wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 10:54 am BST

PDB ID	:	5AFI
EMDB ID	:	EMD-2847
Title	:	2.9A Structure of E. coli ribosome-EF-TU complex by cs-corrected cryo-EM
Authors	:	Fischer, N.; Neumann, P.; Konevega, A.L.; Bock, L.V.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on	:	2015-01-22
Resolution	:	2.90 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 ⓘ 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:

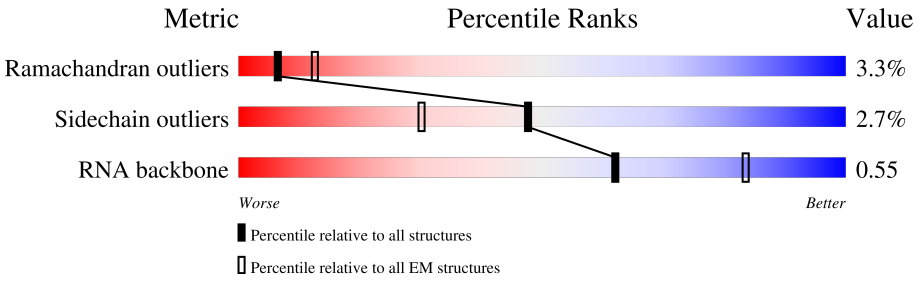
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	a	1539	83% 16% ·
2	b	240	85% 6% 9%
3	c	233	85% · 12%
4	d	206	92% 8%
5	e	167	84% 10% · 6%
6	f	135	68% · · 26%
7	g	179	78% 7% 16%
8	h	130	96% · ·
9	i	130	88% 10% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	j	103	87% 8% 5%
11	k	129	84% 6% 10%
12	l	124	93% 6%
13	m	118	91% 6%
14	n	102	90% 9%
15	o	89	91% 8%
16	p	82	93% 7%
17	q	84	86% 10% 5%
18	r	75	79% 8% 13%
19	s	92	85% 14%
20	t	87	93% 5%
21	u	71	82% 10% 8%
22	v	77	74% 23%
22	w	77	35% 49% 16%
23	x	11	82% 18%
24	y	77	68% 27% 5%
25	z	393	91% 6%
26	A	2903	79% 20%
27	B	120	84% 16%
28	C	273	95% 5%
29	D	209	98%
30	E	201	94% 6%
31	F	179	92% 7%
32	G	177	97%
33	H	149	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	I	142	91% 8%
35	J	142	97%
36	K	123	93% 7%
37	L	144	90% 9%
38	M	136	97%
39	N	127	91% 6%
40	O	117	97%
41	P	115	96%
42	Q	118	97%
43	R	103	97%
44	S	110	93% 6%
45	T	100	87% 5% 7%
46	U	104	94%
47	V	94	97%
48	W	85	86% 12%
49	X	78	97%
50	Y	63	97%
51	Z	59	98%
52	0	57	93% 5%
53	1	55	89% 9%
54	2	46	100%
55	3	65	95%
56	4	38	100%
57	5	165	73% 6% 21%
58	6	70	91% 6%

2 Entry composition (i)

There are 66 unique types of molecules in this entry. The entry contains 152717 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33029	14738	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1704	1081	305	311	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1141	709	218	208	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	100	817	515	148	148	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called P-site fMet-tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
22	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 24 is a RNA chain called A/T-site Phe-tRNAPhe.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	y	77	Total	C	N	O	P	S	0	0
			1643	740	291	534	76	2		

- Molecule 25 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	371	Total	C	N	O	S	1	0
			2881	1824	495	549	13		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total 504	C 323	N 105	O 74	S 2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total 302	C 185	N 65	O 48	S 4	0	0

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	131	Total 988	C 625	N 175	O 183	S 5	0	0

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	66	Total 522	C 323	N 99	O 94	S 6	0	0

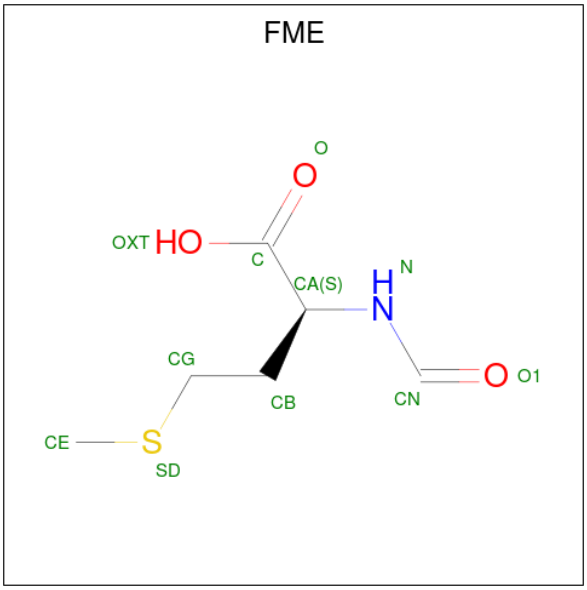
- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	a	83	Total 83	Mg 83	0
59	v	4	Total 4	Mg 4	0
59	z	1	Total 1	Mg 1	0
59	A	234	Total 234	Mg 234	0
59	B	7	Total 7	Mg 7	0
59	N	2	Total 2	Mg 2	0
59	0	1	Total 1	Mg 1	0
59	4	1	Total 1	Mg 1	0

- Molecule 60 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

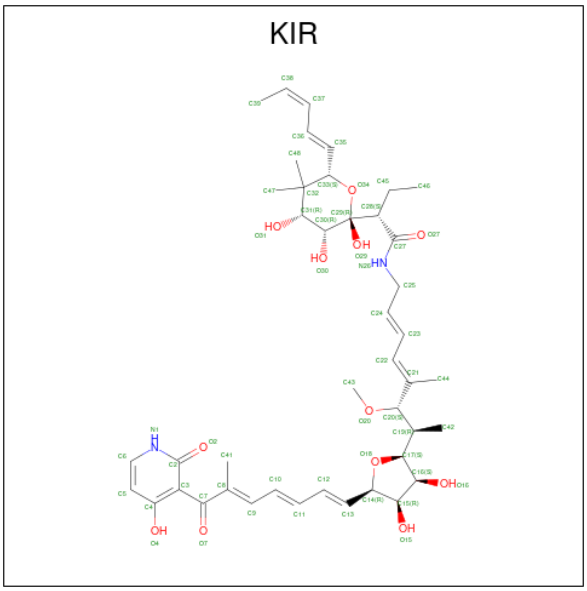
Mol	Chain	Residues	Atoms	AltConf
60	a	1	Total Cl 1 1	0
60	A	1	Total Cl 1 1	0

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



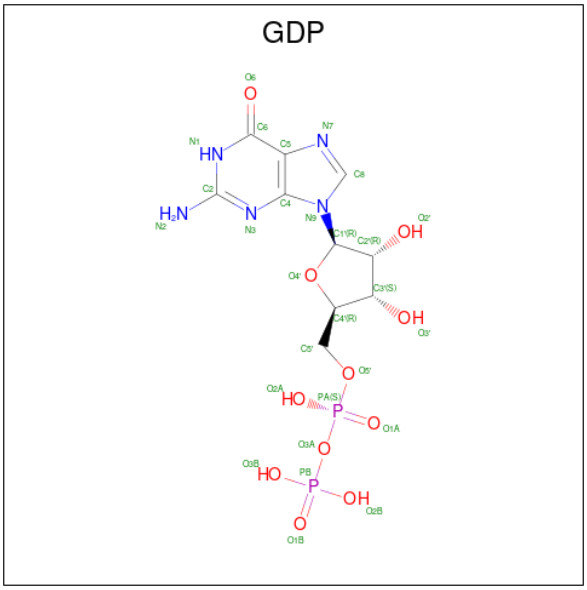
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total 10	C 6	N 1	O 2	S 1	0

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			57	43	2	12	

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 64 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
64	A	1	Total	Na	0
			1	1	
64	B	1	Total	Na	0
			1	1	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
65	4	1	Total	Zn	0
			1	1	
65	6	1	Total	Zn	0
			1	1	

- Molecule 66 is water.

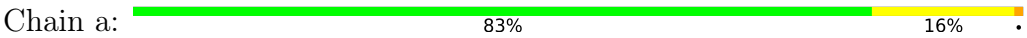
Mol	Chain	Residues	Atoms	AltConf
66	a	9	Total O 9 9	0
66	A	9	Total O 9 9	0
66	D	2	Total O 2 2	0
66	K	1	Total O 1 1	0

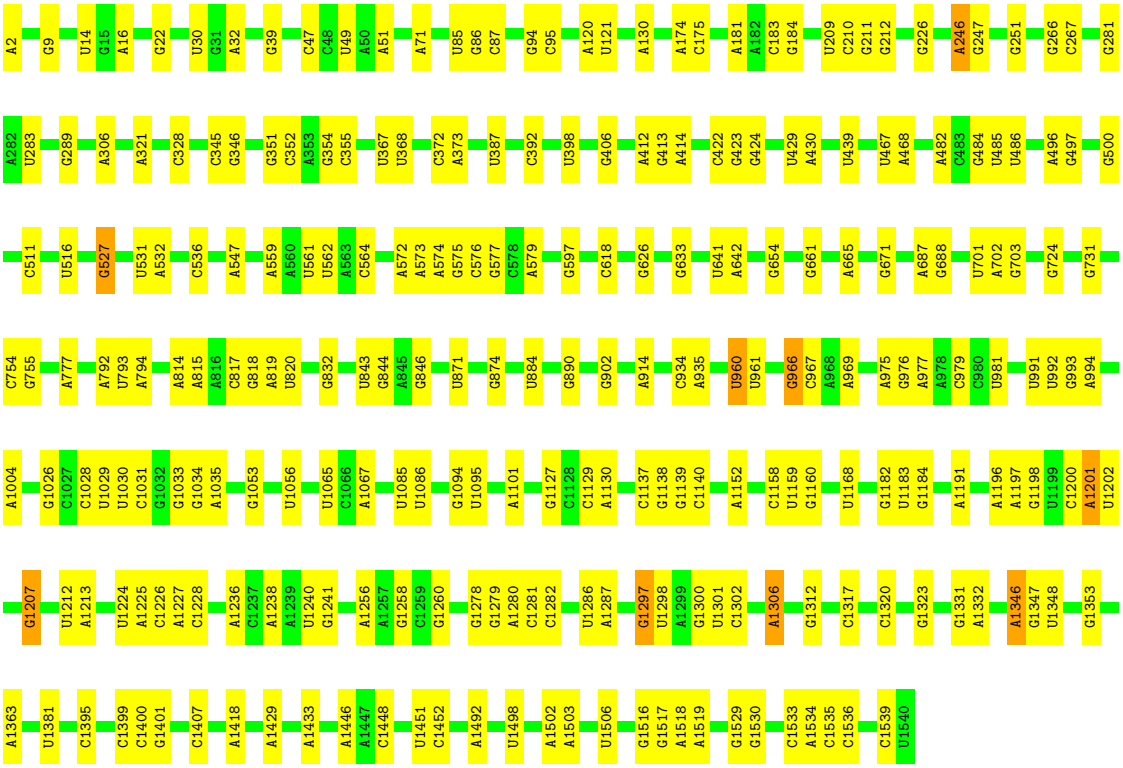
3 Residue-property plots (i)

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

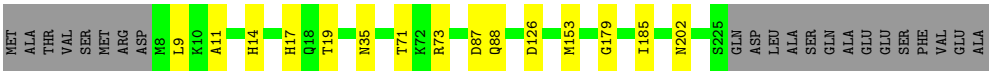
Chain a:





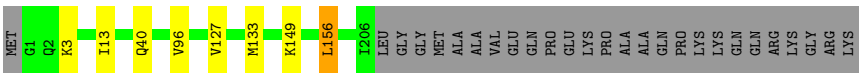
• Molecule 2: 30S ribosomal protein S2

Chain b:



• Molecule 3: 30S ribosomal protein S3

Chain c:



• Molecule 4: 30S ribosomal protein S4

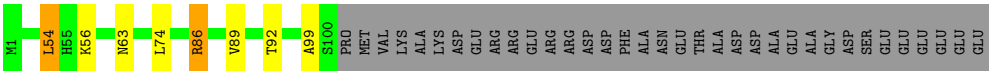
Chain d:

• Molecule 5: 30S ribosomal protein S5

Chain e:

• Molecule 6: 30S ribosomal protein S6

Chain f:

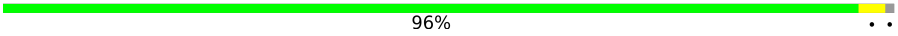


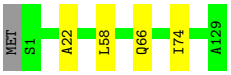
• Molecule 7: 30S ribosomal protein S7

Chain g:

• Molecule 8: 30S ribosomal protein S8

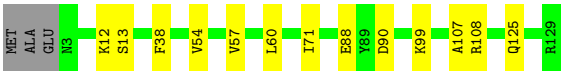
Chain h:





• Molecule 9: 30S ribosomal protein S9

Chain i:

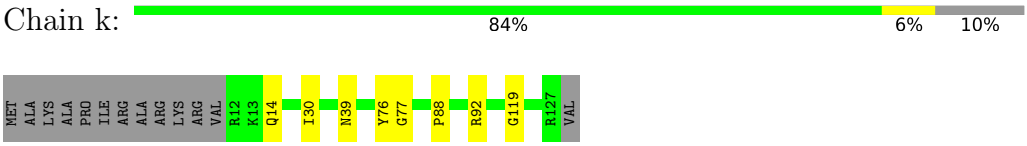


• Molecule 10: 30S ribosomal protein S10

Chain j:

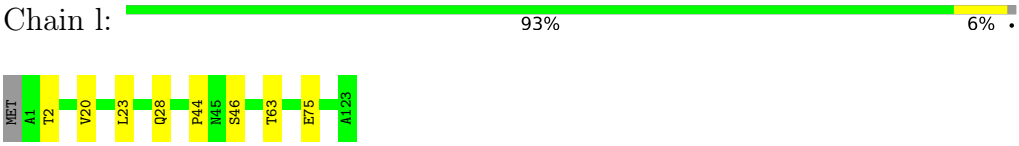
• Molecule 11: 30S ribosomal protein S11

Chain k:



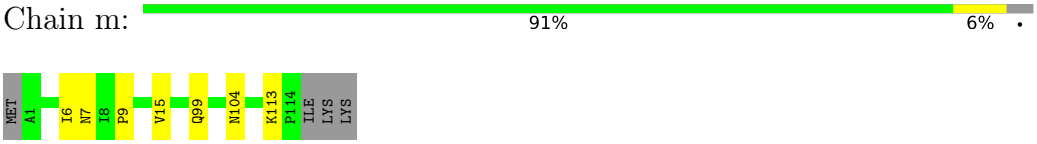
• Molecule 12: 30S ribosomal protein S12

Chain l:



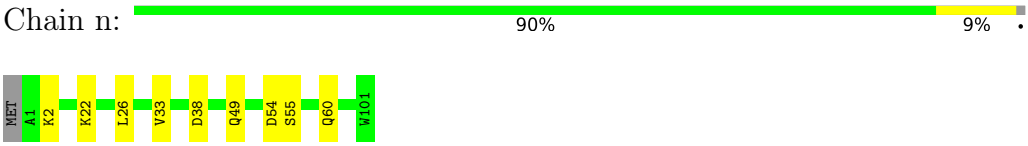
• Molecule 13: 30S ribosomal protein S13

Chain m:



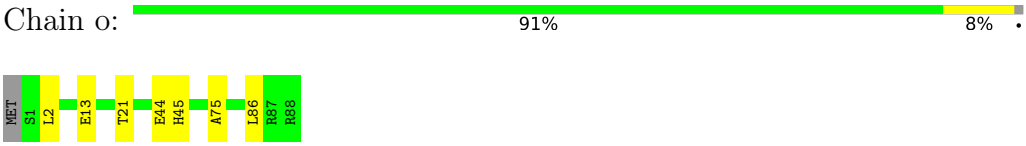
• Molecule 14: 30S ribosomal protein S14

Chain n:



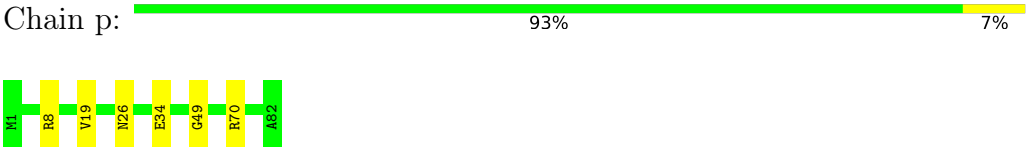
• Molecule 15: 30S ribosomal protein S15

Chain o:



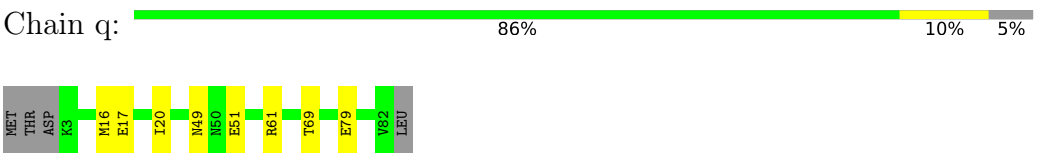
• Molecule 16: 30S ribosomal protein S16

Chain p:



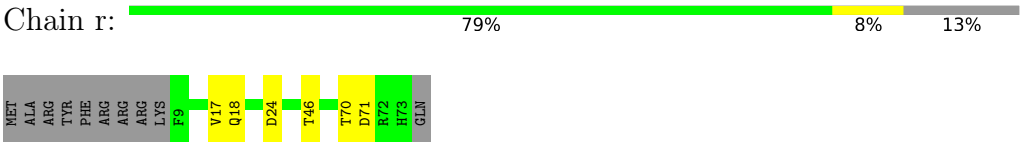
• Molecule 17: 30S ribosomal protein S17

Chain q:



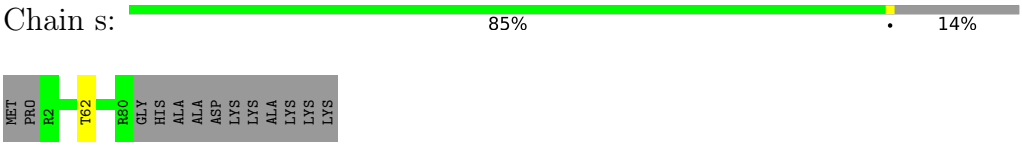
• Molecule 18: 30S ribosomal protein S18

Chain r:



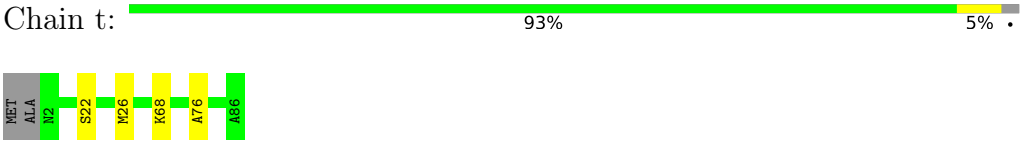
• Molecule 19: 30S ribosomal protein S19

Chain s:



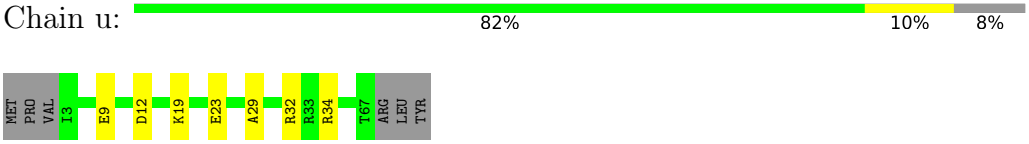
• Molecule 20: 30S ribosomal protein S20

Chain t:



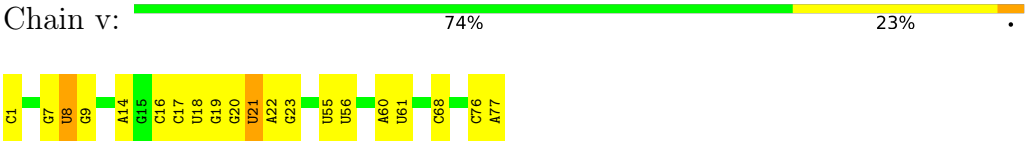
• Molecule 21: 30S ribosomal protein S21

Chain u:



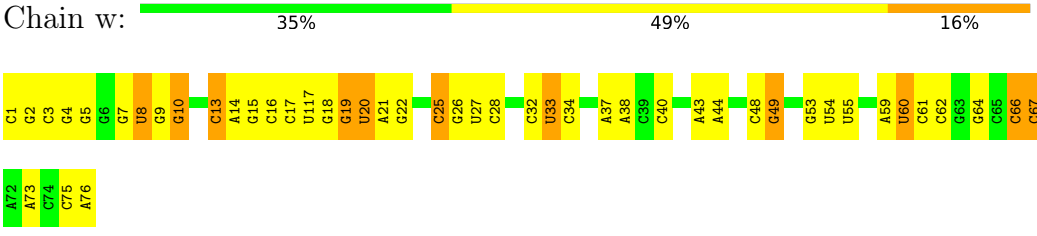
• Molecule 22: P-site fMet-tRNAfMet

Chain v:



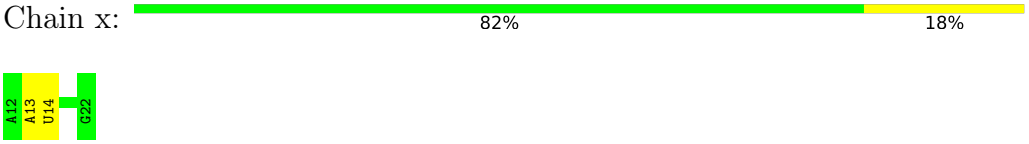
• Molecule 22: P-site fMet-tRNAfMet

Chain w:



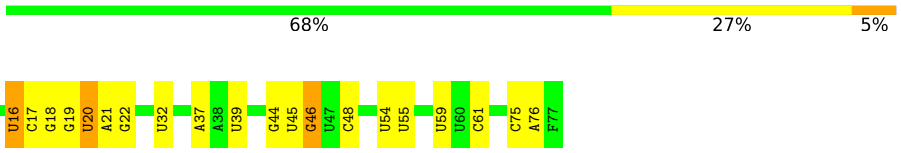
• Molecule 23: mRNA

Chain x:



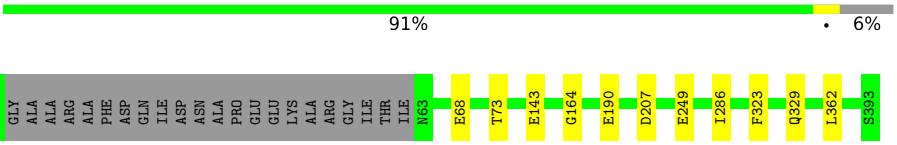
• Molecule 24: A/T-site Phe-tRNAPhe

Chain y:



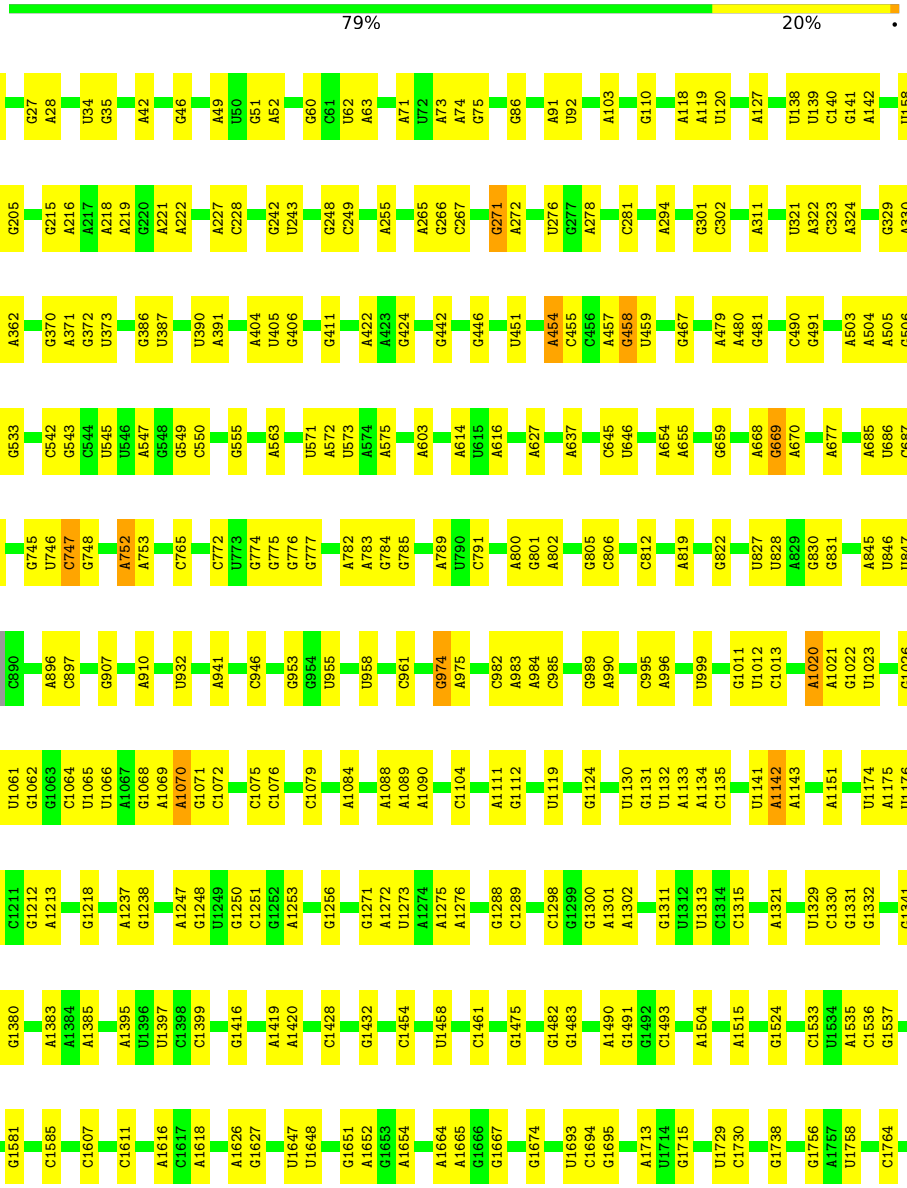
• Molecule 25: Elongation factor Tu 2

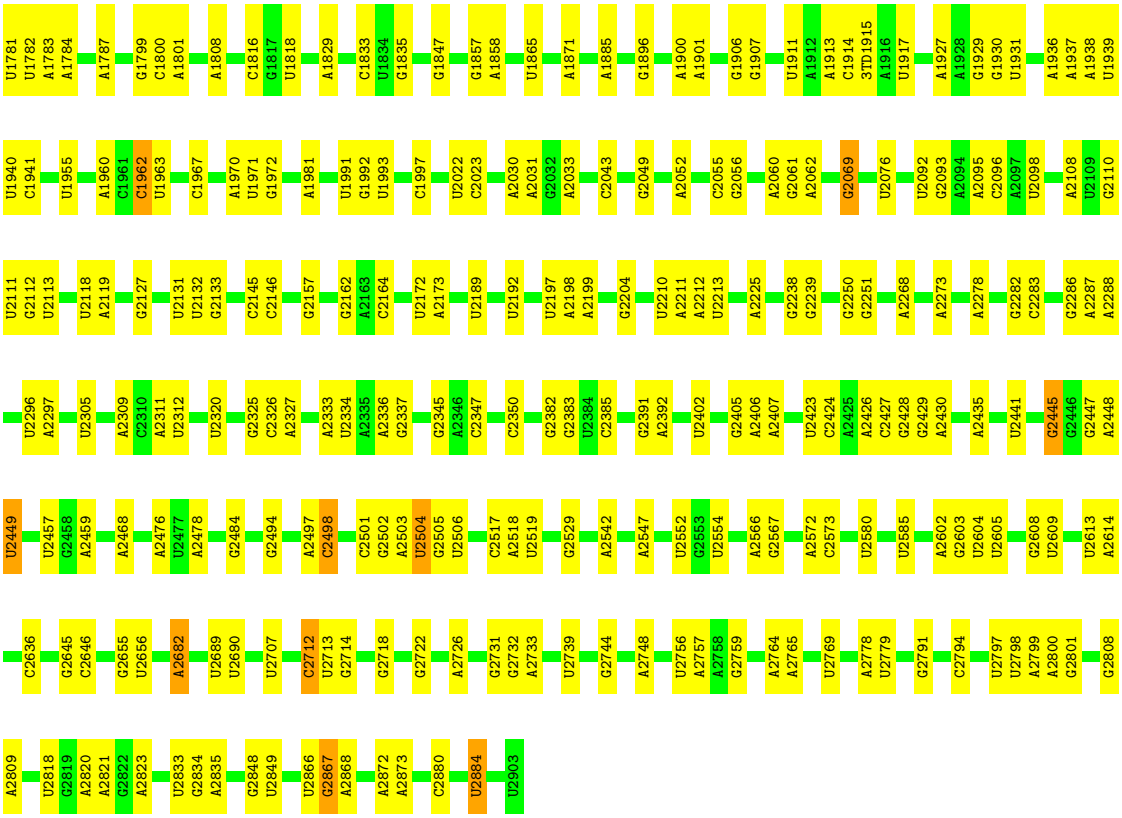
Chain z:



• Molecule 26: 23S ribosomal RNA

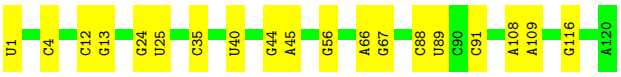
Chain A:





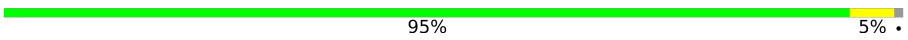
• Molecule 27: 5S ribosomal RNA

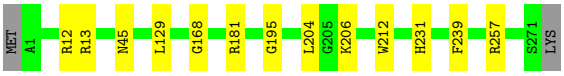
Chain B:



• Molecule 28: 50S ribosomal protein L2

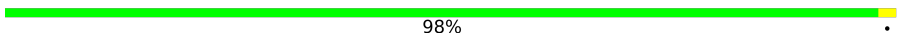
Chain C:





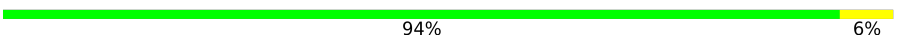
• Molecule 29: 50S ribosomal protein L3

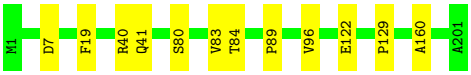
Chain D:



• Molecule 30: 50S ribosomal protein L4

Chain E:



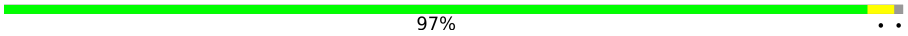


• Molecule 31: 50S ribosomal protein L5

Chain F:

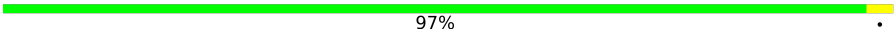
• Molecule 32: 50S ribosomal protein L6

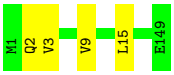
Chain G:



• Molecule 33: 50S ribosomal protein L9

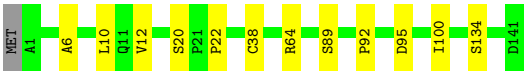
Chain H:





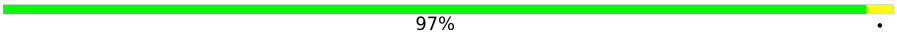
• Molecule 34: 50S ribosomal protein L11

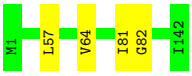
Chain I:



• Molecule 35: 50S ribosomal protein L13

Chain J:



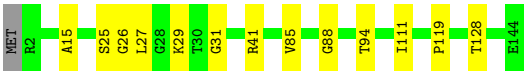


• Molecule 36: 50S ribosomal protein L14

Chain K:

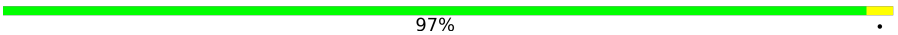
• Molecule 37: 50S ribosomal protein L15

Chain L:



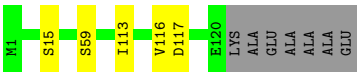
• Molecule 38: 50S ribosomal protein L16

Chain M:



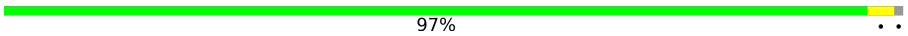
• Molecule 39: 50S ribosomal protein L17

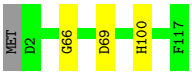
Chain N:



• Molecule 40: 50S ribosomal protein L18

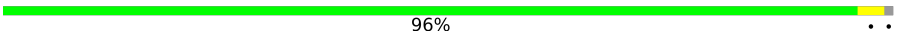
Chain O:

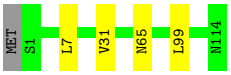




• Molecule 41: 50S ribosomal protein L19

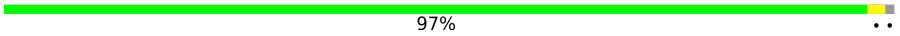
Chain P:

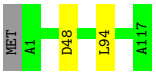




• Molecule 42: 50S ribosomal protein L20

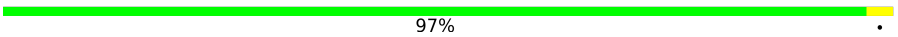
Chain Q:





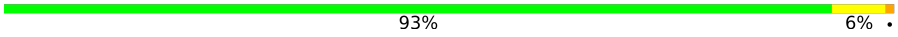
• Molecule 43: 50S ribosomal protein L21

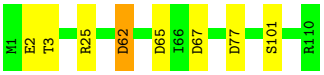
Chain R:



• Molecule 44: 50S ribosomal protein L22

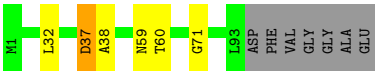
Chain S:





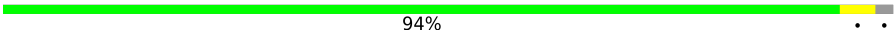
• Molecule 45: 50S ribosomal protein L23

Chain T:



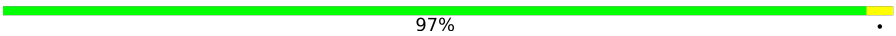
• Molecule 46: 50S ribosomal protein L24

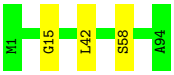
Chain U:



• Molecule 47: 50S ribosomal protein L25

Chain V:



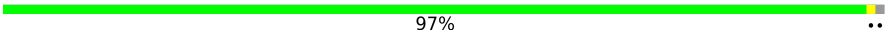


• Molecule 48: 50S ribosomal protein L27

Chain W:

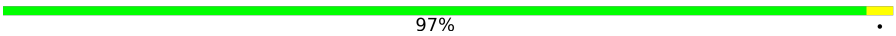
• Molecule 49: 50S ribosomal protein L28

Chain X:



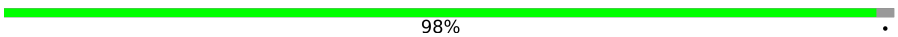
• Molecule 50: 50S ribosomal protein L29

Chain Y:



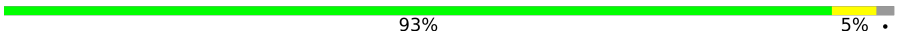
• Molecule 51: 50S ribosomal protein L30

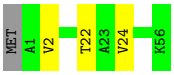
Chain Z:



• Molecule 52: 50S ribosomal protein L32

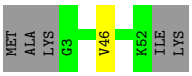
Chain 0:





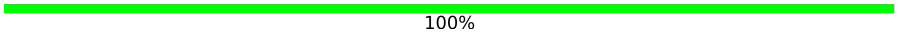
• Molecule 53: 50S ribosomal protein L33

Chain 1:



• Molecule 54: 50S ribosomal protein L34

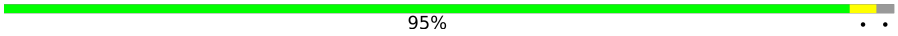
Chain 2:



There are no outlier residues recorded for this chain.

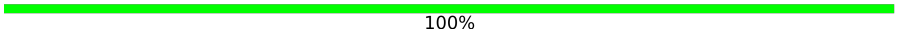
• Molecule 55: 50S ribosomal protein L35

Chain 3:



• Molecule 56: 50S ribosomal protein L36

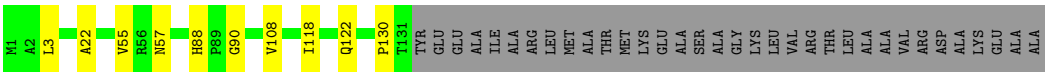
Chain 4:



There are no outlier residues recorded for this chain.

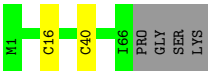
• Molecule 57: 50S ribosomal protein L10

Chain 5:



• Molecule 58: 50S ribosomal protein L31

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	417201	Depositor
Resolution determination method	Not provided	
CTF correction method	LOCAL CTF CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	192000	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, MA6, 3TD, MG, 4OC, NA, ZN, 7MG, KIR, 2MG, PSU, 5MU, 6MZ, 1MG, MIA, 2MA, UR3, OMG, CL, GDP, 5MC, H2U, FME, OMC, OMU

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	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
2	b	0.30	0/1735	0.44	0/2338
3	c	0.32	0/1651	0.46	0/2225
4	d	0.28	0/1665	0.44	0/2227
5	e	0.31	0/1154	0.46	0/1554
6	f	0.35	0/835	0.48	0/1128
7	g	0.36	0/1195	0.50	0/1602
8	h	0.27	0/989	0.45	0/1326
9	i	0.27	0/1034	0.45	0/1375
10	j	0.36	0/796	0.54	0/1077
11	k	0.28	0/885	0.48	0/1195
12	l	0.29	0/969	0.47	0/1300
13	m	0.36	0/892	0.50	0/1193
14	n	0.27	0/811	0.40	0/1081
15	o	0.32	0/722	0.44	0/964
16	p	0.33	0/659	0.45	0/884
17	q	0.27	0/657	0.46	0/881
18	r	0.28	0/511	0.43	0/689
19	s	0.28	0/652	0.44	0/877
20	t	0.38	0/671	0.48	0/888
21	u	0.29	0/500	0.42	0/668
22	v	0.41	1/1747 (0.1%)	0.82	0/2721
22	w	0.98	1/1747 (0.1%)	1.40	24/2721 (0.9%)
23	x	0.62	1/261 (0.4%)	0.85	0/404
24	y	0.39	1/1618 (0.1%)	0.81	0/2514
25	z	0.34	0/2935	0.47	0/3970
26	A	0.46	1/69174 (0.0%)	0.90	50/107910 (0.0%)
27	B	0.38	1/2876 (0.0%)	0.86	0/4483
28	C	0.31	0/2121	0.47	0/2852
29	D	0.35	0/1586	0.48	0/2134
30	E	0.26	0/1571	0.41	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	F	0.30	0/1434	0.47	0/1926
32	G	0.35	0/1343	0.47	0/1816
33	H	0.23	0/1122	0.40	0/1515
34	I	0.23	0/1046	0.44	0/1410
35	J	0.29	0/1152	0.43	0/1551
36	K	0.28	0/947	0.41	0/1268
37	L	0.26	0/1054	0.45	0/1403
38	M	0.32	0/1093	0.46	0/1460
39	N	0.28	0/973	0.44	0/1301
40	O	0.33	0/902	0.44	0/1209
41	P	0.28	0/929	0.43	0/1242
42	Q	0.34	0/960	0.43	0/1278
43	R	0.34	0/829	0.52	0/1107
44	S	0.28	0/864	0.47	0/1156
45	T	0.29	0/744	0.45	0/994
46	U	0.35	0/787	0.44	0/1051
47	V	0.31	0/766	0.45	0/1025
48	W	0.33	0/582	0.47	0/769
49	X	0.28	0/635	0.40	0/848
50	Y	0.33	0/510	0.45	0/677
51	Z	0.25	0/453	0.41	0/605
52	0	0.26	0/450	0.41	0/599
53	1	0.26	0/416	0.41	0/554
54	2	0.29	0/380	0.44	0/498
55	3	0.27	0/513	0.43	0/676
56	4	0.28	0/303	0.40	0/397
57	5	0.25	0/1001	0.45	0/1350
58	6	0.33	0/531	0.54	0/709
All	All	0.41	7/164039 (0.0%)	0.80	86/244934 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	1	C	OP3-P	-10.97	1.48	1.61
27	B	1	U	OP3-P	-10.59	1.48	1.61
26	A	1	G	OP3-P	-10.58	1.48	1.61
22	v	1	C	OP3-P	-10.56	1.48	1.61
1	a	2	A	OP3-P	-10.52	1.48	1.61

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	974	G	N1-C6-O6	9.46	125.57	119.90
26	A	1936	A	N1-C6-N6	9.14	124.09	118.60
22	w	13	C	C6-N1-C2	-8.20	117.02	120.30
22	w	62	C	C6-N1-C2	-8.13	117.05	120.30
22	w	62	C	C5-C6-N1	7.73	124.87	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	2 9
3	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	15 45
4	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	2 8
5	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	1 5
6	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1 4
7	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1 3
8	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	6 22
9	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1 4
10	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1 4
11	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2 6
12	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3 11
13	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	2 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2 7
15	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	1 5
16	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5 21
17	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1 4
18	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1 2
19	s	77/92 (84%)	66 (86%)	11 (14%)	0	100 100
20	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	6 22
21	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1 2
25	z	368/393 (94%)	327 (89%)	35 (10%)	6 (2%)	9 32
28	C	269/273 (98%)	243 (90%)	21 (8%)	5 (2%)	8 28
29	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	15 45
30	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	3 14
31	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3 15
32	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	4 18
33	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	5 19
34	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1 3
35	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11 36
36	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	5 21
37	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1 2
38	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	6 24
39	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	5 21
40	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	17 48
41	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	17 48
42	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100 100
43	R	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	7 27
44	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2 5
45	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	4 15
46	U	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	4 17
47	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	6 24
48	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	11 36
49	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	12 37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9 32
51	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
52	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	8 28
53	1	48/55 (87%)	43 (90%)	5 (10%)	0	100 100
54	2	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
55	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9 32
56	4	36/38 (95%)	28 (78%)	8 (22%)	0	100 100
57	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2 6
58	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	9 32
All	All	6215/6613 (94%)	5318 (86%)	691 (11%)	206 (3%)	6 15

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
5	e	122	VAL
6	f	63	ASN
9	i	12	LYS
9	i	71	ILE

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	b	180/198 (91%)	175 (97%)	5 (3%)	43 76
3	c	170/190 (90%)	163 (96%)	7 (4%)	30 64
4	d	172/173 (99%)	166 (96%)	6 (4%)	36 70
5	e	114/126 (90%)	105 (92%)	9 (8%)	12 34
6	f	87/116 (75%)	83 (95%)	4 (5%)	27 60
7	g	124/147 (84%)	122 (98%)	2 (2%)	62 86
8	h	104/105 (99%)	103 (99%)	1 (1%)	76 92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	105/107 (98%)	100 (95%)	5 (5%)	25	58
10	j	86/90 (96%)	84 (98%)	2 (2%)	50	80
11	k	89/99 (90%)	87 (98%)	2 (2%)	52	81
12	l	103/104 (99%)	100 (97%)	3 (3%)	42	76
13	m	92/96 (96%)	90 (98%)	2 (2%)	52	81
14	n	79/84 (94%)	75 (95%)	4 (5%)	24	56
15	o	76/77 (99%)	74 (97%)	2 (3%)	46	77
16	p	65/65 (100%)	61 (94%)	4 (6%)	18	47
17	q	74/78 (95%)	71 (96%)	3 (4%)	30	64
18	r	48/65 (74%)	47 (98%)	1 (2%)	53	81
19	s	70/79 (89%)	69 (99%)	1 (1%)	67	89
20	t	65/66 (98%)	63 (97%)	2 (3%)	40	74
21	u	44/61 (72%)	42 (96%)	2 (4%)	27	61
25	z	311/326 (95%)	304 (98%)	7 (2%)	50	80
28	C	216/218 (99%)	208 (96%)	8 (4%)	34	68
29	D	164/164 (100%)	161 (98%)	3 (2%)	59	85
30	E	165/165 (100%)	160 (97%)	5 (3%)	41	75
31	F	148/150 (99%)	141 (95%)	7 (5%)	26	59
32	G	137/138 (99%)	137 (100%)	0	100	100
33	H	114/114 (100%)	114 (100%)	0	100	100
34	I	109/110 (99%)	106 (97%)	3 (3%)	43	76
35	J	116/116 (100%)	114 (98%)	2 (2%)	60	86
36	K	103/104 (99%)	98 (95%)	5 (5%)	25	57
37	L	102/103 (99%)	100 (98%)	2 (2%)	55	82
38	M	109/109 (100%)	108 (99%)	1 (1%)	78	93
39	N	100/103 (97%)	98 (98%)	2 (2%)	55	82
40	O	86/87 (99%)	84 (98%)	2 (2%)	50	80
41	P	99/100 (99%)	96 (97%)	3 (3%)	41	75
42	Q	89/90 (99%)	87 (98%)	2 (2%)	52	81
43	R	84/84 (100%)	83 (99%)	1 (1%)	71	91
44	S	93/93 (100%)	90 (97%)	3 (3%)	39	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	T	80/84 (95%)	76 (95%)	4 (5%)	24 57
46	U	83/85 (98%)	82 (99%)	1 (1%)	71 91
47	V	78/78 (100%)	77 (99%)	1 (1%)	69 90
48	W	57/63 (90%)	56 (98%)	1 (2%)	59 85
49	X	67/68 (98%)	67 (100%)	0	100 100
50	Y	55/55 (100%)	54 (98%)	1 (2%)	59 85
51	Z	48/49 (98%)	48 (100%)	0	100 100
52	0	47/48 (98%)	45 (96%)	2 (4%)	29 62
53	1	45/49 (92%)	44 (98%)	1 (2%)	52 81
54	2	38/38 (100%)	38 (100%)	0	100 100
55	3	51/52 (98%)	50 (98%)	1 (2%)	55 82
56	4	34/34 (100%)	34 (100%)	0	100 100
57	5	100/123 (81%)	97 (97%)	3 (3%)	41 75
58	6	59/62 (95%)	58 (98%)	1 (2%)	60 86
All	All	5134/5388 (95%)	4995 (97%)	139 (3%)	48 77

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	P	31	VAL
43	R	22	LEU
50	Y	40	SER
14	n	26	LEU
13	m	99	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
35	J	40	HIS
42	Q	71	ASN
50	Y	41	HIS
16	p	26	ASN
15	o	45	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	242 (15%)	0
22	v	76/77 (98%)	17 (22%)	0
22	w	76/77 (98%)	43 (56%)	0
23	x	10/11 (90%)	1 (10%)	0
24	y	74/77 (96%)	19 (25%)	0
26	A	2894/2903 (99%)	542 (18%)	90 (3%)
27	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4784/4804 (99%)	881 (18%)	94 (1%)

5 of 881 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A

5 of 94 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	1399	C
26	A	2282	G
26	A	1626	A
26	A	1930	G
26	A	2333	A

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

52 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	$\#\|Z\| > 2$
1	MA6	a	1518	1	18,26,27	1.13	2 (11%)	19,38,41	1.90	4 (21%)
24	7MG	y	46	24	22,26,27	1.32	4 (18%)	29,39,42	2.53	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	a	516	1,59	18,21,22	1.45	4 (22%)	22,30,33	2.13	5 (22%)
22	5MU	w	54	22	19,22,23	1.27	3 (15%)	28,32,35	2.32	10 (35%)
26	OMU	A	2552	26	19,22,23	1.22	3 (15%)	26,31,34	2.17	7 (26%)
26	PSU	A	2605	26	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
26	1MG	A	745	26	18,26,27	0.80	0	19,39,42	1.07	1 (5%)
26	2MA	A	2503	59,26	17,25,26	1.00	1 (5%)	17,37,40	0.98	2 (11%)
1	2MG	a	966	1	18,26,27	0.88	1 (5%)	16,38,41	1.17	2 (12%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	0.91	0
26	5MC	A	747	26	18,22,23	0.96	2 (11%)	26,32,35	1.38	3 (11%)
26	OMG	A	2251	22,26	18,26,27	1.03	1 (5%)	19,38,41	1.01	1 (5%)
26	PSU	A	2457	26	18,21,22	1.35	2 (11%)	22,30,33	2.06	4 (18%)
24	H2U	y	20	24	18,21,22	0.95	2 (11%)	21,30,33	2.23	1 (4%)
24	4SU	y	8	24	18,21,22	1.76	4 (22%)	26,30,33	2.37	5 (19%)
26	PSU	A	1917	26	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	5MC	a	967	1	18,22,23	0.98	1 (5%)	26,32,35	1.08	2 (7%)
24	PSU	y	55	24	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
26	5MU	A	1939	26	19,22,23	1.37	4 (21%)	28,32,35	2.26	6 (21%)
26	5MC	A	1962	26	18,22,23	0.98	2 (11%)	26,32,35	1.10	2 (7%)
22	H2U	v	21	22	18,21,22	0.92	2 (11%)	21,30,33	1.57	2 (9%)
24	PSU	y	39	24	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
1	2MG	a	1516	1	18,26,27	0.87	1 (5%)	16,38,41	1.12	2 (12%)
26	2MG	A	1835	26	18,26,27	1.01	1 (5%)	16,38,41	1.25	3 (18%)
24	MIA	y	37	24	24,31,32	2.26	3 (12%)	26,44,47	2.83	9 (34%)
26	7MG	A	2069	26	22,26,27	1.40	4 (18%)	29,39,42	2.50	7 (24%)
26	6MZ	A	2030	26	18,25,26	0.92	1 (5%)	16,36,39	2.49	4 (25%)
1	5MC	a	1407	1	18,22,23	0.95	2 (11%)	26,32,35	1.16	3 (11%)
26	6MZ	A	1618	26	18,25,26	0.98	1 (5%)	16,36,39	2.26	4 (25%)
1	MA6	a	1519	1	18,26,27	0.95	1 (5%)	19,38,41	1.89	6 (31%)
1	UR3	a	1498	1	19,22,23	0.93	0	26,32,35	1.59	3 (11%)
22	4SU	v	8	22	18,21,22	1.68	4 (22%)	26,30,33	2.28	5 (19%)
26	PSU	A	746	59,26	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
26	OMC	A	2498	59,26	19,22,23	0.83	1 (5%)	26,31,34	0.87	0
26	PSU	A	2604	26	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
1	2MG	a	1207	1	18,26,27	0.96	1 (5%)	16,38,41	1.15	2 (12%)
26	2MG	A	2445	26	18,26,27	1.01	1 (5%)	16,38,41	1.14	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PSU	A	1911	26	18,21,22	1.33	2 (11%)	22,30,33	1.96	4 (18%)
22	H2U	w	20	22	18,21,22	1.33	3 (16%)	21,30,33	2.54	4 (19%)
1	7MG	a	527	1	22,26,27	1.37	4 (18%)	29,39,42	2.45	7 (24%)
24	PSU	y	32	24	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
22	5MU	v	55	22	19,22,23	1.38	4 (21%)	28,32,35	2.23	5 (17%)
22	PSU	v	56	22	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
22	4SU	w	8	22	18,21,22	1.79	4 (22%)	26,30,33	2.33	4 (15%)
22	PSU	w	55	22	18,21,22	1.49	3 (16%)	22,30,33	2.14	5 (22%)
26	PSU	A	2504	26	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
26	3TD	A	1915	26	18,22,23	1.22	2 (11%)	22,32,35	1.92	3 (13%)
26	H2U	A	2449	26	18,21,22	0.91	2 (11%)	21,30,33	1.67	3 (14%)
26	PSU	A	955	26	18,21,22	1.42	4 (22%)	22,30,33	2.00	4 (18%)
24	H2U	y	16	24	18,21,22	0.97	2 (11%)	21,30,33	1.45	2 (9%)
26	PSU	A	2580	26	18,21,22	1.43	2 (11%)	22,30,33	2.02	4 (18%)
24	5MU	y	54	24	19,22,23	1.39	5 (26%)	28,32,35	2.22	7 (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
1	MA6	a	1518	1	-	4/7/29/30	0/3/3/3
24	7MG	y	46	24	-	3/7/37/38	0/3/3/3
1	PSU	a	516	1,59	-	2/7/25/26	0/2/2/2
22	5MU	w	54	22	-	2/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
26	2MA	A	2503	59,26	-	1/3/25/26	0/3/3/3
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
26	5MC	A	747	26	-	0/7/25/26	0/2/2/2
26	OMG	A	2251	22,26	-	0/5/27/28	0/3/3/3
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
24	H2U	y	20	24	-	5/7/38/39	0/2/2/2
24	4SU	y	8	24	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	1/7/25/26	0/2/2/2
22	H2U	v	21	22	-	1/7/38/39	0/2/2/2
24	PSU	y	39	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
24	MIA	y	37	24	-	3/11/33/34	0/3/3/3
26	7MG	A	2069	26	-	1/7/37/38	0/3/3/3
26	6MZ	A	2030	26	-	2/5/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
26	6MZ	A	1618	26	-	0/5/27/28	0/3/3/3
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
26	PSU	A	746	59,26	-	1/7/25/26	0/2/2/2
26	OMC	A	2498	59,26	-	1/9/27/28	0/2/2/2
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	2/5/27/28	0/3/3/3
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
22	H2U	w	20	22	-	2/7/38/39	0/2/2/2
1	7MG	a	527	1	-	3/7/37/38	0/3/3/3
24	PSU	y	32	24	-	0/7/25/26	0/2/2/2
22	5MU	v	55	22	-	0/7/25/26	0/2/2/2
22	PSU	v	56	22	-	2/7/25/26	0/2/2/2
22	4SU	w	8	22	-	6/7/25/26	0/2/2/2
22	PSU	w	55	22	-	2/7/25/26	0/2/2/2
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	3/7/25/26	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
24	H2U	y	16	24	-	0/7/38/39	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	37	MIA	C2-S10	-7.22	1.69	1.75
24	y	37	MIA	C13-C14	7.20	1.53	1.32
24	y	8	4SU	C4-S4	-4.75	1.59	1.68
22	w	8	4SU	C4-S4	-4.60	1.59	1.68
22	v	8	4SU	C4-S4	-4.42	1.60	1.68

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	20	H2U	C4-N3-C2	-9.51	117.91	125.79
24	y	37	MIA	C12-C13-C14	-9.25	109.14	127.14
24	y	46	7MG	N9-C4-N3	8.84	138.69	125.47
22	w	20	H2U	C4-N3-C2	-8.60	118.66	125.79
26	A	2069	7MG	N9-C4-N3	8.59	138.32	125.47

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	7MG	C3'-C4'-C5'-O5'
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 342 ligands modelled in this entry, 339 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
63	GDP	z	402	59	24,30,30	0.90	1 (4%)	30,47,47	1.45	4 (13%)
61	FME	v	105	-	8,9,10	0.92	1 (12%)	7,9,11	1.50	1 (14%)
62	KIR	z	401	-	56,59,59	0.64	1 (1%)	62,84,84	1.76	14 (22%)

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
63	GDP	z	402	59	-	1/12/32/32	0/3/3/3
61	FME	v	105	-	-	3/7/9/11	-
62	KIR	z	401	-	-	23/54/98/98	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GDP	C6-N1	-2.27	1.34	1.37
62	z	401	KIR	C3-C2	2.14	1.49	1.43
61	v	105	FME	CA-N	2.11	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	z	401	KIR	C23-C22-C21	-6.01	118.50	127.32
62	z	401	KIR	C15-C14-C13	-4.56	107.29	114.64
63	z	402	GDP	PA-O3A-PB	-3.96	119.23	132.83
62	z	401	KIR	C44-C21-C22	-3.63	119.55	124.03
62	z	401	KIR	C5-C4-C3	-3.55	117.84	120.66

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	v	105	FME	O1-CN-N-CA
62	z	401	KIR	C17-C19-C20-C21
62	z	401	KIR	C42-C19-C20-C21

Continued on next page...

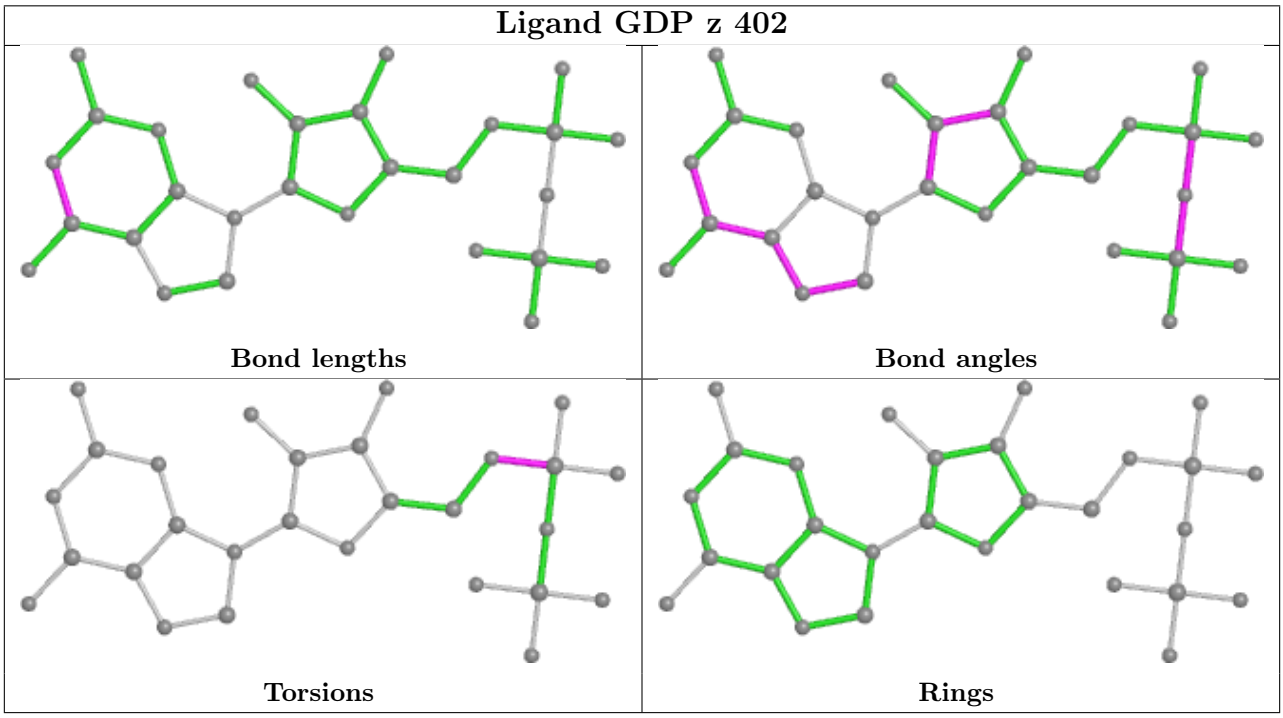
Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	z	401	KIR	C17-C19-C20-O20
62	z	401	KIR	C42-C19-C20-O20

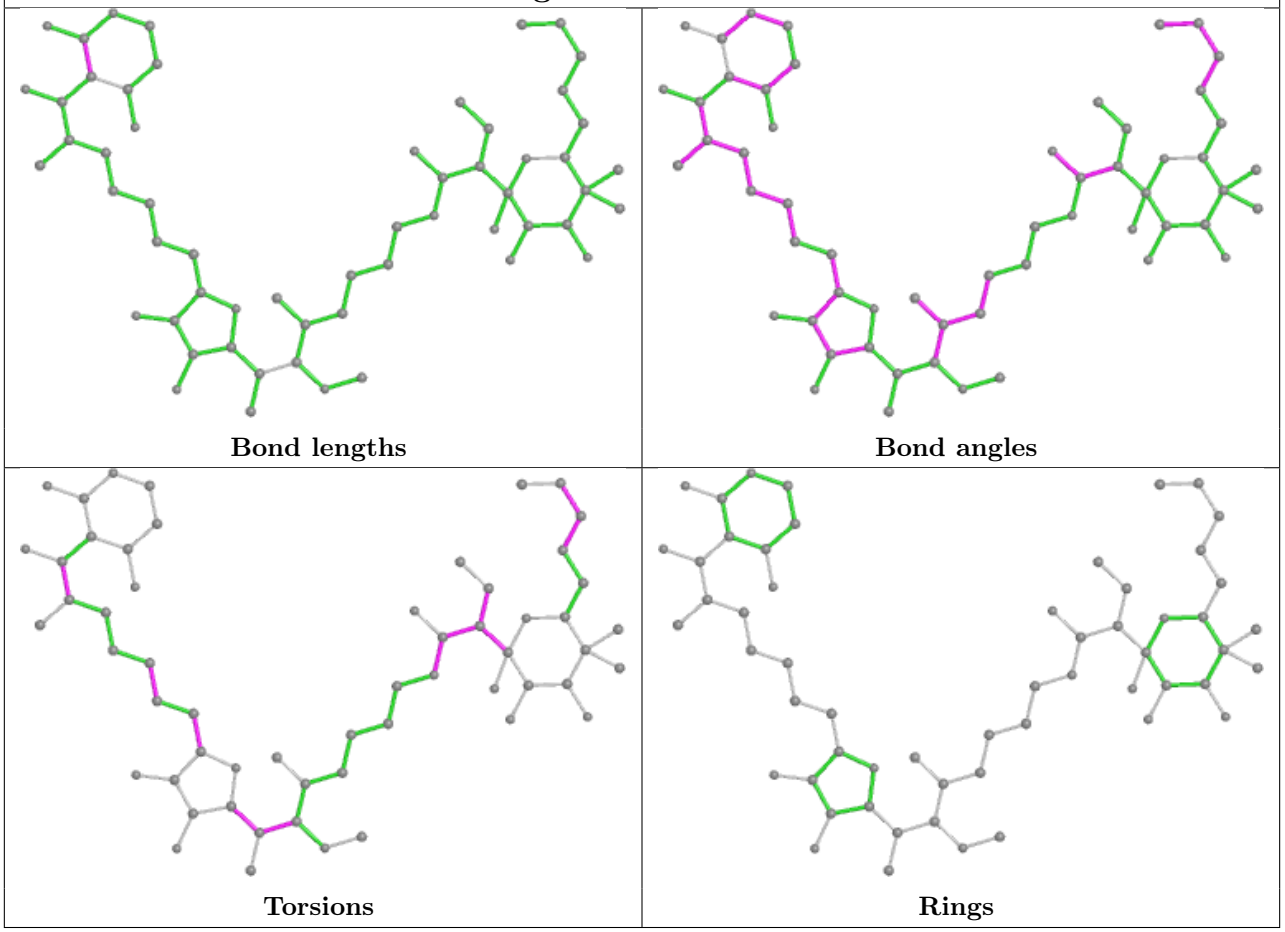
There are no ring outliers.

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 KIR z 401



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-2847. 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.