (93%)	65 (86%)	11 (14%)	3	12
54	GD	76/82 (93%)	65 (86%)	11 (14%)	3	12
55	DB	19/22 (86%)	15 (79%)	4 (21%)	1	3
55	HD	19/22 (86%)	15 (79%)	4 (21%)	1	3
All	All	10120/10672 (95%)	8397 (83%)	1723 (17%)	2	8

5 of 1723 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	WA	47	LEU
8	LB	41	GLN
45	XC	93	GLN
51	ZA	7	THR
5	IB	73	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
47	VA	62	ASN
18	VB	94	ASN
49	BD	46	HIS

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Mol	Chain	Res	Type
53	BB	23	ASN
7	KB	40	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	330 (21%)	13 (0%)
1	EB	1502/1507 (99%)	330 (21%)	13 (0%)
2	B	2876/2880 (99%)	644 (22%)	22 (0%)
2	FB	2876/2880 (99%)	642 (22%)	23 (0%)
3	C	119/120 (99%)	22 (18%)	1 (0%)
3	GB	119/120 (99%)	21 (17%)	1 (0%)
34	HA	9/23 (39%)	5 (55%)	0
34	LC	9/23 (39%)	5 (55%)	0
4	D	76/77 (98%)	25 (32%)	0
4	HB	76/77 (98%)	26 (34%)	0
4	IA	76/77 (98%)	20 (26%)	0
4	MC	76/77 (98%)	20 (26%)	0
All	All	9316/9368 (99%)	2090 (22%)	73 (0%)

5 of 2090 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2602	A
1	EB	723	U
2	FB	1992	G
1	EB	495	A
1	EB	842	C

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
2	5MU	FB	1915	2	15,22,23	1.67	3 (20%)	16,32,35	2.12	2 (12%)
1	5MC	A	967	1	15,22,23	1.40	2 (13%)	19,32,35	1.15	2 (10%)
4	4SU	HB	8	4	14,21,22	6.52	3 (21%)	15,30,33	2.77	2 (13%)
2	5MU	B	1939	2	15,22,23	1.64	4 (26%)	16,32,35	1.63	2 (12%)
1	PSU	A	516	1	17,21,22	1.78	4 (23%)	20,30,33	3.54	6 (30%)
1	5MC	A	1404	1	15,22,23	1.32	1 (6%)	19,32,35	1.14	2 (10%)
1	7MG	EB	527	1	22,26,27	2.27	7 (31%)	28,39,42	1.94	7 (25%)
2	2MU	FB	2552	2	14,22,24	2.32	3 (21%)	14,31,36	1.46	2 (14%)
1	4OC	EB	1402	1	16,23,24	0.87	1 (6%)	17,32,35	2.16	1 (5%)
46	0TD	YC	92	46	4,9,10	1.42	1 (25%)	3,11,13	0.96	0
4	PSU	MC	55	4	17,21,22	1.62	3 (17%)	20,30,33	3.40	5 (25%)
2	5MC	FB	1942	56,2	15,22,23	1.53	2 (13%)	19,32,35	1.44	4 (21%)
1	5MC	EB	967	1	15,22,23	1.41	2 (13%)	19,32,35	1.33	3 (15%)
2	4OC	B	1920	2	15,22,24	0.93	1 (6%)	17,31,35	1.51	3 (17%)
1	M2G	A	966	1	20,27,28	2.25	4 (20%)	22,40,43	1.74	5 (22%)
4	5MU	IA	54	4	15,22,23	1.71	3 (20%)	16,32,35	1.85	1 (6%)
1	5MC	EB	1400	1	15,22,23	1.41	2 (13%)	19,32,35	1.32	2 (10%)
2	PSU	FB	1917	2	17,21,22	1.55	3 (17%)	20,30,33	3.35	6 (30%)
2	PSU	B	1911	2	17,21,22	1.70	3 (17%)	20,30,33	3.81	5 (25%)
1	UR3	A	1498	1	14,22,23	1.60	1 (7%)	15,32,35	0.80	0
1	MA6	EB	1519	1	19,26,27	1.59	3 (15%)	18,38,41	1.22	2 (11%)
2	2MA	FB	2503	56,2	17,25,26	1.50	2 (11%)	19,37,40	1.81	3 (15%)
4	4SU	D	8	4	14,21,22	6.51	3 (21%)	15,30,33	2.77	2 (13%)
2	2MU	B	2552	2	14,22,24	2.46	3 (21%)	14,31,36	1.47	1 (7%)
2	5MU	B	1915	56,2	15,22,23	1.63	3 (20%)	16,32,35	1.61	2 (12%)
1	5MC	A	1407	1	15,22,23	1.33	2 (13%)	19,32,35	1.18	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	EB	1404	1	15,22,23	1.33	2 (13%)	19,32,35	1.22	2 (10%)
1	UR3	EB	1498	1	14,22,23	1.57	1 (7%)	15,32,35	0.83	0
4	PSU	IA	55	4	17,21,22	1.63	3 (17%)	20,30,33	3.42	5 (25%)
1	7MG	A	527	1	22,26,27	2.18	7 (31%)	28,39,42	1.85	8 (28%)
4	5MU	D	54	4	15,22,23	1.70	3 (20%)	16,32,35	1.88	2 (12%)
2	PSU	B	2605	2	17,21,22	1.83	3 (17%)	20,30,33	3.54	6 (30%)
46	0TD	UA	92	46	4,9,10	1.68	1 (25%)	3,11,13	1.40	1 (33%)
2	5MC	B	1942	2	15,22,23	1.34	2 (13%)	19,32,35	1.56	4 (21%)
4	4SU	IA	8	4	14,21,22	6.51	3 (21%)	15,30,33	2.75	2 (13%)
4	5MU	HB	54	4	15,22,23	1.65	3 (20%)	16,32,35	1.85	2 (12%)
4	4SU	MC	8	4	14,21,22	6.52	3 (21%)	15,30,33	2.73	2 (13%)
4	5MU	MC	54	4	15,22,23	1.78	3 (20%)	16,32,35	2.02	1 (6%)
1	2MG	A	1207	1	19,26,27	2.45	2 (10%)	21,38,41	1.84	7 (33%)
1	MA6	A	1518	1	19,26,27	1.69	3 (15%)	18,38,41	1.57	2 (11%)
1	M2G	EB	966	1	20,27,28	2.21	4 (20%)	22,40,43	1.72	5 (22%)
1	PSU	EB	516	1	17,21,22	1.72	4 (23%)	20,30,33	3.67	6 (30%)
2	PSU	FB	2605	2	17,21,22	1.51	3 (17%)	20,30,33	3.18	6 (30%)
1	MA6	A	1519	1	19,26,27	1.72	3 (15%)	18,38,41	1.23	2 (11%)
1	5MC	A	1400	1	15,22,23	1.47	2 (13%)	19,32,35	1.24	2 (10%)
2	5MC	B	1962	2	15,22,23	1.38	2 (13%)	19,32,35	1.28	3 (15%)
2	OMG	FB	2251	2,4	18,26,27	1.81	2 (11%)	20,38,41	1.65	5 (25%)
2	5MU	FB	1939	2	15,22,23	1.53	3 (20%)	16,32,35	1.77	3 (18%)
1	MA6	EB	1518	1	19,26,27	1.77	3 (15%)	18,38,41	1.69	3 (16%)
2	4OC	FB	1920	2	15,22,24	0.89	1 (6%)	17,31,35	1.43	3 (17%)
2	5MC	FB	1962	2	15,22,23	1.52	2 (13%)	19,32,35	1.32	4 (21%)
1	2MG	EB	1207	1,56	19,26,27	2.46	2 (10%)	21,38,41	1.98	7 (33%)
2	OMG	B	2251	2	18,26,27	1.90	4 (22%)	20,38,41	1.76	5 (25%)
2	2MA	B	2503	2	17,25,26	1.47	4 (23%)	19,37,40	2.07	3 (15%)
2	PSU	B	1917	2	17,21,22	1.37	3 (17%)	20,30,33	3.26	6 (30%)
2	PSU	FB	1911	2	17,21,22	1.74	4 (23%)	20,30,33	3.27	5 (25%)
1	4OC	A	1402	1	16,23,24	0.86	1 (6%)	17,32,35	1.92	2 (11%)
4	PSU	HB	55	4	17,21,22	1.71	4 (23%)	20,30,33	3.44	5 (25%)
4	PSU	D	55	4	17,21,22	1.65	4 (23%)	20,30,33	3.47	5 (25%)
4	5MC	D	32	4	15,22,23	1.45	2 (13%)	19,32,35	1.45	3 (15%)
1	5MC	EB	1407	1	15,22,23	1.39	2 (13%)	19,32,35	1.22	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5MC	HB	32	4	15,22,23	1.44	2 (13%)	19,32,35	1.37	3 (15%)
4	5MC	MC	32	4	15,22,23	1.44	2 (13%)	19,32,35	1.66	5 (26%)
4	5MC	IA	32	4	15,22,23	1.51	2 (13%)	19,32,35	1.72	4 (21%)

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
2	5MU	FB	1915	2	-	0/5/25/26	0/2/2/2
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
4	4SU	HB	8	4	-	1/5/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/5/25/26	0/2/2/2
1	PSU	A	516	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	7MG	EB	527	1	-	3/7/37/38	0/3/3/3
2	2MU	FB	2552	2	-	1/7/27/28	0/2/2/2
1	4OC	EB	1402	1	-	4/9/29/30	0/2/2/2
46	0TD	YC	92	46	-	1/3/12/14	-
4	PSU	MC	55	4	-	0/7/25/26	0/2/2/2
2	5MC	FB	1942	56,2	-	0/5/25/26	0/2/2/2
1	5MC	EB	967	1	-	0/5/25/26	0/2/2/2
2	4OC	B	1920	2	-	1/7/27/30	0/2/2/2
1	M2G	A	966	1	-	1/7/29/30	0/3/3/3
4	5MU	IA	54	4	-	0/5/25/26	0/2/2/2
1	5MC	EB	1400	1	-	0/5/25/26	0/2/2/2
2	PSU	FB	1917	2	-	2/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/5/25/26	0/2/2/2
1	MA6	EB	1519	1	-	6/7/29/30	0/3/3/3
2	2MA	FB	2503	56,2	-	1/3/25/26	0/3/3/3
4	4SU	D	8	4	-	1/5/25/26	0/2/2/2
2	2MU	B	2552	2	-	1/7/27/28	0/2/2/2
2	5MU	B	1915	56,2	-	0/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	5MC	EB	1404	1	-	0/5/25/26	0/2/2/2
1	UR3	EB	1498	1	-	2/5/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	3/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MU	D	54	4	-	0/5/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
46	0TD	UA	92	46	-	1/3/12/14	-
2	5MC	B	1942	2	-	0/5/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/5/25/26	0/2/2/2
4	5MU	HB	54	4	-	0/5/25/26	0/2/2/2
4	4SU	MC	8	4	-	0/5/25/26	0/2/2/2
4	5MU	MC	54	4	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	5/7/29/30	0/3/3/3
1	M2G	EB	966	1	-	1/7/29/30	0/3/3/3
1	PSU	EB	516	1	-	1/7/25/26	0/2/2/2
2	PSU	FB	2605	2	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	6/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	0/5/25/26	0/2/2/2
2	5MC	B	1962	2	-	2/5/25/26	0/2/2/2
2	OMG	FB	2251	2,4	-	2/5/27/28	0/3/3/3
2	5MU	FB	1939	2	-	0/5/25/26	0/2/2/2
1	MA6	EB	1518	1	-	5/7/29/30	0/3/3/3
2	4OC	FB	1920	2	-	1/7/27/30	0/2/2/2
2	5MC	FB	1962	2	-	1/5/25/26	0/2/2/2
1	2MG	EB	1207	1,56	-	4/5/27/28	0/3/3/3
2	OMG	B	2251	2	-	3/5/27/28	0/3/3/3
2	2MA	B	2503	2	-	1/3/25/26	0/3/3/3
2	PSU	B	1917	2	-	2/7/25/26	0/2/2/2
2	PSU	FB	1911	2	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
4	PSU	HB	55	4	-	1/7/25/26	0/2/2/2
4	PSU	D	55	4	-	1/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/5/25/26	0/2/2/2
1	5MC	EB	1407	1	-	0/5/25/26	0/2/2/2
4	5MC	HB	32	4	-	0/5/25/26	0/2/2/2
4	5MC	MC	32	4	-	0/5/25/26	0/2/2/2
4	5MC	IA	32	4	-	0/5/25/26	0/2/2/2

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	MC	8	4SU	C4-S4	-23.84	1.23	1.67
4	HB	8	4SU	C4-S4	-23.81	1.23	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IA	8	4SU	C4-S4	-23.80	1.23	1.67
4	D	8	4SU	C4-S4	-23.79	1.23	1.67
1	A	1207	2MG	C2-N2	8.06	1.40	1.34

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1911	PSU	N1-C2-N3	-13.20	117.93	128.43
1	EB	516	PSU	N1-C2-N3	-12.81	118.25	128.43
1	A	516	PSU	N1-C2-N3	-12.35	118.61	128.43
2	B	2605	PSU	N1-C2-N3	-11.99	118.90	128.43
4	MC	55	PSU	N1-C2-N3	-11.57	119.23	128.43

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	HB	8	4SU	O4'-C1'-N1-C6
1	EB	527	7MG	C3'-C4'-C5'-O5'
2	FB	2552	2MU	C1'-C2'-O2'-C6'
1	EB	1402	4OC	N3-C4-N4-CM4
1	EB	1402	4OC	C5-C4-N4-CM4

There are no ring outliers.

38 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FB	1915	5MU	1	0
1	A	967	5MC	2	0
4	HB	8	4SU	2	0
2	B	1939	5MU	3	0
2	FB	2552	2MU	2	0
1	EB	1402	4OC	2	0
46	YC	92	0TD	3	0
4	MC	55	PSU	1	0
1	EB	967	5MC	2	0
2	B	1920	4OC	4	0
1	EB	1400	5MC	1	0
1	A	1498	UR3	1	0
1	EB	1519	MA6	3	0
2	FB	2503	2MA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	8	4SU	2	0
2	B	2552	2MU	1	0
2	B	1915	5MU	3	0
1	EB	1404	5MC	1	0
1	EB	1498	UR3	1	0
4	IA	55	PSU	1	0
4	D	54	5MU	3	0
46	UA	92	0TD	2	0
4	HB	54	5MU	3	0
4	MC	8	4SU	1	0
1	A	1207	2MG	3	0
1	A	1518	MA6	2	0
1	EB	516	PSU	1	0
1	A	1519	MA6	4	0
1	A	1400	5MC	1	0
2	B	1962	5MC	1	0
1	EB	1518	MA6	1	0
2	FB	1920	4OC	2	0
2	FB	1962	5MC	1	0
1	EB	1207	2MG	1	0
2	B	2503	2MA	1	0
1	A	1402	4OC	2	0
4	HB	55	PSU	1	0
4	D	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1695 ligands modelled in this entry, 1693 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	FB	9001	-	25,31,31	3.34	9 (36%)	23,43,43	2.28	9 (39%)
57	BLS	B	9001	-	25,31,31	3.32	10 (40%)	23,43,43	2.11	10 (43%)

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	FB	9001	-	-	4/17/38/38	0/2/2/2
57	BLS	B	9001	-	-	4/17/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FB	9001	BLS	C14-N12	8.72	1.54	1.35
57	B	9001	BLS	C14-N12	8.36	1.53	1.35
57	FB	9001	BLS	C7-N6	7.24	1.49	1.34
57	B	9001	BLS	C7-N6	7.05	1.49	1.34
57	B	9001	BLS	O5'-C5'	6.00	1.51	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	FB	9001	BLS	O5'-C1'-C2'	-5.79	110.00	113.13
57	FB	9001	BLS	C1'-C2'-C3'	-4.63	116.46	122.52
57	B	9001	BLS	C1'-C2'-C3'	-4.10	117.15	122.52
57	B	9001	BLS	O5'-C1'-C2'	-3.50	111.24	113.13
57	B	9001	BLS	C13-N12-C11	3.43	122.85	115.89

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

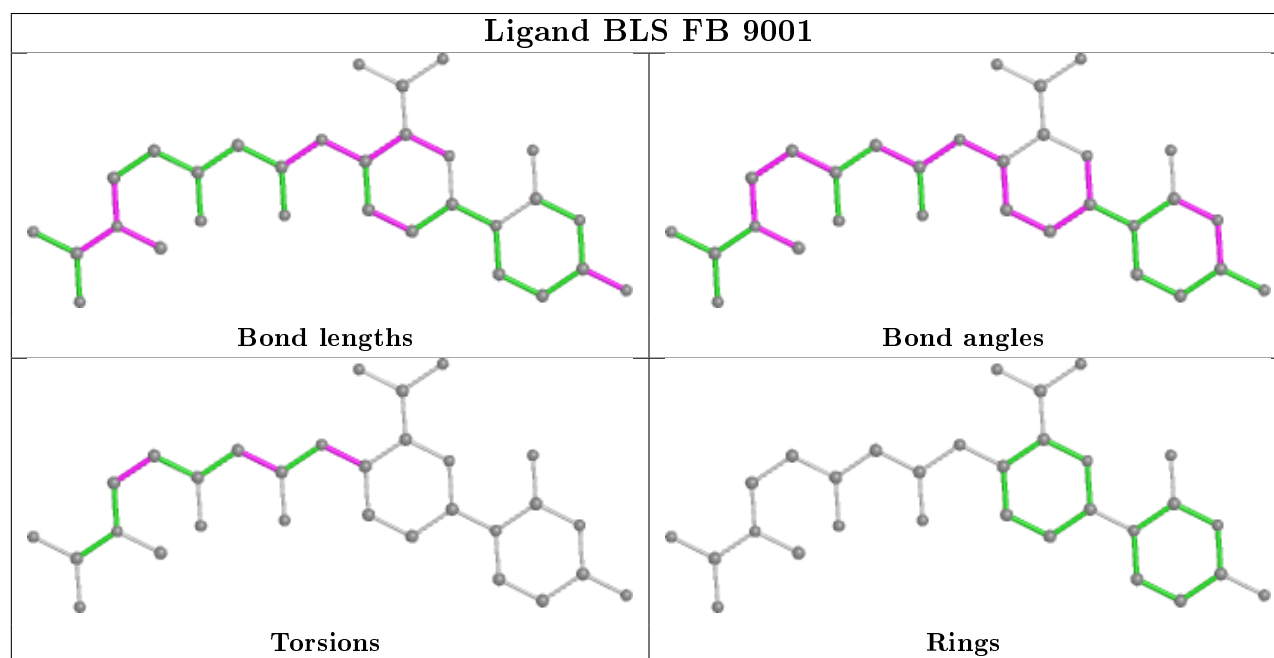
Mol	Chain	Res	Type	Atoms
57	FB	9001	BLS	N6-C7-C8-C9
57	FB	9001	BLS	O7-C7-C8-C9
57	FB	9001	BLS	C9-C10-C11-N12
57	B	9001	BLS	N6-C7-C8-C9
57	B	9001	BLS	O7-C7-C8-C9

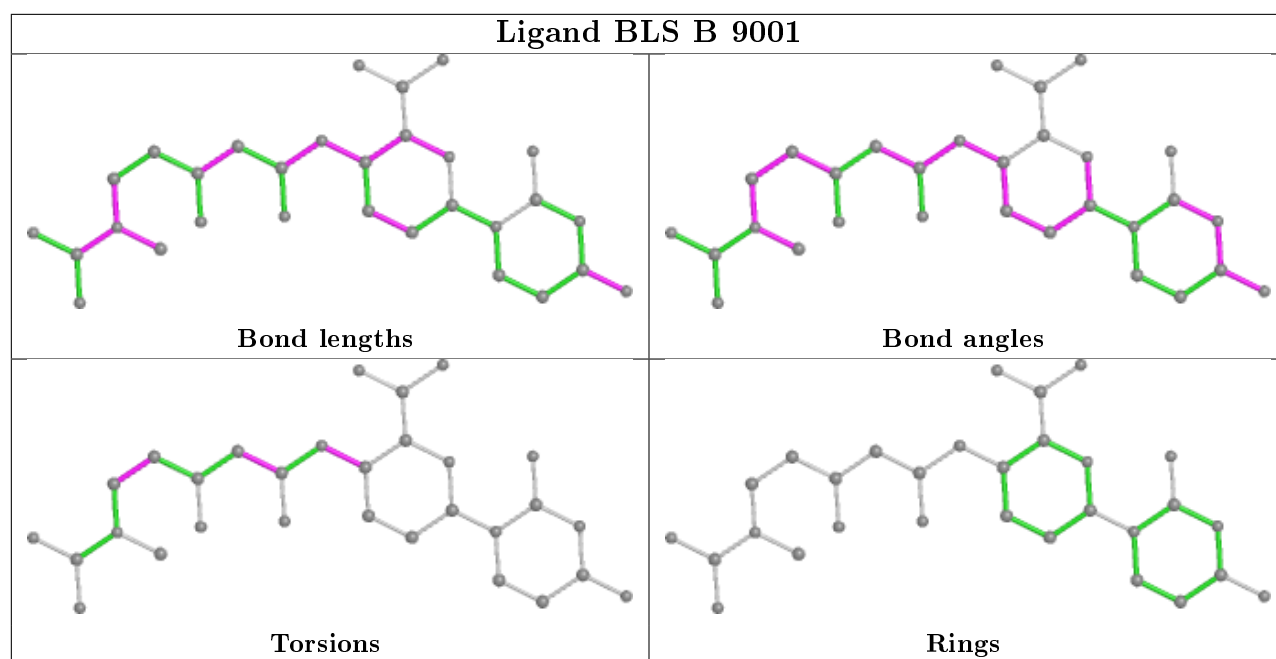
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	FB	9001	BLS	1	0
57	B	9001	BLS	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

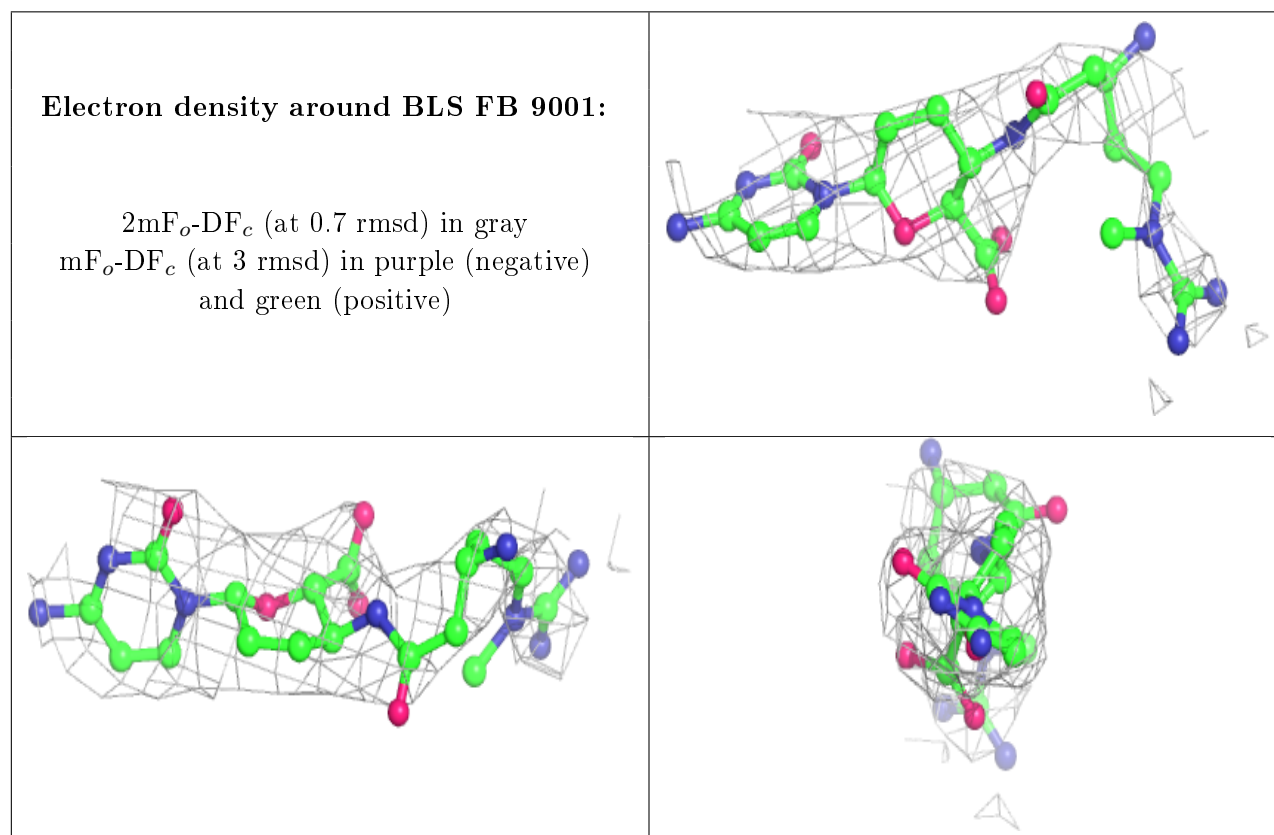
6.3 Carbohydrates [i](#)

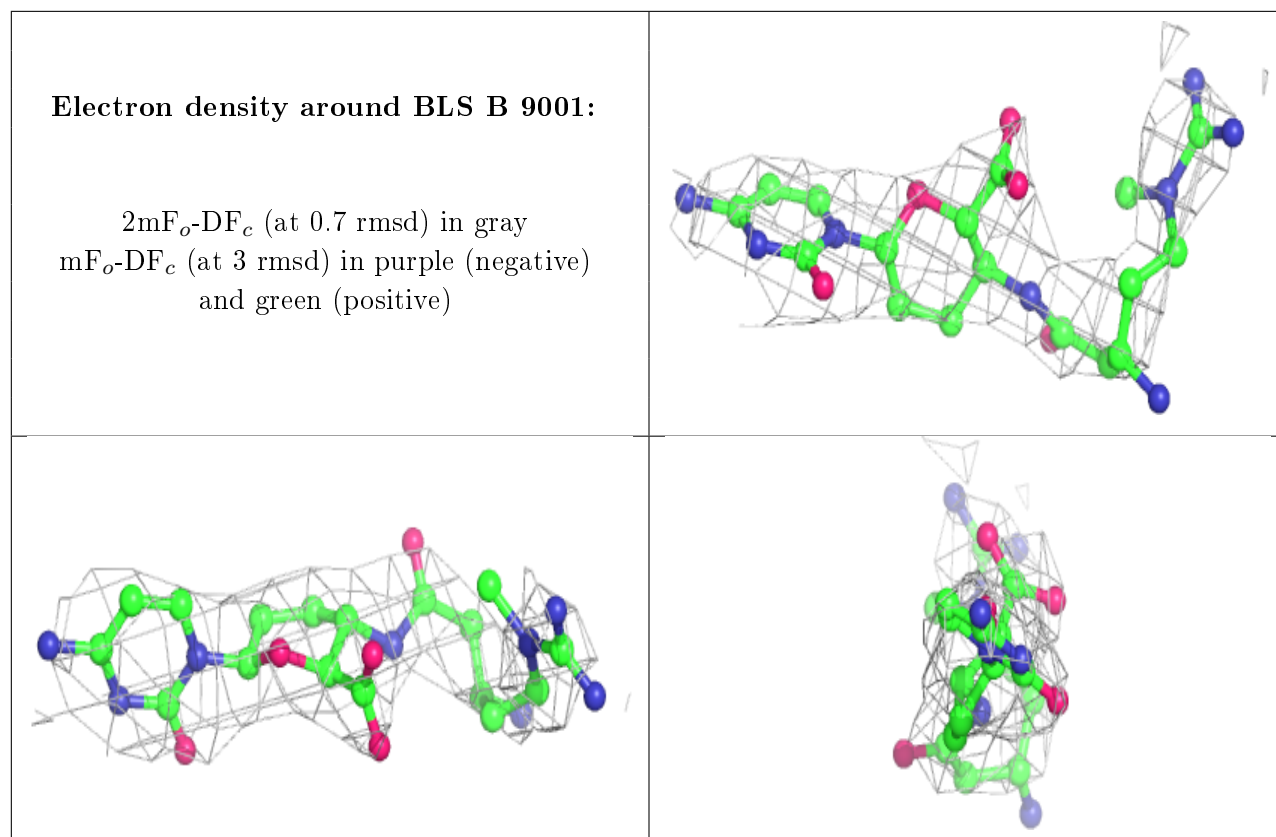
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

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.