



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:12 PM 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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

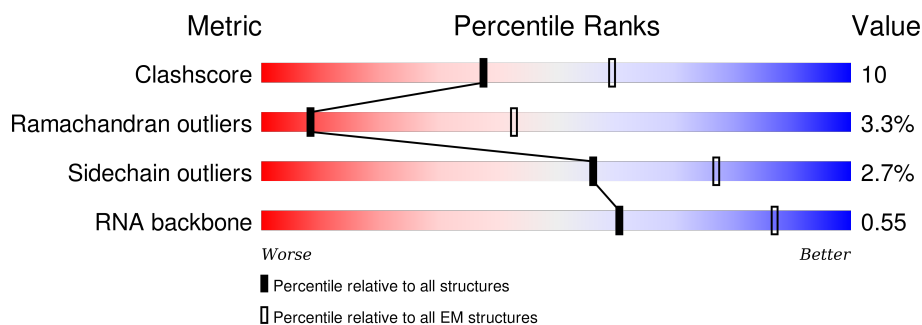
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.














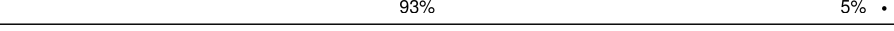







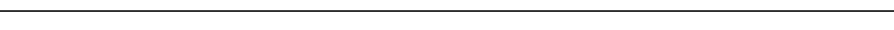

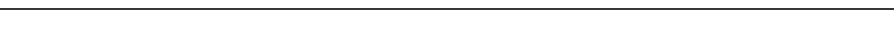
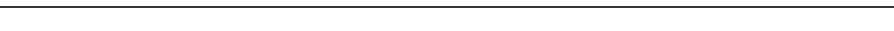


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	a	1539	84% 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% • •













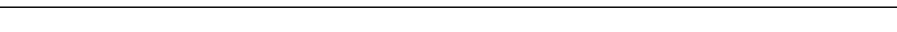

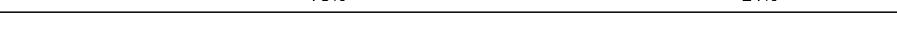

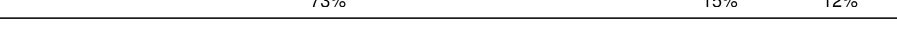








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Mol	Chain	Length	Quality of chain
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	102	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	v	78	
23	w	77	
24	x	11	
25	y	77	
26	z	393	
27	A	2903	
28	B	120	
29	C	273	
30	D	209	
31	E	201	
32	F	179	
33	G	177	

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Mol	Chain	Length	Quality of chain
34	H	149	 80% 18% .
35	I	142	 63% 33% . .
36	J	142	 73% 26% .
37	K	123	 68% 28% . .
38	L	144	 63% 34% . .
39	M	136	 75% 24% .
40	N	127	 68% 26% . 6%
41	O	117	 82% 16% . .
42	P	115	 79% 19% . .
43	Q	118	 75% 25% .
44	R	103	 80% 20%
45	S	110	 70% 27% .
46	T	100	 67% 23% . 7%
47	U	104	 73% 24% . .
48	V	94	 71% 28% .
49	W	85	 73% 15% 12%
50	X	78	 78% 19% . .
51	Y	63	 75% 24% .
52	Z	59	 80% 19% .
53	0	57	 68% 26% . .
54	1	55	 78% 13% 9%
55	2	46	 70% 30%
56	3	65	 72% 25% . .
57	4	38	 61% 39%
58	5	165	 52% 25% . 21%

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Mol	Chain	Length	Quality of chain
59	6	70	<div><div></div><div>71%</div><div>21%</div><div>• 6%</div></div>

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 152718 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
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

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

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

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

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

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

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

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

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

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

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

- 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
			505	318	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-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	78	Total	C	N	O	P	S	0	0
			1654	739	298	538	77	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	77	FME	-	initiating methionine	GB 147949

- Molecule 23 is a RNA chain called E-site tRNA^{fMet}.

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

- Molecule 24 is a RNA chain called mRNA.

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

- Molecule 25 is a RNA chain called A/T-site Phe-tRNA^{Phe}.

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

- Molecule 26 is a protein called Elongation factor Tu 2.

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

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 28 is a RNA chain called 5S ribosomal RNA (120-MER).

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	0	56	Total	C	N	O	S	0
			444	269	94	80	1	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 58 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 59 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	D	1	Total	Mg	0
			1	1	
60	B	7	Total	Mg	0
			7	7	

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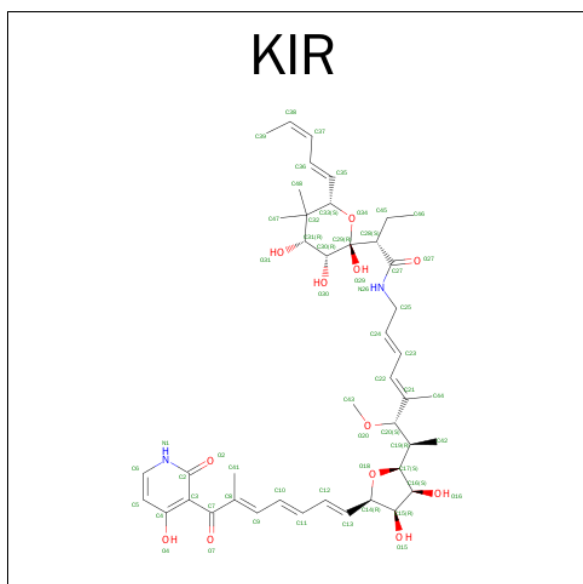
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Mol	Chain	Residues	Atoms		AltConf
60	a	83	Total	Mg	0
			83	83	
60	z	1	Total	Mg	0
			1	1	
60	A	234	Total	Mg	0
			234	234	
60	4	1	Total	Mg	0
			1	1	
60	v	4	Total	Mg	0
			4	4	
60	N	1	Total	Mg	0
			1	1	

- Molecule 61 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: C₄₃H₆₀N₂O₁₂).



- # GDP

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

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

- Molecule 66 is water.

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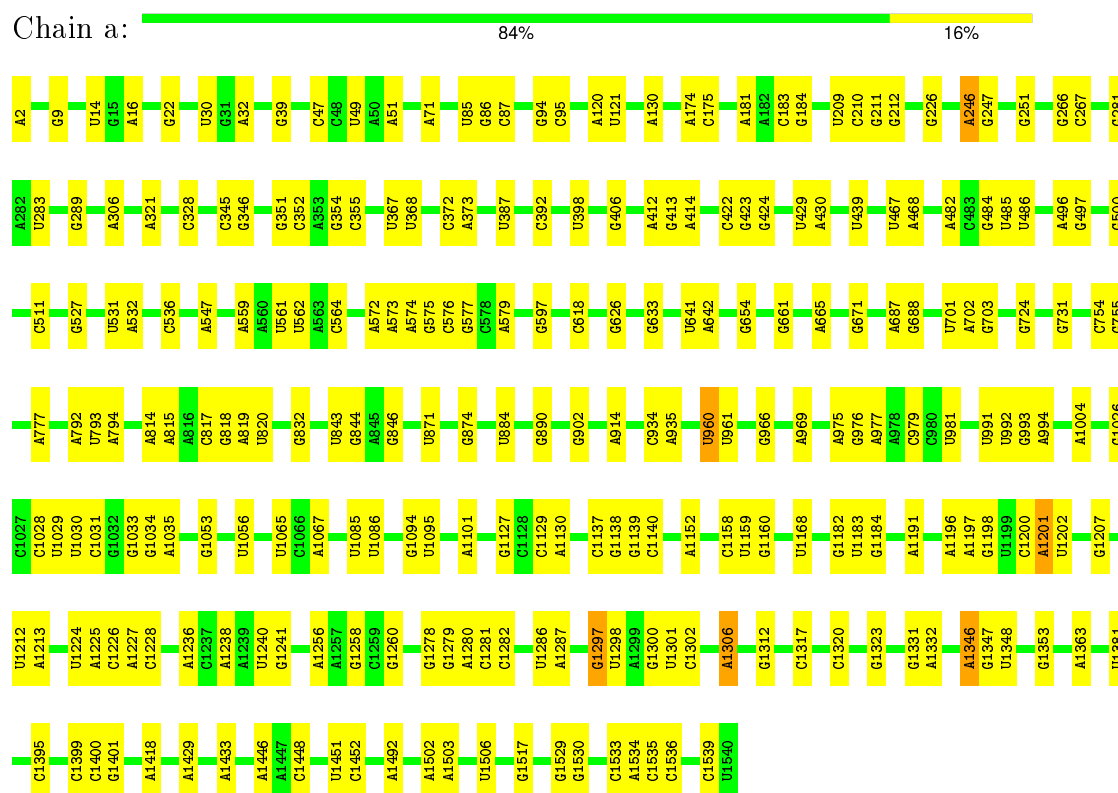
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Mol	Chain	Residues	Atoms		AltConf
66	A	9	Total 9	O 9	0
66	D	2	Total 2	O 2	0
66	K	1	Total 1	O 1	0

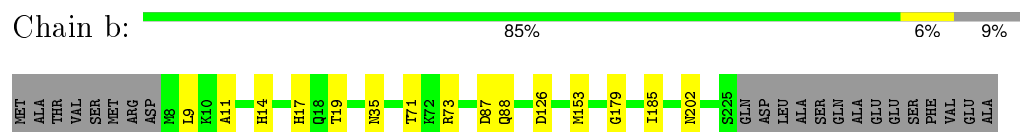
3 Residue-property plots

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

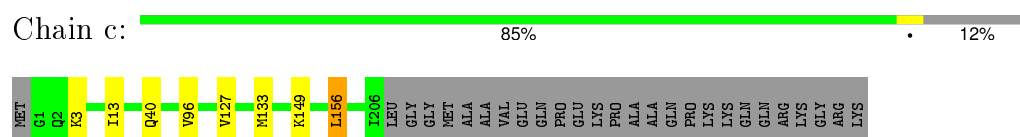
• Molecule 1: 16S ribosomal RNA



• Molecule 2: 30S ribosomal protein S2

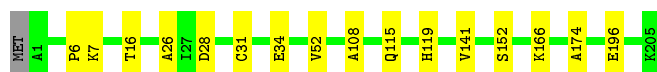


• Molecule 3: 30S ribosomal protein S3




• Molecule 4: 30S ribosomal protein S4

Chain d:  92% 8%



- Molecule 5: 30S ribosomal protein S5

Chain e:  84% 10% 6%




- Molecule 6: 30S ribosomal protein S6

Chain f:  68% 26%



- Molecule 7: 30S ribosomal protein S7

Chain g:  78% 7% 16%




- Molecule 8: 30S ribosomal protein S8

Chain h:  96%




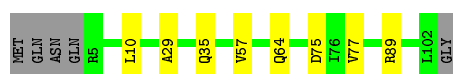
- Molecule 9: 30S ribosomal protein S9

Chain i:  88% 10%




- Molecule 10: 30S ribosomal protein S10

Chain j:  87% 8% 5%



- Molecule 11: 30S ribosomal protein S11

Chain k:  84% 6% 10%



- Molecule 12: 30S ribosomal protein S12

Chain l: 93% 6% .



- Molecule 13: 30S ribosomal protein S13

Chain m: 91% 6% .



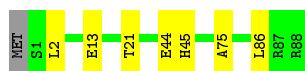
- Molecule 14: 30S ribosomal protein S14

Chain n: 90% 9% .



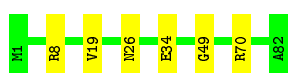
- Molecule 15: 30S ribosomal protein S15

Chain o: 91% 8% .



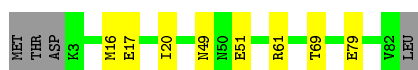
- Molecule 16: 30S ribosomal protein S16

Chain p: 93% 7% .



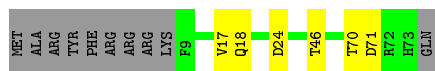
- Molecule 17: 30S ribosomal protein S17

Chain q: 86% 10% 5% .




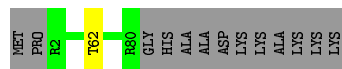
- Molecule 18: 30S ribosomal protein S18

Chain r: 79% 8% 13% .



- Molecule 19: 30S ribosomal protein S19

Chain s:  85% 14%




- Molecule 20: 30S ribosomal protein S20

Chain t:  93% 5%



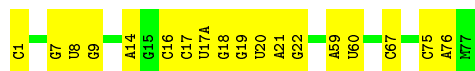
- Molecule 21: 30S ribosomal protein S21

Chain u:  82% 10% 8%



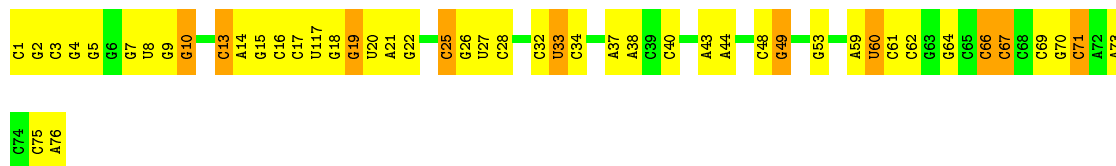
- Molecule 22: P-site fMet-tRNA^{fMet}

Chain v:  77% 23%




- Molecule 23: E-site tRNA^{fMet}

Chain w:  38% 49% 13%



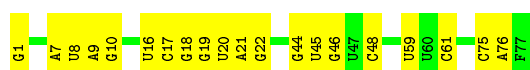
- Molecule 24: mRNA

Chain x:  82% 18%




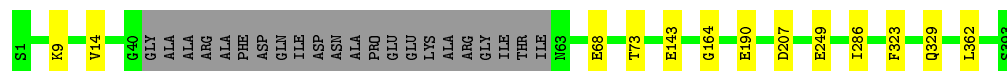
- Molecule 25: A/T-site Phe-tRNA^{Phe}

Chain y:  74% 26%



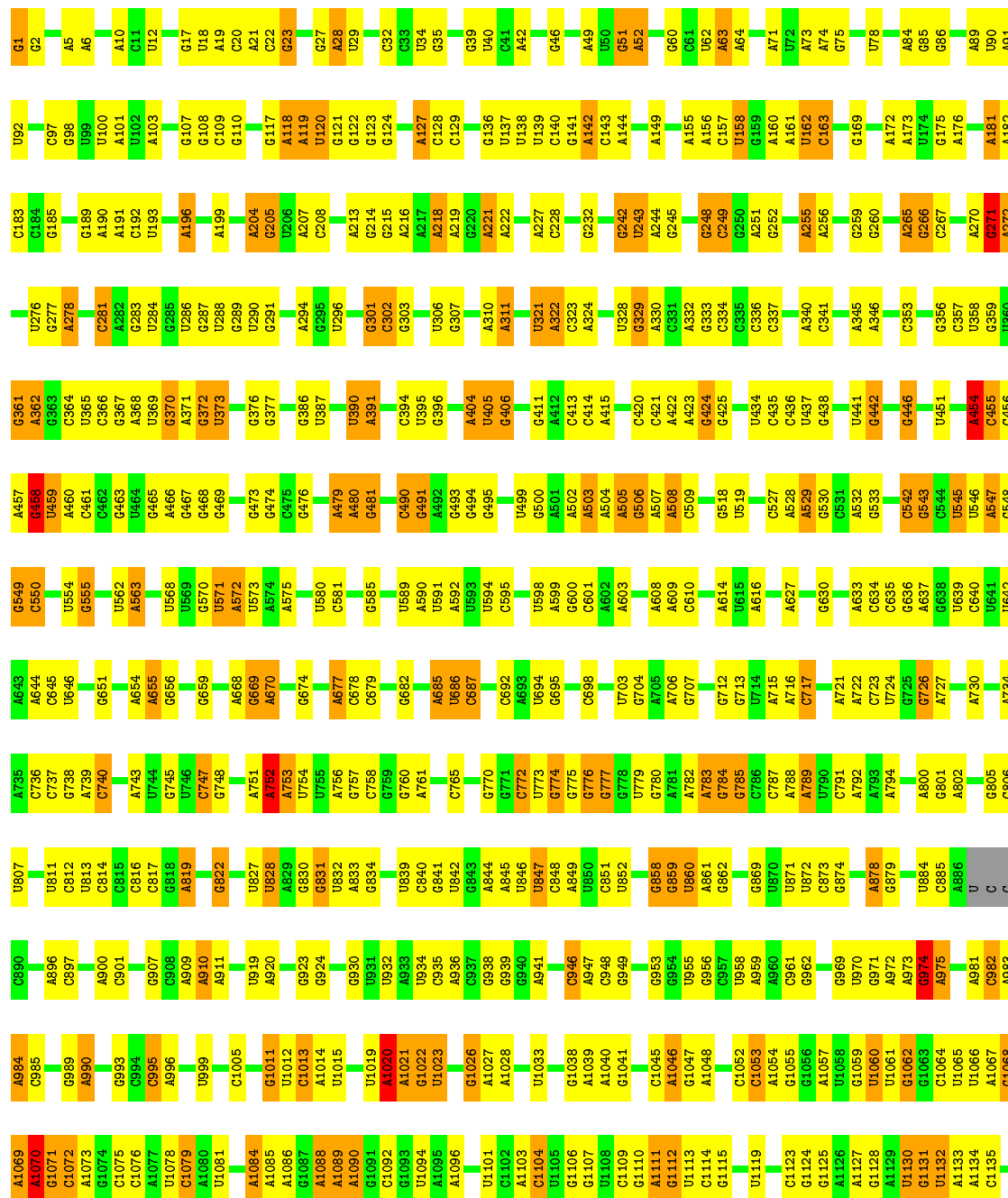
- Molecule 26: Elongation factor Tu 2

Chain z:  91% 6%

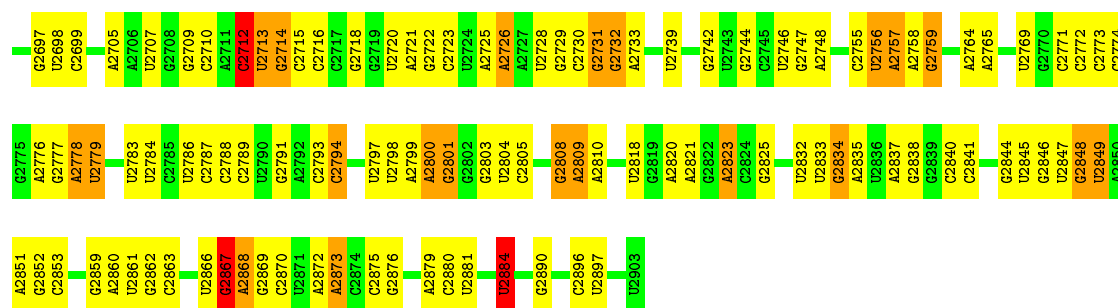


- Molecule 27: 23S ribosomal RNA

Chain A:  53% 37% 9%

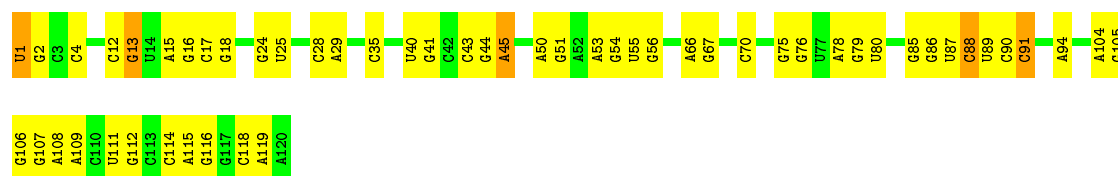


U2489	U2584	U2497	U2398	G2035	C1941	C1844	A1746	C1646	G1538	A1434			G1248	G1139
G2490	U2585	G2494	A2392	G2036	C1942	G1845	U1747	U1647	U1539	G1435	U1340	U1249	C1250	C1140
	A2587		C2394	G2207	U1943	G1846	C1748	G1649	U1542	U1443	A1342	G1251	A1142	A1141
A2497				G2208	G1945	A1848	U1751	G1651	G1543	G1444	G1343	G1252	A1143	
C2498	A2590	C2498	U2399	G2209	U1951	G1857	U1752	G1652	A1544		U1344	A1253		A1151
	G2591			G2210	U1952	A1858	G1753	A1652	A1548	G1447	C1345	G1256		C1152
G2592	G2592	U2402	U2308	G2211	A1953		A1754	G1653	A1549	G1448	U1352			C1153
	G2599		A2309	G2212	U1954	U1865	A1755	G1654	G1555	C1454		G1266	G1160	
G2593		G2405	G2310	U2220	U1955	A1866	G1756	A1664		U1458	G1361	U1267		
U2504	A2602	A2406	A2311	G2221	U1956	G1867	U1758	A1665	C1558		C1362	A1268	U1174	
G2505	G2603	A2407	U2312	G2222	C1957	G1868	A1759	G1666	U1559	C1461	C1363	G1270	A1175	
U2506		U2408	G2313	G2223	C1958	G1869	C1760	G1667			G1364	G1271	U1176	
		G2409		G2224	U1959	C1870					A1365	A1272	U1177	
				G2225	A1960	A1871	C1764	G1674	U1562	A1469	A1366	G1273	G1177	
				G2226	C1961	A1872	A1773		U1563	A1470	A1367	A1274	G1178	
				G2227	U1962	G1873			C1564	G1475	G1368	A1275	U1180	
				G2228	U1963		U1779	G1681	C1565	A1476	A1378	A1276	U1181	
				G2229	G1964	A1877	U1780	G1682	U1566	A1477		G1277	U1182	
				G2230	C1967	G1879	U1781	U1683	G1567	G1478	G1380	G1278	U1183	
				G2231		U1880	U1782	G1684	G1568			G1279	U1184	
				G2232	A1970	C1881	A1783	C1685	A1569	G1482	A1383		G1185	
				G2233	U1971	U1882	A1784			G1483	A1384	G1283	G1186	
				G2234	G1972	U1883			U1578		A1385		G1187	
				G2235	G1973	A1884	A1787	A1689	U1579	U1486	C1386	A1287	U1188	
				G2236	G1974	A1885	C1788	A1690	A1580	U1487	A1387	G1288	A1189	
				G2237	U1982	A1895	A1789	U1693	G1581			C1289	G1190	
				G2238	U1983	G1896	A1794	C1694	C1585	A1490	A1396	G1292	U1198	
				G2239	G1988	C1900	C1795	G1695	A1586	G1493	U1397	C1293	U1199	
				G2240	G1989	A1901	U1796		G1587	C1398			C1200	
				G2241	C1990	U1901	G1797	A1701	A1590	U1400	C1399	C1297	U1201	
				G2242	G1991	G1906	U1798	G1702	A1591	G1401		C1298	U1202	
				G2243	U1992	G1907	G1799	A1591	C1592			G1299	U1203	
				G2244	U1993	G1907	C1800	A1713		U1504	U1405	G1300	A1204	
				G2245	U2092	A1801	A1801	U1714	A1597		U1406	A1302	A1205	
				G2246	G2093					U1509			G1206	
				G2247	A2094	G1913	C1806	U1716	A1610	G1510			G1210	
				G2248	A2095	G1914	G1807	U1717	C1604	G1511	G1410	C1306	G1211	
				G2249	C2096	G1915	A1808	G1718	C1605	C1512	U1411		G1212	
				G2250	A2097	U1917	A1809		C1606	U1513	U1412	G1310	G1213	
				G2251	U2098			G1726	C1607	G1514	U1413	G1311	A1213	
				G2252	G2099	U1923	A1815	C1727	A1610	U1515	C1414	U1312		
				G2253	G2100	C1924	C1816	U1728	A1611	G1524	U1415	U1313	G1218	
				G2254	A2101	G1927	G1817	U1729	C1611	A1525	G1416	C1314	U1222	
				G2255	G2102	U1928	U1818	C1730	C1612	A1526	C1417	C1315	U1223	
				G2256	C2103	G1929	A1819	G1731	G1613	G1527	G1418	U1316		
				G2257	C2104	U1930	U1820		A1614	G1527	A1419	G1317		
				G2258	U2105	U1931			C1615	A1528	A1420	U1318	G1235	
				G2259	U2106	G1932	G1824	U1737	A1616	G1421	G1421	U1319	G1236	
				G2260	G2107	U1933	U1825	G1738	A1626	G1530	C1422	C1320	A1237	
				G2261	A2108	G1933	G1826	A1739	A1532	A1321			G1238	
				G2262	U2109			G1740	G1627	C1428			G1239	
				G2263	U2110	A1936	A1829	C1741		G1429		A1328	U1240	
				G2264	U2111	A1937		U1742	U1636	U1533	G1430	U1329	C1243	
				G2265	G2112	U1938	C1833	G1743	A1637	A1535	A1431	G1330	G1243	
				G2266	U2113	U1939		A1744	C1536	G1432		G1331		
				G2267	A2114	U1940	C1843	A1745	G1645	G1537	A1433	G1332	A1247	



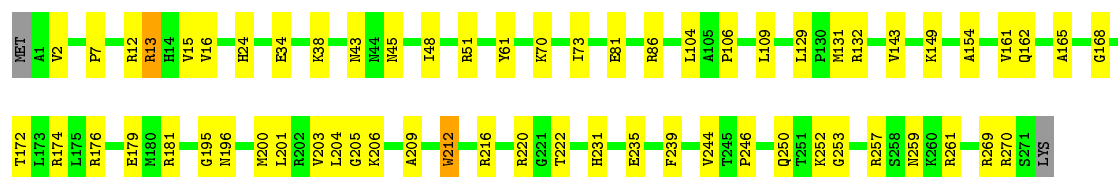
- Molecule 28: 5S ribosomal RNA (120-MER)

Chain B: 55% 41%



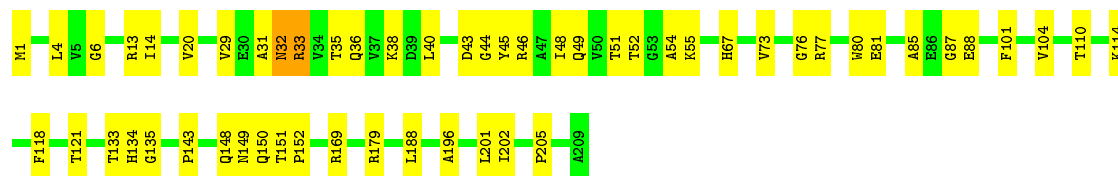
- Molecule 29: 50S ribosomal protein L2

Chain C: 77% 22%



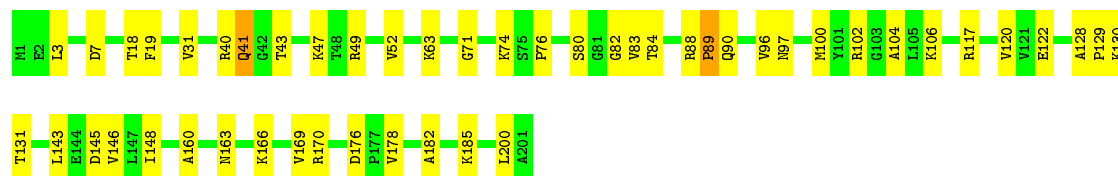
- Molecule 30: 50S ribosomal protein L3

Chain D: 74% 25%

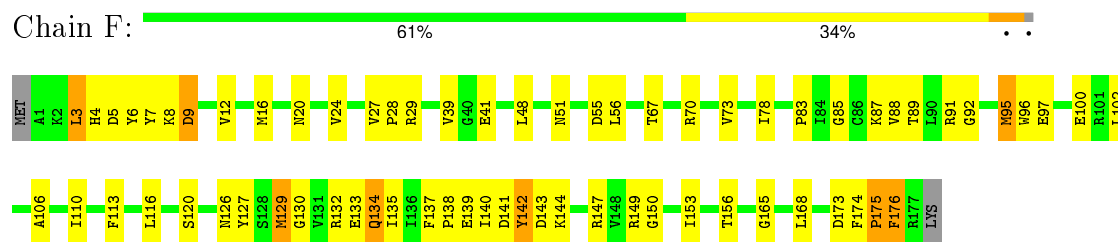


- Molecule 31: 50S ribosomal protein L4

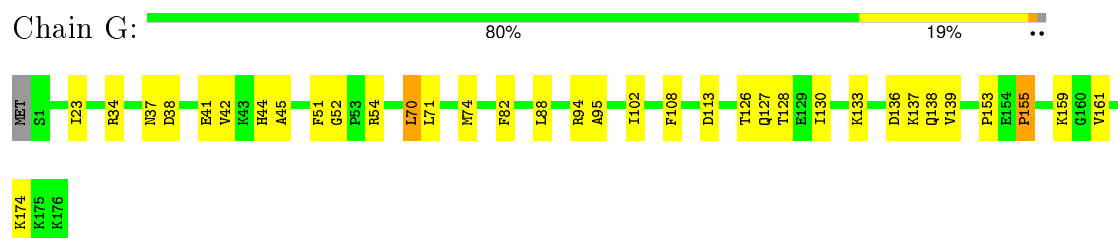
Chain E: 76% 23%



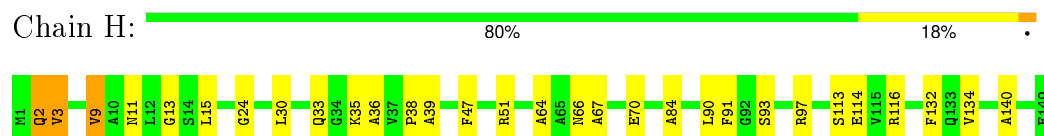
- Molecule 32: 50S ribosomal protein L5



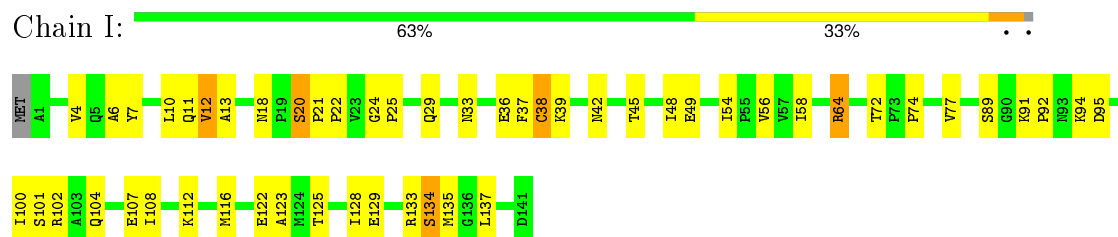
- Molecule 33: 50S ribosomal protein L6



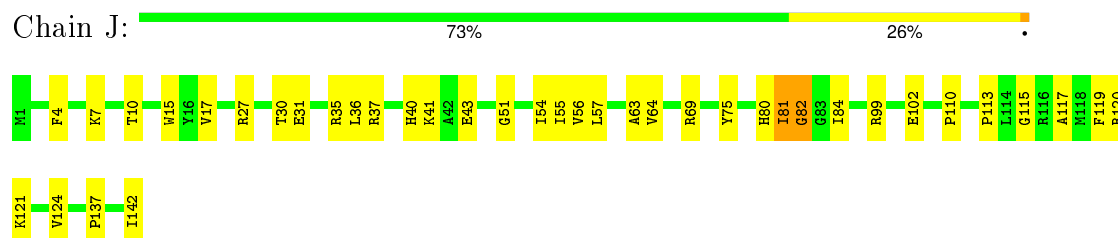
- Molecule 34: 50S ribosomal protein L9



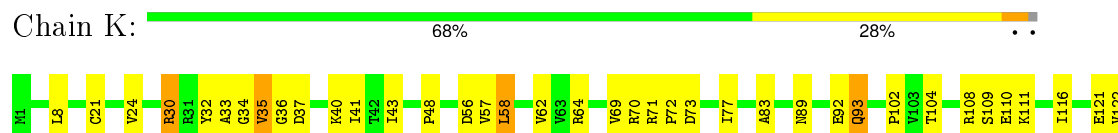
- Molecule 35: 50S ribosomal protein L11



- Molecule 36: 50S ribosomal protein L13

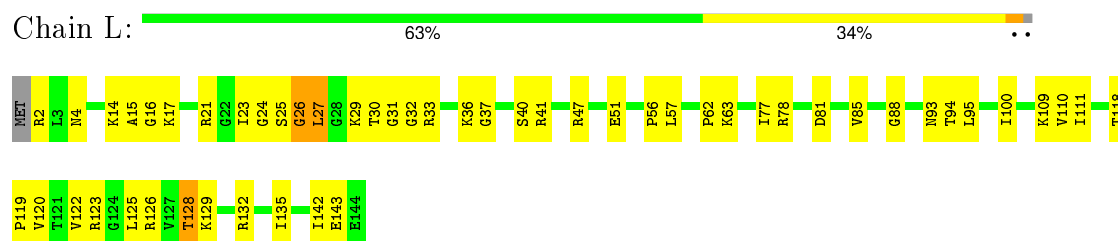


- Molecule 37: 50S ribosomal protein L14

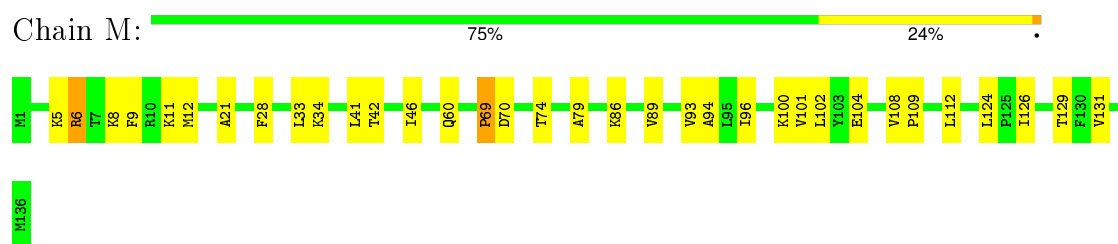


LEU

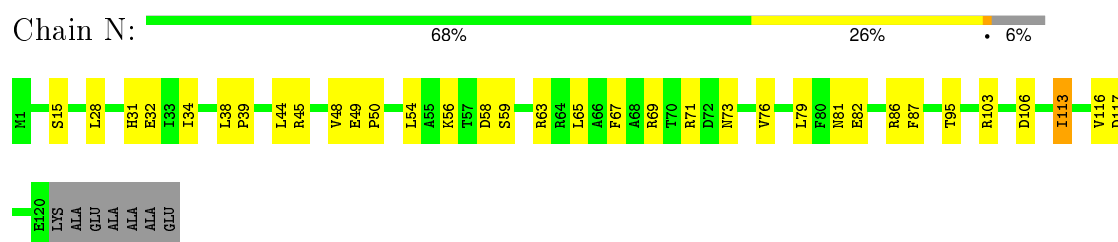
- Molecule 38: 50S ribosomal protein L15



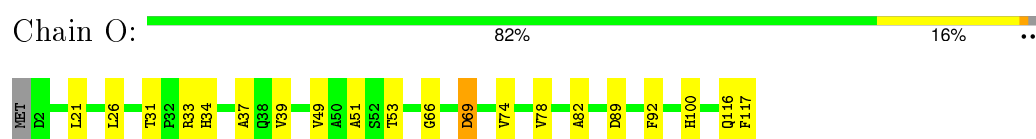
- Molecule 39: 50S ribosomal protein L16



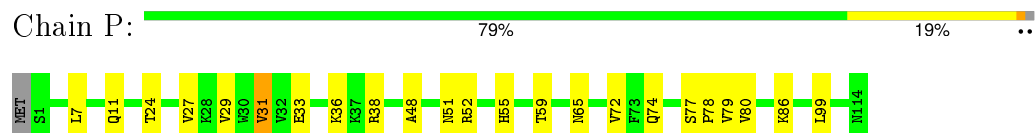
- Molecule 40: 50S ribosomal protein L17



- Molecule 41: 50S ribosomal protein L18



- Molecule 42: 50S ribosomal protein L19

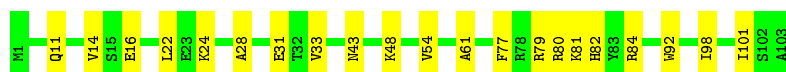
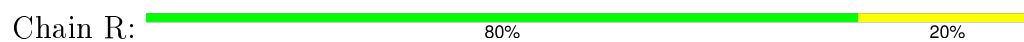


- Molecule 43: 50S ribosomal protein L20

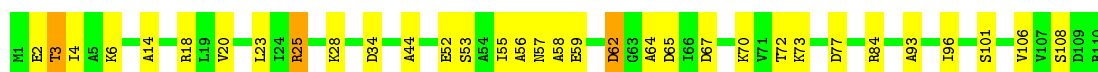




- Molecule 44: 50S ribosomal protein L21



- Molecule 45: 50S ribosomal protein L22



- Molecule 46: 50S ribosomal protein L23



- Molecule 47: 50S ribosomal protein L24



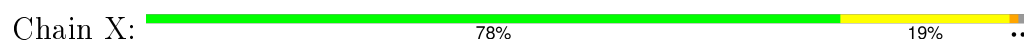
- Molecule 48: 50S ribosomal protein L25



- Molecule 49: 50S ribosomal protein L27



- Molecule 50: 50S ribosomal protein L28




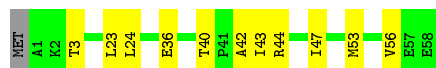
- Molecule 51: 50S ribosomal protein L29

Chain Y:  75% 24%



- Molecule 52: 50S ribosomal protein L30

Chain Z:  80% 19%




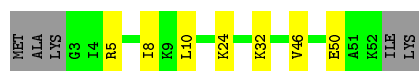
- Molecule 53: 50S ribosomal protein L32

Chain 0:  68% 26%



- Molecule 54: 50S ribosomal protein L33

Chain 1:  78% 13% 9%



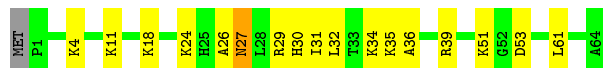
- Molecule 55: 50S ribosomal protein L34

Chain 2:  70% 30%



- Molecule 56: 50S ribosomal protein L35

Chain 3:  72% 25%



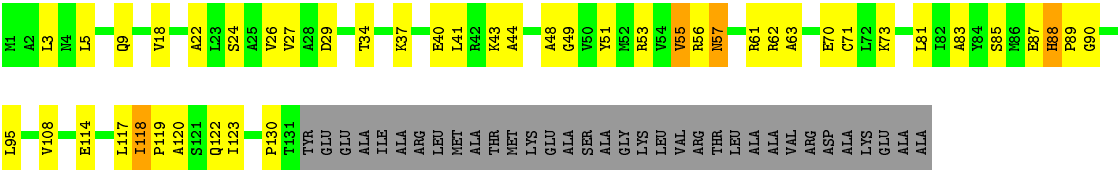
- Molecule 57: 50S ribosomal protein L36

Chain 4:  61% 39%

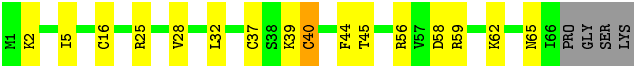


- Molecule 58: 50S ribosomal protein L10

Chain 5:  52% 25% 21%



• Molecule 59: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	LOCAL CTF CORRECTION	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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: MA6, MIA, 2MA, 2MG, 5MU, 1MG, 3TD, NA, UR3, 7MG, GDP, ZN, OMU, CL, 6MZ, FME, OMC, MG, OMG, H2U, KIR, 5MC, 4OC, 4SU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	a	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
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
2	b	0.30	0/1735	0.44	0/2338
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
23	w	0.98	1/1747 (0.1%)	1.40	24/2721 (0.9%)
24	x	0.62	1/261 (0.4%)	0.85	0/404
25	y	0.39	1/1618 (0.1%)	0.81	0/2514
26	z	0.34	0/2935	0.47	0/3970
27	A	0.46	1/69174 (0.0%)	0.90	50/107910 (0.0%)
28	B	0.38	1/2876 (0.0%)	0.86	0/4483
29	C	0.31	0/2121	0.47	0/2852
3	c	0.32	0/1651	0.46	0/2225
30	D	0.35	0/1586	0.48	0/2134
31	E	0.26	0/1571	0.41	0/2113
32	F	0.30	0/1434	0.47	0/1926
33	G	0.35	0/1343	0.47	0/1816
34	H	0.23	0/1122	0.40	0/1515
35	I	0.23	0/1046	0.44	0/1410
36	J	0.29	0/1152	0.43	0/1551
37	K	0.28	0/947	0.41	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	L	0.26	0/1054	0.45	0/1403
39	M	0.32	0/1093	0.46	0/1460
4	d	0.28	0/1665	0.44	0/2227
40	N	0.28	0/973	0.44	0/1301
41	O	0.33	0/902	0.44	0/1209
42	P	0.28	0/929	0.43	0/1242
43	Q	0.34	0/960	0.43	0/1278
44	R	0.34	0/829	0.52	0/1107
45	S	0.28	0/864	0.47	0/1156
46	T	0.29	0/744	0.45	0/994
47	U	0.35	0/787	0.44	0/1051
48	V	0.31	0/766	0.45	0/1025
49	W	0.33	0/582	0.47	0/769
5	e	0.31	0/1154	0.46	0/1554
50	X	0.28	0/635	0.40	0/848
51	Y	0.33	0/510	0.45	0/677
52	Z	0.25	0/453	0.41	0/605
53	0	0.26	0/450	0.41	0/599
54	1	0.26	0/416	0.41	0/554
55	2	0.29	0/380	0.44	0/498
56	3	0.27	0/513	0.43	0/676
57	4	0.28	0/303	0.40	0/397
58	5	0.25	0/1001	0.45	0/1350
59	6	0.33	0/531	0.54	0/709
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
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)
23	w	1	C	OP3-P	-10.97	1.48	1.61
28	B	1	U	OP3-P	-10.59	1.48	1.61
27	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(°)	Ideal(°)
27	A	974	G	N1-C6-O6	9.46	125.57	119.90
27	A	1936	A	N1-C6-N6	9.14	124.09	118.60
23	w	13	C	C6-N1-C2	-8.20	117.02	120.30
23	w	62	C	C6-N1-C2	-8.13	117.05	120.30
23	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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16645	0	0
2	b	1704	0	1732	0	0
3	c	1624	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1141	0	1170	0	0
6	f	817	0	808	0	0
7	g	1181	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	786	0	828	0	0
11	k	869	0	878	0	0
12	l	955	0	1019	0	0
13	m	883	0	944	0	0
14	n	799	0	841	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	648	0	691	0	0
18	r	505	0	502	0	0
19	s	637	0	665	0	0
20	t	665	0	714	0	0
21	u	495	0	486	0	0
22	v	1654	0	849	0	0
23	w	1644	0	840	0	0
24	x	234	0	118	0	0
25	y	1643	0	850	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	z	2881	0	2894	0	0
27	A	62276	0	31346	830	0
28	B	2572	0	1302	27	0
29	C	2082	0	2157	39	0
30	D	1565	0	1616	37	0
31	E	1552	0	1619	28	0
32	F	1410	0	1447	47	0
33	G	1323	0	1374	22	0
34	H	1111	0	1148	18	0
35	I	1032	0	1088	34	0
36	J	1129	0	1162	31	0
37	K	938	0	1012	22	0
38	L	1045	0	1117	36	0
39	M	1074	0	1157	20	0
40	N	960	0	1000	24	0
41	O	892	0	923	12	0
42	P	917	0	965	16	0
43	Q	947	0	1022	22	0
44	R	816	0	839	13	0
45	S	857	0	922	23	0
46	T	738	0	807	17	0
47	U	779	0	834	17	0
48	V	753	0	780	16	0
49	W	575	0	592	9	0
50	X	625	0	655	12	0
51	Y	509	0	543	11	0
52	Z	449	0	491	7	0
53	0	444	0	461	15	0
54	1	409	0	440	4	0
55	2	377	0	418	18	0
56	3	504	0	574	16	0
57	4	302	0	341	12	0
58	5	988	0	1025	31	0
59	6	522	0	520	12	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
60	A	234	0	0	0	0
60	B	7	0	0	0	0
60	D	1	0	0	0	0
60	N	1	0	0	0	0
60	a	83	0	0	0	0
60	v	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	z	1	0	0	0	0
61	A	1	0	0	0	0
61	a	1	0	0	0	0
62	z	57	0	60	0	0
63	z	28	0	12	0	0
64	A	1	0	0	0	0
64	B	1	0	0	0	0
65	4	1	0	0	0	0
65	6	1	0	0	0	0
66	A	9	0	0	1	0
66	D	2	0	0	0	0
66	K	1	0	0	0	0
66	a	9	0	0	0	0
All	All	152718	0	103399	1338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1338 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:X:17:ARG:HE	50:X:23:ALA:HB2	1.29	0.97
27:A:704:G:H2'	27:A:726:G:H22	1.31	0.94
27:A:1055:G:H1	27:A:1104:C:H42	1.11	0.94
32:F:134:GLN:NE2	32:F:149:ARG:O	2.06	0.87
27:A:585:G:N7	43:Q:5:ARG:NH1	2.26	0.83

There are no symmetry-related clashes.

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%)	3	11
3	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	19	54
4	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	3	10
5	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	2	6
6	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	5
7	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	4
8	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	7	29
9	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	2	5
10	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	2	5
11	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	8
12	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	14
13	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	3	12
14	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	9
15	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	2	6
16	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7	27
17	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	2	5
18	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	3
19	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
20	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	7	29
21	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	3
26	z	368/393 (94%)	327 (89%)	35 (10%)	6 (2%)	12	40
29	C	269/273 (98%)	243 (90%)	21 (8%)	5 (2%)	10	35
30	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	19	54
31	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	4	18
32	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	5	19
33	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	6	23
34	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	6	25
35	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	4
36	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	44
37	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	7	27
38	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	3
39	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	8	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	7	27
41	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	21	57
42	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	21	57
43	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
44	R	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	9	33
45	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	7
46	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	5	20
47	U	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	5	22
48	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8	31
49	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	14	44
50	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	15	46
51	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	40
52	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
53	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	10	35
54	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
55	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
56	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	12	40
57	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
58	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	7
59	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	12	40
All	All	6215/6613 (94%)	5318 (86%)	691 (11%)	206 (3%)	8	20

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 ⓘ

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%)	51	84
3	c	170/190 (90%)	163 (96%)	7 (4%)	37	73
4	d	172/173 (99%)	166 (96%)	6 (4%)	43	78
5	e	114/126 (90%)	105 (92%)	9 (8%)	15	41
6	f	87/116 (75%)	83 (95%)	4 (5%)	33	69
7	g	124/147 (84%)	122 (98%)	2 (2%)	70	91
8	h	104/105 (99%)	103 (99%)	1 (1%)	82	95
9	i	105/107 (98%)	100 (95%)	5 (5%)	31	67
10	j	86/90 (96%)	84 (98%)	2 (2%)	58	87
11	k	89/99 (90%)	87 (98%)	2 (2%)	60	88
12	l	103/104 (99%)	100 (97%)	3 (3%)	50	83
13	m	92/96 (96%)	90 (98%)	2 (2%)	60	88
14	n	79/84 (94%)	75 (95%)	4 (5%)	29	65
15	o	76/77 (99%)	74 (97%)	2 (3%)	54	85
16	p	65/65 (100%)	61 (94%)	4 (6%)	23	55
17	q	74/78 (95%)	71 (96%)	3 (4%)	37	73
18	r	48/65 (74%)	47 (98%)	1 (2%)	61	88
19	s	70/79 (89%)	69 (99%)	1 (1%)	74	93
20	t	65/66 (98%)	63 (97%)	2 (3%)	47	82
21	u	44/61 (72%)	42 (96%)	2 (4%)	34	70
26	z	311/326 (95%)	304 (98%)	7 (2%)	58	87
29	C	216/218 (99%)	208 (96%)	8 (4%)	41	77
30	D	164/164 (100%)	161 (98%)	3 (2%)	66	90
31	E	165/165 (100%)	160 (97%)	5 (3%)	48	83
32	F	148/150 (99%)	141 (95%)	7 (5%)	32	68
33	G	137/138 (99%)	137 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	I	109/110 (99%)	106 (97%)	3 (3%)	51	84
36	J	116/116 (100%)	114 (98%)	2 (2%)	68	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	K	103/104 (99%)	98 (95%)	5 (5%)	31	67
38	L	102/103 (99%)	100 (98%)	2 (2%)	63	88
39	M	109/109 (100%)	108 (99%)	1 (1%)	84	96
40	N	100/103 (97%)	98 (98%)	2 (2%)	63	88
41	O	86/87 (99%)	84 (98%)	2 (2%)	58	87
42	P	99/100 (99%)	96 (97%)	3 (3%)	48	83
43	Q	89/90 (99%)	87 (98%)	2 (2%)	60	88
44	R	84/84 (100%)	83 (99%)	1 (1%)	78	94
45	S	93/93 (100%)	90 (97%)	3 (3%)	46	81
46	T	80/84 (95%)	76 (95%)	4 (5%)	30	65
47	U	83/85 (98%)	82 (99%)	1 (1%)	78	94
48	V	78/78 (100%)	77 (99%)	1 (1%)	76	94
49	W	57/63 (90%)	56 (98%)	1 (2%)	66	90
50	X	67/68 (98%)	67 (100%)	0	100	100
51	Y	55/55 (100%)	54 (98%)	1 (2%)	66	90
52	Z	48/49 (98%)	48 (100%)	0	100	100
53	0	47/48 (98%)	45 (96%)	2 (4%)	35	71
54	1	45/49 (92%)	44 (98%)	1 (2%)	60	88
55	2	38/38 (100%)	38 (100%)	0	100	100
56	3	51/52 (98%)	50 (98%)	1 (2%)	63	88
57	4	34/34 (100%)	34 (100%)	0	100	100
58	5	100/123 (81%)	97 (97%)	3 (3%)	48	83
59	6	59/62 (95%)	58 (98%)	1 (2%)	68	91
All	All	5134/5388 (95%)	4995 (97%)	139 (3%)	56	84

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

Mol	Chain	Res	Type
19	s	62	THR
29	C	129	LEU
48	V	42	LEU
20	t	26	MET
26	z	190	GLU

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

Mol	Chain	Res	Type
19	s	51	HIS
26	z	135	ASN
51	Y	41	HIS
19	s	56	HIS
26	z	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	242 (15%)	0
22	v	76/78 (97%)	17 (22%)	0
23	w	76/77 (98%)	43 (56%)	0
24	x	10/11 (90%)	1 (10%)	0
25	y	74/77 (96%)	19 (25%)	0
27	A	2894/2903 (99%)	542 (18%)	90 (3%)
28	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4784/4805 (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
27	A	1124	G
27	A	1275	A
27	A	2798	U
27	A	1130	U
27	A	1142	A

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

53 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$
27	6MZ	A	1618	27	17,25,26	1.11	1 (5%)	15,36,39	2.55	2 (13%)
27	2MG	A	1835	27	18,26,27	0.91	2 (11%)	21,38,41	2.08	6 (28%)
27	PSU	A	1911	27	15,21,22	1.45	1 (6%)	16,30,33	2.11	4 (25%)
27	3TD	A	1915	27	15,22,23	1.29	3 (20%)	17,32,35	1.57	3 (17%)
27	PSU	A	1917	27	15,21,22	1.43	1 (6%)	16,30,33	2.31	4 (25%)
27	5MU	A	1939	27	13,22,23	0.71	1 (7%)	16,32,35	2.31	2 (12%)
27	5MC	A	1962	27	14,22,23	1.32	1 (7%)	17,32,35	0.99	1 (5%)
27	6MZ	A	2030	27	17,25,26	1.02	1 (5%)	15,36,39	2.87	3 (20%)
27	7MG	A	2069	27	20,26,27	1.17	2 (10%)	23,39,42	3.18	6 (26%)
27	OMG	A	2251	27,22	18,26,27	0.94	2 (11%)	21,38,41	2.10	4 (19%)
27	2MG	A	2445	27	18,26,27	0.88	2 (11%)	21,38,41	2.34	7 (33%)
27	H2U	A	2449	27	17,21,22	0.96	2 (11%)	23,30,33	2.05	5 (21%)
27	PSU	A	2457	27	15,21,22	1.80	1 (6%)	16,30,33	2.20	4 (25%)
27	OMC	A	2498	60,27	15,22,23	0.79	1 (6%)	20,31,34	1.45	1 (5%)
27	2MA	A	2503	60,27	17,25,26	1.58	3 (17%)	18,37,40	2.70	1 (5%)
27	PSU	A	2504	27	15,21,22	1.51	1 (6%)	16,30,33	2.40	4 (25%)
27	OMU	A	2552	27	14,22,23	0.70	0	19,31,34	1.49	1 (5%)
27	PSU	A	2580	27	15,21,22	1.70	2 (13%)	16,30,33	2.21	3 (18%)
27	PSU	A	2604	27	15,21,22	1.61	2 (13%)	16,30,33	2.47	4 (25%)
27	PSU	A	2605	27	15,21,22	1.26	2 (13%)	16,30,33	2.39	4 (25%)
27	1MG	A	745	27	17,26,27	1.49	3 (17%)	19,39,42	0.84	0
27	PSU	A	746	60,27	15,21,22	1.37	1 (6%)	16,30,33	2.11	3 (18%)
27	5MC	A	747	27	14,22,23	1.36	1 (7%)	17,32,35	1.36	3 (17%)
27	PSU	A	955	27	15,21,22	1.62	4 (26%)	16,30,33	2.28	4 (25%)
1	2MG	a	1207	1	18,26,27	1.20	2 (11%)	21,38,41	2.22	6 (28%)
1	4OC	a	1402	1	15,23,24	0.59	0	21,32,35	1.66	3 (14%)
1	5MC	a	1407	1	14,22,23	1.26	1 (7%)	17,32,35	1.00	1 (5%)
1	UR3	a	1498	1	13,22,23	0.69	0	18,32,35	0.75	0
1	2MG	a	1516	1	18,26,27	1.21	2 (11%)	21,38,41	2.28	6 (28%)

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	1.12	1 (5%)	15,38,41	2.43	2 (13%)
1	MA6	a	1519	1	18,26,27	0.91	1 (5%)	15,38,41	2.67	4 (26%)
1	PSU	a	516	1,60	15,21,22	1.50	3 (20%)	16,30,33	2.07	3 (18%)
1	7MG	a	527	1	20,26,27	1.26	2 (10%)	23,39,42	3.12	6 (26%)
1	2MG	a	966	1	18,26,27	1.14	2 (11%)	21,38,41	2.22	6 (28%)
1	5MC	a	967	1	14,22,23	1.20	1 (7%)	17,32,35	1.08	1 (5%)
22	H2U	v	20	22	17,21,22	0.95	2 (11%)	23,30,33	1.91	4 (17%)
22	5MU	v	54	22	13,22,23	0.56	0	16,32,35	2.39	2 (12%)
22	PSU	v	55	22	15,21,22	1.18	1 (6%)	16,30,33	2.25	4 (25%)
22	FME	v	77	-	8,9,10	0.93	1 (12%)	5,9,11	1.60	1 (20%)
22	4SU	v	8	22	12,21,22	0.69	0	15,30,33	1.07	1 (6%)
23	H2U	w	20	23	17,21,22	1.37	4 (23%)	23,30,33	3.36	5 (21%)
23	5MU	w	54	23	13,22,23	0.61	0	16,32,35	2.69	3 (18%)
23	PSU	w	55	23	15,21,22	1.54	3 (20%)	16,30,33	2.28	4 (25%)
23	4SU	w	8	23	12,21,22	0.78	1 (8%)	15,30,33	1.09	1 (6%)
25	H2U	y	16	25	17,21,22	1.00	2 (11%)	23,30,33	1.81	2 (8%)
25	H2U	y	20	25	17,21,22	0.98	2 (11%)	23,30,33	2.36	4 (17%)
25	PSU	y	32	25	15,21,22	1.38	1 (6%)	16,30,33	2.24	4 (25%)
25	MIA	y	37	25	22,31,32	1.75	2 (9%)	26,44,47	1.67	6 (23%)
25	PSU	y	39	25	15,21,22	1.45	1 (6%)	16,30,33	2.39	4 (25%)
25	7MG	y	46	25	20,26,27	1.51	2 (10%)	23,39,42	3.22	5 (21%)
25	5MU	y	54	25	13,22,23	0.66	1 (7%)	16,32,35	2.30	2 (12%)
25	PSU	y	55	25	15,21,22	1.31	1 (6%)	16,30,33	2.32	4 (25%)
25	4SU	y	8	25	12,21,22	0.78	0	15,30,33	0.86	1 (6%)

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
27	6MZ	A	1618	27	-	0/5/27/28	0/3/3/3
27	2MG	A	1835	27	-	0/5/27/28	0/3/3/3
27	PSU	A	1911	27	-	0/7/25/26	0/2/2/2
27	3TD	A	1915	27	-	0/7/25/26	0/2/2/2
27	PSU	A	1917	27	-	0/7/25/26	0/2/2/2
27	5MU	A	1939	27	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	5MC	A	1962	27	-	0/3/25/26	0/2/2/2
27	6MZ	A	2030	27	-	0/5/27/28	0/3/3/3
27	7MG	A	2069	27	-	0/7/37/38	0/3/3/3
27	OMG	A	2251	27,22	-	0/5/27/28	0/3/3/3
27	2MG	A	2445	27	-	0/5/27/28	0/3/3/3
27	H2U	A	2449	27	-	0/7/38/39	0/2/2/2
27	PSU	A	2457	27	-	0/7/25/26	0/2/2/2
27	OMC	A	2498	60,27	-	0/5/27/28	0/2/2/2
27	2MA	A	2503	60,27	-	0/3/25/26	0/3/3/3
27	PSU	A	2504	27	-	0/7/25/26	0/2/2/2
27	OMU	A	2552	27	-	0/5/27/28	0/2/2/2
27	PSU	A	2580	27	-	0/7/25/26	0/2/2/2
27	PSU	A	2604	27	-	0/7/25/26	0/2/2/2
27	PSU	A	2605	27	-	0/7/25/26	0/2/2/2
27	1MG	A	745	27	-	0/3/25/26	0/3/3/3
27	PSU	A	746	60,27	-	0/7/25/26	0/2/2/2
27	5MC	A	747	27	-	0/3/25/26	0/2/2/2
27	PSU	A	955	27	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1,60	-	0/7/25/26	0/2/2/2
1	7MG	a	527	1	-	0/7/37/38	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	FME	v	77	-	-	1/6/9/11	0/0/0/0
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
23	H2U	w	20	23	-	0/7/38/39	0/2/2/2
23	5MU	w	54	23	-	0/3/25/26	0/2/2/2
23	PSU	w	55	23	-	0/7/25/26	0/2/2/2
23	4SU	w	8	23	-	0/3/25/26	0/2/2/2
25	H2U	y	16	25	-	0/7/38/39	0/2/2/2
25	H2U	y	20	25	-	0/7/38/39	0/2/2/2
25	PSU	y	32	25	-	0/7/25/26	0/2/2/2
25	MIA	y	37	25	-	0/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	y	39	25	-	0/7/25/26	0/2/2/2
25	7MG	y	46	25	-	0/7/37/38	0/3/3/3
25	5MU	y	54	25	-	0/3/25/26	0/2/2/2
25	PSU	y	55	25	-	0/7/25/26	0/2/2/2
25	4SU	y	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	37	MIA	C2-S10	-7.15	1.69	1.75
27	A	2457	PSU	C5-C1'	-6.03	1.47	1.52
27	A	2580	PSU	C5-C1'	-5.43	1.47	1.52
27	A	2604	PSU	C5-C1'	-5.18	1.47	1.52
27	A	955	PSU	C5-C1'	-4.88	1.48	1.52

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	w	20	H2U	C5-C6-N1	-11.65	98.00	110.76
25	y	46	7MG	C5-C4-N3	-8.74	117.84	126.74
25	y	20	H2U	C4-N3-C2	-8.68	117.91	125.77
1	a	1519	MA6	N3-C2-N1	-8.18	122.45	128.87
1	a	527	7MG	C5-C4-N3	-7.86	118.73	126.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	v	77	FME	O1-CN-N-CA

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1917	PSU	1	0
27	A	1962	5MC	1	0
27	A	2030	6MZ	1	0
27	A	2445	2MG	1	0
27	A	2449	H2U	1	0
27	A	2498	OMC	1	0
27	A	2552	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	745	1MG	1	0
27	A	747	5MC	1	0
27	A	955	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 341 ligands modelled in this entry, 339 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$
62	KIR	z	401	-	54,59,59	0.63	1 (1%)	52,84,84	1.97	12 (23%)
63	GDP	z	402	60	24,30,30	1.12	2 (8%)	26,47,47	1.93	5 (19%)

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
62	KIR	z	401	-	-	0/54/98/98	0/3/3/3
63	GDP	z	402	60	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	z	401	KIR	C2-C3	2.28	1.49	1.44
63	z	402	GDP	C5-C4	2.91	1.47	1.40
63	z	402	GDP	C6-C5	3.61	1.48	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	z	401	KIR	C23-C22-C21	-7.49	118.50	127.69
62	z	401	KIR	C15-C14-C13	-4.53	107.29	114.52
62	z	401	KIR	C5-C4-C3	-4.42	117.84	120.63
63	z	402	GDP	C5-C6-N1	-4.04	118.25	123.52
62	z	401	KIR	C39-C38-C37	-3.91	118.60	125.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.