



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 09:37 PM EDT

PDB ID : 6BOK
Title : E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-11-20
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

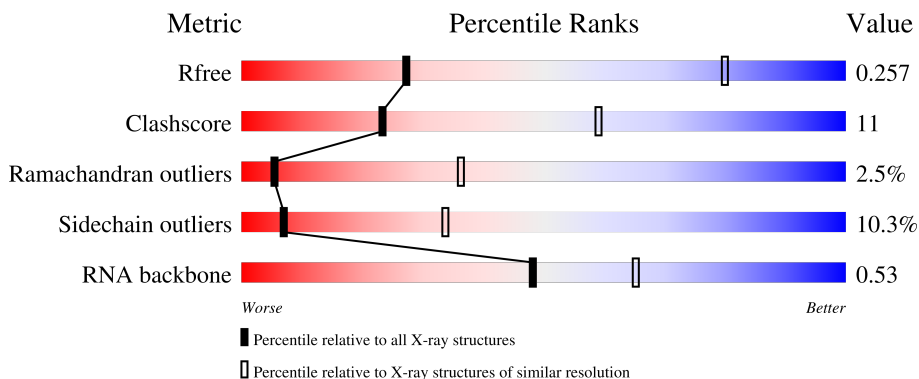
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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.




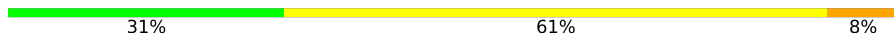











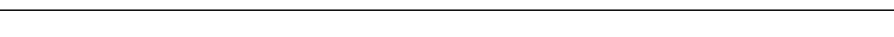
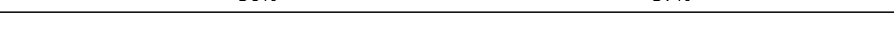
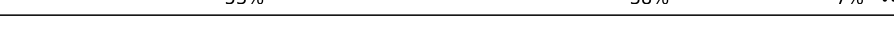



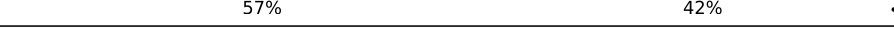





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RNA backbone	3102	1008 (4.10-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1507	49% 41% 9% .
1	DB	1507	49% 41% 9% .
2	B	2880	43% 41% 14% .
2	EB	2880	47% 39% 12% .
3	C	120	52% 37% 9% .
3	FB	120	53% 39% 7% .


























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

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

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Mol	Chain	Length	Quality of chain
28	BA	71	56% 34% 7% .
28	EC	71	58% 32% 7% .
29	CA	60	62% 32% 5% .
29	FC	60	60% 33% 5% .
30	DA	54	65% 31% ..
30	GC	54	65% 31% ..
31	EA	49	53% 37% 8% .
31	HC	49	49% 43% 6% .
32	FA	65	66% 23% 9% .
32	IC	65	60% 31% 8% .
33	GA	37	51% 46% .
33	JC	37	49% 49% .
34	HA	27	11% 15% 11% . 59%
34	KC	27	7% 22% 11% 59%
35	JA	256	50% 33% 7% . 9%
35	MC	256	48% 36% 7% . 9%
36	KA	239	54% 28% . 14%
36	NC	239	54% 28% 5% 14%
37	LA	209	58% 33% 7% .
37	OC	209	57% 34% 7% .
38	MA	162	51% 38% . 7%
38	PC	162	49% 39% 6% 7%
39	NA	101	47% 46% 8%
39	QC	101	52% 38% 10%
40	OA	156	66% 31% ..


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Mol	Chain	Length	Quality of chain
40	RC	156	65% 31% ..
41	PA	138	51% 43% 5%
41	SC	138	50% 46% .
42	QA	128	57% 34% 7% ..
42	TC	128	60% 30% 8% ..
43	RA	105	51% 41% . 7%
43	UC	105	50% 42% . 7%
44	SA	129	60% 29% . 10%
44	VC	129	60% 29% . 10%
45	TA	132	61% 26% 5% 8%
45	WC	132	60% 27% 5% 8%
46	UA	126	49% 37% 7% 7%
46	XC	126	48% 38% 6% 7%
47	VA	61	66% 31% ..
47	YC	61	70% 28% .
48	WA	89	55% 38% 6% .
48	ZC	89	60% 34% 6% .
49	AD	88	65% 26% .. 6%
49	XA	88	66% 26% .. 6%
50	BD	105	68% 23% . 6%
50	YA	105	69% 22% . 6%
51	CD	88	55% 20% 5% 20%
51	ZA	88	58% 17% 5% 20%
52	AB	93	52% 33% . 11%
52	DD	93	48% 38% . 11%

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Mol	Chain	Length	Quality of chain
53	BB	106	
53	ED	106	
54	CB	27	
54	FD	27	
55	GD	365	
55	HD	365	

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	DB	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
			Total	C	N	O	P			
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	EB	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
EB	154A	C	UNK	conflict	GB 46197919

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

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

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
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	GB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	LC	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	HB	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	IB	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	JB	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	KB	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	LB	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	MB	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	NB	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	OB	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	PB	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
			Total	C	N	O	S			
14	QB	141	1121	715	212	187	7	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	WB	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	XB	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	YB	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	ZB	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	AC	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
AC	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	BC	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	CC	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	DC	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	EC	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	FC	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	GC	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	HC	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	IC	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	JC	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	KC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
35	MC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
36	NC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
37	OC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
38	PC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
39	QC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	RC	155	1257	781	252	218	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	PA	138	1116	705	215	193	3	0	0	0
41	SC	138	1116	705	215	193	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	QA	127	1011	639	198	174	0	0	0
42	TC	127	1011	639	198	174	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	RA	98	794	499	156	138	1	0	0	0
43	UC	98	794	499	156	138	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	SA	116	864	537	164	160	3	0	0	0
44	VC	116	864	537	164	160	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	TA	122	958	604	193	159	2	0	0	0
45	WC	122	958	604	193	159	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
46	XC	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	VA	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
47	YC	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
48	ZC	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
49	AD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
50	BD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	ZA	70	Total	C	N	O	0	0	0
			574	367	112	95			
51	CD	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	AB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
52	DD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
53	ED	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	CB	24	Total	C	N	O	0	0	0
			208	128	50	30			
54	FD	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	GD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			
55	HD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GD	?	-	ASP	deletion	UNP B7MKB3
GD	?	-	ARG	deletion	UNP B7MKB3
GD	?	-	SER	deletion	UNP B7MKB3

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	A	160	Total Mg 160 160	0	0
56	B	514	Total Mg 514 514	0	0
56	C	23	Total Mg 23 23	0	0
56	D	6	Total Mg 6 6	0	0
56	E	4	Total Mg 4 4	0	0
56	F	1	Total Mg 1 1	0	0
56	G	4	Total Mg 4 4	0	0
56	H	1	Total Mg 1 1	0	0
56	I	3	Total Mg 3 3	0	0
56	J	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	K	2	Total Mg 2 2	0	0
56	L	7	Total Mg 7 7	0	0
56	M	4	Total Mg 4 4	0	0
56	N	3	Total Mg 3 3	0	0
56	O	1	Total Mg 1 1	0	0
56	P	2	Total Mg 2 2	0	0
56	Q	3	Total Mg 3 3	0	0
56	R	4	Total Mg 4 4	0	0
56	S	3	Total Mg 3 3	0	0
56	T	2	Total Mg 2 2	0	0
56	U	2	Total Mg 2 2	0	0
56	V	5	Total Mg 5 5	0	0
56	W	12	Total Mg 12 12	0	0
56	Y	4	Total Mg 4 4	0	0
56	Z	3	Total Mg 3 3	0	0
56	CA	1	Total Mg 1 1	0	0
56	EA	1	Total Mg 1 1	0	0
56	FA	1	Total Mg 1 1	0	0
56	HA	1	Total Mg 1 1	0	0
56	IA	8	Total Mg 8 8	0	0
56	JA	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	KA	1	Total 1	Mg 1	0	0
56	LA	1	Total 1	Mg 1	0	0
56	MA	3	Total 3	Mg 3	0	0
56	NA	2	Total 2	Mg 2	0	0
56	OA	3	Total 3	Mg 3	0	0
56	PA	2	Total 2	Mg 2	0	0
56	RA	2	Total 2	Mg 2	0	0
56	SA	1	Total 1	Mg 1	0	0
56	TA	3	Total 3	Mg 3	0	0
56	VA	2	Total 2	Mg 2	0	0
56	WA	3	Total 3	Mg 3	0	0
56	YA	2	Total 2	Mg 2	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	AB	1	Total 1	Mg 1	0	0
56	BB	1	Total 1	Mg 1	0	0
56	DB	177	Total 177	Mg 177	0	0
56	EB	395	Total 395	Mg 395	0	0
56	FB	17	Total 17	Mg 17	0	0
56	GB	5	Total 5	Mg 5	0	0
56	HB	8	Total 8	Mg 8	0	0
56	IB	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	JB	2	Total 2	Mg 2	0	0
56	KB	1	Total 1	Mg 1	0	0
56	LB	5	Total 5	Mg 5	0	0
56	MB	2	Total 2	Mg 2	0	0
56	NB	1	Total 1	Mg 1	0	0
56	OB	3	Total 3	Mg 3	0	0
56	PB	2	Total 2	Mg 2	0	0
56	QB	3	Total 3	Mg 3	0	0
56	RB	5	Total 5	Mg 5	0	0
56	SB	1	Total 1	Mg 1	0	0
56	TB	5	Total 5	Mg 5	0	0
56	VB	1	Total 1	Mg 1	0	0
56	WB	3	Total 3	Mg 3	0	0
56	XB	2	Total 2	Mg 2	0	0
56	YB	3	Total 3	Mg 3	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	AC	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	DC	1	Total 1	Mg 1	0	0
56	FC	1	Total 1	Mg 1	0	0
56	HC	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	IC	2	Total 2	Mg 2	0	0
56	JC	1	Total 1	Mg 1	0	0
56	KC	1	Total 1	Mg 1	0	0
56	LC	8	Total 8	Mg 8	0	0
56	MC	3	Total 3	Mg 3	0	0
56	PC	2	Total 2	Mg 2	0	0
56	QC	2	Total 2	Mg 2	0	0
56	RC	2	Total 2	Mg 2	0	0
56	SC	1	Total 1	Mg 1	0	0
56	TC	2	Total 2	Mg 2	0	0
56	UC	1	Total 1	Mg 1	0	0
56	WC	2	Total 2	Mg 2	0	0
56	XC	2	Total 2	Mg 2	0	0
56	YC	1	Total 1	Mg 1	0	0
56	ZC	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BD	2	Total 2	Mg 2	0	0
56	CD	2	Total 2	Mg 2	0	0
56	ED	1	Total 1	Mg 1	0	0
56	GD	5	Total 5	Mg 5	0	0
56	HD	3	Total 3	Mg 3	0	0

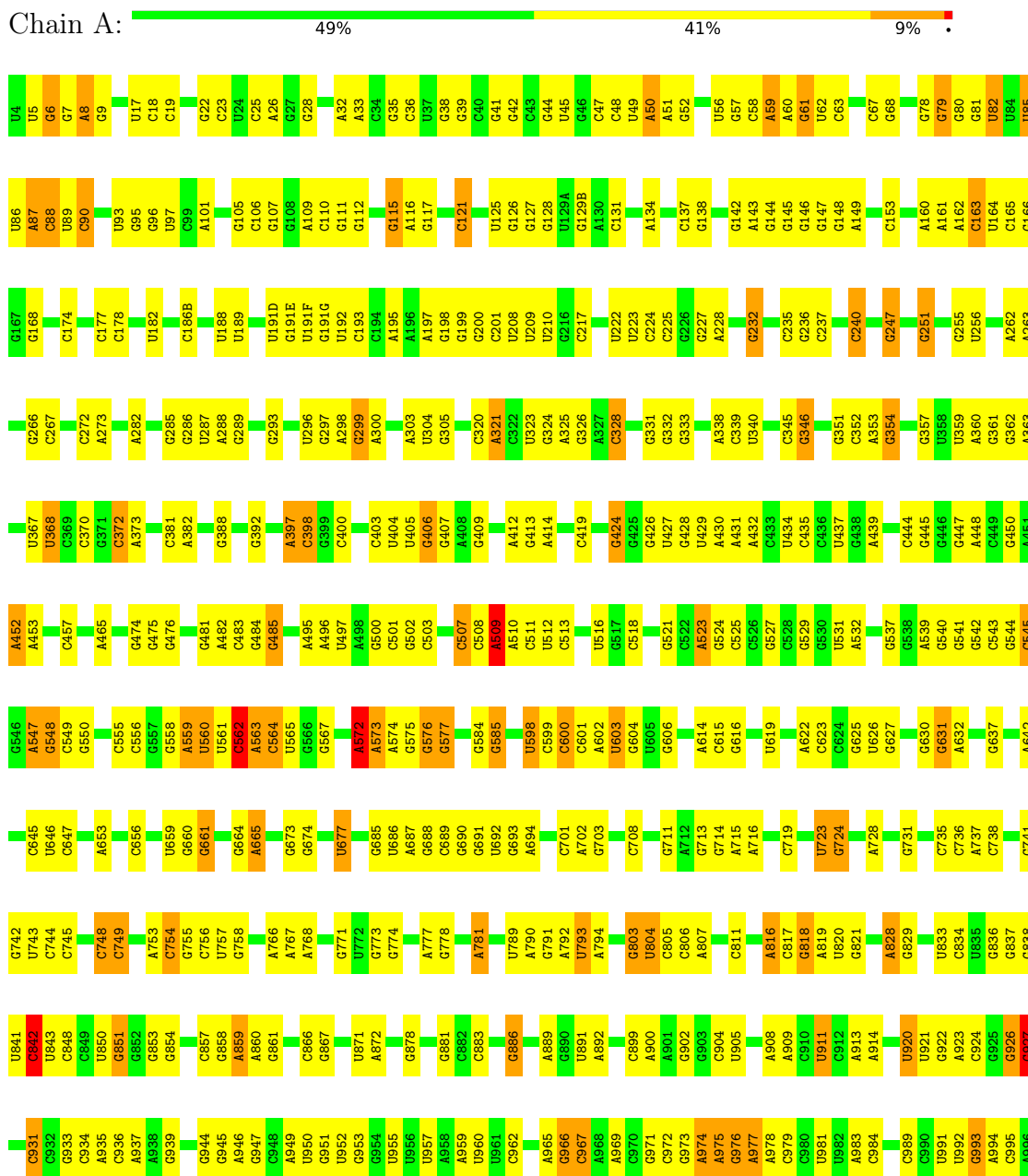
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

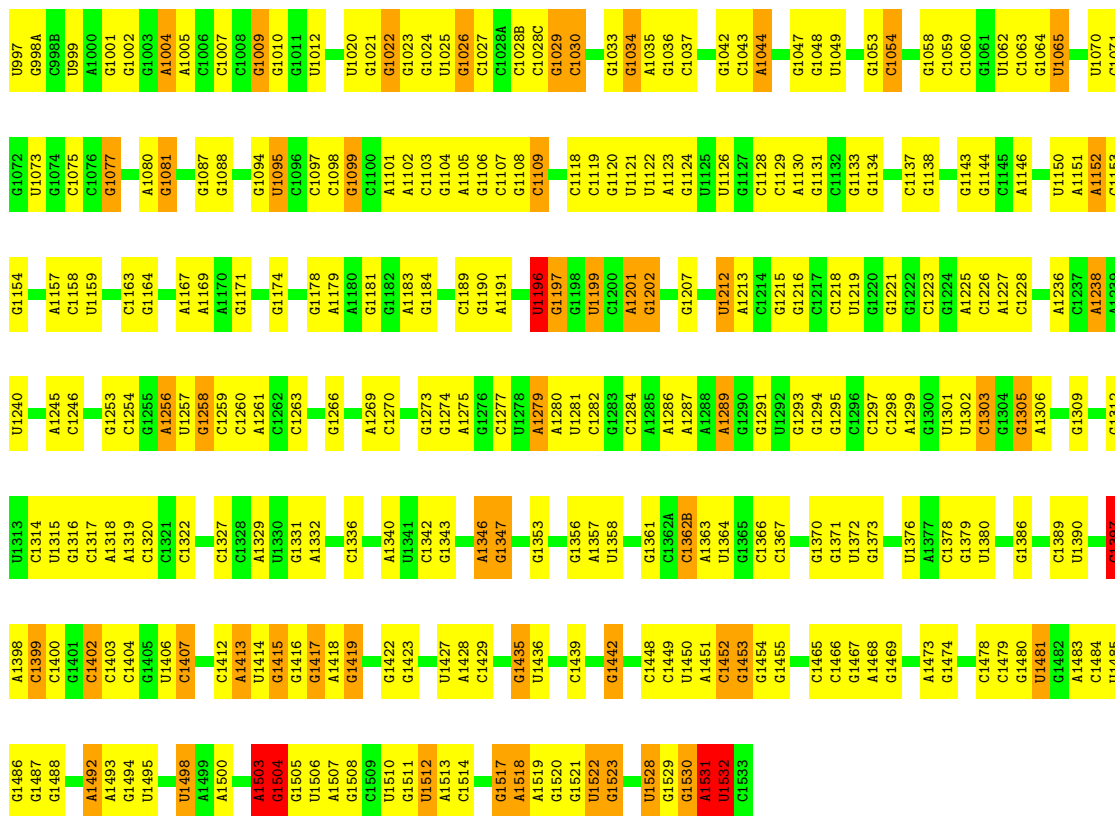
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	V	1	Total 1	Zn 1	0	0
57	BA	1	Total 1	Zn 1	0	0
57	CA	1	Total 1	Zn 1	0	0
57	DA	1	Total 1	Zn 1	0	0
57	GA	1	Total 1	Zn 1	0	0
57	YB	1	Total 1	Zn 1	0	0
57	EC	1	Total 1	Zn 1	0	0
57	FC	1	Total 1	Zn 1	0	0
57	GC	1	Total 1	Zn 1	0	0
57	JC	1	Total 1	Zn 1	0	0

3 Residue-property plots [i](#)

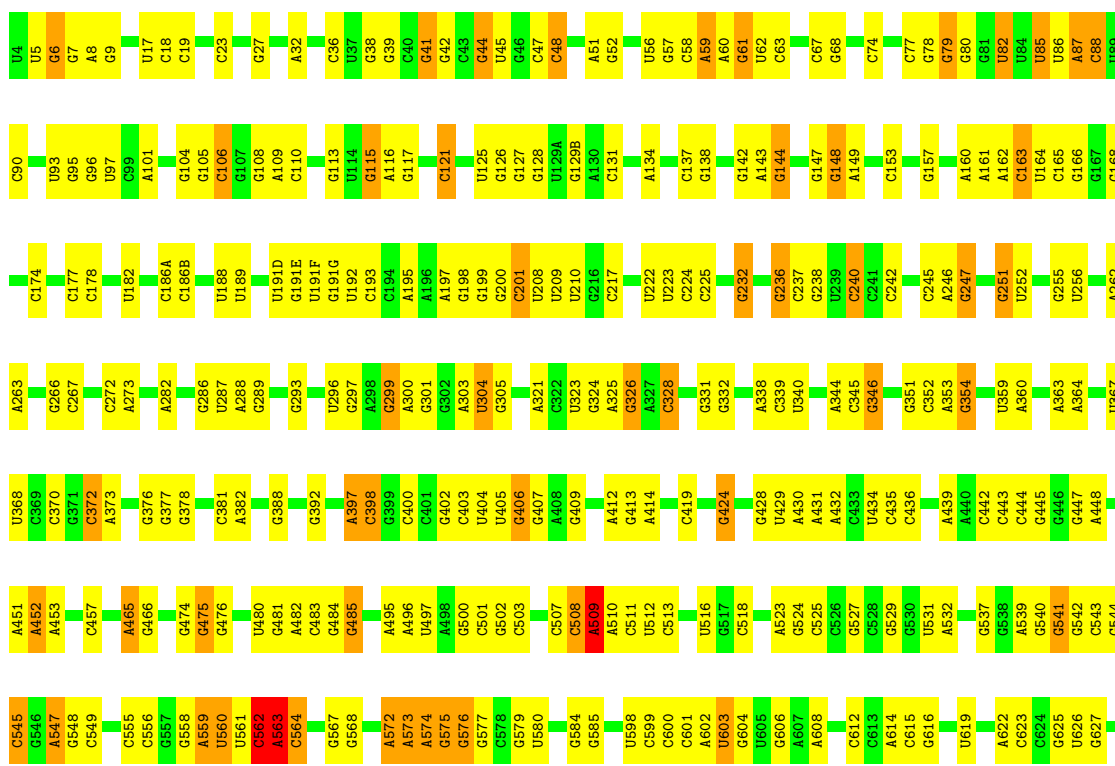
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

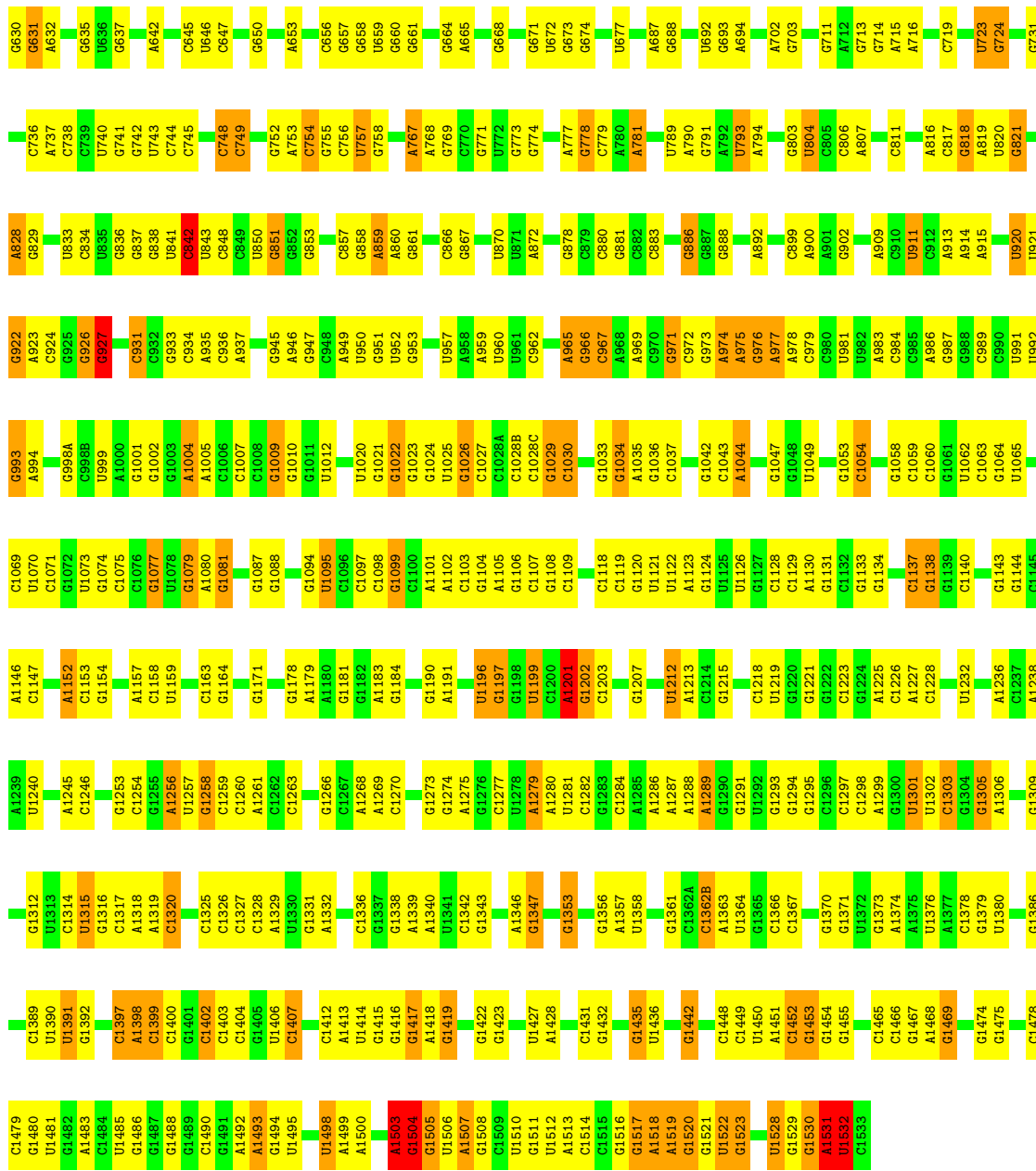
- Molecule 1: 16S ribosomal RNA



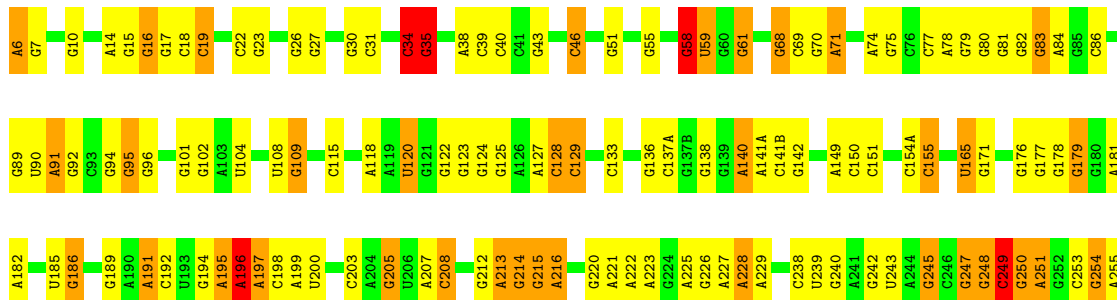


● Molecule 1: 16S ribosomal RNA



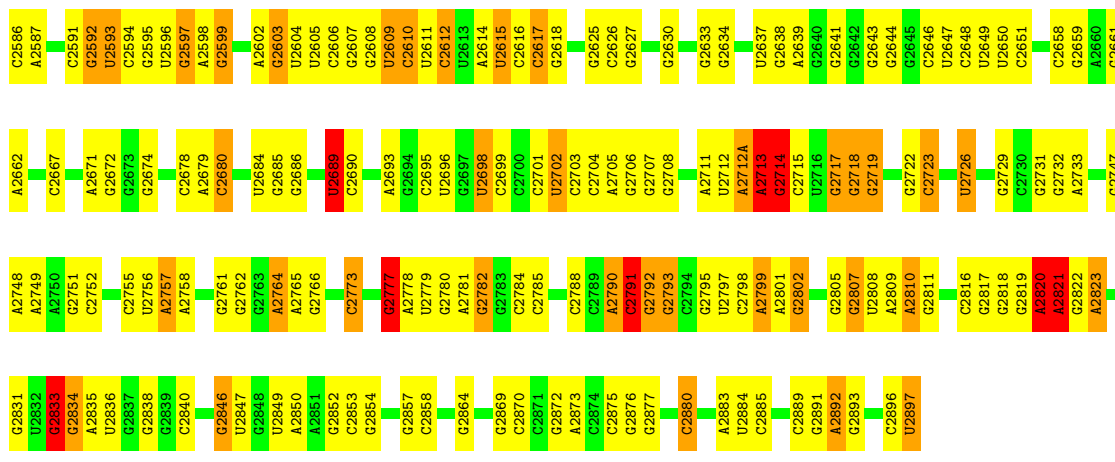


• Molecule 2: 23S ribosomal RNA

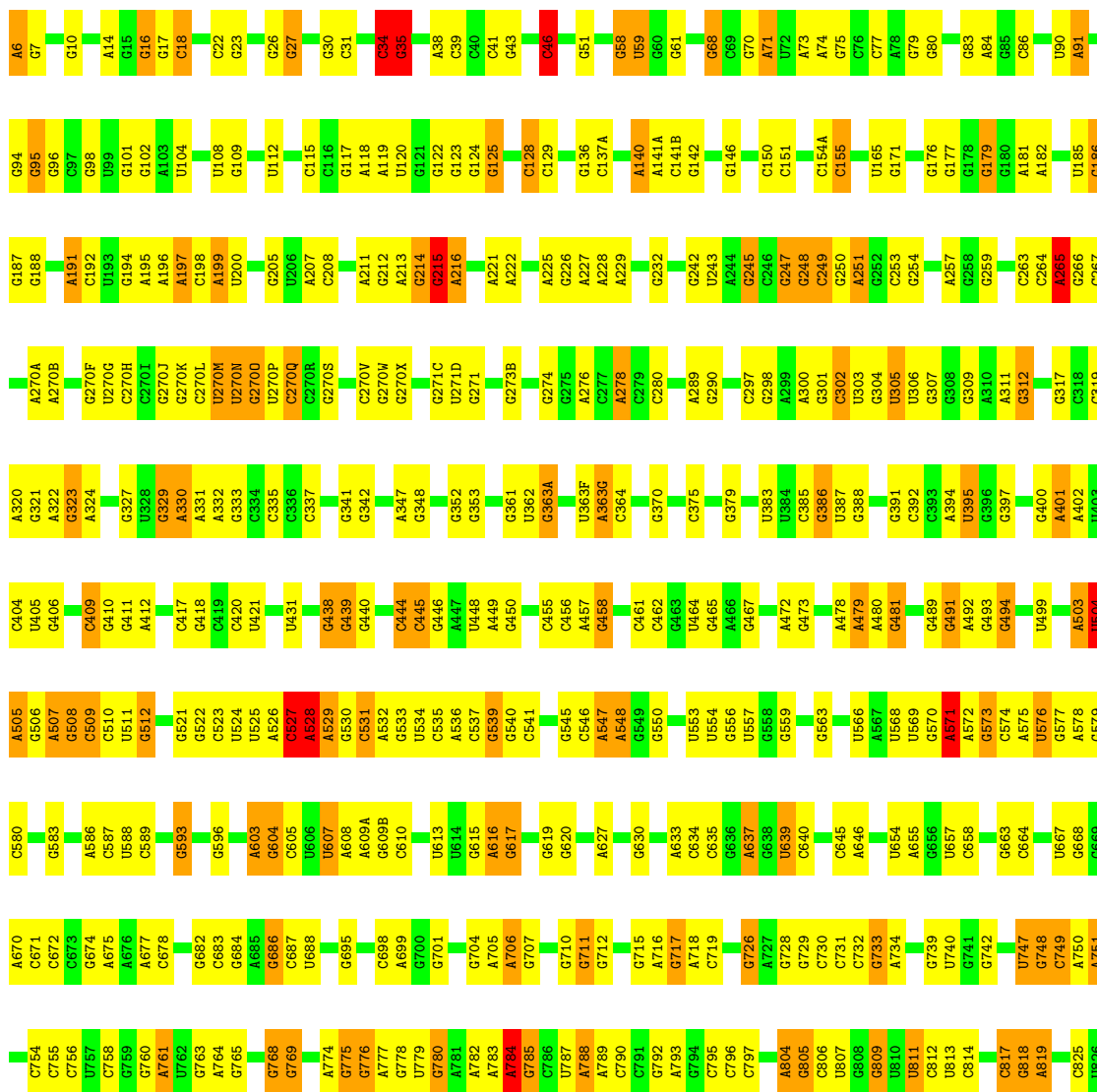


G1325	U1082	G1164	U1083	U1088	A933	G854	A782	G710	A632	G558	A479	G396	G312	G259
U1326	U1083	U1166	U1083	U1083	G954	G855	A783	G711	A633	G559	A480	G397	C313	G262
G1327	A1084	G1173	A1084	A1085	C935	C856	A784	G712	C634	U662	G481	G400	G317	C263
G1328	A1085	G1174	A1085	A1086	C936	C857	A785	G713	C635	U663	C484	A401	C318	C264
A1331	A1086	G1175	A1086	A1087	U937	U858	C786	U714	G636	C564	C485	A402	C319	A265
G1332	A1088	G1176	A1088	A1088	G938	U859	C787	U715	A637	C565	C486	U603	A320	
G1333	G1089	A1177	G1089	A1088	G939	U860	A788	G715	G638	U666	C404	C409	A321	
G1334	A1178	G1177	G1089	A1088	A940	A861	A789	G716	U639	U667	G489	C410	A322	A270A
G1259	C1092	C1178	G1092	A1088	A941	G862	C790	A717	G640	A567	G491	C409	A323	U270G
G1260	G1093	C1179	G1093	A1088	A942	G865	C791	A718	C645	U568	G492	C409	A324	U270G
G1261	G1094	C1180	G1093	A1088	U943	G866	C792	A719	C646	U569	G493	C409	A325	C270H
G1264	U1094	G1185	U1094	A1088	A944	A866	A793	U724	G647	A571	G494	C410	A326	C270I
A1265	A1095	G1186	A1095	A1088	A945	G869	C795	G725	G648	A572	G499	C411	A329	G270J
A1266	A1096	G1187	A1096	A1088	G946	G870	C796	G726	G649	C574	G500	A412	A330	G270K
A1267	A1097	U1187	A1097	A1088	G947	U871	C797	A727	C653	C575	U499	A412	A331	C270L
A1268	A1098	U1188	A1098	A1088	G948	U872	C798	G728	U654	U576	G503	C417	A332	U270M
A1269	A1099	U1189	A1099	A1088	G949	U873	C799	G729	U655	U577	G504	C418	A332	U270M
A1270	G1100	G1190	G1100	A1088	G952	C876	A800	G730	U656	U578	U505	C419	A333	G270N
C1271	U1101	G1193	U1101	A1088	G953	U877	G801	C731	A655	C578	U506	C420	A334	U270P
A1272	C1104	C1196	C1104	A1088	G954	U878	G802	C732	A656	U579	U507	C421	A335	C270Q
A1273	U1105	C1196	U1105	A1088	G955	U879	G803	G733	A657	C580	U508	A422	A337	G270S
A1274	G1106	C1202	G1106	A1088	G956	U880	A804	A734	U658	C581	U509	C422	A341	G270T
A1275	G1107	G1203	G1107	A1088	A957	U881	A805	A735	C658	C582	C510	C423	A342	G270U
A1276	G1203	G1203	G1203	A1088	U958	U882	C806	U740	G663	C583	C511	C433	A343	G270V
G1277	A1204	A1204	A1204	A1088	A960	U883	C807	U741	C664	C584	C512	G438	A344	G270W
A1278	G1205	U1205	G1205	A1088	A961	G886	C808	G744	U667	C585	U511	G439	A345	G270X
U1282	U1206	U1206	U1206	A1088	C961	U887	G809	G745	U668	A586	U512	G440	A347	G270Y
U1282	G1206	G1206	G1206	A1088	G962	U888	U810	G746	U669	U587	G520	G441	A348	G271C
A1286	U1209	G1209	U1209	A1088	U963	C888	U811	A747	U670	U588	G521	G442	A349	G271D
A1287	G1210	G1210	G1210	A1088	G964	C889	U812	U747	A670	C589	G522	G443		
A1288	A1210	A1210	A1210	A1088	U965	U890	U813	G748	C671	C592	C523	C444		
A1289	U1211	U1211	U1211	A1088	C970	U892	C814	C749	U674	U524	U524	C445		
U1288	A1126	G1212	A1126	A1088	C971	C893	C817	A750	A675	U525	U525	G446		
C1291	A1128	G1215	A1128	A1088	G972	U894	C818	A751	A676	U526	A526	G450		
U1292	U1130	G1216	U1130	A1088	A973	U895	C819	A752	A677	C527	A528	G451		
C1293	U1131	G1217	U1131	A1088	G974A	U896	C820	C754	A677	C528	A529	C451		
C1297	G1135	G1218	G1135	A1088	C974B	C897	A820	C755	G682	C601	C529	C455		
C1298	U1136	G1219	U1136	A1088	G978	U900	C825	C756	A685	C603	G530	C456		
G1299	G1137	A1220	G1137	A1088	G979	A901	C826	U757	A686	G604	C531	C457		
U1300	G1138	A1221	G1138	A1088	A980	U907	U827	C758	G686	C605	A532	G463		
A1301	G1139	G1224	G1139	A1088	C981	U908	U828	A761	C687	U606	G533	G464		
A1302	U1065	G1225	U1065	A1088	C982	C908	U829	U762	U688	U607	U534	G465		
G1303	U1066	G1226	U1066	A1088	A983	A909	G832	C763	A689	C602	C535	G466		
C1304	A1143	A1226	A1143	A1088	C986	A910	C836	U764	G690	A603	A536	C467		
A1307	G1144	G1227	G1144	A1088	G989	A911	U826	A764	C691	G604	C537	C468		
G1310	G1149	G1231	G1149	A1088	G989	U913	C837	G765	C692	C606	G539	G469		
C1314	C1152	U1234	C1152	A1088	G993	C914	U839	G769	G695	C610	C541	G472		
C1315	C1153	G1236	C1153	A1088	A996	A917	C844	G770	G696	U613	G540	A473		
C1384	G1154	G1236	G1154	A1088	A996	A918	G845	A774	C697	U614	G541	A474		
G1385	A1155	U1240	A1155	A1088	G1002	G921	U847	G775	U700	G615	C542	A475		
C1392	A1156	C1243	A1156	A1088	G1003	U922	U848	G776	G701	A616	G543	A476		
A1393	G1157	G1243	G1157	A1088	C1004	C923	A849	A777	G697	U617	C544	G477		
A1394	C1158	G1244	C1158	A1088	C1005	G929	G850	G778	C698	C628	U553	G478		
A1395	C1161	G1245	C1161	A1088	C1006	U929	U851	U779	G700	G629	U554	U475		
G1394	A1246	G1246	A1246	A1088	C1007	G932	G852	G780	A705	G630	U555	U476		
G1396	G1394	G1246	G1394	A1088	C1008	U932	G853	A781	G707	A631	U557	A478		

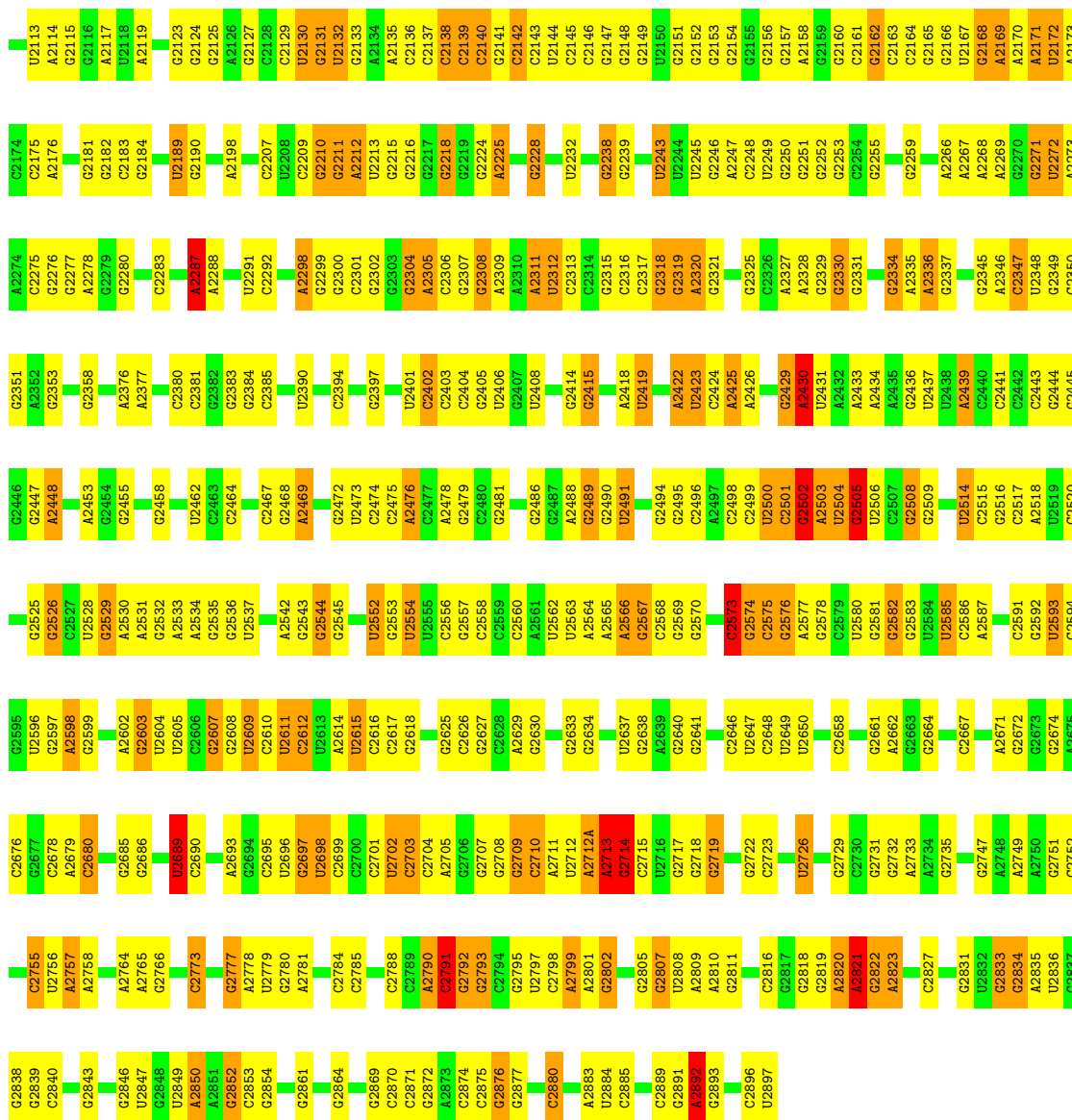
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C2520	A2451	G2052	G1973	G1906	G1811	A1729	G1642	G1566	U1489	C1402
G2525	C2452	G2053	C1974	C1908	A1812	U1730	G1643	A1569	C1493	U1405
C2526	A2453	A2054	G1975	G1908	G1813	G1731	G1646	G1573	A1494	U1406
U2528	G2454	G2055	U1976	U1911	G1814	A1732	G1647	G1573	U1497	C1407
G2529	A2455	G2056	G1979	A1912	A1815	C1742	C1648	U1578	C1501	C1408
U2530	G2458	A2057	G1980	A1914	G1817	G1743	G1651	G1581	A1508	G1410
A2531	C2461	A2058	A1981	C1914	A1818	G1750	A1652	C1582	A1508	C1409
C2532	G2462	A2059	C1982	U1915	A1819	G1751	A1653	C1583	A1509	C1409
A2533	U2463	A2060	C1983	A1916	G1820	C1752	A1654	C1585	A1510	G1417
G2534	C2464	G2061	G1984	U1917	A1821	G1753	A1654	C1586	A1511	G1416
G2535	G2465	A2062	G1989	A1918	G1822	C1754	C1657	A1587	A1512	A1419
U2536	A2466	C2063	G1992	A1919	A1823	A1755	C1658	C1588	U1512	U1420
U2537	C2468	G2064	G1992	G1920	G1824	A1756	U1659	C1589	C1513	G1421
A2541	G2469	C2065	U1993	G1921	A1825	U1757	C1660	U1590	C1513	G1422
A2542	U2472	G2066	G1997	U1922	G1826	C1761	G1661	C1592	U1516	G1425
G2543	C2473	C2067	U1998	C1923	A1827	A1762	A1664	C1593	G1517	G1426
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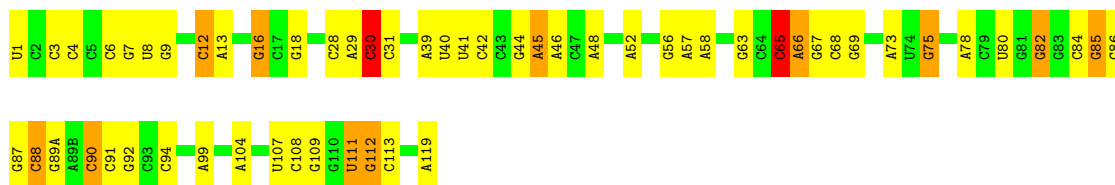
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• Molecule 3: 5S ribosomal RNA

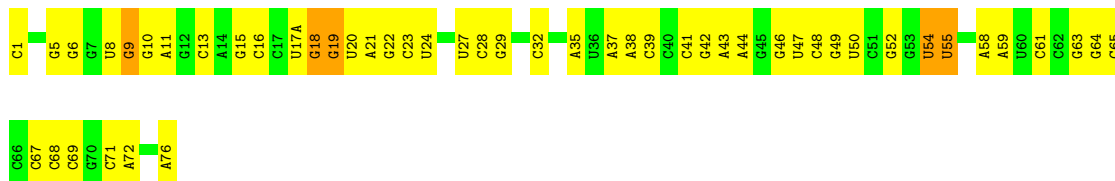


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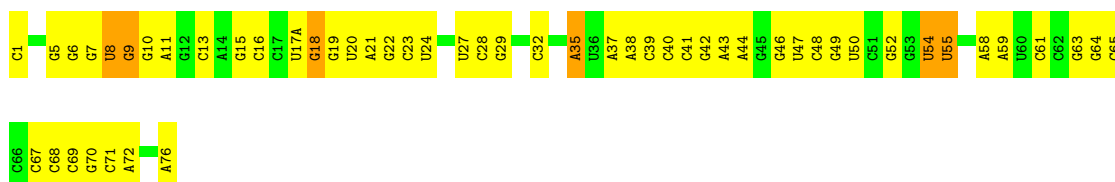
- Molecule 4: 16S ribosomal RNA



- Molecule 4: 16S ribosomal RNA



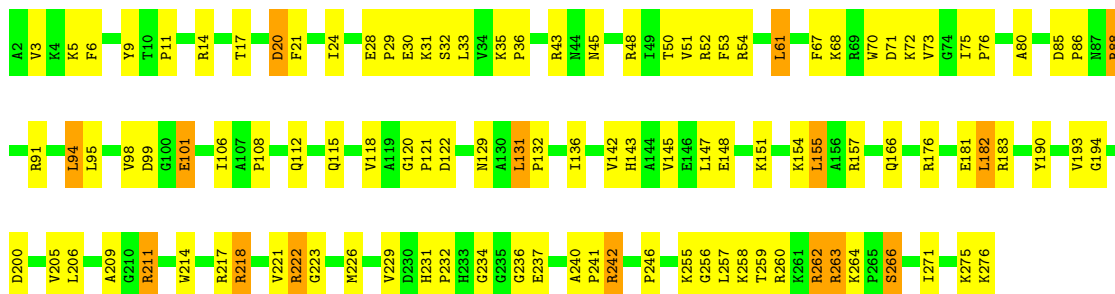
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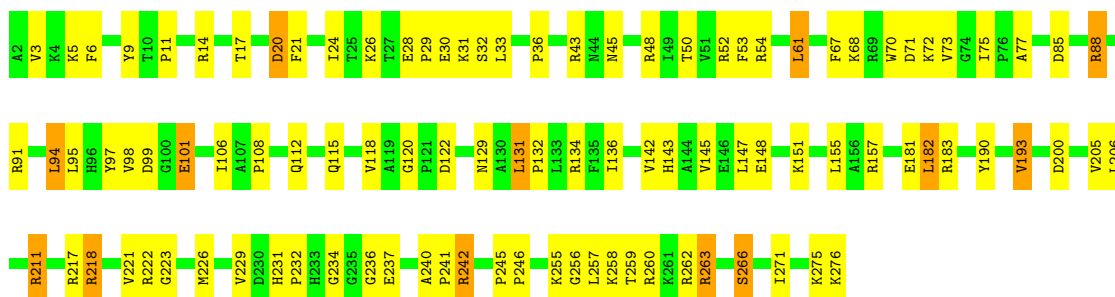
- Molecule 4: 16S ribosomal RNA



- Molecule 5: 50S ribosomal protein L2



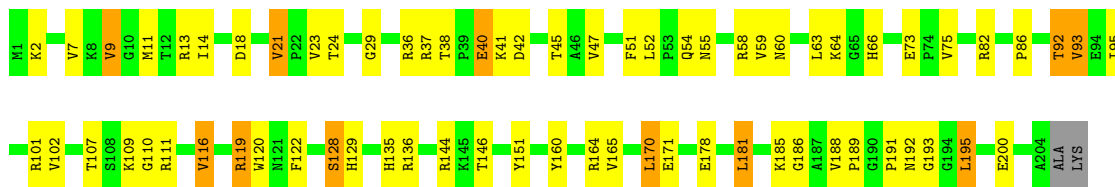
• Molecule 5: 50S ribosomal protein L2

Chain HB:  63% 32% 5%

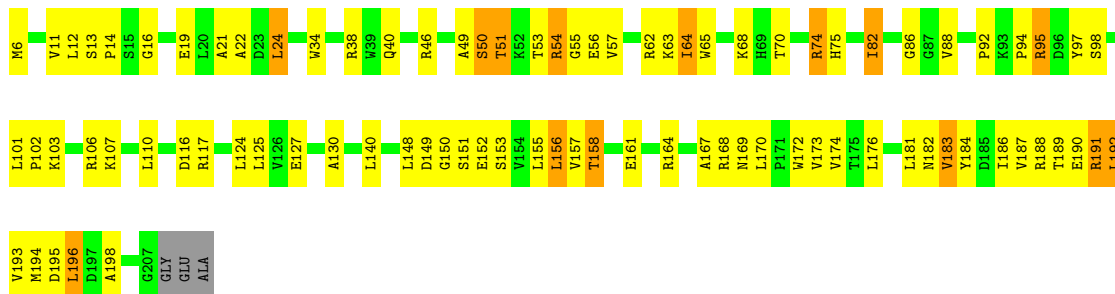
• Molecule 6: 50S ribosomal protein L3

Chain F:  62% 32% 5%

• Molecule 6: 50S ribosomal protein L3

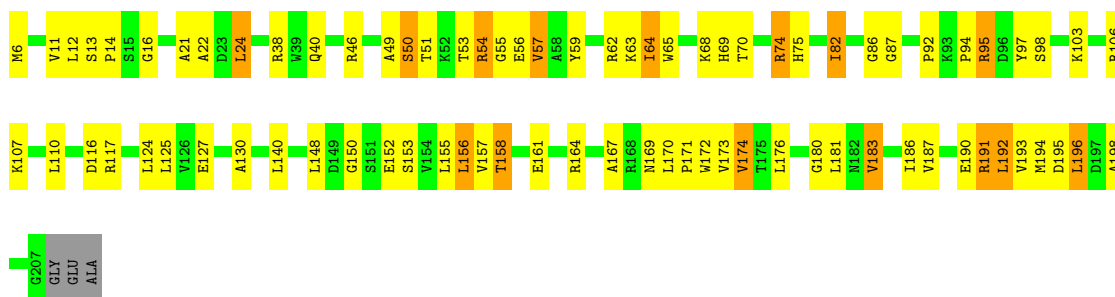
Chain IB:  66% 28% 5%

• Molecule 7: 50S ribosomal protein L4

Chain G:  56% 36% 7%

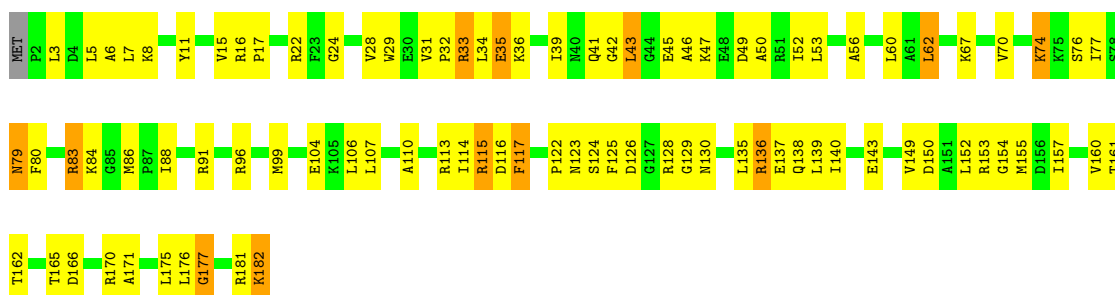
- Molecule 7: 50S ribosomal protein L4

Chain JB:  60% 32% 7%



- Molecule 8: 50S ribosomal protein L5

Chain H:  50% 43% 7%



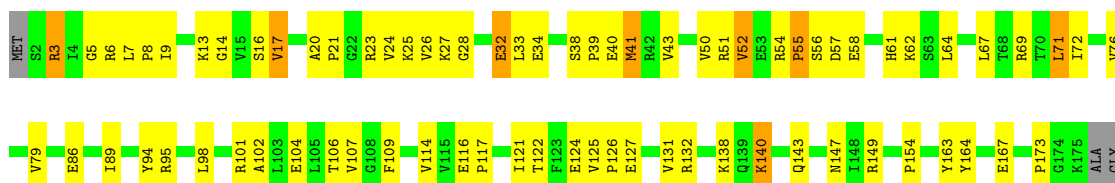
- Molecule 8: 50S ribosomal protein L5

Chain KB:  54% 39% 7%



- Molecule 9: 50S ribosomal protein L6

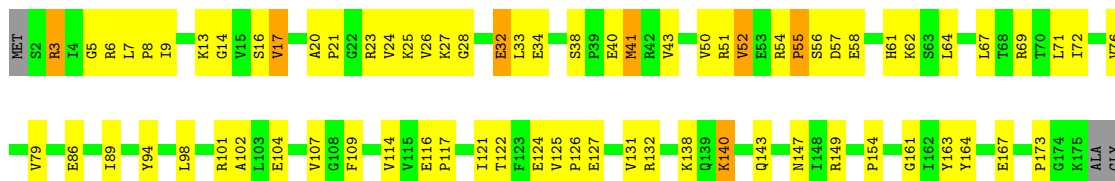
Chain I:  55% 37% 8%



ALA
LYS
LYS

- Molecule 9: 50S ribosomal protein L6

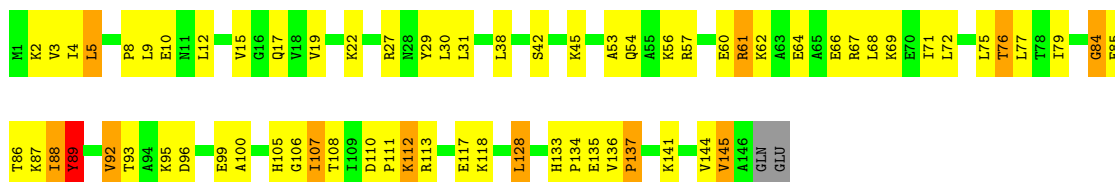
Chain LB:  56% 37%



ALA
LYS
LYS

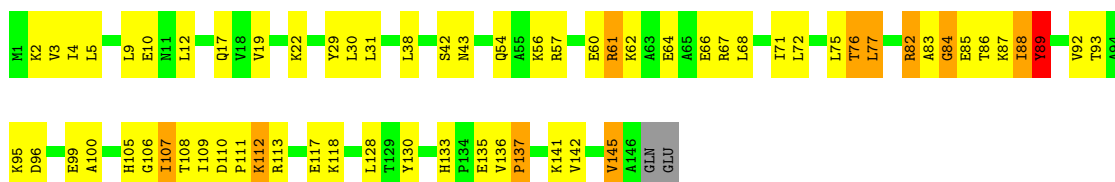
- Molecule 10: 50S ribosomal protein L9

Chain J:  53% 38% 7%



- Molecule 10: 50S ribosomal protein L9

Chain MB:  55% 36% 7%



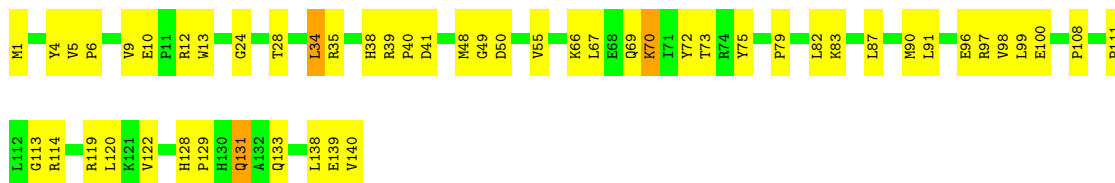
- Molecule 11: 50S ribosomal protein L13

Chain K:  63% 34%



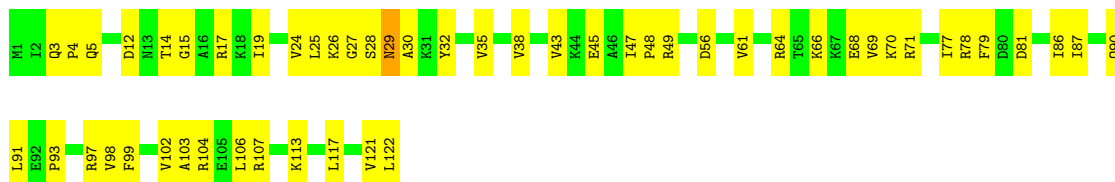
- Molecule 11: 50S ribosomal protein L13

Chain NB:  63% 35%



- Molecule 12: 50S ribosomal protein L14

Chain L: 57% 42%



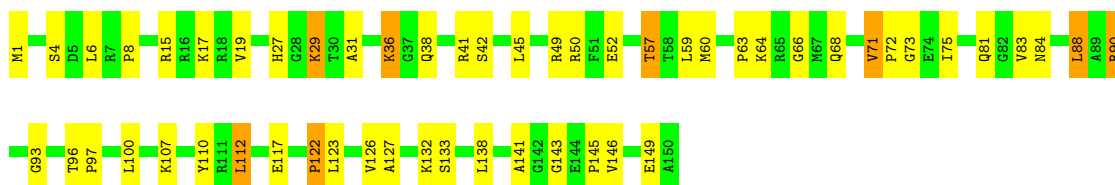
- Molecule 12: 50S ribosomal protein L14

Chain OB: 59% 41%



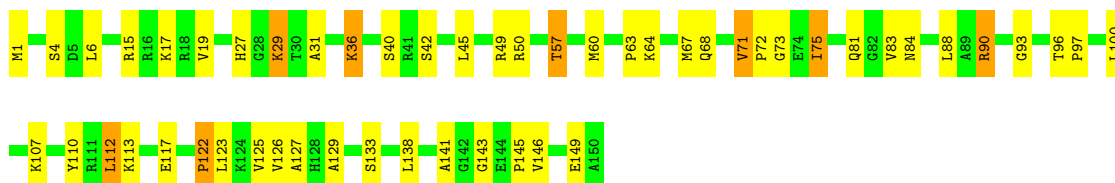
- Molecule 13: 50S ribosomal protein L15

Chain M: 64% 31% 5%



- Molecule 13: 50S ribosomal protein L15

Chain PB: 65% 29% 5%



- Molecule 14: 50S ribosomal protein L16

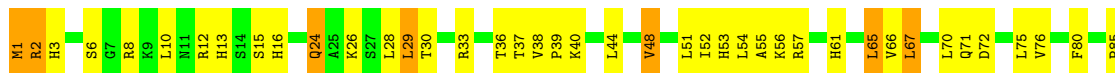
Chain N: 72% 21% 6%



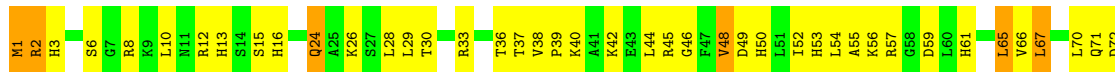
• Molecule 14: 50S ribosomal protein L16



• Molecule 15: 50S ribosomal protein L17



• Molecule 15: 50S ribosomal protein L17



• Molecule 16: 50S ribosomal protein L18

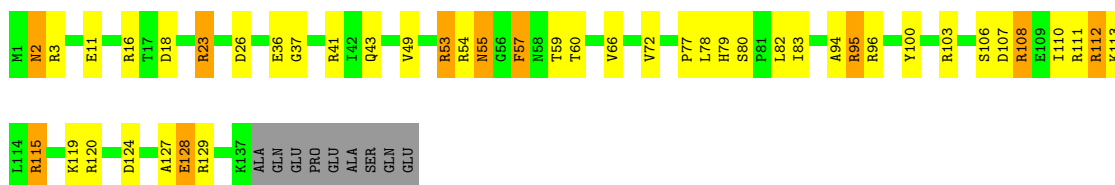


• Molecule 16: 50S ribosomal protein L18



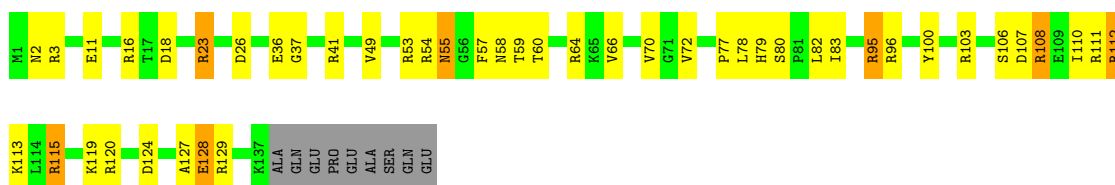
- Molecule 17: 50S ribosomal protein L19

Chain Q: 



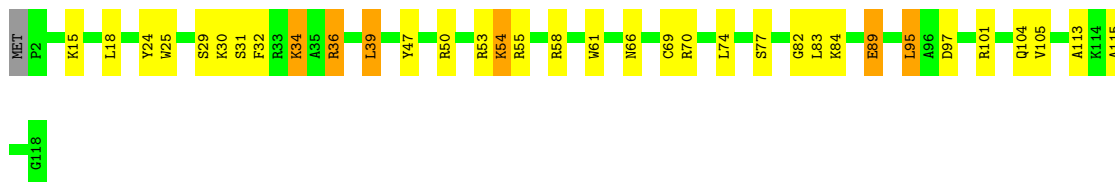
- Molecule 17: 50S ribosomal protein L19

Chain TB: 



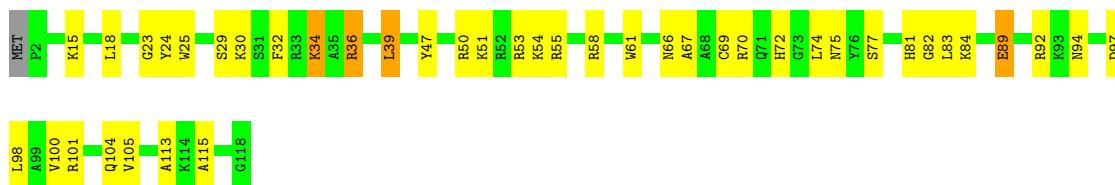
- Molecule 18: 50S ribosomal protein L20

Chain R: 



- Molecule 18: 50S ribosomal protein L20

Chain UB: 



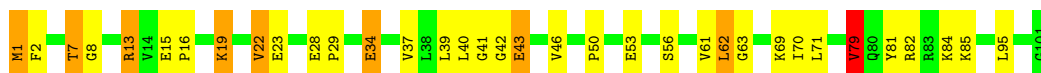
- Molecule 19: 50S ribosomal protein L21

Chain S: 



- Molecule 19: 50S ribosomal protein L21

Chain VB:  65% 26% 8%



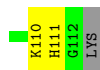
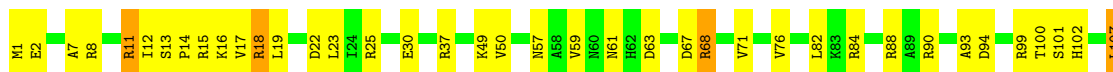
- Molecule 20: 50S ribosomal protein L22

Chain T:  59% 35%



- Molecule 20: 50S ribosomal protein L22

Chain WB:  63% 33%




- Molecule 21: 50S ribosomal protein L23

Chain U:  78% 20%



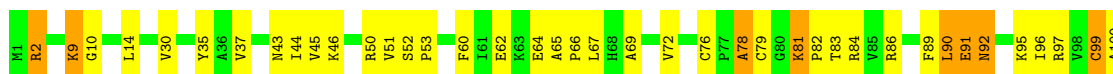
- Molecule 21: 50S ribosomal protein L23

Chain XB:  77% 22%



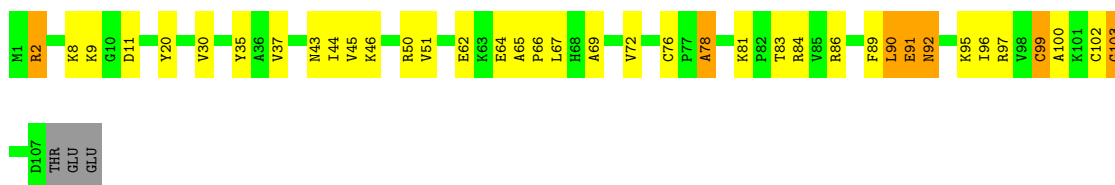
- Molecule 22: 50S ribosomal protein L24

Chain V:  59% 30% 8%



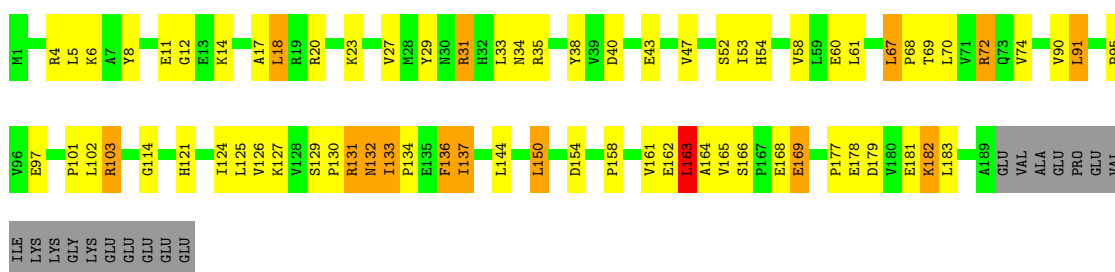
- Molecule 22: 50S ribosomal protein L24

Chain YB:  63% 28% 6%



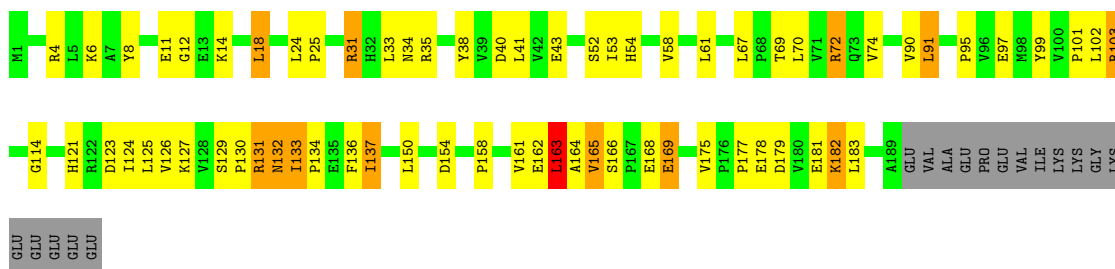
- Molecule 23: 50S ribosomal protein L25

Chain W:  57% 28% 7% 8%



- Molecule 23: 50S ribosomal protein L25

Chain ZB:  59% 27% 6% 8%



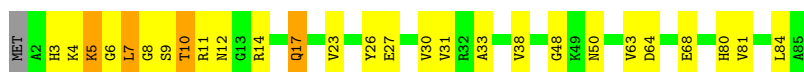
- Molecule 24: 50S ribosomal protein L27

Chain X:  65% 31%

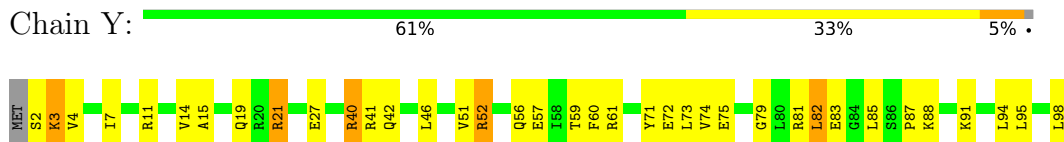


- Molecule 24: 50S ribosomal protein L27

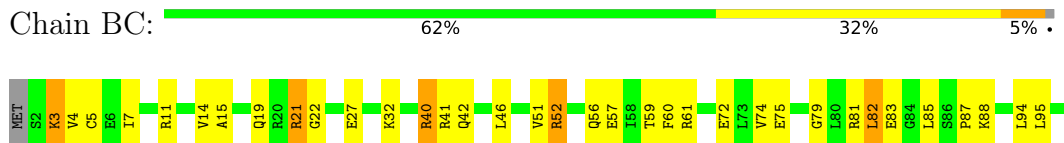
Chain AC:  67% 27% 5%



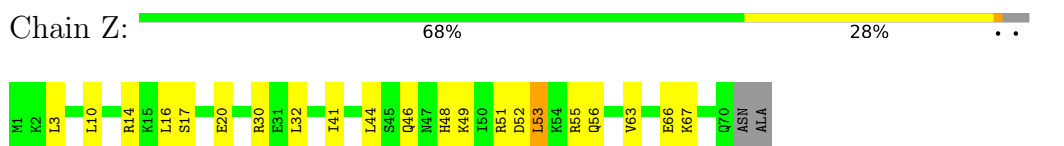
- Molecule 25: 50S ribosomal protein L28



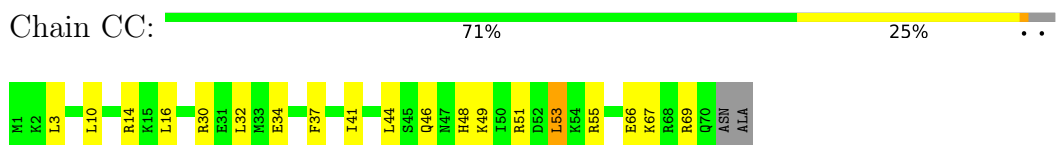
- Molecule 25: 50S ribosomal protein L28



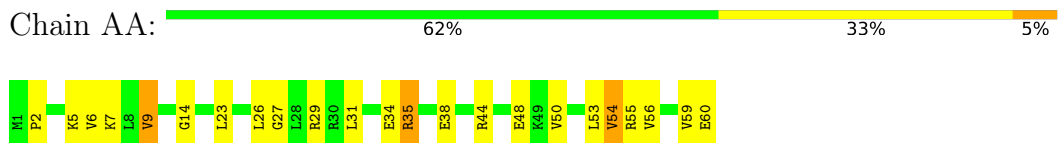
- Molecule 26: 50S ribosomal protein L29



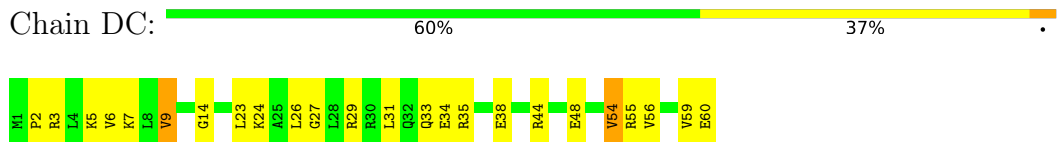
- Molecule 26: 50S ribosomal protein L29



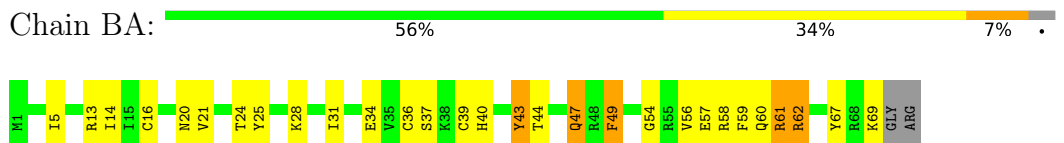
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31

Chain EC:  58% 32% 7%



- Molecule 29: 50S ribosomal protein L32

Chain CA:  62% 32% 5%



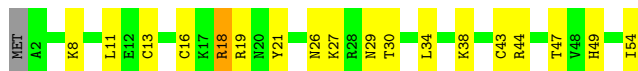
- Molecule 29: 50S ribosomal protein L32

Chain FC:  60% 33% 5%



- Molecule 30: 50S ribosomal protein L33

Chain DA:  65% 31%



- Molecule 30: 50S ribosomal protein L33

Chain GC:  65% 31%



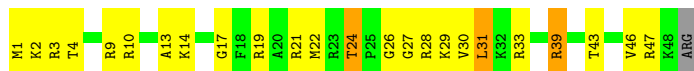
- Molecule 31: 50S ribosomal protein L34

Chain EA:  53% 37% 8%

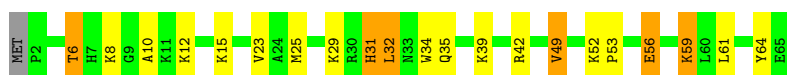


- Molecule 31: 50S ribosomal protein L34

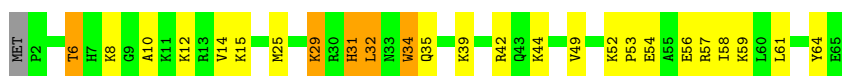
Chain HC:  49% 43% 6%



- Molecule 32: 50S ribosomal protein L35



• Molecule 32: 50S ribosomal protein L35



• Molecule 33: 50S ribosomal protein L36



• Molecule 33: 50S ribosomal protein L36



• Molecule 34: mRNA



• Molecule 34: mRNA

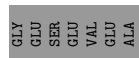
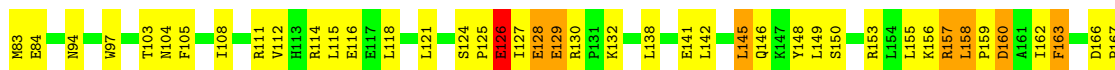
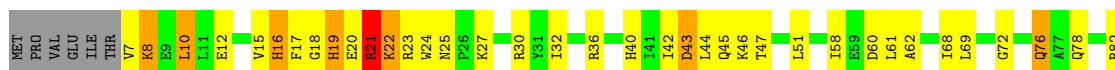


• Molecule 35: 30S ribosomal protein S2

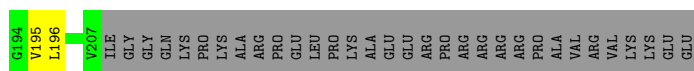




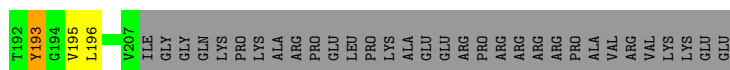
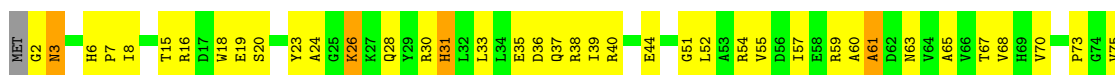
• Molecule 35: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S3

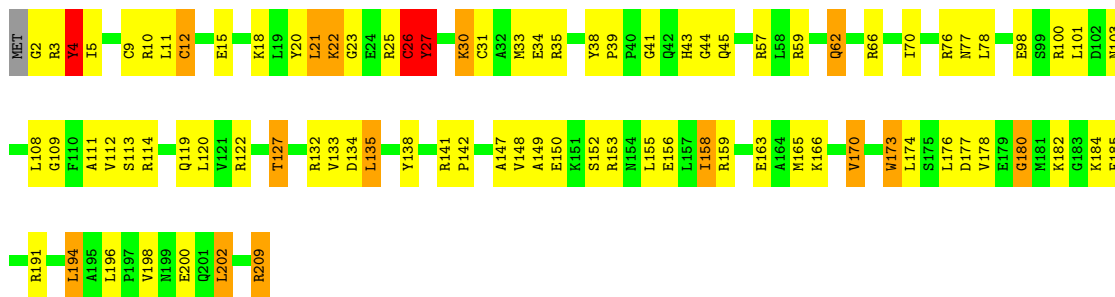


• Molecule 36: 30S ribosomal protein S3

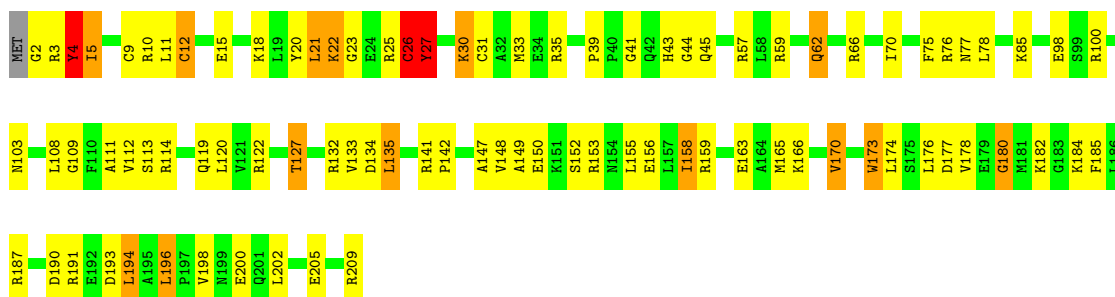


• Molecule 37: 30S ribosomal protein S4

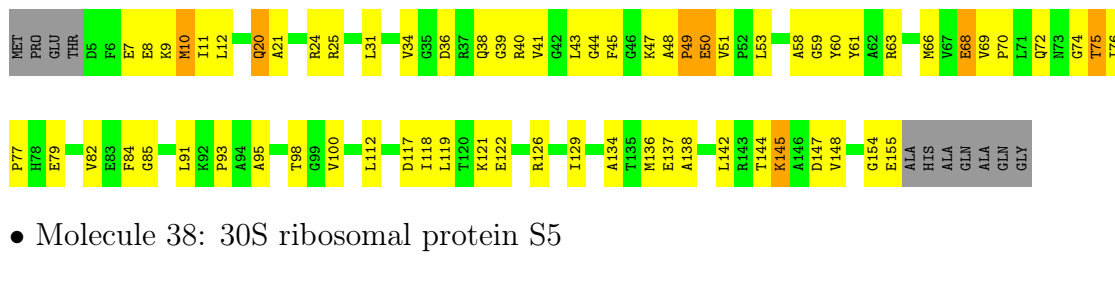




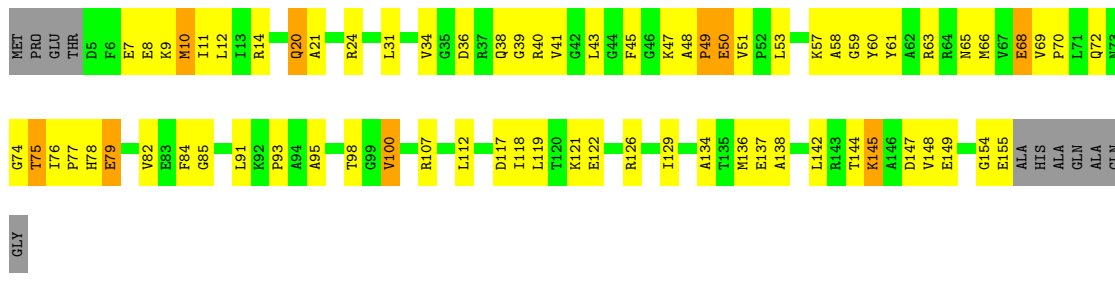
• Molecule 37: 30S ribosomal protein S4



• Molecule 38: 30S ribosomal protein S5

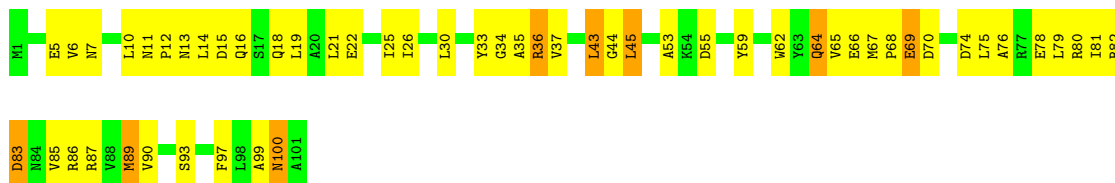


• Molecule 38: 30S ribosomal protein S5

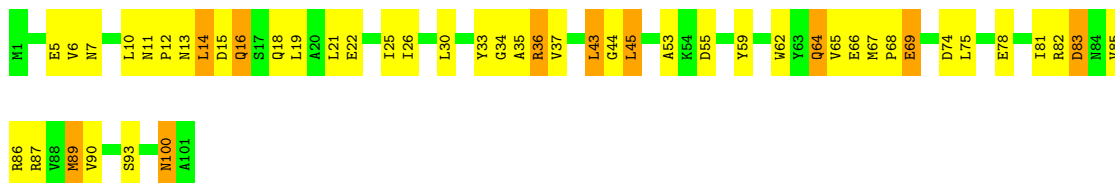


• Molecule 39: 30S ribosomal protein S6

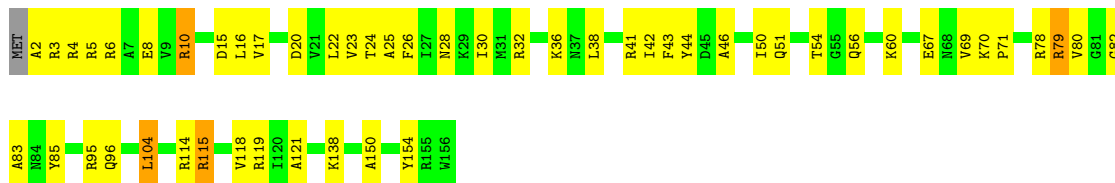




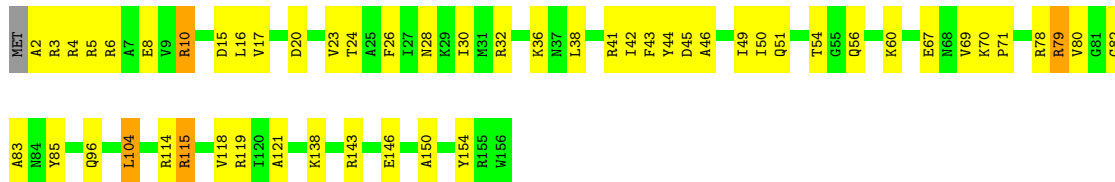
• Molecule 39: 30S ribosomal protein S6



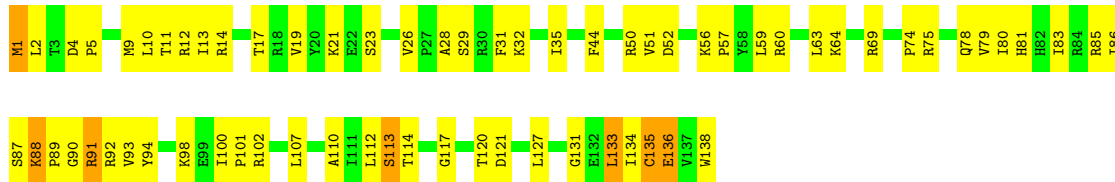
• Molecule 40: 30S ribosomal protein S7



• Molecule 40: 30S ribosomal protein S7

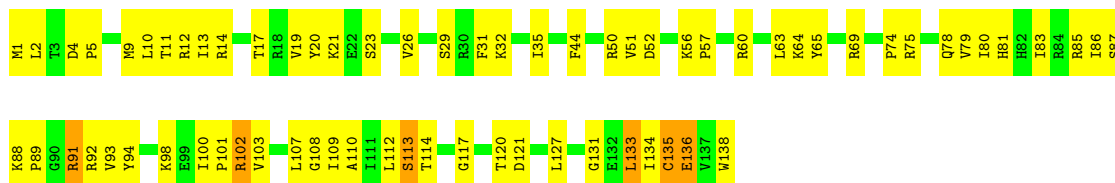


• Molecule 41: 30S ribosomal protein S8

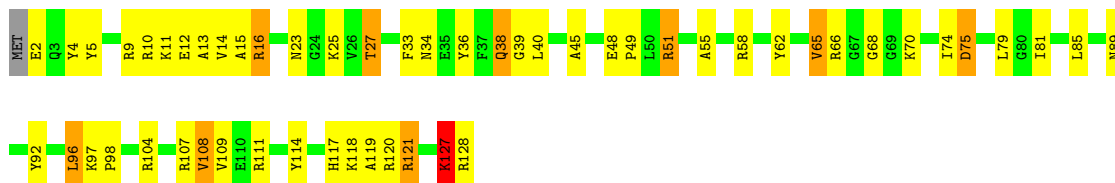


• Molecule 41: 30S ribosomal protein S8

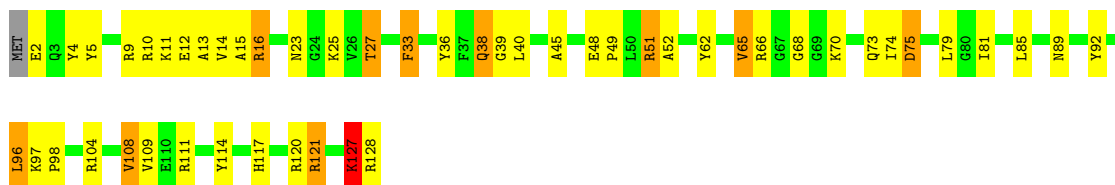




• Molecule 42: 30S ribosomal protein S9



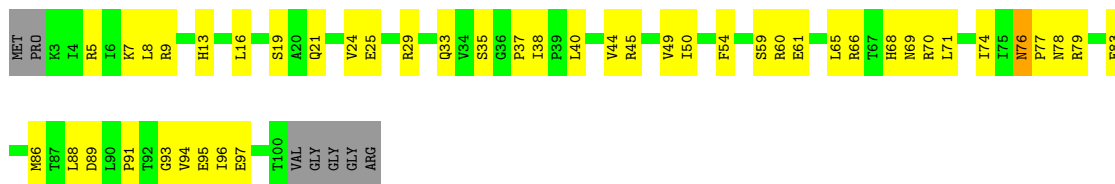
• Molecule 42: 30S ribosomal protein S9



• Molecule 43: 30S ribosomal protein S10

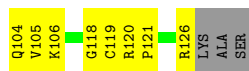
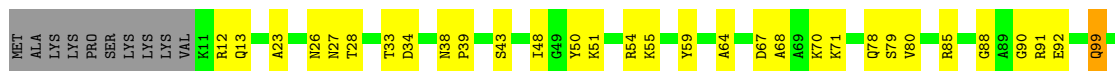


• Molecule 43: 30S ribosomal protein S10

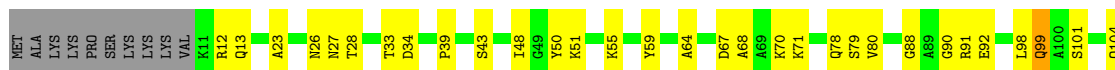


• Molecule 44: 30S ribosomal protein S11

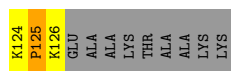
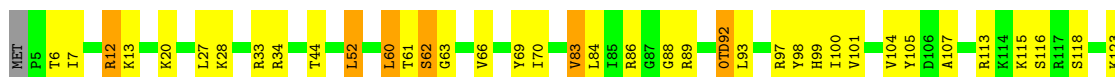




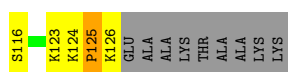
• Molecule 44: 30S ribosomal protein S11



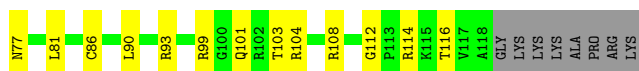
• Molecule 45: 30S ribosomal protein S12



• Molecule 45: 30S ribosomal protein S12

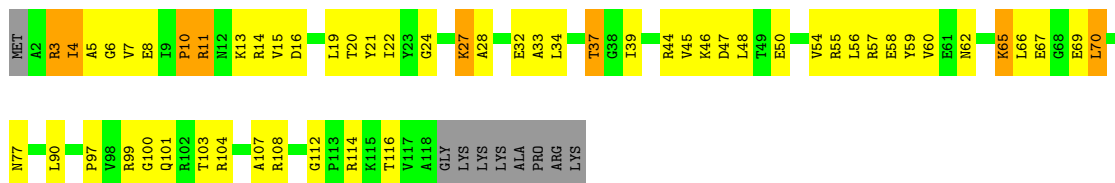


• Molecule 46: 30S ribosomal protein S13



• Molecule 46: 30S ribosomal protein S13





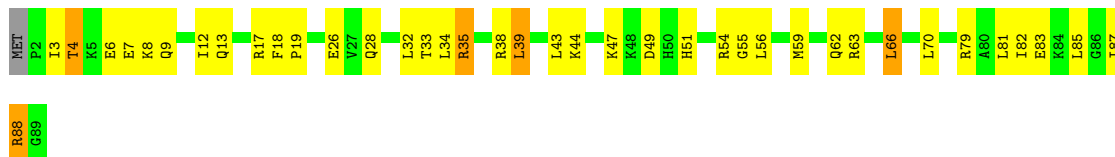
• Molecule 47: 30S ribosomal protein S14 type Z



• Molecule 47: 30S ribosomal protein S14 type Z



• Molecule 48: 30S ribosomal protein S15



• Molecule 48: 30S ribosomal protein S15



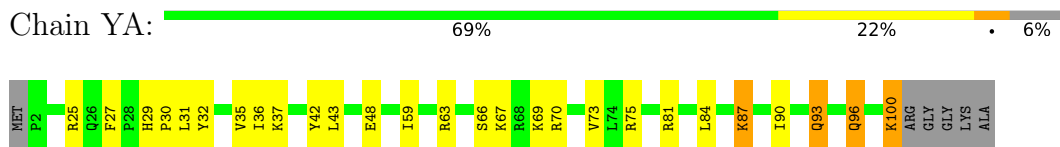
• Molecule 49: 30S ribosomal protein S16



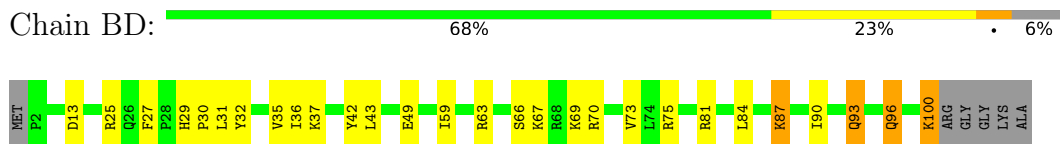
• Molecule 49: 30S ribosomal protein S16



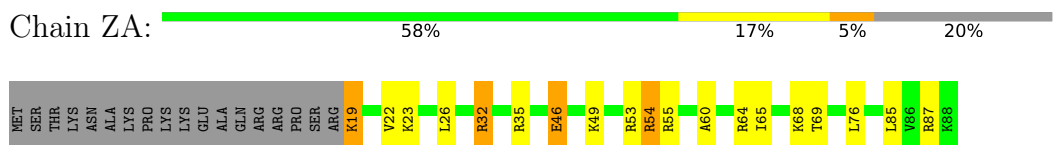
• Molecule 50: 30S ribosomal protein S17



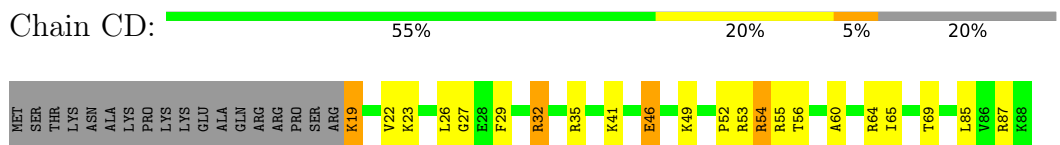
• Molecule 50: 30S ribosomal protein S17



• Molecule 51: 30S ribosomal protein S18



• Molecule 51: 30S ribosomal protein S18

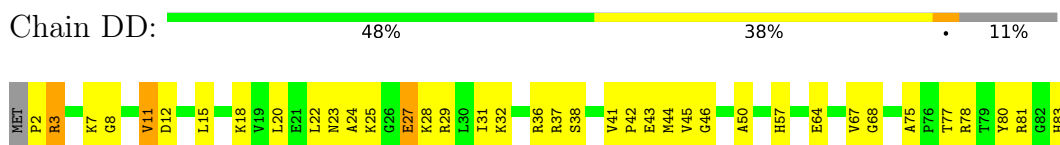


• Molecule 52: 30S ribosomal protein S19



LYS
LYS
LYS

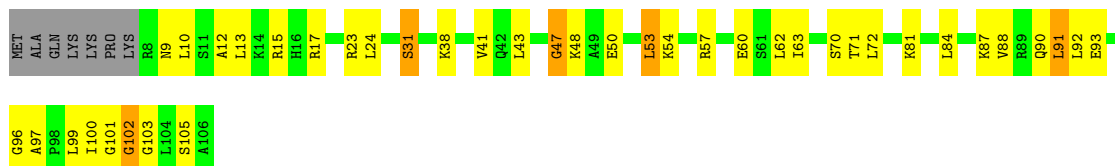
• Molecule 52: 30S ribosomal protein S19



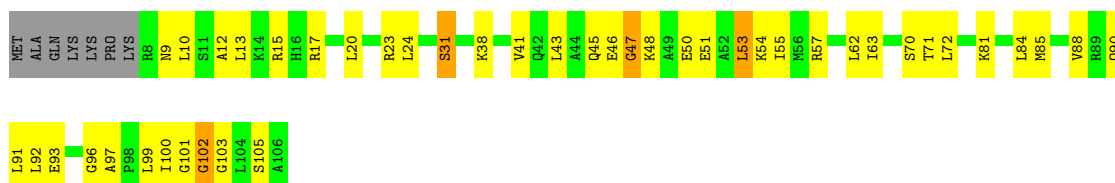
ALA
LYS
ALA
THR
LYS
LYS
LYS

• Molecule 53: 30S ribosomal protein S20

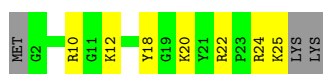




- Molecule 53: 30S ribosomal protein S20



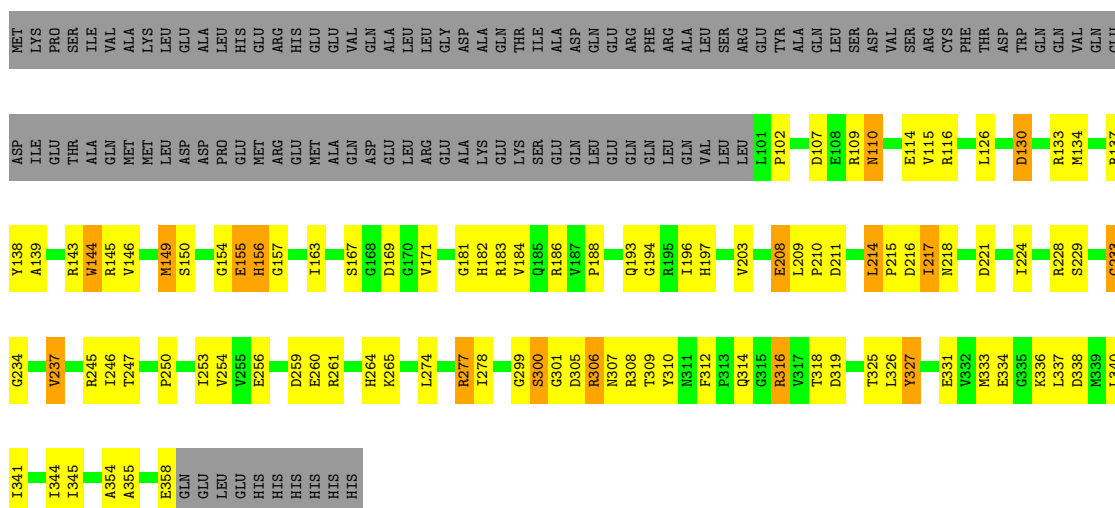
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: Peptide chain release factor 1



- Molecule 55: Peptide chain release factor 1

Chain HD: 43% 22% 5% 30%

MET	ASP	D130	D221	M339
LYS	ILE	M134	I224	L340
PRO	THR	R137	R228	I341
SER	ALA	Y138	S229	I345
ILE	GLN	A139	G233	A354
VAL	VAL	R143	G234	A355
ALA	MET	W144	V237	E358
LYS	MET	R145	R245	GLN
LEU	ARG	V146	I246	LEU
LEU	ARG	M149	I253	GLU
GLU	GLU	S150	E256	LEU
HIS	GLU	G154	K265	GLU
HIS	GLU	E155	L274	LEU
GLU	ALA	H156	R277	HIS
VAL	GLN	G157	I278	HIS
VAL	ASP	G163	Q287	HIS
GLN	GLU	K165	G299	HIS
ALA	ALA	I166	S300	
ALA	ASP	A164	G301	
LEU	LEU	I168	D305	
LEU	LEU	S167	R306	
GLY	ARG	G168	N307	
GLY	ARG	G170	R308	
ASP	GLN	V171	T309	
ASP	LYS	E178	Y310	
GLN	GLU	G181	R311	
GLN	LEU	H182	F312	
GLU	GLU	R183	Q314	
GLU	GLN	V184	G315	
ARG	GLN	Q185	R316	
PHE	LEU	R186	V317	
ARG	VAL	V187	T318	
ARG	LEU	P188	D319	
GLU	LEU	Q193	T325	
TYR	LEU	G194	L326	
ALA	P102	R195	Y327	
GLN	D107	I196	E331	
LEU	E108	H197	V332	
SER	R109	V203	M333	
SER	M110	E208	E334	
ASP	ASP	L209	G335	
VAL	VAL	P210	K336	
SER	F111	D211	L337	
VAL	F112	L214	D338	
ARG	L113	P215		
ARG	E114	D216		
CHS	V115	I217		
CHS	R116	N218		
PHE	R119			
THR	ASP			
THR	T119			
TRP	E123			
GLN	L126			
GLN				
VAL				
GLN				
GLU				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.82Å 450.45Å 615.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 68.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.55) 99.9 (68.93-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.58Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.221 , 0.257	Depositor DCC
R_{free} test set	13965 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	124.9	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299566	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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 i

5.1 Standard geometry i

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

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	0.66	8/35961 (0.0%)	1.15	147/56125 (0.3%)
1	DB	0.69	5/35961 (0.0%)	1.18	176/56125 (0.3%)
2	B	1.01	76/69214 (0.1%)	1.49	1088/108048 (1.0%)
2	EB	0.88	60/69214 (0.1%)	1.38	770/108048 (0.7%)
3	C	0.69	0/2881	1.20	18/4494 (0.4%)
3	FB	0.61	0/2881	1.09	11/4494 (0.2%)
4	D	0.47	0/1744	0.88	0/2719
4	GB	0.48	0/1744	0.88	0/2719
4	IA	0.74	0/1744	1.17	7/2719 (0.3%)
4	LC	0.70	1/1744 (0.1%)	1.12	5/2719 (0.2%)
5	E	0.78	4/2195 (0.2%)	0.74	0/2955
5	HB	0.70	3/2195 (0.1%)	0.72	0/2955
6	F	0.63	0/1596	0.67	0/2153
6	IB	0.57	0/1596	0.65	0/2153
7	G	0.70	0/1621	0.69	0/2194
7	JB	0.61	0/1621	0.65	0/2194
8	H	0.44	0/1496	0.57	0/2013
8	KB	0.40	0/1496	0.56	0/2013
9	I	0.52	0/1356	0.56	0/1834
9	LB	0.38	0/1356	0.52	0/1834
10	J	0.51	0/1152	0.58	0/1559
10	MB	0.47	0/1152	0.58	0/1559
11	K	0.62	0/1148	0.66	0/1547
11	NB	0.51	0/1148	0.63	0/1547
12	L	0.67	0/942	0.68	0/1268
12	OB	0.67	0/942	0.67	0/1268
13	M	0.64	0/1162	0.69	0/1544
13	PB	0.56	0/1162	0.67	0/1544
14	N	0.67	0/1142	0.63	0/1525
14	QB	0.60	0/1142	0.63	0/1525
15	O	0.60	0/982	0.72	0/1312
15	RB	0.57	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	P	0.45	0/887	0.58	0/1180
16	SB	0.40	0/887	0.53	0/1180
17	Q	0.61	0/1157	0.65	0/1544
17	TB	0.58	0/1157	0.65	0/1544
18	R	0.67	0/982	0.68	0/1306
18	UB	0.57	0/982	0.65	0/1306
19	S	0.65	0/790	0.67	0/1057
19	VB	0.56	0/790	0.65	0/1057
20	T	0.74	0/901	0.73	0/1209
20	WB	0.65	0/901	0.69	0/1209
21	U	0.76	0/764	0.69	0/1025
21	XB	0.63	0/764	0.65	0/1025
22	V	0.64	0/827	0.66	0/1103
22	YB	0.60	0/827	0.65	0/1103
23	W	0.49	0/1527	0.58	0/2073
23	ZB	0.43	0/1527	0.55	0/2073
24	AC	0.61	0/671	0.71	0/892
24	X	0.71	0/671	0.73	0/892
25	BC	0.65	0/768	0.71	0/1021
25	Y	0.70	0/768	0.72	0/1021
26	CC	0.57	0/594	0.60	0/785
26	Z	0.68	0/594	0.64	0/785
27	AA	0.60	0/482	0.62	0/646
27	DC	0.57	0/482	0.63	0/646
28	BA	0.42	0/565	0.46	0/761
28	EC	0.39	0/565	0.46	0/761
29	CA	0.60	0/474	0.63	0/640
29	FC	0.55	0/474	0.64	0/640
30	DA	0.41	0/460	0.50	0/613
30	GC	0.40	0/460	0.48	0/613
31	EA	0.79	0/426	0.89	3/561 (0.5%)
31	HC	0.69	0/426	0.78	1/561 (0.2%)
32	FA	0.74	1/525 (0.2%)	0.68	0/691
32	IC	0.61	0/525	0.66	0/691
33	GA	0.45	0/310	0.53	0/407
33	JC	0.46	0/310	0.53	0/407
34	HA	1.01	0/247	1.24	3/382 (0.8%)
34	KC	1.01	0/247	1.14	0/382
35	JA	0.41	0/1935	0.55	0/2609
35	MC	0.41	0/1935	0.54	0/2609
36	KA	0.41	0/1636	0.53	0/2205
36	NC	0.40	0/1636	0.53	0/2205
37	LA	0.51	1/1733 (0.1%)	0.60	1/2318 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	OC	0.58	1/1733 (0.1%)	0.62	1/2318 (0.0%)
38	MA	0.48	0/1171	0.61	0/1576
38	PC	0.51	0/1171	0.63	0/1576
39	NA	0.53	0/856	0.59	0/1154
39	QC	0.50	0/856	0.59	0/1154
40	OA	0.42	0/1276	0.51	0/1709
40	RC	0.44	0/1276	0.52	0/1709
41	PA	0.45	0/1136	0.59	0/1527
41	SC	0.46	0/1136	0.60	0/1527
42	QA	0.36	0/1029	0.49	0/1378
42	TC	0.36	0/1029	0.49	0/1378
43	RA	0.38	0/807	0.49	0/1085
43	UC	0.38	0/807	0.49	0/1085
44	SA	0.52	0/879	0.61	0/1187
44	VC	0.50	0/879	0.61	0/1187
45	TA	0.55	0/963	0.63	0/1287
45	WC	0.56	0/963	0.63	0/1287
46	UA	0.38	0/943	0.53	0/1265
46	XC	0.38	0/943	0.52	0/1265
47	VA	0.42	0/501	0.54	0/664
47	YC	0.39	0/501	0.53	0/664
48	WA	0.50	0/745	0.56	0/992
48	ZC	0.51	0/745	0.56	0/992
49	AD	0.49	0/716	0.58	0/963
49	XA	0.40	0/716	0.55	0/963
50	BD	0.53	0/836	0.58	0/1117
50	YA	0.52	0/836	0.59	0/1117
51	CD	0.50	0/579	0.55	0/768
51	ZA	0.52	0/579	0.57	0/768
52	AB	0.36	0/680	0.51	0/915
52	DD	0.35	0/680	0.51	0/915
53	BB	0.40	0/764	0.52	0/1006
53	ED	0.44	0/764	0.55	0/1006
54	CB	0.35	0/212	0.46	0/277
54	FD	0.36	0/212	0.46	0/277
55	GD	0.54	0/2012	0.62	0/2713
55	HD	0.48	0/2012	0.60	0/2713
All	All	0.77	160/322204 (0.0%)	1.18	2231/481240 (0.5%)

The worst 5 of 160 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1762	A	N9-C4	14.42	1.46	1.37
2	EB	1762	A	N9-C4	13.35	1.45	1.37
2	B	1142(B)	A	N9-C4	-10.33	1.31	1.37
1	A	1503	A	N9-C4	9.28	1.43	1.37
1	A	1531	A	N9-C4	9.11	1.43	1.37

The worst 5 of 2231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2053	G	N1-C6-O6	19.40	131.54	119.90
2	EB	2053	G	C5-C6-O6	-15.62	119.23	128.60
2	B	2053	G	N1-C6-O6	15.42	129.15	119.90
2	B	2593	U	N3-C4-C5	-14.85	105.69	114.60
2	B	1602	U	N3-C4-C5	-14.74	105.75	114.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	505	0
1	DB	32394	0	16367	492	0
2	B	62031	0	31275	829	0
2	EB	62031	0	31275	802	0
3	C	2576	0	1305	35	0
3	FB	2576	0	1305	35	0
4	D	1642	0	841	26	0
4	GB	1642	0	841	29	0
4	IA	1642	0	841	12	0
4	LC	1642	0	841	10	0
5	E	2145	0	2234	91	0
5	HB	2145	0	2234	78	0
6	F	1563	0	1629	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	IB	1563	0	1629	55	0
7	G	1586	0	1632	65	0
7	JB	1586	0	1632	61	0
8	H	1471	0	1526	67	0
8	KB	1471	0	1526	62	0
9	I	1330	0	1407	57	0
9	LB	1330	0	1407	51	0
10	J	1137	0	1225	50	0
10	MB	1137	0	1225	40	0
11	K	1121	0	1195	34	0
11	NB	1121	0	1195	31	0
12	L	932	0	994	32	0
12	OB	932	0	994	27	0
13	M	1145	0	1228	40	0
13	PB	1145	0	1228	35	0
14	N	1121	0	1179	36	0
14	QB	1121	0	1179	42	0
15	O	968	0	1033	39	0
15	RB	968	0	1033	43	0
16	P	877	0	938	28	0
16	SB	877	0	938	29	0
17	Q	1143	0	1211	37	0
17	TB	1143	0	1211	33	0
18	R	964	0	1022	25	0
18	UB	964	0	1022	30	0
19	S	779	0	852	28	0
19	VB	779	0	852	29	0
20	T	890	0	951	34	0
20	WB	890	0	951	26	0
21	U	750	0	814	14	0
21	XB	750	0	814	14	0
22	V	814	0	907	28	0
22	YB	814	0	907	25	0
23	W	1495	0	1521	51	0
23	ZB	1495	0	1521	50	0
24	AC	662	0	688	23	0
24	X	662	0	688	23	0
25	BC	761	0	837	28	0
25	Y	761	0	837	30	0
26	CC	592	0	654	16	0
26	Z	592	0	654	16	0
27	AA	477	0	529	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DC	477	0	529	16	0
28	BA	552	0	537	23	0
28	EC	552	0	537	22	0
29	CA	460	0	484	17	0
29	FC	460	0	484	19	0
30	DA	453	0	477	11	0
30	GC	453	0	477	11	0
31	EA	418	0	467	17	0
31	HC	418	0	467	17	0
32	FA	517	0	582	17	0
32	IC	517	0	582	19	0
33	GA	307	0	338	15	0
33	JC	307	0	337	16	0
34	HA	220	0	108	7	0
34	KC	220	0	108	9	0
35	JA	1900	0	1951	69	0
35	MC	1900	0	1951	69	0
36	KA	1612	0	1677	49	0
36	NC	1612	0	1677	48	0
37	LA	1703	0	1765	74	0
37	OC	1703	0	1765	68	0
38	MA	1155	0	1213	45	0
38	PC	1155	0	1213	51	0
39	NA	843	0	857	44	0
39	QC	843	0	857	40	0
40	OA	1257	0	1296	38	0
40	RC	1257	0	1296	42	0
41	PA	1116	0	1177	49	0
41	SC	1116	0	1177	48	0
42	QA	1011	0	1043	43	0
42	TC	1011	0	1043	43	0
43	RA	794	0	840	25	0
43	UC	794	0	840	27	0
44	SA	864	0	881	25	0
44	VC	864	0	881	21	0
45	TA	958	0	1047	31	0
45	WC	958	0	1047	31	0
46	UA	933	0	992	50	0
46	XC	933	0	992	47	0
47	VA	492	0	533	20	0
47	YC	492	0	533	17	0
48	WA	734	0	771	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	ZC	734	0	771	27	0
49	AD	700	0	720	20	0
49	XA	700	0	720	20	0
50	BD	823	0	893	24	0
50	YA	823	0	893	21	0
51	CD	574	0	644	17	0
51	ZA	574	0	644	19	0
52	AB	665	0	686	28	0
52	DD	665	0	686	29	0
53	BB	762	0	859	27	0
53	ED	762	0	859	27	0
54	CB	208	0	221	4	0
54	FD	208	0	221	12	0
55	GD	1980	0	1942	69	0
55	HD	1980	0	1942	63	0
56	A	160	0	0	0	0
56	AB	1	0	0	0	0
56	AC	2	0	0	0	0
56	AD	1	0	0	0	0
56	B	514	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	C	23	0	0	0	0
56	CA	1	0	0	0	0
56	CD	2	0	0	0	0
56	D	6	0	0	0	0
56	DB	177	0	0	0	0
56	DC	1	0	0	0	0
56	E	4	0	0	0	0
56	EA	1	0	0	0	0
56	EB	395	0	0	0	0
56	ED	1	0	0	0	0
56	F	1	0	0	0	0
56	FA	1	0	0	0	0
56	FB	17	0	0	0	0
56	FC	1	0	0	0	0
56	G	4	0	0	0	0
56	GB	5	0	0	0	0
56	GD	5	0	0	0	0
56	H	1	0	0	0	0
56	HA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	HB	8	0	0	0	0
56	HC	1	0	0	0	0
56	HD	3	0	0	0	0
56	I	3	0	0	0	0
56	IA	8	0	0	0	0
56	IB	3	0	0	0	0
56	IC	2	0	0	0	0
56	J	5	0	0	0	0
56	JA	3	0	0	0	0
56	JB	2	0	0	0	0
56	JC	1	0	0	0	0
56	K	2	0	0	0	0
56	KA	1	0	0	0	0
56	KB	1	0	0	0	0
56	KC	1	0	0	0	0
56	L	7	0	0	0	0
56	LA	1	0	0	0	0
56	LB	5	0	0	0	0
56	LC	8	0	0	0	0
56	M	4	0	0	0	0
56	MA	3	0	0	0	0
56	MB	2	0	0	0	0
56	MC	3	0	0	0	0
56	N	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	O	1	0	0	0	0
56	OA	3	0	0	0	0
56	OB	3	0	0	0	0
56	P	2	0	0	0	0
56	PA	2	0	0	0	0
56	PB	2	0	0	0	0
56	PC	2	0	0	0	0
56	Q	3	0	0	0	0
56	QB	3	0	0	0	0
56	QC	2	0	0	0	0
56	R	4	0	0	0	0
56	RA	2	0	0	0	0
56	RB	5	0	0	0	0
56	RC	2	0	0	0	0
56	S	3	0	0	0	0
56	SA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	T	2	0	0	0	0
56	TA	3	0	0	0	0
56	TB	5	0	0	0	0
56	TC	2	0	0	0	0
56	U	2	0	0	0	0
56	UC	1	0	0	0	0
56	V	5	0	0	0	0
56	VA	2	0	0	0	0
56	VB	1	0	0	0	0
56	W	12	0	0	0	0
56	WA	3	0	0	0	0
56	WB	3	0	0	0	0
56	WC	2	0	0	0	0
56	XB	2	0	0	0	0
56	XC	2	0	0	0	0
56	Y	4	0	0	0	0
56	YA	2	0	0	0	0
56	YB	3	0	0	0	0
56	YC	1	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	BA	1	0	0	0	0
57	CA	1	0	0	0	0
57	DA	1	0	0	0	0
57	EC	1	0	0	0	0
57	FC	1	0	0	0	0
57	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	JC	1	0	0	0	0
57	V	1	0	0	0	0
57	YB	1	0	0	0	0
All	All	299566	0	203671	5481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5481 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)
37:LA:18:LYS:NZ	37:LA:31:CYS:SG	2.10	1.23
37:OC:18:LYS:NZ	37:OC:31:CYS:SG	2.10	1.23
37:OC:12:CYS:SG	37:OC:18:LYS:NZ	2.24	1.11
10:J:60:GLU:HG3	10:J:61:ARG:HH12	1.11	1.09
10:MB:60:GLU:HG3	10:MB:61:ARG:HH12	1.19	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	8	43
5	HB	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	8	43
6	F	202/206 (98%)	180 (89%)	20 (10%)	2 (1%)	15	55
6	IB	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	15	55
7	G	200/205 (98%)	187 (94%)	9 (4%)	4 (2%)	7	42
7	JB	200/205 (98%)	186 (93%)	10 (5%)	4 (2%)	7	42
8	H	179/182 (98%)	152 (85%)	20 (11%)	7 (4%)	3	27
8	KB	179/182 (98%)	151 (84%)	22 (12%)	6 (3%)	3	31
9	I	172/180 (96%)	155 (90%)	14 (8%)	3 (2%)	9	45
9	LB	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	9	45
10	J	144/148 (97%)	118 (82%)	17 (12%)	9 (6%)	1	17
10	MB	144/148 (97%)	118 (82%)	16 (11%)	10 (7%)	1	15
11	K	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	22	62
11	NB	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	22	62
12	L	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	9	45
12	OB	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	9	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	148/150 (99%)	132 (89%)	11 (7%)	5 (3%)	3	31
13	PB	148/150 (99%)	131 (88%)	12 (8%)	5 (3%)	3	31
14	N	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	48
14	QB	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	11	48
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	45
15	RB	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	45
16	P	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8	42
16	SB	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	8	42
17	Q	135/146 (92%)	118 (87%)	12 (9%)	5 (4%)	3	28
17	TB	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	4	33
18	R	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	57
18	UB	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	57
19	S	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7	42
19	VB	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	7	42
20	T	110/113 (97%)	104 (94%)	4 (4%)	2 (2%)	8	43
20	WB	110/113 (97%)	103 (94%)	5 (4%)	2 (2%)	8	43
21	U	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	14	54
21	XB	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	14	54
22	V	105/110 (96%)	89 (85%)	11 (10%)	5 (5%)	2	22
22	YB	105/110 (96%)	91 (87%)	9 (9%)	5 (5%)	2	22
23	W	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	29	67
23	ZB	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	29	67
24	AC	82/85 (96%)	70 (85%)	10 (12%)	2 (2%)	6	37
24	X	82/85 (96%)	69 (84%)	11 (13%)	2 (2%)	6	37
25	BC	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	14	54
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	14	54
26	CC	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
26	Z	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
27	AA	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	9	45
27	DC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	9	45
28	BA	67/71 (94%)	47 (70%)	19 (28%)	1 (2%)	10	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	EC	67/71 (94%)	47 (70%)	20 (30%)	0	100	100
29	CA	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	43
29	FC	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	43
30	DA	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	GC	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	HC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	IC	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	GA	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
33	JC	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
35	JA	232/256 (91%)	189 (82%)	29 (12%)	14 (6%)	1	17
35	MC	232/256 (91%)	188 (81%)	30 (13%)	14 (6%)	1	17
36	KA	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	3	27
36	NC	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	3	27
37	LA	206/209 (99%)	179 (87%)	20 (10%)	7 (3%)	3	31
37	OC	206/209 (99%)	182 (88%)	16 (8%)	8 (4%)	3	27
38	MA	149/162 (92%)	132 (89%)	11 (7%)	6 (4%)	3	26
38	PC	149/162 (92%)	132 (89%)	10 (7%)	7 (5%)	2	22
39	NA	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	7	42
39	QC	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	7	42
40	OA	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	23
40	RC	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	23
41	PA	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	10	47
41	SC	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22	62
42	QA	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	6	37
42	TC	125/128 (98%)	105 (84%)	16 (13%)	4 (3%)	4	31
43	RA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	4	32
43	UC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	4	32
44	SA	114/129 (88%)	101 (89%)	10 (9%)	3 (3%)	5	35
44	VC	114/129 (88%)	101 (89%)	9 (8%)	4 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	TA	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	31
45	WC	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	31
46	UA	115/126 (91%)	102 (89%)	12 (10%)	1 (1%)	17	57
46	XC	115/126 (91%)	102 (89%)	11 (10%)	2 (2%)	9	45
47	VA	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
47	YC	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
48	WA	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	38
48	ZC	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	6	38
49	AD	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	13	52
49	XA	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	13	52
50	BD	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
50	YA	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	CD	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	10	47
51	ZA	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	47
52	AB	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	21
52	DD	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	21
53	BB	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	3	26
53	ED	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	3	26
54	CB	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
54	FD	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
55	GD	253/365 (69%)	207 (82%)	35 (14%)	11 (4%)	2	24
55	HD	253/365 (69%)	206 (81%)	37 (15%)	10 (4%)	3	26
All	All	11990/12846 (93%)	10568 (88%)	1121 (9%)	301 (2%)	5	36

5 of 301 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	LYS
6	F	192	ASN
7	G	21	ALA
7	G	130	ALA
8	H	74	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	217/217 (100%)	197 (91%)	20 (9%)	9	38
5	HB	217/217 (100%)	197 (91%)	20 (9%)	9	38
6	F	165/166 (99%)	145 (88%)	20 (12%)	5	26
6	IB	165/166 (99%)	145 (88%)	20 (12%)	5	26
7	G	161/162 (99%)	142 (88%)	19 (12%)	5	28
7	JB	161/162 (99%)	142 (88%)	19 (12%)	5	28
8	H	154/156 (99%)	134 (87%)	20 (13%)	4	24
8	KB	154/156 (99%)	136 (88%)	18 (12%)	5	28
9	I	144/148 (97%)	130 (90%)	14 (10%)	8	35
9	LB	144/148 (97%)	130 (90%)	14 (10%)	8	35
10	J	122/124 (98%)	105 (86%)	17 (14%)	3	21
10	MB	122/124 (98%)	106 (87%)	16 (13%)	4	23
11	K	119/119 (100%)	107 (90%)	12 (10%)	7	34
11	NB	119/119 (100%)	108 (91%)	11 (9%)	9	38
12	L	100/100 (100%)	91 (91%)	9 (9%)	9	39
12	OB	100/100 (100%)	90 (90%)	10 (10%)	7	35
13	M	116/116 (100%)	103 (89%)	13 (11%)	6	30
13	PB	116/116 (100%)	101 (87%)	15 (13%)	4	24
14	N	111/111 (100%)	99 (89%)	12 (11%)	6	32
14	QB	111/111 (100%)	98 (88%)	13 (12%)	5	28
15	O	101/101 (100%)	89 (88%)	12 (12%)	5	27
15	RB	101/101 (100%)	89 (88%)	12 (12%)	5	27
16	P	87/88 (99%)	83 (95%)	4 (5%)	27	61
16	SB	87/88 (99%)	83 (95%)	4 (5%)	27	61
17	Q	121/128 (94%)	112 (93%)	9 (7%)	13	45
17	TB	121/128 (94%)	113 (93%)	8 (7%)	16	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	93/94 (99%)	83 (89%)	10 (11%)	6	32
18	UB	93/94 (99%)	84 (90%)	9 (10%)	8	35
19	S	82/82 (100%)	70 (85%)	12 (15%)	3	20
19	VB	82/82 (100%)	72 (88%)	10 (12%)	5	26
20	T	91/92 (99%)	81 (89%)	10 (11%)	6	31
20	WB	91/92 (99%)	81 (89%)	10 (11%)	6	31
21	U	77/78 (99%)	73 (95%)	4 (5%)	23	58
21	XB	77/78 (99%)	73 (95%)	4 (5%)	23	58
22	V	87/91 (96%)	81 (93%)	6 (7%)	15	48
22	YB	87/91 (96%)	81 (93%)	6 (7%)	15	48
23	W	163/179 (91%)	142 (87%)	21 (13%)	4	24
23	ZB	163/179 (91%)	143 (88%)	20 (12%)	4	26
24	AC	66/67 (98%)	57 (86%)	9 (14%)	3	22
24	X	66/67 (98%)	57 (86%)	9 (14%)	3	22
25	BC	81/83 (98%)	70 (86%)	11 (14%)	3	22
25	Y	81/83 (98%)	70 (86%)	11 (14%)	3	22
26	CC	66/67 (98%)	62 (94%)	4 (6%)	18	53
26	Z	66/67 (98%)	62 (94%)	4 (6%)	18	53
27	AA	52/52 (100%)	48 (92%)	4 (8%)	13	44
27	DC	52/52 (100%)	49 (94%)	3 (6%)	20	55
28	BA	59/63 (94%)	51 (86%)	8 (14%)	3	22
28	EC	59/63 (94%)	51 (86%)	8 (14%)	3	22
29	CA	51/52 (98%)	46 (90%)	5 (10%)	8	35
29	FC	51/52 (98%)	46 (90%)	5 (10%)	8	35
30	DA	51/52 (98%)	47 (92%)	4 (8%)	12	43
30	GC	51/52 (98%)	46 (90%)	5 (10%)	8	35
31	EA	41/42 (98%)	35 (85%)	6 (15%)	3	20
31	HC	41/42 (98%)	35 (85%)	6 (15%)	3	20
32	FA	54/55 (98%)	47 (87%)	7 (13%)	4	24
32	IC	54/55 (98%)	48 (89%)	6 (11%)	6	31
33	GA	34/34 (100%)	30 (88%)	4 (12%)	5	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	JC	34/34 (100%)	30 (88%)	4 (12%)	5	28
35	JA	202/220 (92%)	177 (88%)	25 (12%)	4	25
35	MC	202/220 (92%)	177 (88%)	25 (12%)	4	25
36	KA	160/188 (85%)	146 (91%)	14 (9%)	10	40
36	NC	160/188 (85%)	145 (91%)	15 (9%)	8	37
37	LA	180/181 (99%)	159 (88%)	21 (12%)	5	28
37	OC	180/181 (99%)	157 (87%)	23 (13%)	4	24
38	MA	116/123 (94%)	100 (86%)	16 (14%)	3	22
38	PC	116/123 (94%)	99 (85%)	17 (15%)	3	19
39	NA	90/90 (100%)	80 (89%)	10 (11%)	6	31
39	QC	90/90 (100%)	79 (88%)	11 (12%)	5	26
40	OA	126/127 (99%)	120 (95%)	6 (5%)	25	60
40	RC	126/127 (99%)	120 (95%)	6 (5%)	25	60
41	PA	119/119 (100%)	107 (90%)	12 (10%)	7	34
41	SC	119/119 (100%)	108 (91%)	11 (9%)	9	38
42	QA	98/99 (99%)	86 (88%)	12 (12%)	5	26
42	TC	98/99 (99%)	86 (88%)	12 (12%)	5	26
43	RA	88/92 (96%)	81 (92%)	7 (8%)	12	43
43	UC	88/92 (96%)	81 (92%)	7 (8%)	12	43
44	SA	88/99 (89%)	85 (97%)	3 (3%)	37	69
44	VC	88/99 (89%)	85 (97%)	3 (3%)	37	69
45	TA	102/108 (94%)	95 (93%)	7 (7%)	15	48
45	WC	102/108 (94%)	95 (93%)	7 (7%)	15	48
46	UA	94/101 (93%)	82 (87%)	12 (13%)	4	24
46	XC	94/101 (93%)	83 (88%)	11 (12%)	5	28
47	VA	49/50 (98%)	47 (96%)	2 (4%)	30	64
47	YC	49/50 (98%)	47 (96%)	2 (4%)	30	64
48	WA	79/80 (99%)	72 (91%)	7 (9%)	9	39
48	ZC	79/80 (99%)	72 (91%)	7 (9%)	9	39
49	AD	72/74 (97%)	66 (92%)	6 (8%)	11	41
49	XA	72/74 (97%)	66 (92%)	6 (8%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	BD	94/97 (97%)	86 (92%)	8 (8%)	10	41
50	YA	94/97 (97%)	86 (92%)	8 (8%)	10	41
51	CD	61/77 (79%)	56 (92%)	5 (8%)	11	42
51	ZA	61/77 (79%)	56 (92%)	5 (8%)	11	42
52	AB	72/80 (90%)	65 (90%)	7 (10%)	8	35
52	DD	72/80 (90%)	65 (90%)	7 (10%)	8	35
53	BB	76/82 (93%)	70 (92%)	6 (8%)	12	43
53	ED	76/82 (93%)	70 (92%)	6 (8%)	12	43
54	CB	19/22 (86%)	18 (95%)	1 (5%)	22	58
54	FD	19/22 (86%)	18 (95%)	1 (5%)	22	58
55	GD	206/305 (68%)	179 (87%)	27 (13%)	4	23
55	HD	206/305 (68%)	179 (87%)	27 (13%)	4	23
All	All	10114/10666 (95%)	9077 (90%)	1037 (10%)	7	34

5 of 1037 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	WC	52	LEU
49	AD	67	THR
45	WC	44	THR
39	NA	69	GLU
38	MA	136	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
10	MB	54	GLN
55	HD	236	HIS
23	ZB	75	ASN
55	HD	197	HIS
50	BD	26	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	228 (15%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	DB	1502/1507 (99%)	223 (14%)	10 (0%)
2	B	2876/2880 (99%)	498 (17%)	15 (0%)
2	EB	2876/2880 (99%)	496 (17%)	15 (0%)
3	C	119/120 (99%)	18 (15%)	0
3	FB	119/120 (99%)	17 (14%)	0
34	HA	9/27 (33%)	4 (44%)	1 (11%)
34	KC	9/27 (33%)	4 (44%)	1 (11%)
4	D	76/77 (98%)	13 (17%)	0
4	GB	76/77 (98%)	13 (17%)	0
4	IA	76/77 (98%)	7 (9%)	0
4	LC	76/77 (98%)	7 (9%)	0
All	All	9316/9376 (99%)	1528 (16%)	52 (0%)

5 of 1528 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	8	A
1	A	9	G
1	A	32	A

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	DB	560	U
1	DB	1201	A
2	EB	2422	A
1	DB	563	A
1	DB	723	U

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

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	EB	1939	2	19,22,23	2.19	4 (21%)	28,32,35	2.57	8 (28%)
2	PSU	EB	2605	2	18,21,22	1.44	2 (11%)	22,30,33	1.54	4 (18%)
1	M2G	DB	966	1	20,27,28	2.48	5 (25%)	22,40,43	1.27	3 (13%)
45	0TD	TA	92	45	7,9,10	1.50	1 (14%)	6,11,13	3.26	3 (50%)
4	5MC	IA	32	4	18,22,23	1.80	3 (16%)	26,32,35	1.23	3 (11%)
2	5MC	B	1942	2	18,22,23	1.50	3 (16%)	26,32,35	1.40	4 (15%)
4	PSU	D	55	4	18,21,22	1.70	2 (11%)	22,30,33	1.38	2 (9%)
4	4SU	IA	8	4	18,21,22	4.63	7 (38%)	26,30,33	5.01	11 (42%)
2	5MU	B	1939	2	19,22,23	2.25	3 (15%)	28,32,35	2.44	8 (28%)
2	OMG	EB	2251	2,4	18,26,27	2.23	5 (27%)	19,38,41	1.41	4 (21%)
4	5MU	LC	54	4	19,22,23	2.20	3 (15%)	28,32,35	1.80	7 (25%)
2	PSU	B	2605	2	18,21,22	1.55	3 (16%)	22,30,33	1.57	4 (18%)
4	4SU	D	8	4	18,21,22	4.68	7 (38%)	26,30,33	5.20	10 (38%)
1	5MC	A	967	1	18,22,23	1.68	3 (16%)	26,32,35	1.33	3 (11%)
4	5MC	D	32	4	18,22,23	1.68	3 (16%)	26,32,35	0.98	2 (7%)
2	5MC	EB	1962	2,56	18,22,23	1.66	4 (22%)	26,32,35	1.26	2 (7%)
4	5MU	GB	54	4	19,22,23	2.05	3 (15%)	28,32,35	2.10	8 (28%)
2	PSU	B	1917	2	18,21,22	1.72	3 (16%)	22,30,33	1.71	5 (22%)
1	5MC	A	1404	1	18,22,23	1.72	3 (16%)	26,32,35	1.22	1 (3%)
2	5MU	B	1915	2	19,22,23	1.93	3 (15%)	28,32,35	2.43	6 (21%)
1	MA6	DB	1519	1	19,26,27	1.47	3 (15%)	18,38,41	1.28	2 (11%)
2	4OC	EB	1920	2	19,22,24	1.06	1 (5%)	26,31,35	0.84	0
1	2MG	DB	1207	1	18,26,27	2.37	3 (16%)	16,38,41	1.29	2 (12%)
4	5MU	D	54	4	19,22,23	2.08	3 (15%)	28,32,35	1.97	8 (28%)
2	PSU	EB	1917	2	18,21,22	1.66	2 (11%)	22,30,33	1.69	5 (22%)
4	PSU	GB	55	4	18,21,22	1.60	3 (16%)	22,30,33	1.47	3 (13%)
4	5MC	LC	32	4	18,22,23	1.78	3 (16%)	26,32,35	1.29	3 (11%)
1	PSU	A	516	1	18,21,22	1.88	3 (16%)	22,30,33	1.38	4 (18%)
1	7MG	A	527	1	22,26,27	3.18	7 (31%)	29,39,42	1.98	8 (27%)
1	UR3	A	1498	1	19,22,23	1.77	2 (10%)	26,32,35	1.34	3 (11%)
2	5MC	B	1962	2	18,22,23	1.64	3 (16%)	26,32,35	1.32	2 (7%)
1	M2G	A	966	1	20,27,28	2.53	5 (25%)	22,40,43	1.35	4 (18%)
1	PSU	DB	516	1	18,21,22	1.77	3 (16%)	22,30,33	1.27	3 (13%)
1	4OC	DB	1402	1	20,23,24	1.08	2 (10%)	26,32,35	1.58	7 (26%)
1	5MC	A	1400	1	18,22,23	1.73	3 (16%)	26,32,35	1.22	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1207	1	18,26,27	2.36	3 (16%)	16,38,41	1.24	2 (12%)
1	5MC	DB	1404	1	18,22,23	1.76	3 (16%)	26,32,35	1.29	3 (11%)
45	0TD	WC	92	45	7,9,10	1.70	1 (14%)	6,11,13	3.08	3 (50%)
2	2MA	EB	2503	2	17,25,26	1.36	2 (11%)	17,37,40	1.06	2 (11%)
4	4SU	LC	8	4	18,21,22	4.57	7 (38%)	26,30,33	5.81	11 (42%)
4	PSU	LC	55	4	18,21,22	1.85	3 (16%)	22,30,33	1.59	5 (22%)
2	5MU	EB	1915	2	19,22,23	2.00	3 (15%)	28,32,35	2.28	5 (17%)
1	5MC	DB	967	1	18,22,23	1.74	4 (22%)	26,32,35	1.34	3 (11%)
4	5MU	IA	54	56,4	19,22,23	2.12	3 (15%)	28,32,35	2.18	10 (35%)
2	OMG	B	2251	2,4	18,26,27	2.26	3 (16%)	19,38,41	1.23	2 (10%)
1	MA6	DB	1518	1	19,26,27	1.43	3 (15%)	18,38,41	1.53	2 (11%)
1	MA6	A	1518	1	19,26,27	1.53	3 (15%)	18,38,41	1.41	2 (11%)
1	7MG	DB	527	1	22,26,27	3.14	7 (31%)	29,39,42	2.15	9 (31%)
2	2MA	B	2503	2	17,25,26	1.33	2 (11%)	17,37,40	1.17	2 (11%)
1	5MC	A	1407	1	18,22,23	1.59	3 (16%)	26,32,35	1.24	1 (3%)
1	4OC	A	1402	1	20,23,24	1.11	2 (10%)	26,32,35	1.31	5 (19%)
2	2MU	EB	2552	2,56	19,22,24	2.56	4 (21%)	26,31,36	2.19	6 (23%)
2	5MC	EB	1942	2	18,22,23	1.59	3 (16%)	26,32,35	1.45	4 (15%)
4	5MC	GB	32	4	18,22,23	1.64	3 (16%)	26,32,35	1.14	3 (11%)
1	5MC	DB	1407	1	18,22,23	1.64	3 (16%)	26,32,35	1.15	2 (7%)
2	4OC	B	1920	2	19,22,24	1.16	1 (5%)	26,31,35	0.85	0
4	PSU	IA	55	4	18,21,22	1.85	2 (11%)	22,30,33	1.74	4 (18%)
2	PSU	EB	1911	2	18,21,22	1.53	2 (11%)	22,30,33	1.93	6 (27%)
1	5MC	DB	1400	1	18,22,23	1.66	3 (16%)	26,32,35	1.27	4 (15%)
4	4SU	GB	8	4	18,21,22	4.51	7 (38%)	26,30,33	6.01	9 (34%)
1	MA6	A	1519	1	19,26,27	1.58	3 (15%)	18,38,41	1.28	2 (11%)
1	UR3	DB	1498	1	19,22,23	1.90	1 (5%)	26,32,35	1.26	3 (11%)
2	2MU	B	2552	2	19,22,24	2.71	4 (21%)	26,31,36	2.14	7 (26%)
2	PSU	B	1911	2	18,21,22	1.47	2 (11%)	22,30,33	1.59	4 (18%)

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	EB	1939	2	-	0/7/25/26	0/2/2/2
2	PSU	EB	2605	2	-	0/7/25/26	0/2/2/2
1	M2G	DB	966	1	-	0/7/29/30	0/3/3/3
45	0TD	TA	92	45	-	4/7/12/14	-
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
2	OMG	EB	2251	2,4	-	1/5/27/28	0/3/3/3
4	5MU	LC	54	4	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
2	5MC	EB	1962	2,56	-	0/7/25/26	0/2/2/2
4	5MU	GB	54	4	-	0/7/25/26	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2
1	MA6	DB	1519	1	-	3/7/29/30	0/3/3/3
2	4OC	EB	1920	2	-	3/9/27/30	0/2/2/2
1	2MG	DB	1207	1	-	0/5/27/28	0/3/3/3
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
2	PSU	EB	1917	2	-	0/7/25/26	0/2/2/2
4	PSU	GB	55	4	-	0/7/25/26	0/2/2/2
4	5MC	LC	32	4	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	PSU	DB	516	1	-	0/7/25/26	0/2/2/2
1	4OC	DB	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	DB	1404	1	-	0/7/25/26	0/2/2/2
45	0TD	WC	92	45	-	5/7/12/14	-
2	2MA	EB	2503	2	-	2/3/25/26	0/3/3/3
4	4SU	LC	8	4	-	0/7/25/26	0/2/2/2
4	PSU	LC	55	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	EB	1915	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	967	1	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	56,4	-	0/7/25/26	0/2/2/2
2	OMG	B	2251	2,4	-	1/5/27/28	0/3/3/3
1	MA6	DB	1518	1	-	2/7/29/30	0/3/3/3
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	7MG	DB	527	1	-	2/7/37/38	0/3/3/3
2	2MA	B	2503	2	-	2/3/25/26	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
2	2MU	EB	2552	2,56	-	0/9/27/28	0/2/2/2
2	5MC	EB	1942	2	-	0/7/25/26	0/2/2/2
4	5MC	GB	32	4	-	0/7/25/26	0/2/2/2
1	5MC	DB	1407	1	-	0/7/25/26	0/2/2/2
2	4OC	B	1920	2	-	4/9/27/30	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
2	PSU	EB	1911	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	1400	1	-	2/7/25/26	0/2/2/2
4	4SU	GB	8	4	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	DB	1498	1	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	0/9/27/28	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	4SU	C4-N3	12.43	1.50	1.37
4	LC	8	4SU	C4-N3	12.16	1.50	1.37
4	IA	8	4SU	C4-N3	11.78	1.50	1.37
4	GB	8	4SU	C4-N3	11.67	1.50	1.37
4	IA	8	4SU	O2-C2	11.58	1.44	1.23

The worst 5 of 276 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GB	8	4SU	C4-N3-C2	-19.62	108.28	127.34
4	LC	8	4SU	C4-N3-C2	-16.78	111.03	127.34
4	LC	8	4SU	C1'-N1-C2	13.81	142.57	117.57
4	GB	8	4SU	C1'-N1-C2	11.30	138.02	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	IA	8	4SU	S4-C4-N3	-11.22	109.15	120.21

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
2	B	1920	4OC	C1'-C2'-O2'-CM2
2	B	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1939	5MU	1	0
1	DB	966	M2G	1	0
45	TA	92	0TD	3	0
4	D	55	PSU	1	0
2	B	1939	5MU	2	0
1	A	967	5MC	1	0
4	GB	54	5MU	1	0
2	B	1915	5MU	1	0
1	DB	1519	MA6	1	0
4	D	54	5MU	1	0
2	EB	1917	PSU	1	0
4	GB	55	PSU	1	0
1	A	1498	UR3	1	0
1	A	966	M2G	1	0
1	DB	1402	4OC	1	0
45	WC	92	0TD	3	0
2	EB	2503	2MA	4	0
2	EB	1915	5MU	1	0
1	DB	967	5MC	1	0
1	DB	1518	MA6	1	0
1	A	1518	MA6	1	0
2	B	2503	2MA	3	0
1	A	1407	5MC	1	0
1	A	1402	4OC	2	0
2	EB	2552	2MU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1942	5MC	1	0
1	DB	1407	5MC	1	0
2	B	1920	4OC	1	0
4	GB	8	4SU	1	0
1	DB	1498	UR3	1	0
2	B	2552	2MU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1528 ligands modelled in this entry, 1528 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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