wwPDB EM Validation Summary Report (i)

Mar 31, 2025 – 06:10 PM JST

PDB ID	:	5ZLU / pdb_00005zlu
EMDB ID	:	EMD-6934
Title	:	Ribosome Structure bound to ABC-F protein.
Authors	:	Su, W.X.; Kumar, V.; Ero, R.; Andrew, S.W.W.; Jian, S.; Yong-Gui, G.
Deposited on	:	2018-03-29
Resolution	:	3.60 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

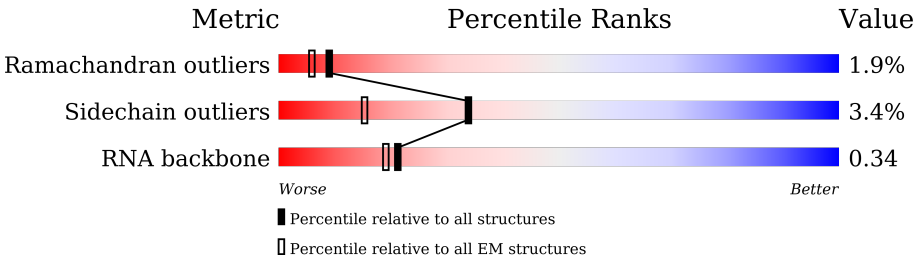
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	W	25	24% 72%
2	A	104	90% 7%
3	B	73	96%
4	C	106	91% 7%
5	D	93	84% 12%
6	E	105	89% 7%
7	F	27	89% 11%
8	G	1514	64% 32%
9	H	256	82% 5% 13%

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Mol	Chain	Length	Quality of chain
10	I	239	85% 14%
11	J	209	95% 5%
12	K	162	91% 7%
13	L	101	94% 6%
14	M	156	96%
15	N	138	96%
16	O	128	95%
17	P	129	90% 8%
18	Q	132	92% 6%
19	R	126	87% 10%
20	S	61	84% 15%
21	T	89	97%
22	U	88	93% 6%
23	V	2875	54% 38% 7%
24	X	123	62% 32% 7%
25	Y	229	90% 9%
26	Z	276	93% 5%
27	a	206	97%
28	b	210	94% 5%
29	c	182	84% 12%
30	d	180	84% 12%
31	e	173	65% 6% 27%
32	f	147	74% 15% 9%
33	g	140	76% 7% 16%
34	h	122	86% 13%

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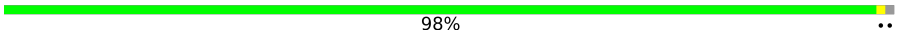
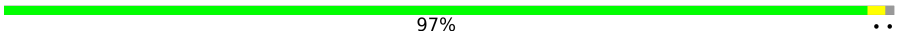
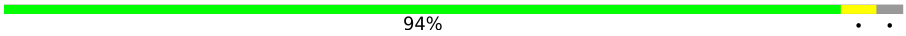
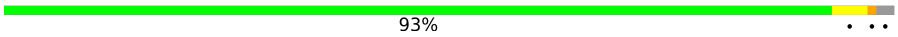
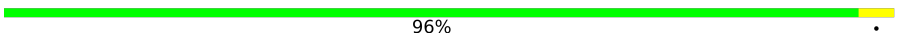
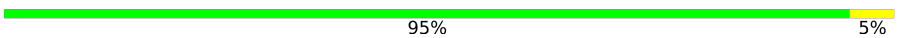
Mol	Chain	Length	Quality of chain
35	i	150	
36	j	141	
37	k	118	
38	l	112	
39	m	146	
40	n	118	
41	o	101	
42	p	113	
43	q	96	
44	r	110	
45	s	206	
46	t	85	
47	u	67	
48	v	60	
49	CC	71	
49	w	71	
50	x	60	
51	y	54	
52	z	49	
53	AA	65	
54	BB	37	
55	DD	77	
56	EE	497	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 150313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA (25-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	W	7	149	67	26	49	7	0	0

- Molecule 2 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	97	808	519	149	138	2	0	0

- Molecule 3 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	B	73	597	380	118	99	0	0

- Molecule 4 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	99	763	470	162	129	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	82	656	419	121	113	3	0	1

- Molecule 6 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	98	794	499	156	138	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 8 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	1514	Total	C	N	O	P	0	0
			32534	14481	6019	10520	1514		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	222	Total	C	N	O	S	0	0
			1810	1154	328	323	5		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 20 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	2875	Total	C	N	O	P	0	0
			61917	27558	11575	19909	2875		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	273	Total	C	N	O	S	0	0
			2126	1341	424	358	3		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	179	Total	C	N	O	S	0	0
			1455	929	266	256	4		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	176	Total	C	N	O	S	0	0
			1335	847	250	237	1		

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	126	Total	C	N	O	0	0
			621	369	126	126		

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	117	Total	C	N	O	S	0	0
			931	603	171	154	3		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	145	Total	C	N	O	S	0	0
			1108	689	226	191	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	l	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	q	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	80	Total	C	N	O	S	0	0
			629	389	132	107	1		

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	AltConf	Trace
49	w	71	Total C N O S 581 364 108 104 5	0	0
49	CC	32	Total C N O 157 93 32 32	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
50	x	57	Total C N O S 445 279 87 74 5	0	0

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	AltConf	Trace
51	y	49	Total C N O S 422 262 87 69 4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	7	LEU	ILE	see sequence details	UNP P35871

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	AltConf	Trace
52	z	49	Total C N O S 430 263 108 57 2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	AltConf	Trace
53	AA	64	Total C N O S 515 331 102 79 3	0	0

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	AltConf	Trace
54	BB	37	Total C N O S 307 188 68 47 4	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	DD	77	Total	C	N	O	P	S	0	0
			1648	736	301	533	77	1		

- Molecule 56 is a protein called Macrolide efflux protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	490	Total	C	N	O	S	0	0
			3841	2415	668	742	16		

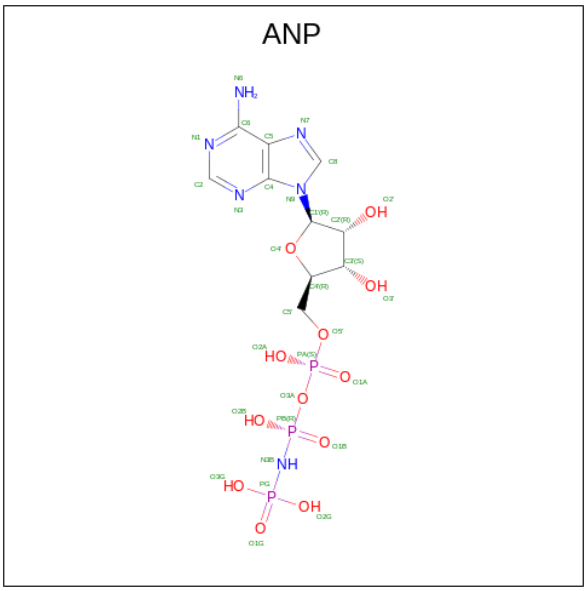
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	492	HIS	-	expression tag	UNP A0A1I9WCL8
EE	493	HIS	-	expression tag	UNP A0A1I9WCL8
EE	494	HIS	-	expression tag	UNP A0A1I9WCL8
EE	495	HIS	-	expression tag	UNP A0A1I9WCL8
EE	496	HIS	-	expression tag	UNP A0A1I9WCL8
EE	497	HIS	-	expression tag	UNP A0A1I9WCL8

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

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total	Mg	0
			1	1	
57	i	1	Total	Mg	0
			1	1	

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



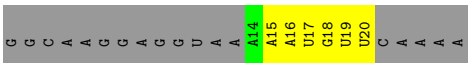
Mol	Chain	Residues	Atoms					AltConf
58	EE	1	Total	C	N	O	P	0
			31	10	6	12	3	
58	EE	1	Total	C	N	O	P	0
			31	10	6	12	3	

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.

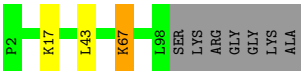
- Molecule 1: RNA (25-mer)

Chain W:



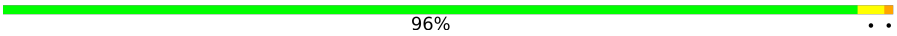
- Molecule 2: 30S ribosomal protein S17

Chain A:



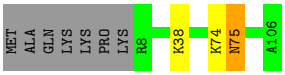
- Molecule 3: 30S ribosomal protein S18

Chain B:



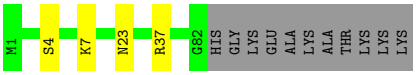
- Molecule 4: 30S ribosomal protein S20

Chain C:



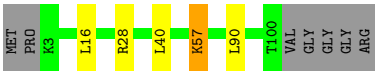
- Molecule 5: 30S ribosomal protein S19

Chain D:



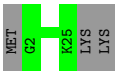
- Molecule 6: 30S ribosomal protein S10

Chain E:



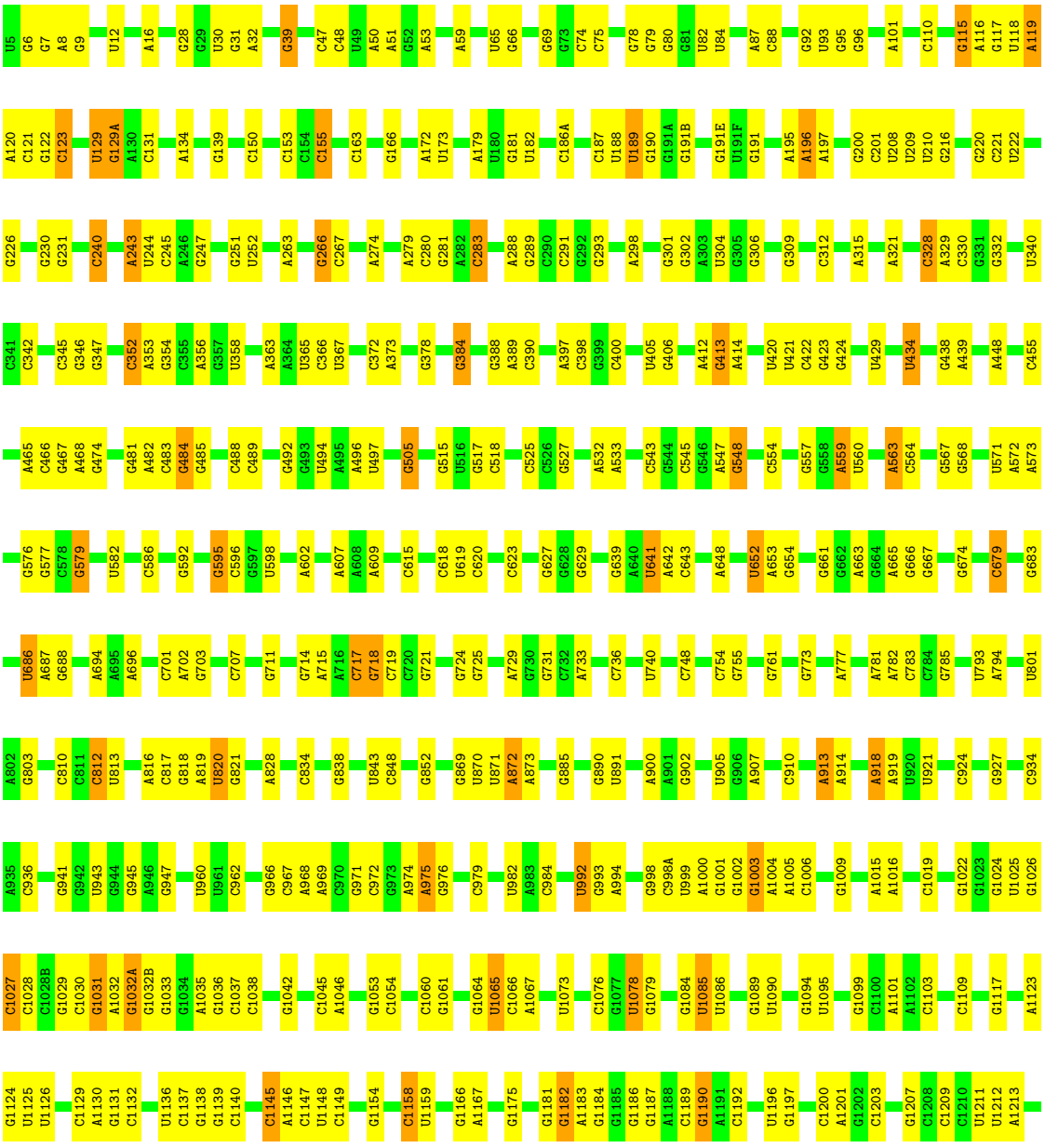
• Molecule 7: 30S ribosomal protein Thx

Chain F:



• Molecule 8: 16S ribosomal RNA

Chain G:



• Molecule 9: 30S ribosomal protein S2

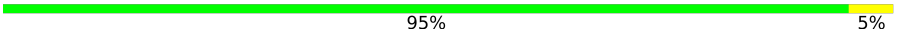
Chain H:

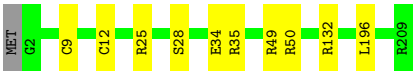
• Molecule 10: 30S ribosomal protein S3

Chain I:

• Molecule 11: 30S ribosomal protein S4

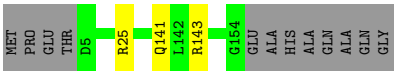
Chain J:





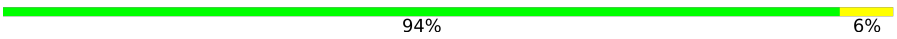
• Molecule 12: 30S ribosomal protein S5

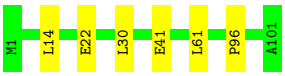
Chain K:



• Molecule 13: 30S ribosomal protein S6

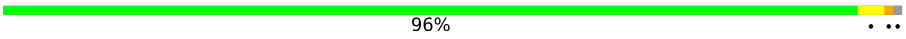
Chain L:

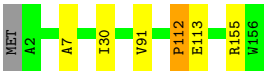




• Molecule 14: 30S ribosomal protein S7

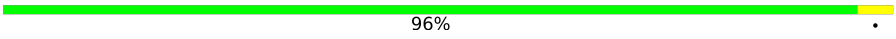
Chain M:





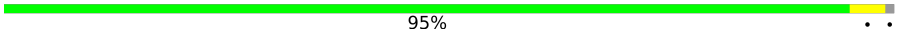
• Molecule 15: 30S ribosomal protein S8

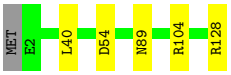
Chain N:



• Molecule 16: 30S ribosomal protein S9

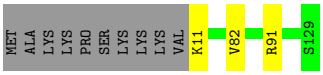
Chain O:





• Molecule 17: 30S ribosomal protein S11

Chain P:

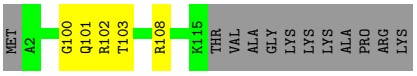


• Molecule 18: 30S ribosomal protein S12

Chain Q:

• Molecule 19: 30S ribosomal protein S13

Chain R:

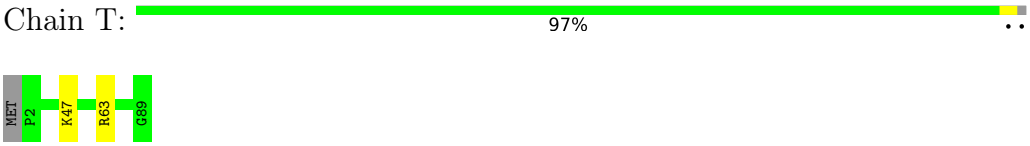


• Molecule 20: 30S ribosomal protein S14 type Z

Chain S:

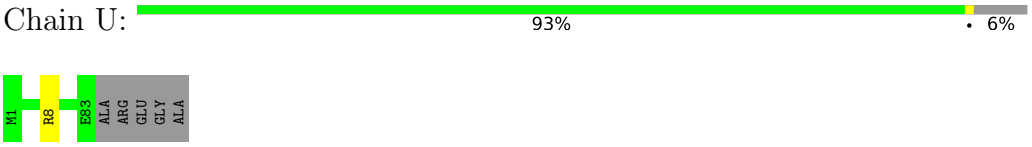
• Molecule 21: 30S ribosomal protein S15

Chain T:



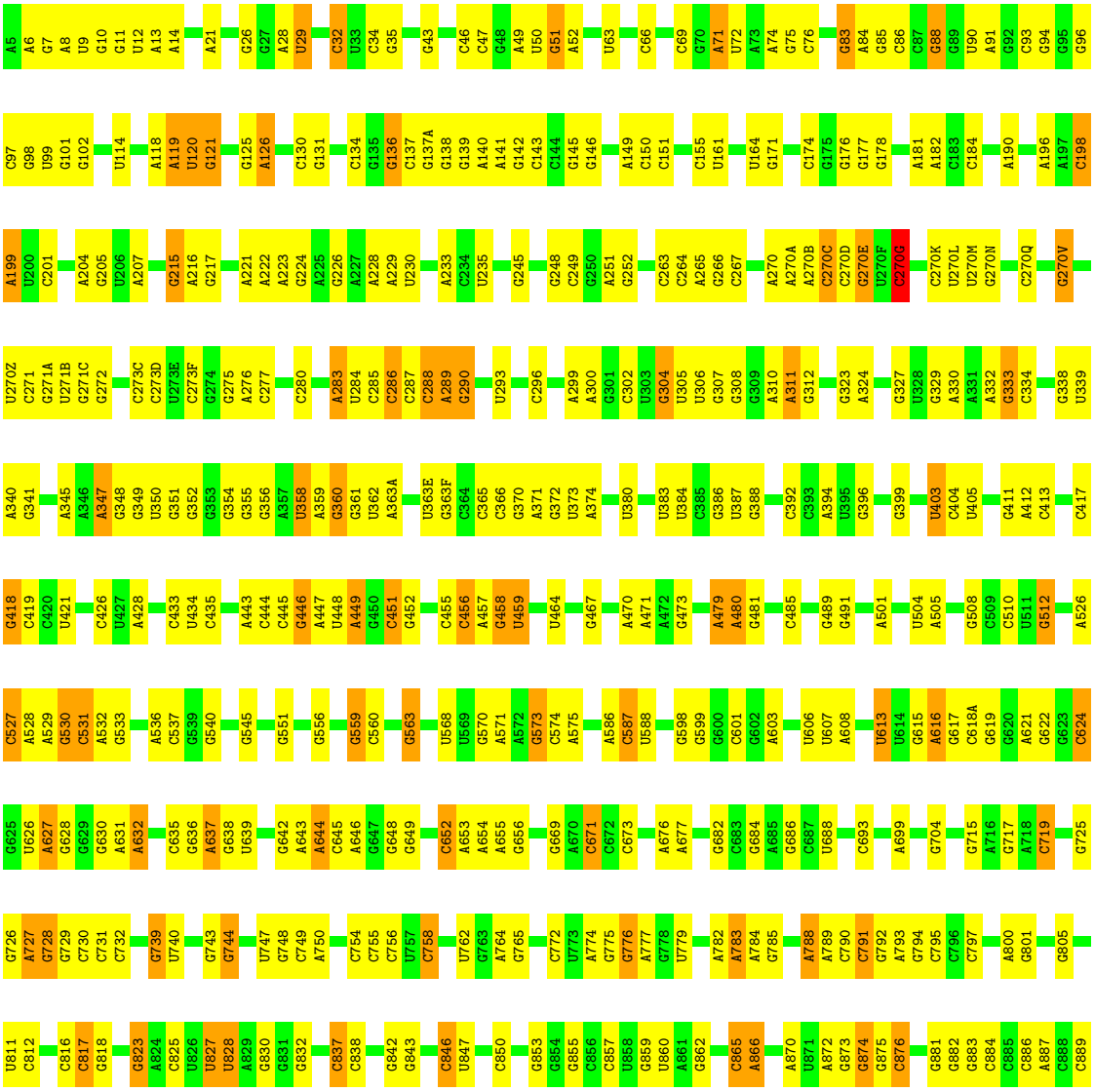
• Molecule 22: 30S ribosomal protein S16

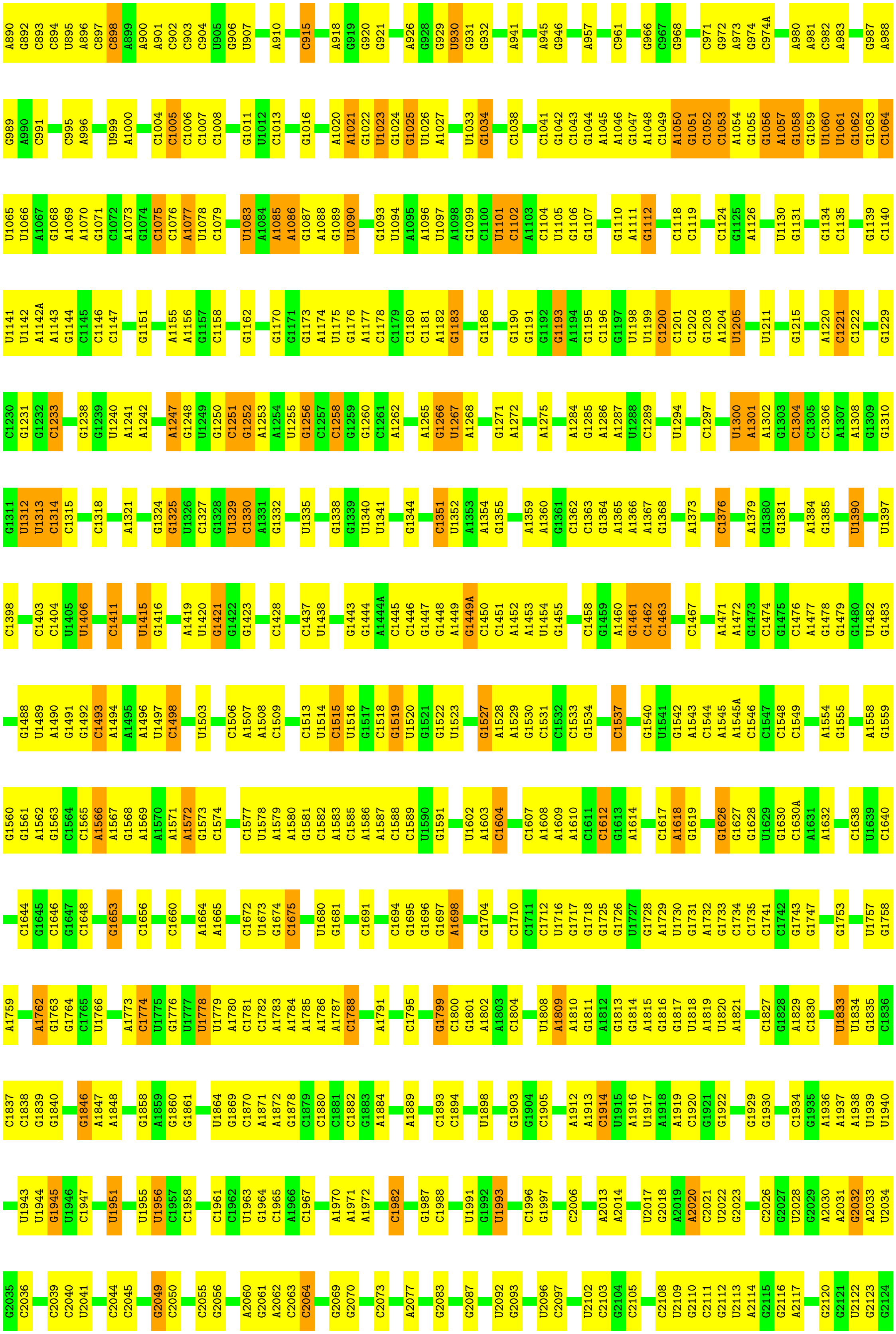
Chain U:

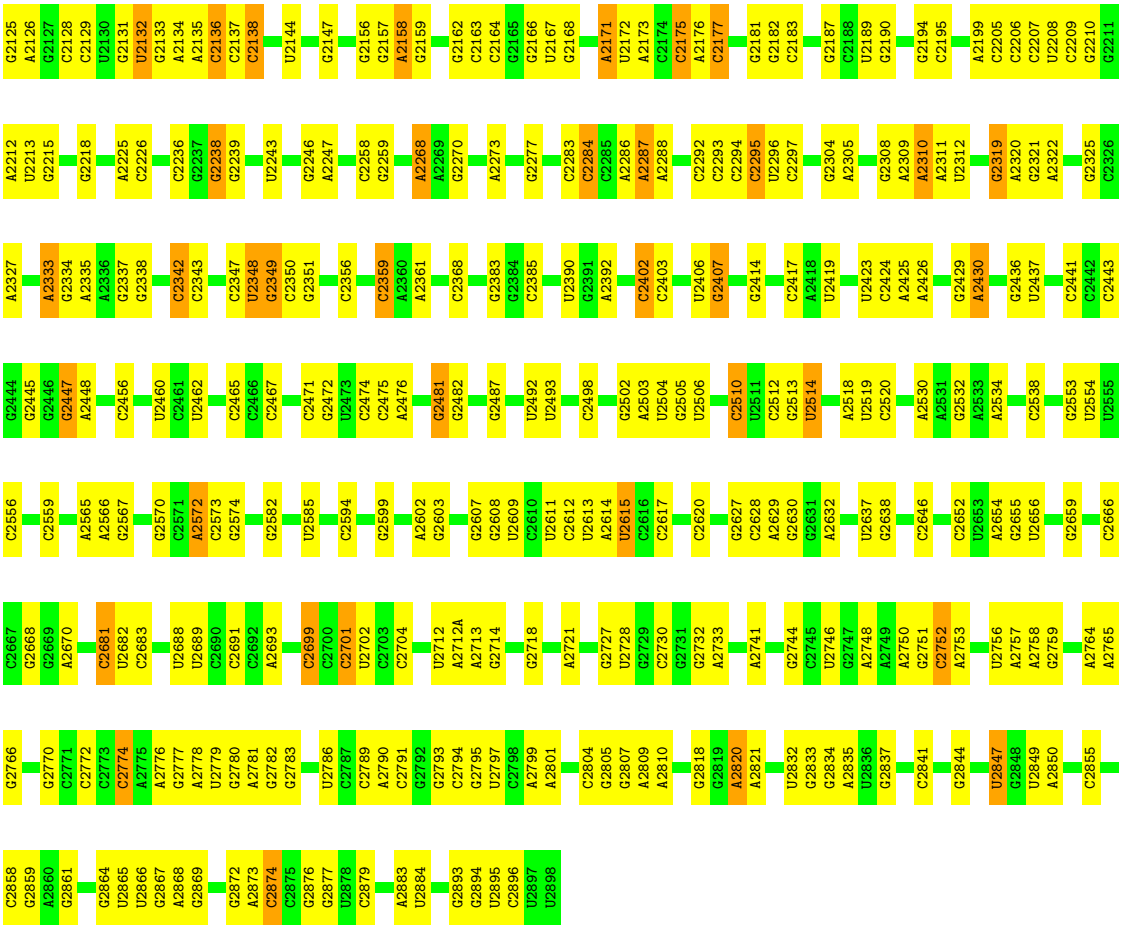


• Molecule 23: 23S ribosomal RNA

Chain V:

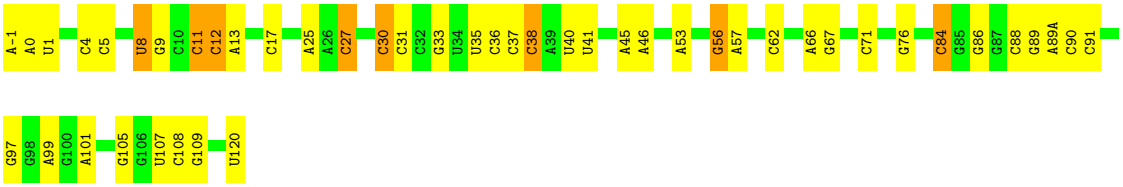






• Molecule 24: 5S ribosomal RNA

Chain X:

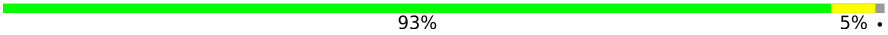


• Molecule 25: 50S ribosomal protein L1

Chain Y:

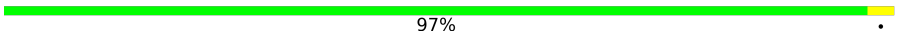
• Molecule 26: 50S ribosomal protein L2

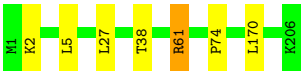
Chain Z:



• Molecule 27: 50S ribosomal protein L3

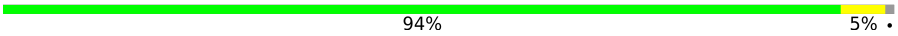
Chain a:





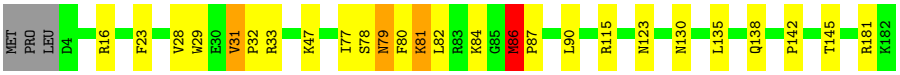
• Molecule 28: 50S ribosomal protein L4

Chain b:



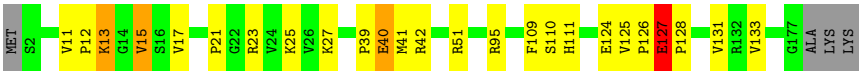
• Molecule 29: 50S ribosomal protein L5

Chain c:



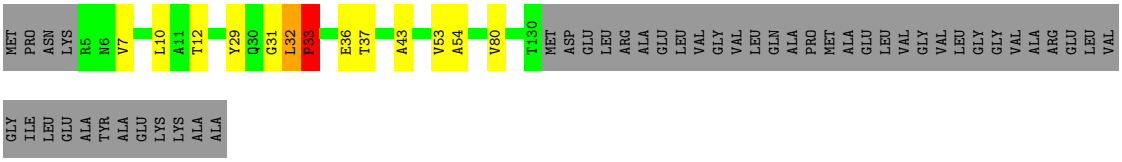
• Molecule 30: 50S ribosomal protein L6

Chain d:



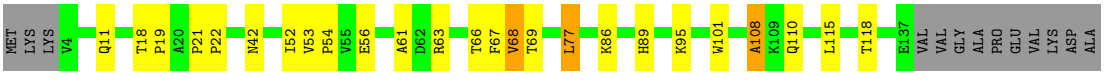
• Molecule 31: 50S ribosomal protein L10

Chain e:



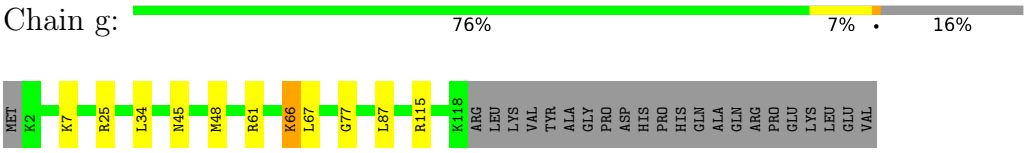
• Molecule 32: 50S ribosomal protein L11

Chain f:



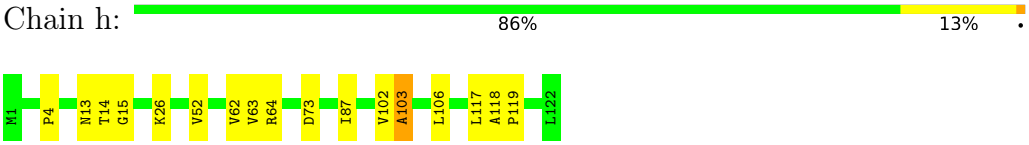
• Molecule 33: 50S ribosomal protein L13

Chain g:



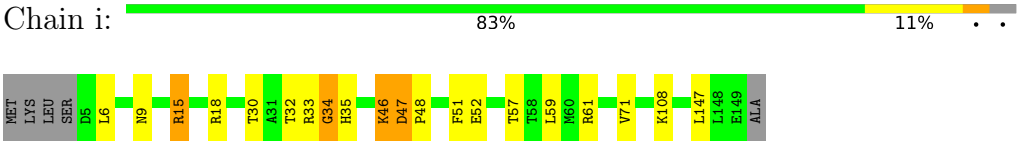
• Molecule 34: 50S ribosomal protein L14

Chain h:



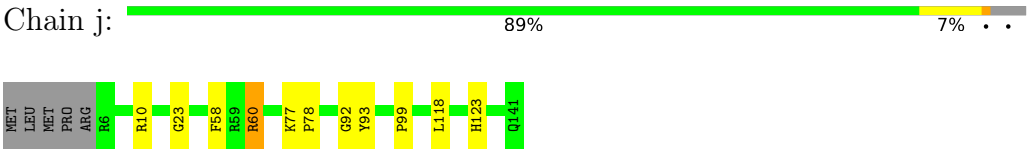
• Molecule 35: 50S ribosomal protein L15

Chain i:



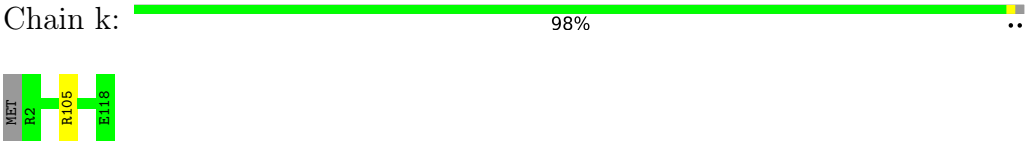
• Molecule 36: 50S ribosomal protein L16

Chain j:



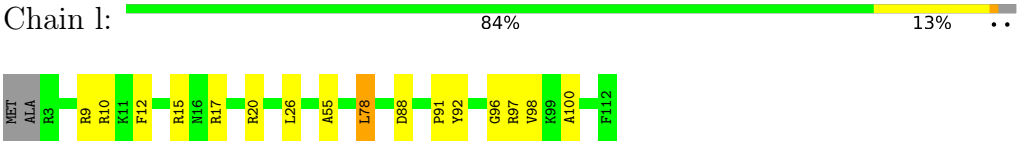
• Molecule 37: 50S ribosomal protein L17

Chain k:



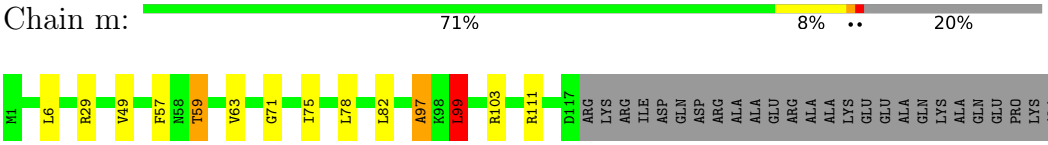
• Molecule 38: 50S ribosomal protein L18

Chain l:



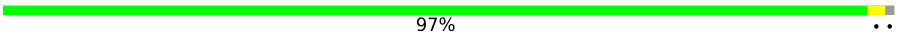
• Molecule 39: 50S ribosomal protein L19

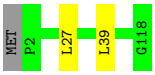
Chain m:



• Molecule 40: 50S ribosomal protein L20

Chain n:



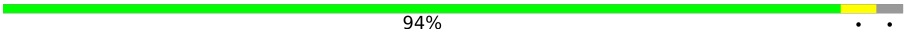


• Molecule 41: 50S ribosomal protein L21

Chain o:

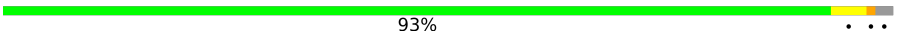
• Molecule 42: 50S ribosomal protein L22

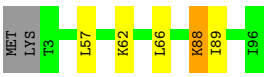
Chain p:



• Molecule 43: 50S ribosomal protein L23

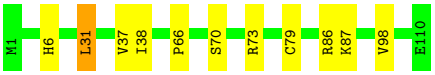
Chain q:





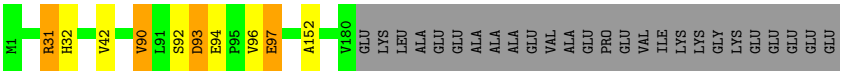
• Molecule 44: 50S ribosomal protein L24

Chain r:



• Molecule 45: 50S ribosomal protein L25

Chain s:

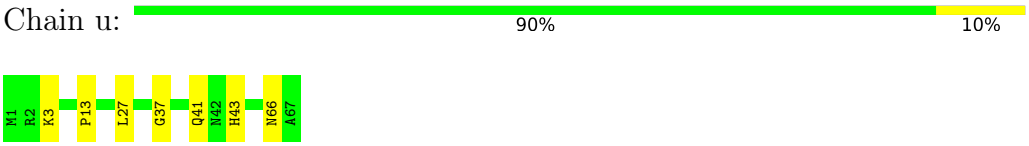


• Molecule 46: 50S ribosomal protein L27

Chain t:

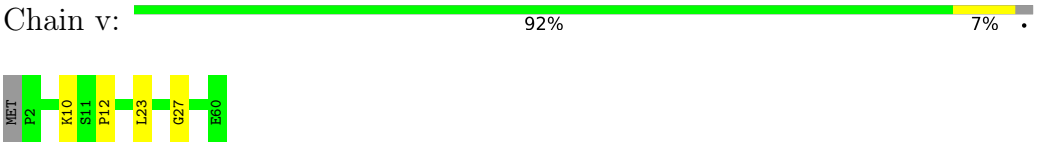
• Molecule 47: 50S ribosomal protein L29

Chain u:



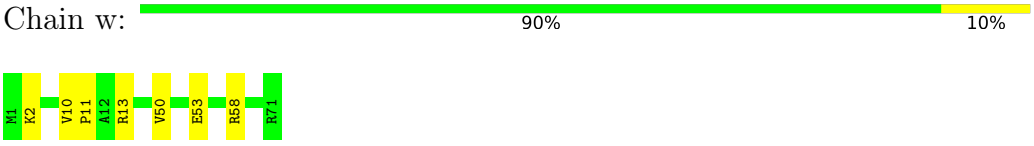
• Molecule 48: 50S ribosomal protein L30

Chain v:



• Molecule 49: 50S ribosomal protein L31

Chain w:

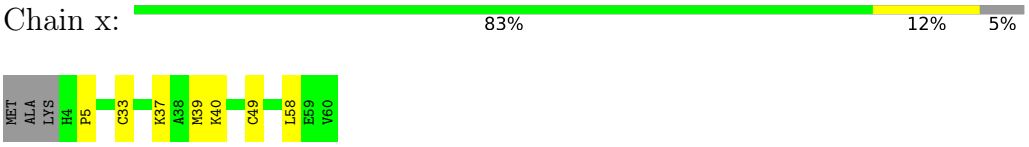


• Molecule 49: 50S ribosomal protein L31

Chain CC:

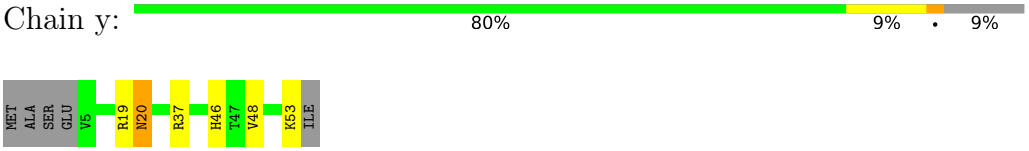
• Molecule 50: 50S ribosomal protein L32

Chain x:



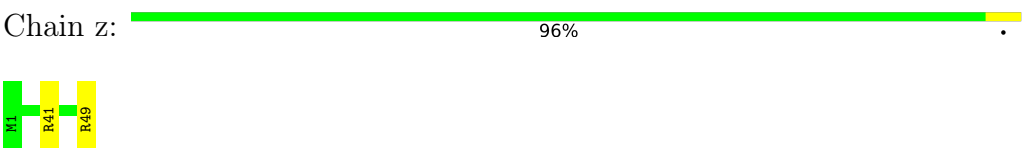
• Molecule 51: 50S ribosomal protein L33

Chain y:



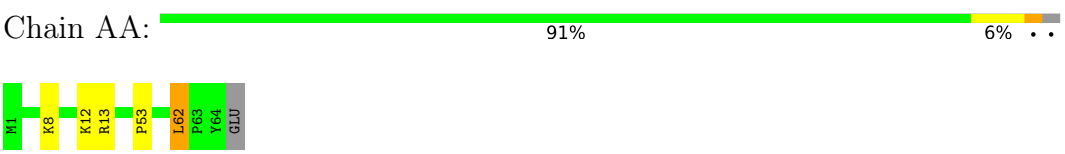
• Molecule 52: 50S ribosomal protein L34

Chain z:



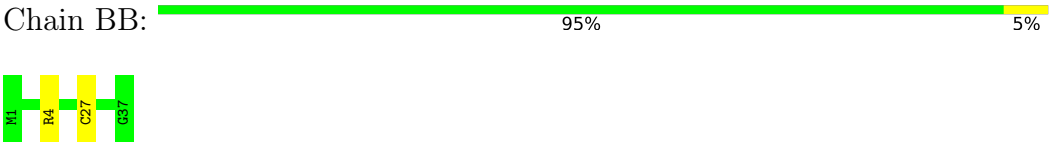
• Molecule 53: 50S ribosomal protein L35

Chain AA:



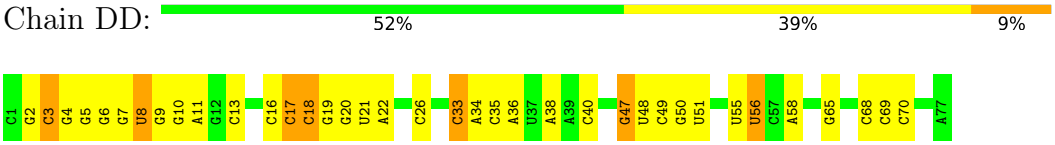
• Molecule 54: 50S ribosomal protein L36

Chain BB:



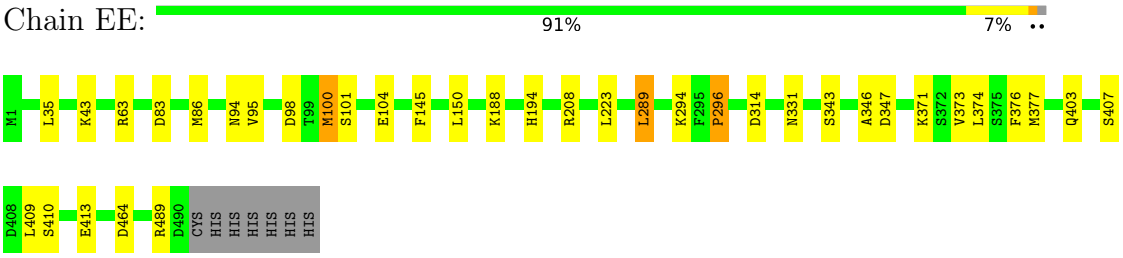
• Molecule 55: P-site tRNA

Chain DD:



• Molecule 56: Macrolide efflux protein

Chain EE:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

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: 4SU, MG, PSU, 5MU, ANP, OMC, 7MG

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	W	0.25	0/166	0.74	0/256
2	A	0.38	0/821	0.69	2/1098 (0.2%)
3	B	0.32	0/603	0.77	1/799 (0.1%)
4	C	0.31	0/765	0.63	0/1007
5	D	0.36	0/670	0.69	0/903
6	E	0.32	0/807	0.72	1/1085 (0.1%)
7	F	0.32	0/212	0.57	0/277
8	G	0.67	2/36416 (0.0%)	1.15	241/56835 (0.4%)
9	H	0.33	0/1842	0.72	3/2479 (0.1%)
10	I	0.34	0/1636	0.64	1/2205 (0.0%)
11	J	0.41	1/1733 (0.1%)	0.75	3/2318 (0.1%)
12	K	0.38	0/1162	0.69	0/1564
13	L	0.34	0/856	0.76	3/1154 (0.3%)
14	M	0.36	0/1276	0.67	1/1709 (0.1%)
15	N	0.36	0/1136	0.70	2/1527 (0.1%)
16	O	0.34	0/1029	0.71	1/1379 (0.1%)
17	P	0.32	0/900	0.67	0/1213
18	Q	0.40	0/986	0.76	0/1320
19	R	0.34	0/924	0.71	0/1238
20	S	0.29	0/501	0.50	0/664
21	T	0.33	0/745	0.63	0/992
22	U	0.35	0/716	0.63	0/963
23	V	0.86	11/69349 (0.0%)	1.27	775/108263 (0.7%)
24	X	0.64	1/2954 (0.0%)	1.23	24/4606 (0.5%)
25	Y	0.43	1/1775 (0.1%)	0.79	3/2393 (0.1%)
26	Z	0.47	0/2176	0.78	3/2933 (0.1%)
27	a	0.48	0/1611	0.82	3/2171 (0.1%)
28	b	0.46	0/1660	0.80	1/2247 (0.0%)
29	c	0.33	0/1479	0.83	3/1989 (0.2%)
30	d	0.35	0/1360	0.98	4/1838 (0.2%)
31	e	0.41	0/620	0.81	2/861 (0.2%)
32	f	0.34	0/1012	0.85	5/1373 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.40	0/952	0.80	3/1283 (0.2%)
34	h	0.47	0/942	0.91	2/1268 (0.2%)
35	i	0.41	0/1125	0.88	4/1497 (0.3%)
36	j	0.47	0/1100	0.87	1/1470 (0.1%)
37	k	0.41	0/974	0.74	0/1302
38	l	0.32	0/887	0.69	2/1180 (0.2%)
39	m	0.43	0/990	0.89	3/1325 (0.2%)
40	n	0.46	0/982	0.72	1/1306 (0.1%)
41	o	0.41	0/790	0.90	1/1057 (0.1%)
42	p	0.43	0/886	0.67	0/1189
43	q	0.41	0/756	0.81	2/1015 (0.2%)
44	r	0.37	0/857	0.91	2/1142 (0.2%)
45	s	0.37	0/1467	0.72	1/1992 (0.1%)
46	t	0.39	0/637	0.69	1/848 (0.1%)
47	u	0.34	0/569	0.72	2/751 (0.3%)
48	v	0.47	0/474	0.79	1/635 (0.2%)
49	CC	0.26	0/156	0.53	0/215
49	w	0.49	0/594	0.96	0/795
50	x	0.44	0/459	0.79	0/621
51	y	0.48	0/429	0.85	0/572
52	z	0.55	0/438	0.84	0/575
53	AA	0.50	0/523	0.88	0/690
54	BB	0.43	0/310	0.88	1/407 (0.2%)
55	DD	0.46	0/1724	1.16	24/2687 (0.9%)
56	EE	0.34	0/3892	0.70	4/5224 (0.1%)
All	All	0.69	16/162811 (0.0%)	1.11	1137/242705 (0.5%)

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
3	B	0	3
4	C	0	1
5	D	0	1
6	E	0	4
9	H	0	2
11	J	0	2
12	K	0	1
13	L	0	2
14	M	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	N	0	1
16	O	0	2
18	Q	0	1
19	R	0	1
23	V	0	6
25	Y	0	4
26	Z	0	8
27	a	0	2
28	b	0	5
29	c	0	4
30	d	0	2
31	e	0	8
32	f	0	2
33	g	0	2
34	h	0	10
35	i	0	8
36	j	0	6
38	l	0	1
39	m	0	8
41	o	0	4
43	q	0	2
44	r	0	7
46	t	0	1
47	u	0	2
48	v	0	1
49	w	0	2
50	x	0	1
51	y	0	1
52	z	0	1
53	AA	0	2
56	EE	0	6
All	All	0	129

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	1449(A)	G	O3'-P	-15.61	1.42	1.61
23	V	1146	C	O3'-P	11.89	1.75	1.61
24	X	-1	A	OP3-P	-10.17	1.49	1.61
8	G	93	U	O3'-P	-8.97	1.50	1.61
8	G	1167	A	O3'-P	-7.78	1.51	1.61

The worst 5 of 1137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	11	VAL	C-N-CD	-21.67	72.92	120.60
23	V	1449(A)	G	O3'-P-O5'	-19.38	67.19	104.00
23	V	1061	U	OP1-P-OP2	18.30	147.06	119.60
23	V	155	C	O3'-P-O5'	-18.02	69.77	104.00
23	V	2349	G	C8-N9-C4	-17.62	99.35	106.40

There are no chirality outliers.

5 of 129 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	44	LEU	Peptide
3	B	83	GLU	Peptide
3	B	86	VAL	Peptide
4	C	75	ASN	Peptide
5	D	4	SER	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	95/104 (91%)	82 (86%)	12 (13%)	1 (1%)	12 45
3	B	71/73 (97%)	59 (83%)	12 (17%)	0	100 100
4	C	97/106 (92%)	85 (88%)	10 (10%)	2 (2%)	5 33
5	D	80/93 (86%)	64 (80%)	16 (20%)	0	100 100
6	E	96/105 (91%)	81 (84%)	14 (15%)	1 (1%)	13 46
7	F	22/27 (82%)	20 (91%)	2 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	H	220/256 (86%)	195 (89%)	23 (10%)	2 (1%)	14 48
10	I	204/239 (85%)	174 (85%)	30 (15%)	0	100 100
11	J	206/209 (99%)	178 (86%)	27 (13%)	1 (0%)	25 59
12	K	148/162 (91%)	129 (87%)	18 (12%)	1 (1%)	19 53
13	L	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	13 46
14	M	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	10 41
15	N	136/138 (99%)	118 (87%)	17 (12%)	1 (1%)	19 53
16	O	125/128 (98%)	97 (78%)	28 (22%)	0	100 100
17	P	117/129 (91%)	103 (88%)	14 (12%)	0	100 100
18	Q	122/132 (92%)	96 (79%)	25 (20%)	1 (1%)	16 51
19	R	112/126 (89%)	86 (77%)	23 (20%)	3 (3%)	4 28
20	S	58/61 (95%)	39 (67%)	18 (31%)	1 (2%)	7 37
21	T	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
22	U	81/88 (92%)	70 (86%)	11 (14%)	0	100 100
25	Y	226/229 (99%)	179 (79%)	39 (17%)	8 (4%)	3 24
26	Z	271/276 (98%)	232 (86%)	38 (14%)	1 (0%)	30 63
27	a	204/206 (99%)	162 (79%)	42 (21%)	0	100 100
28	b	206/210 (98%)	156 (76%)	48 (23%)	2 (1%)	13 46
29	c	177/182 (97%)	121 (68%)	45 (25%)	11 (6%)	1 13
30	d	174/180 (97%)	135 (78%)	27 (16%)	12 (7%)	1 11
31	e	124/173 (72%)	79 (64%)	39 (32%)	6 (5%)	2 17
32	f	132/147 (90%)	86 (65%)	34 (26%)	12 (9%)	0 7
33	g	115/140 (82%)	92 (80%)	21 (18%)	2 (2%)	7 37
34	h	120/122 (98%)	76 (63%)	39 (32%)	5 (4%)	2 20
35	i	143/150 (95%)	95 (66%)	41 (29%)	7 (5%)	2 17
36	j	134/141 (95%)	94 (70%)	37 (28%)	3 (2%)	5 32
37	k	115/118 (98%)	97 (84%)	18 (16%)	0	100 100
38	l	108/112 (96%)	82 (76%)	23 (21%)	3 (3%)	4 27
39	m	115/146 (79%)	78 (68%)	34 (30%)	3 (3%)	4 28
40	n	115/118 (98%)	103 (90%)	12 (10%)	0	100 100
41	o	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	13 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	p	108/113 (96%)	92 (85%)	15 (14%)	1 (1%)	14 48
43	q	92/96 (96%)	76 (83%)	14 (15%)	2 (2%)	5 32
44	r	108/110 (98%)	66 (61%)	40 (37%)	2 (2%)	6 35
45	s	178/206 (86%)	128 (72%)	41 (23%)	9 (5%)	1 16
46	t	78/85 (92%)	64 (82%)	13 (17%)	1 (1%)	10 41
47	u	65/67 (97%)	55 (85%)	9 (14%)	1 (2%)	8 39
48	v	57/60 (95%)	46 (81%)	10 (18%)	1 (2%)	7 35
49	CC	30/71 (42%)	18 (60%)	12 (40%)	0	100 100
49	w	69/71 (97%)	43 (62%)	23 (33%)	3 (4%)	2 19
50	x	55/60 (92%)	35 (64%)	18 (33%)	2 (4%)	3 23
51	y	47/54 (87%)	29 (62%)	17 (36%)	1 (2%)	5 33
52	z	47/49 (96%)	40 (85%)	7 (15%)	0	100 100
53	AA	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2 17
54	BB	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
56	EE	488/497 (98%)	386 (79%)	98 (20%)	4 (1%)	16 51
All	All	6425/6914 (93%)	5084 (79%)	1218 (19%)	123 (2%)	9 35

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	75	ASN
9	H	78	GLN
25	Y	161	ILE
25	Y	179	SER
29	c	31	VAL

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	92/96 (96%)	91 (99%)	1 (1%)	70 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	B	64/64 (100%)	64 (100%)	0	100 100
4	C	76/82 (93%)	75 (99%)	1 (1%)	65 81
5	D	72/80 (90%)	69 (96%)	3 (4%)	25 54
6	E	88/92 (96%)	88 (100%)	0	100 100
7	F	19/22 (86%)	19 (100%)	0	100 100
9	H	191/220 (87%)	186 (97%)	5 (3%)	41 65
10	I	160/188 (85%)	157 (98%)	3 (2%)	52 73
11	J	180/181 (99%)	176 (98%)	4 (2%)	47 69
12	K	115/123 (94%)	114 (99%)	1 (1%)	75 87
13	L	90/90 (100%)	90 (100%)	0	100 100
14	M	126/127 (99%)	124 (98%)	2 (2%)	58 76
15	N	119/119 (100%)	118 (99%)	1 (1%)	79 88
16	O	98/99 (99%)	96 (98%)	2 (2%)	50 72
17	P	90/99 (91%)	87 (97%)	3 (3%)	33 61
18	Q	104/109 (95%)	104 (100%)	0	100 100
19	R	92/101 (91%)	91 (99%)	1 (1%)	70 83
20	S	49/50 (98%)	41 (84%)	8 (16%)	2 12
21	T	79/80 (99%)	77 (98%)	2 (2%)	42 66
22	U	72/74 (97%)	71 (99%)	1 (1%)	62 79
25	Y	180/181 (99%)	174 (97%)	6 (3%)	33 61
26	Z	215/218 (99%)	209 (97%)	6 (3%)	38 64
27	a	166/166 (100%)	163 (98%)	3 (2%)	54 74
28	b	164/166 (99%)	160 (98%)	4 (2%)	44 67
29	c	152/156 (97%)	139 (91%)	13 (9%)	8 33
30	d	142/148 (96%)	130 (92%)	12 (8%)	8 33
32	f	101/111 (91%)	92 (91%)	9 (9%)	8 32
33	g	99/119 (83%)	94 (95%)	5 (5%)	20 49
34	h	100/100 (100%)	99 (99%)	1 (1%)	73 85
35	i	112/116 (97%)	107 (96%)	5 (4%)	23 53
36	j	106/111 (96%)	104 (98%)	2 (2%)	52 73
37	k	100/101 (99%)	99 (99%)	1 (1%)	73 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	l	87/88 (99%)	76 (87%)	11 (13%)	3 19
39	m	105/127 (83%)	101 (96%)	4 (4%)	28 57
40	n	93/94 (99%)	92 (99%)	1 (1%)	70 83
41	o	82/82 (100%)	79 (96%)	3 (4%)	29 58
42	p	90/92 (98%)	87 (97%)	3 (3%)	33 61
43	q	76/78 (97%)	76 (100%)	0	100 100
44	r	91/91 (100%)	90 (99%)	1 (1%)	70 83
45	s	159/179 (89%)	155 (98%)	4 (2%)	42 66
46	t	63/67 (94%)	61 (97%)	2 (3%)	34 61
47	u	62/62 (100%)	60 (97%)	2 (3%)	34 61
48	v	51/52 (98%)	50 (98%)	1 (2%)	50 72
49	w	63/63 (100%)	61 (97%)	2 (3%)	34 61
50	x	50/52 (96%)	46 (92%)	4 (8%)	10 35
51	y	47/52 (90%)	42 (89%)	5 (11%)	5 26
52	z	42/42 (100%)	41 (98%)	1 (2%)	44 67
53	AA	54/55 (98%)	53 (98%)	1 (2%)	52 73
54	BB	34/34 (100%)	33 (97%)	1 (3%)	37 63
56	EE	412/419 (98%)	386 (94%)	26 (6%)	15 44
All	All	5274/5518 (96%)	5097 (97%)	177 (3%)	34 60

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	l	98	VAL
51	y	20	ASN
39	m	111	ARG
45	s	93	ASP
54	BB	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
43	q	31	HIS
51	y	32	ASN
43	q	41	ASN

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Mol	Chain	Res	Type
47	u	66	ASN
56	EE	285	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	W	6/25 (24%)	6 (100%)	1 (16%)
23	V	2874/2875 (99%)	1140 (39%)	83 (2%)
24	X	122/123 (99%)	41 (33%)	1 (0%)
55	DD	76/77 (98%)	31 (40%)	4 (5%)
8	G	1513/1514 (99%)	479 (31%)	37 (2%)
All	All	4591/4614 (99%)	1697 (36%)	126 (2%)

5 of 1697 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	W	15	A
1	W	16	A
1	W	17	U
1	W	18	G
1	W	19	U

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	V	451	C
23	V	2319	G
23	V	827	U
23	V	2238	G
23	V	2712	U

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

5 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	$\#\|Z\|>2$
55	PSU	DD	56	55	18,21,22	1.00	1 (5%)	22,30,33	1.67	5 (22%)
55	OMC	DD	33	55	19,22,23	0.82	0	26,31,34	1.04	1 (3%)
55	5MU	DD	55	55	19,22,23	4.61	5 (26%)	28,32,35	3.70	10 (35%)
55	7MG	DD	47	55	22,26,27	1.32	3 (13%)	29,39,42	2.65	8 (27%)
55	4SU	DD	8	55	18,21,22	1.72	4 (22%)	26,30,33	2.31	6 (23%)

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
55	PSU	DD	56	55	-	2/7/25/26	0/2/2/2
55	OMC	DD	33	55	-	2/9/27/28	0/2/2/2
55	5MU	DD	55	55	-	1/7/25/26	0/2/2/2
55	7MG	DD	47	55	-	1/7/37/38	0/3/3/3
55	4SU	DD	8	55	-	1/7/25/26	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DD	55	5MU	C2-N1	11.06	1.56	1.38
55	DD	55	5MU	C4-N3	-9.89	1.20	1.38
55	DD	55	5MU	C4-C5	9.87	1.61	1.44
55	DD	55	5MU	C6-N1	7.96	1.51	1.38
55	DD	8	4SU	C4-S4	-4.46	1.59	1.68

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DD	55	5MU	C5-C4-N3	12.26	125.78	115.31
55	DD	55	5MU	C5-C6-N1	-9.85	113.21	123.34
55	DD	47	7MG	N9-C4-N3	9.15	139.16	125.47
55	DD	8	4SU	C4-N3-C2	-6.88	120.66	127.34
55	DD	8	4SU	C5-C4-N3	5.94	120.20	114.69

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	DD	8	4SU	O4'-C4'-C5'-O5'
55	DD	33	OMC	O4'-C4'-C5'-O5'
55	DD	33	OMC	C3'-C4'-C5'-O5'
55	DD	56	PSU	C3'-C4'-C5'-O5'
55	DD	56	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
58	ANP	EE	501	56	29,33,33	1.86	5 (17%)	31,52,52	1.88	8 (25%)
58	ANP	EE	502	-	29,33,33	1.86	5 (17%)	31,52,52	1.89	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ANP	EE	501	56	-	7/14/38/38	0/3/3/3
58	ANP	EE	502	-	-	6/14/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	EE	501	ANP	PB-N3B	4.63	1.75	1.63
58	EE	502	ANP	PB-N3B	4.62	1.75	1.63
58	EE	502	ANP	PG-N3B	4.62	1.75	1.63
58	EE	501	ANP	PG-N3B	4.60	1.75	1.63
58	EE	502	ANP	PG-O1G	3.37	1.51	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	EE	502	ANP	O1G-PG-N3B	-4.85	104.63	111.77
58	EE	501	ANP	O1G-PG-N3B	-4.84	104.64	111.77
58	EE	501	ANP	O2B-PB-O1B	4.04	118.40	109.92
58	EE	502	ANP	O2B-PB-O1B	4.04	118.40	109.92
58	EE	502	ANP	PB-O3A-PA	-3.46	120.44	132.62

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

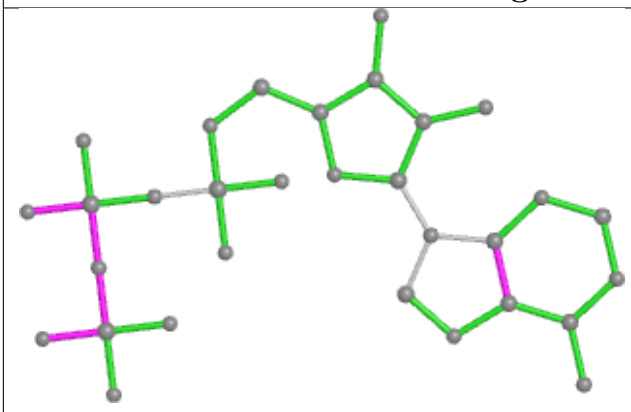
Mol	Chain	Res	Type	Atoms
58	EE	501	ANP	PB-N3B-PG-O1G
58	EE	501	ANP	PG-N3B-PB-O1B
58	EE	501	ANP	C3'-C4'-C5'-O5'
58	EE	502	ANP	PB-N3B-PG-O1G
58	EE	502	ANP	PA-O3A-PB-O1B

There are no ring outliers.

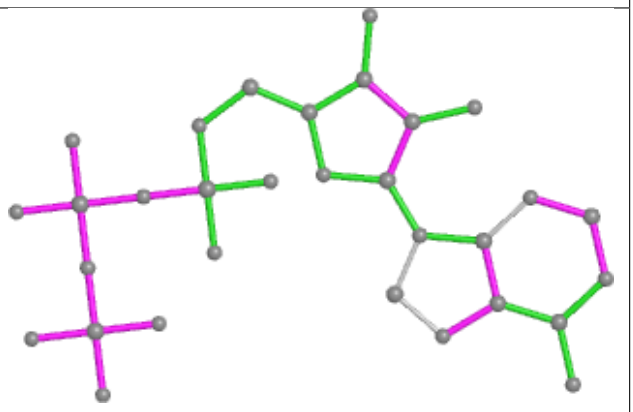
No monomer is involved in short contacts.

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

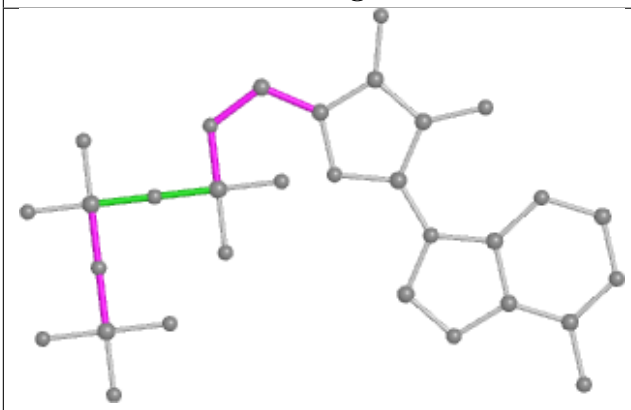
Ligand ANP EE 501



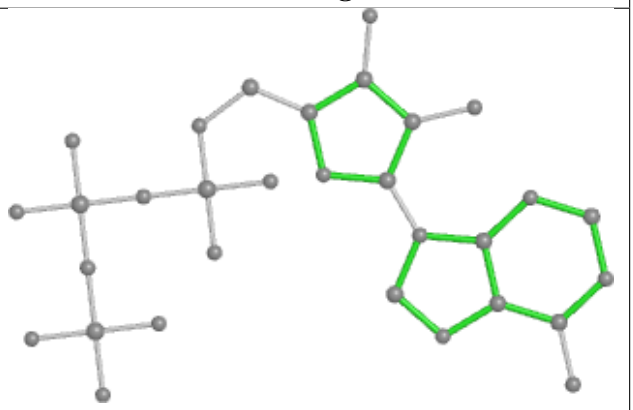
Bond lengths



Bond angles

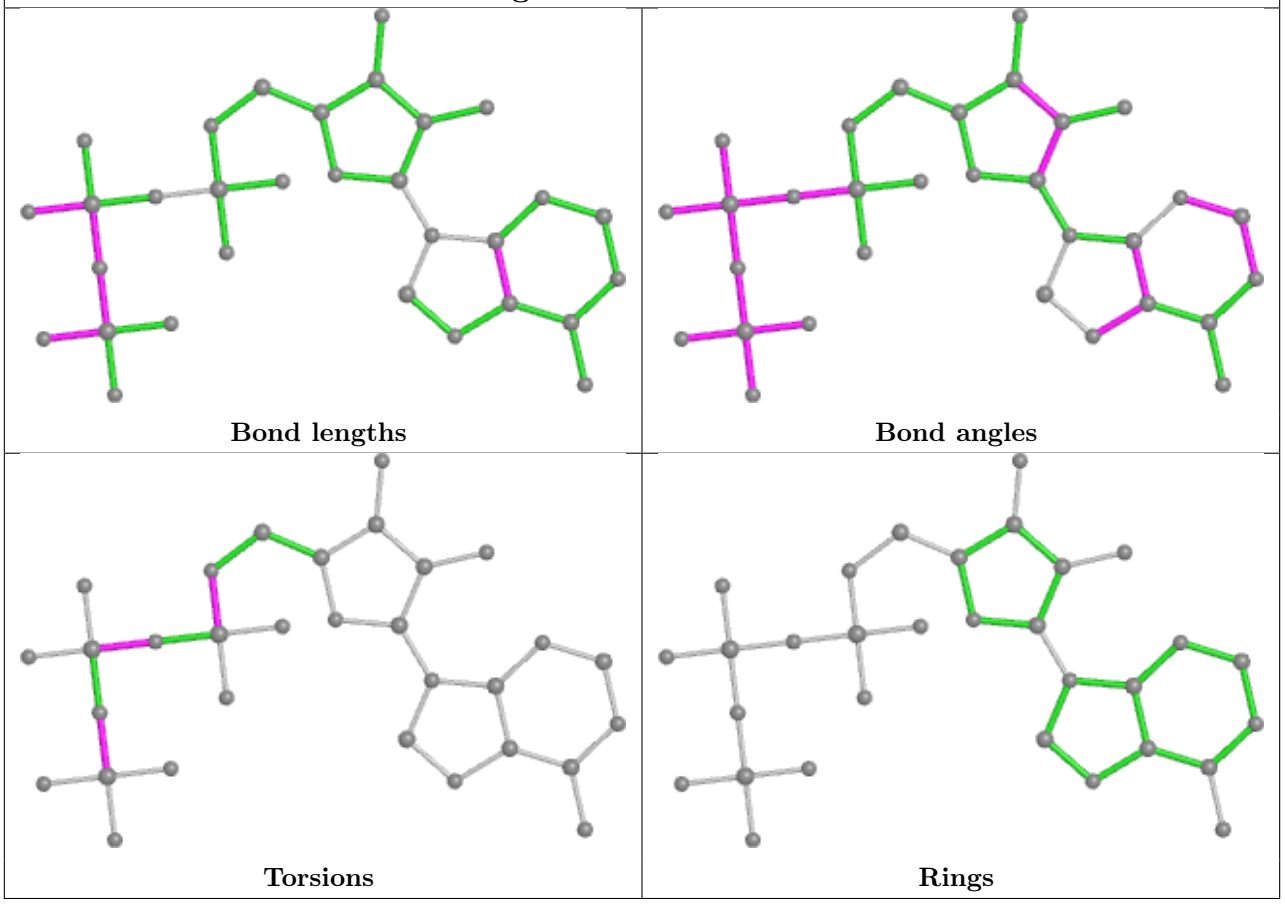


Torsions



Rings

Ligand ANP EE 502



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-6934. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.