



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:32 AM EST

PDB ID : 3J79
EMDB ID : EMD-2660
Title : Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, large subunit
Authors : Wong, W.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condron, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.
Deposited on : 2014-06-02
Resolution : 3.20 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.dev43
MolProbity : 4.02b-467
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) : 2.31.3

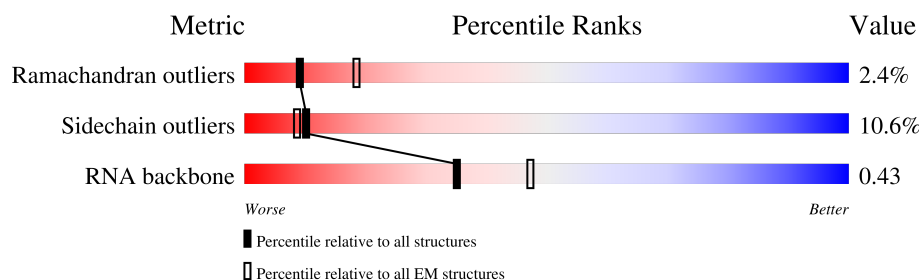
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.








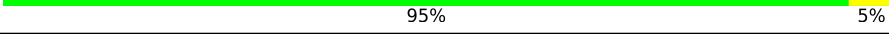


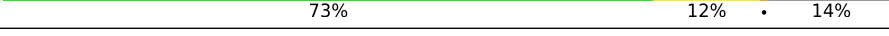

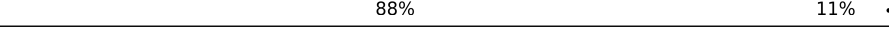
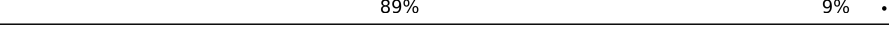

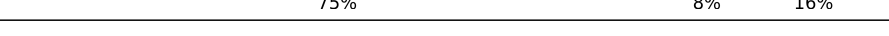

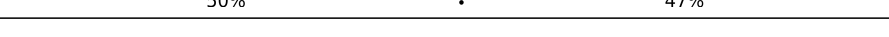
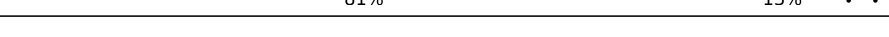

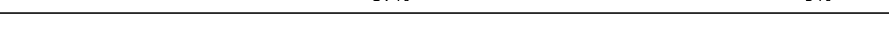






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	3788	
2	B	119	
3	C	159	
4	D	260	
5	E	386	
6	F	411	
7	G	173	
8	H	190	
9	I	221	

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Mol	Chain	Length	Quality of chain
10	J	283	
11	K	202	
12	L	215	
13	M	139	
14	N	165	
15	O	148	
16	P	205	
17	Q	219	
18	R	294	
19	S	187	
20	T	182	
21	U	184	
22	V	161	
23	W	203	
24	X	139	
25	Y	190	
26	Z	126	
27	0	162	
28	1	146	
29	2	127	
30	3	124	
31	4	67	
32	5	257	
33	6	108	
34	7	120	

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Mol	Chain	Length	Quality of chain
35	8	131	 80%15%5%
36	9	140	 60%12%26%
37	a	150	 63%8%29%
38	b	112	 79%5%15%
39	c	92	 83%14%
40	d	87	 75%8%17%
41	e	51	 71%14%16%
42	f	128	 36%60%
43	g	39	 90%5%5%
44	h	96	 83%5%11%
45	i	104	 81%11%9%

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 124514 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3191	Total	C	N	O	P	0	0
			67935	30426	12044	22274	3191		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2525	1128	461	818	118		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	P	0	0
			3224	1444	589	1040	151		

- Molecule 4 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1866	1166	374	317	9		

- Molecule 5 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total	C	N	O	S	0	0
			3061	1948	575	521	17		

- Molecule 6 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	390	Total	C	N	O	S	0	0
			3094	1962	594	527	11		

- Molecule 7 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	124	Total	C	N	O	S	0	0
			1010	636	197	171	6		

- Molecule 8 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1460	938	261	255	6		

- Molecule 9 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	207	Total	C	N	O	S	0	0
			1684	1096	298	285	5		

- Molecule 10 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	229	Total	C	N	O	S	0	0
			1873	1210	337	319	7		

- Molecule 11 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1659	1064	311	276	8		

- Molecule 12 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1761	1119	349	290	3		

- Molecule 13 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 14 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1197	779	210	202	6		

- Molecule 15 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 16 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 17 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	189	Total	C	N	O	S	0	0
			1544	984	291	261	8		

- Molecule 18 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	252	Total	C	N	O	S	0	0
			2045	1297	384	358	6		

- Molecule 19 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	186	Total	C	N	O	S	0	0
			1502	958	299	240	5		

- Molecule 20 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	181	Total	C	N	O	S	0	0
			1505	949	308	244	4		

- Molecule 21 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	180	Total	C	N	O	S	0	0
			1496	946	289	254	7		

- Molecule 22 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	155	Total	C	N	O	S	0	0
			1275	814	241	214	6		

- Molecule 23 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	170	Total	C	N	O	S	0	0
			1318	824	266	221	7		

- Molecule 24 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			824	548	135	139	2		

- Molecule 25 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	101	Total	C	N	O	S	0	0
			796	502	144	144	6		

- Molecule 26 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	121	Total	C	N	O	S	0	0
			1000	626	206	165	3		

- Molecule 27 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	62	Total	C	N	O	S	0	0
			521	336	97	87	1		

- Molecule 28 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 29 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	104	Total	C	N	O	S	0	0
			830	529	151	147	3		

- Molecule 30 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	119	Total	C	N	O	S	0	0
			994	635	194	163	2		

- Molecule 31 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 32 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 33 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	98	Total	C	N	O	S	0	0
			740	462	132	139	7		

- Molecule 34 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			793	508	151	129	5		

- Molecule 35 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	125	Total	C	N	O	S	0	0
			1036	660	206	163	7		

- Molecule 36 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	103	Total	C	N	O	S	0	0
			844	543	163	135	3		

- Molecule 37 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	106	Total	C	N	O	S	0	0
			858	530	184	138	6		

- Molecule 38 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	95	Total	C	N	O		0	0
			756	477	150	129			

- Molecule 39 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	89	Total	C	N	O	S	0	0
			705	439	150	111	5		

- Molecule 40 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	72	Total	C	N	O	S	0	0
			603	395	107	99	2		

- Molecule 41 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 42 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	51	Total	C	N	O	S	0	0
			413	255	87	66	5		

- Molecule 43 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	37	Total	C	N	O	S	0	0
			342	210	86	44	2		

- Molecule 44 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	85	Total	C	N	O	S	0	0
			658	417	127	107	7		

- Molecule 45 is a protein called 60S ribosomal protein eL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	95	Total	C	N	O	S	0	0
			778	490	152	127	9		

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	153	Total	Mg	0
			153	153	
46	B	3	Total	Mg	0
			3	3	
46	C	5	Total	Mg	0
			5	5	
46	M	1	Total	Mg	0
			1	1	
46	Q	1	Total	Mg	0
			1	1	

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

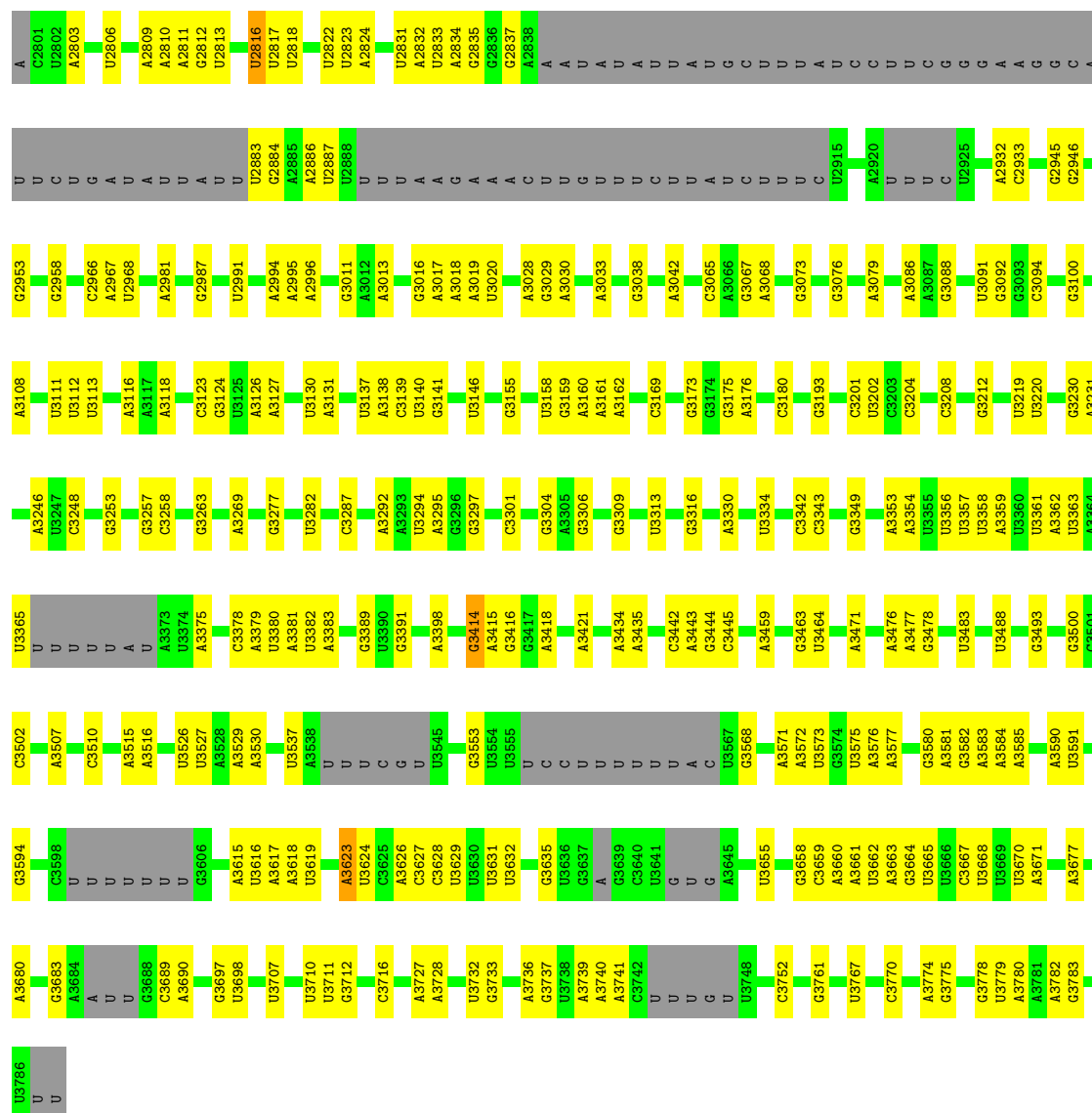
Mol	Chain	Residues	Atoms		AltConf
47	a	1	Total	Zn	0
			1	1	
47	c	1	Total	Zn	0
			1	1	

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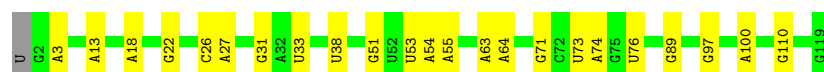
Mol	Chain	Residues	Atoms		AltConf
47	f	1	Total 1	Zn 1	0
47	h	1	Total 1	Zn 1	0
47	i	1	Total 1	Zn 1	0





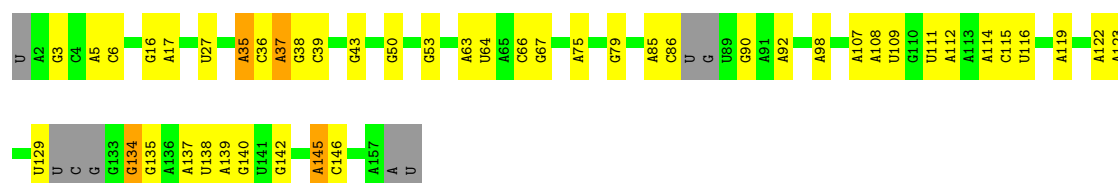
- Molecule 2: 5S ribosomal RNA

Chain B: 80% 19%

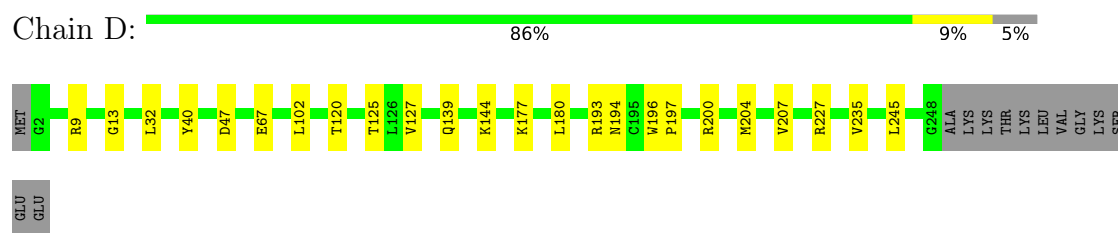


- Molecule 3: 5.8S ribosomal RNA

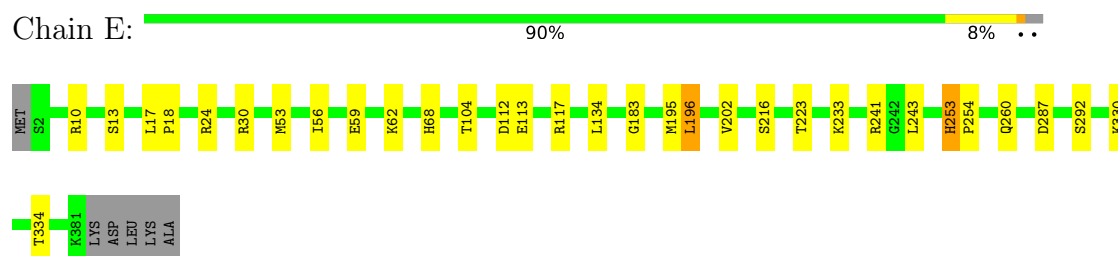
Chain C: 66% 26% 5%



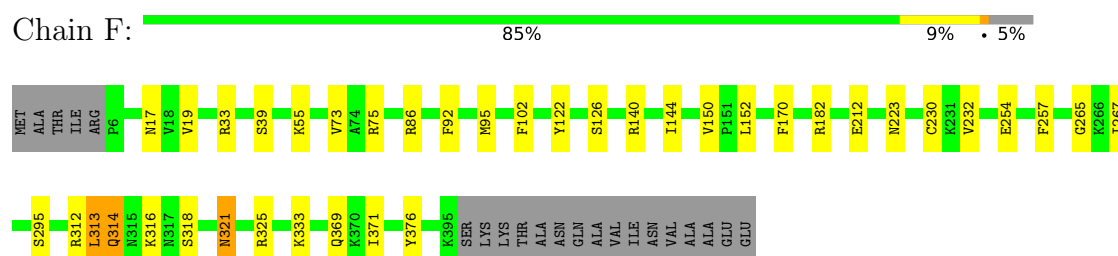
- Molecule 4: 60S ribosomal protein uL2



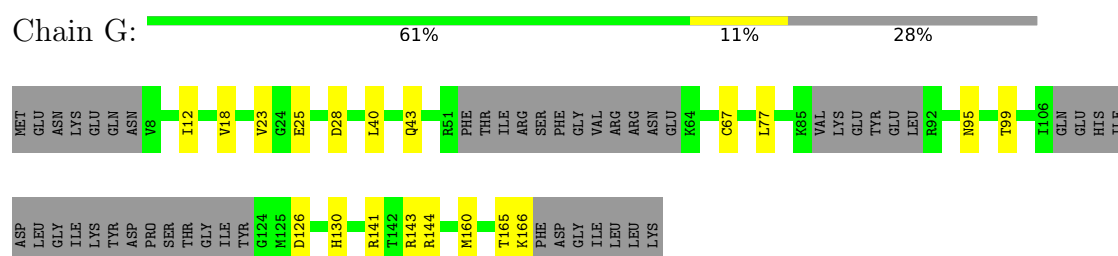
- Molecule 5: 60S ribosomal protein uL3



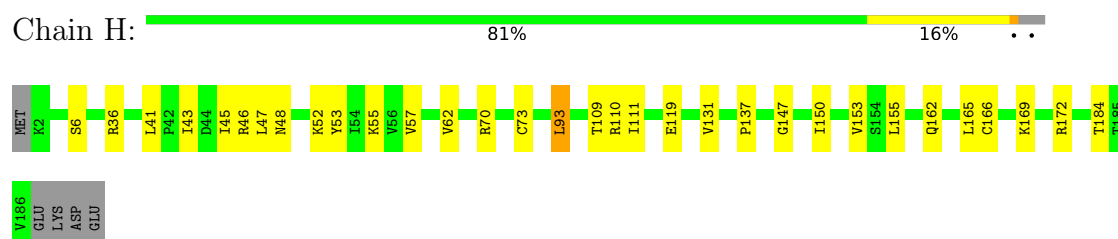
- Molecule 6: 60S ribosomal protein uL4



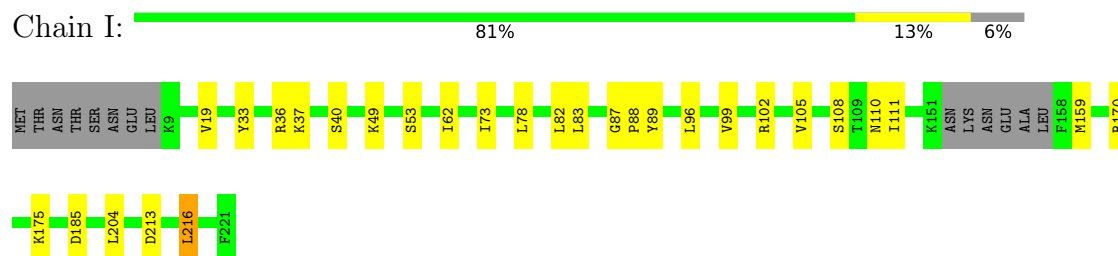
- Molecule 7: 60S ribosomal protein uL5



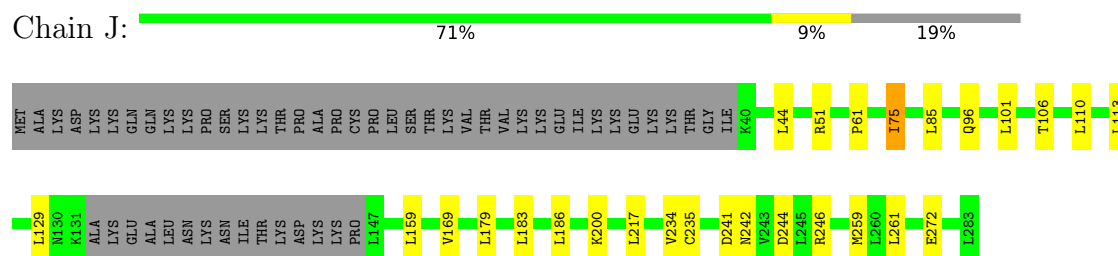
- Molecule 8: 60S ribosomal protein uL6



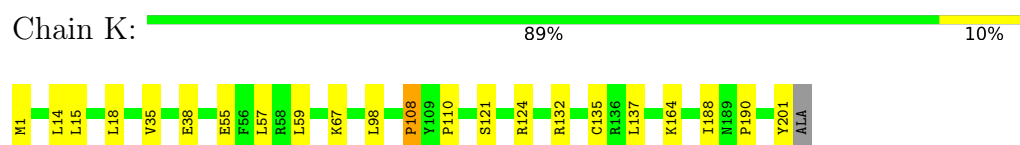
- Molecule 9: 60S ribosomal protein eL6



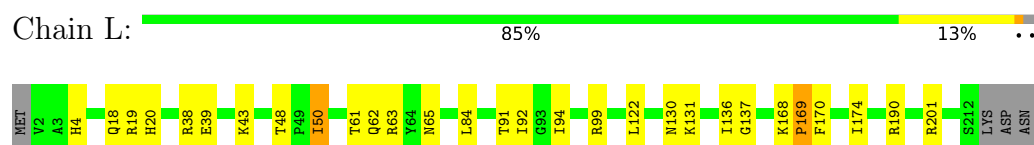
- Molecule 10: 60S ribosomal protein eL8



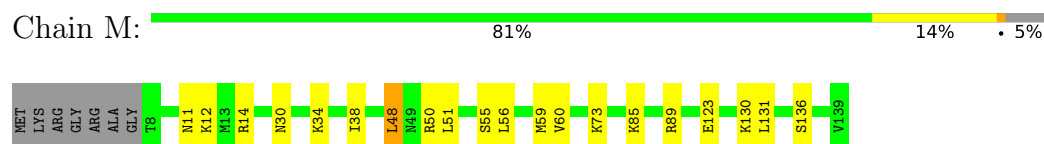
- Molecule 11: 60S ribosomal protein uL13



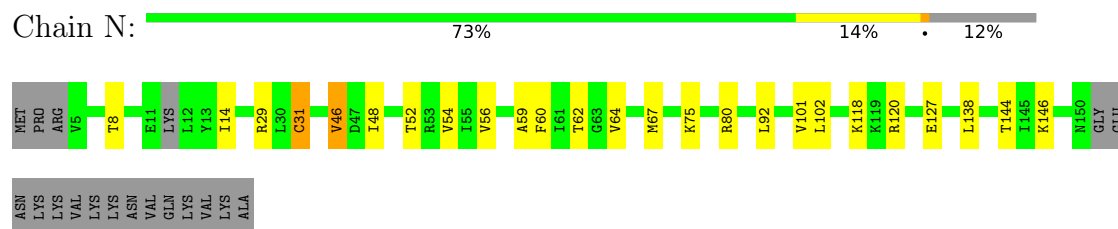
- Molecule 12: 60S ribosomal protein eL13



- Molecule 13: 60S ribosomal protein uL14



- Molecule 14: 60S ribosomal protein eL14




- Molecule 15: 60S ribosomal protein uL15

Chain O:  95% 5% .




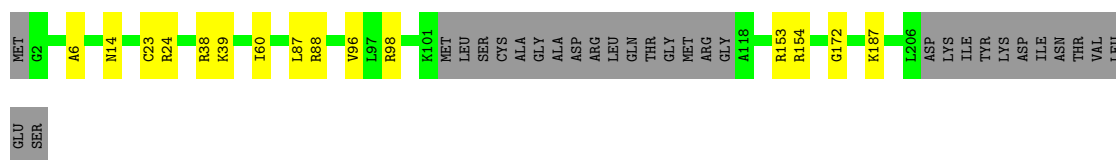
- Molecule 16: 60S ribosomal protein eL15

Chain P:  89% 10% .



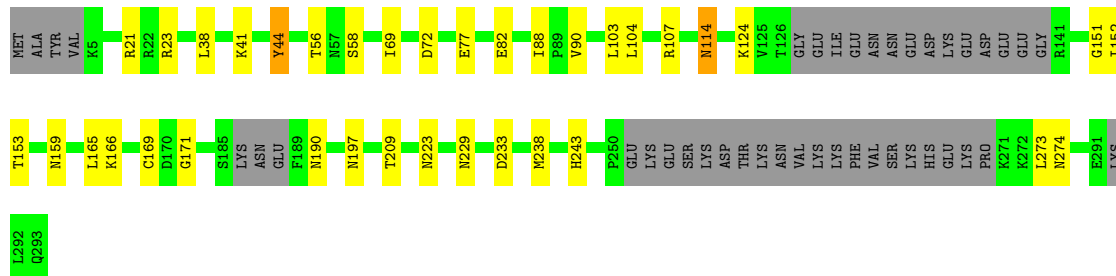
- Molecule 17: 60S ribosomal protein uL16

Chain Q:  79% 7% 14%




- Molecule 18: 60S ribosomal protein uL18

Chain R:  73% 12% 14%




- Molecule 19: 60S ribosomal protein eL18

Chain S:  88% 12% .



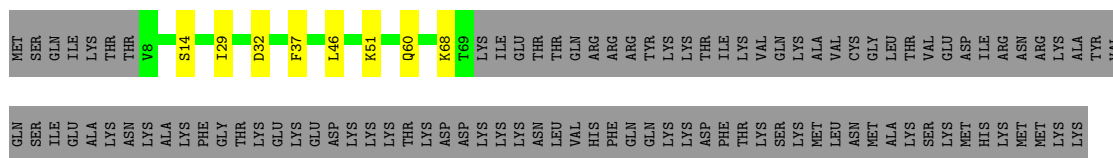
- Molecule 20: 60S ribosomal protein eL19

Chain T:  88% 11% .




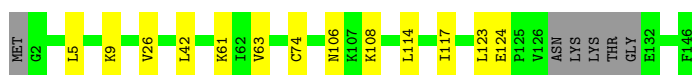
- Molecule 27: 60S ribosomal protein eL24

Chain 0:  33% 5% 62%




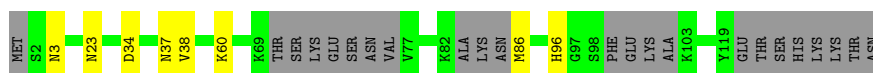
- Molecule 28: 60S ribosomal protein eL27

Chain 1:  87% 9% .




- Molecule 29: 60S ribosomal protein eL28

Chain 2:  76% 6% 18%




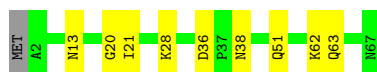
- Molecule 30: 60S ribosomal protein uL29

Chain 3:  82% 12% . .




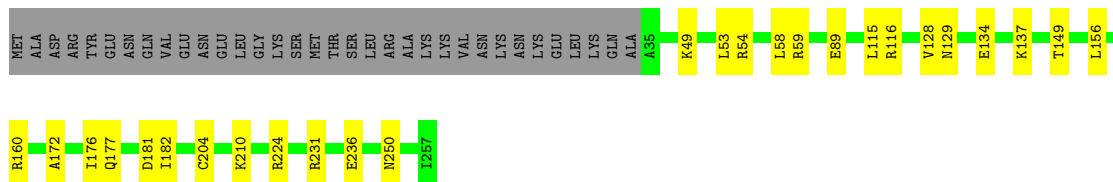
- Molecule 31: 60S ribosomal protein eL29

Chain 4:  85% 13% .



- Molecule 32: 60S ribosomal protein uL30

Chain 5:  77% 10% 13%

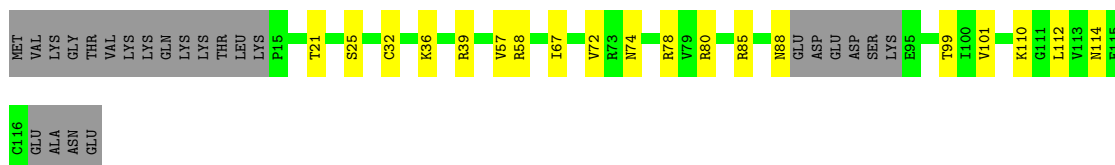


- Molecule 33: 60S ribosomal protein eL30

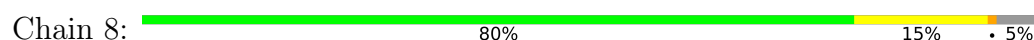
Chain 6:  75% 16% 9%



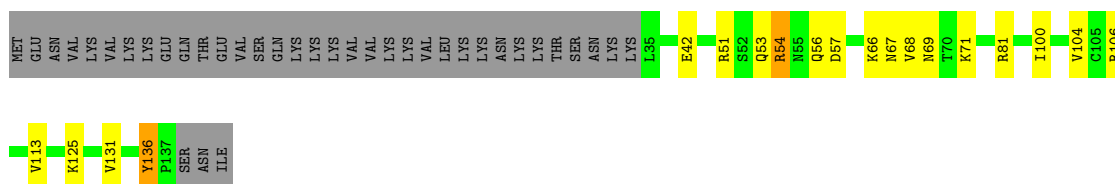
- Molecule 34: 60S ribosomal protein eL31



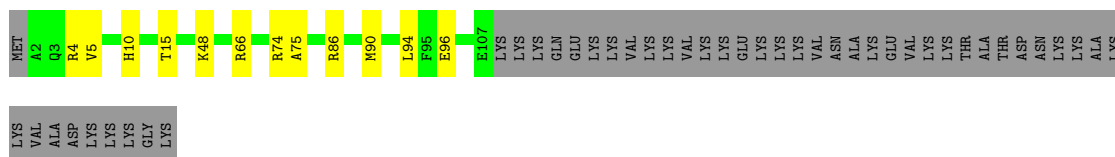
- Molecule 35: 60S ribosomal protein eL32



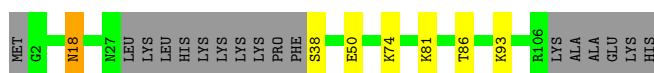
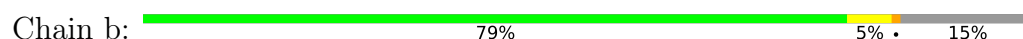
- Molecule 36: 60S ribosomal protein eL33



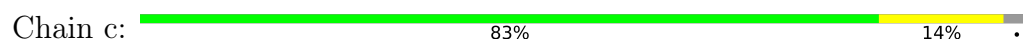
- Molecule 37: 60S ribosomal protein eL34



- Molecule 38: 60S ribosomal protein eL36



- Molecule 39: 60S ribosomal protein eL37

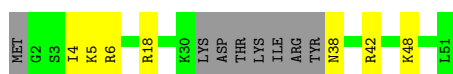




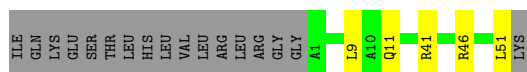
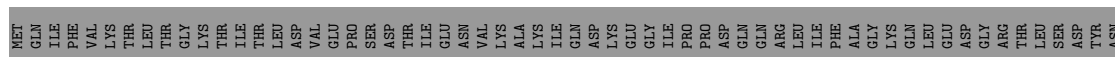
- Molecule 40: 60S ribosomal protein eL38



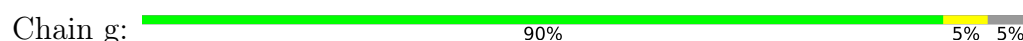
- Molecule 41: 60S ribosomal protein eL39



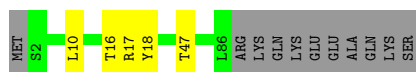
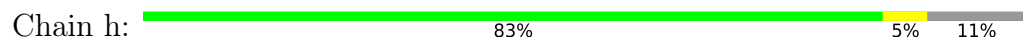
- Molecule 42: 60S ribosomal protein eL40



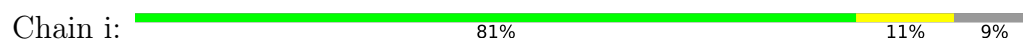
- Molecule 43: 60S ribosomal protein eL41



- Molecule 44: 60S ribosomal protein eL43



- Molecule 45: 60S ribosomal protein eL44



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (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: ZN, MG

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	0.30	1/75991 (0.0%)	0.73	35/118299 (0.0%)
2	B	0.26	0/2826	0.69	0/4404
3	C	0.28	0/3608	0.74	4/5615 (0.1%)
4	D	0.48	0/1901	0.82	1/2544 (0.0%)
5	E	0.43	0/3129	0.74	0/4195
6	F	0.42	0/3144	0.80	2/4205 (0.0%)
7	G	0.43	0/1020	0.80	0/1349
8	H	0.42	0/1485	0.77	1/2009 (0.0%)
9	I	0.41	0/1707	0.75	0/2274
10	J	0.41	0/1901	0.74	0/2537
11	K	0.45	0/1689	0.81	0/2260
12	L	0.44	0/1793	0.80	0/2387
13	M	0.45	0/1012	0.73	0/1363
14	N	0.45	0/1213	0.81	0/1616
15	O	0.44	0/1199	0.76	0/1597
16	P	0.44	0/1735	0.83	2/2320 (0.1%)
17	Q	0.41	0/1579	0.73	0/2113
18	R	0.43	0/2074	0.79	0/2773
19	S	0.43	0/1530	0.80	0/2040
20	T	0.46	0/1521	0.80	0/2012
21	U	0.43	0/1526	0.73	0/2043
22	V	0.40	0/1300	0.70	0/1732
23	W	0.45	0/1338	0.78	0/1793
24	X	0.40	0/841	0.66	0/1125
25	Y	0.41	0/805	0.74	0/1074
26	Z	0.39	0/1012	0.78	1/1339 (0.1%)
27	0	0.46	0/533	0.76	0/711
28	1	0.37	0/1151	0.68	0/1531
29	2	0.41	0/839	0.64	0/1114
30	3	0.44	0/1004	0.82	0/1329
31	4	0.43	0/564	0.77	0/737
32	5	0.45	0/1917	0.83	0/2562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.42	0/748	0.83	0/1001
34	7	0.44	0/805	0.82	0/1073
35	8	0.45	0/1053	0.79	0/1399
36	9	0.48	0/864	0.87	0/1160
37	a	0.38	0/871	0.77	0/1161
38	b	0.46	0/762	0.83	0/1008
39	c	0.47	0/718	0.84	0/946
40	d	0.42	0/611	0.71	0/812
41	e	0.48	0/396	0.84	0/521
42	f	0.45	0/418	0.83	0/556
43	g	0.45	0/347	0.95	0/448
44	h	0.43	0/667	0.73	0/887
45	i	0.41	0/788	0.71	0/1032
All	All	0.36	1/133935 (0.0%)	0.75	46/197006 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	E	0	3
6	F	0	1
9	I	0	1
11	K	0	1
14	N	0	1
23	W	0	1
32	5	0	1
33	6	0	1
36	9	0	1
39	c	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2463	U	O3'-P	-5.46	1.54	1.61

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1805	U	C2'-C3'-O3'	8.69	128.62	109.50
1	A	289	A	C2'-C3'-O3'	8.40	127.98	109.50
3	C	145	A	C2'-C3'-O3'	8.31	127.79	109.50
3	C	37	A	C2'-C3'-O3'	8.03	127.16	109.50
1	A	652	A	C2'-C3'-O3'	7.52	126.05	109.50

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	196	TRP	Peptide
5	E	17	LEU	Peptide
5	E	195	MET	Peptide
5	E	253	HIS	Peptide
6	F	150	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	245/260 (94%)	225 (92%)	15 (6%)	5 (2%)	7	38
5	E	378/386 (98%)	345 (91%)	26 (7%)	7 (2%)	8	39
6	F	388/411 (94%)	359 (92%)	20 (5%)	9 (2%)	6	34
7	G	116/173 (67%)	106 (91%)	7 (6%)	3 (3%)	5	31
8	H	183/190 (96%)	150 (82%)	26 (14%)	7 (4%)	3	22
9	I	203/221 (92%)	179 (88%)	15 (7%)	9 (4%)	2	19
10	J	225/283 (80%)	203 (90%)	16 (7%)	6 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	199/202 (98%)	185 (93%)	10 (5%)	4 (2%)	7	38
12	L	209/215 (97%)	183 (88%)	17 (8%)	9 (4%)	2	20
13	M	130/139 (94%)	119 (92%)	8 (6%)	3 (2%)	6	34
14	N	144/165 (87%)	135 (94%)	5 (4%)	4 (3%)	5	29
15	O	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
16	P	202/205 (98%)	185 (92%)	11 (5%)	6 (3%)	4	28
17	Q	185/219 (84%)	157 (85%)	22 (12%)	6 (3%)	4	26
18	R	244/294 (83%)	218 (89%)	17 (7%)	9 (4%)	3	22
19	S	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	5	30
20	T	179/182 (98%)	172 (96%)	4 (2%)	3 (2%)	9	42
21	U	178/184 (97%)	166 (93%)	9 (5%)	3 (2%)	9	42
22	V	153/161 (95%)	134 (88%)	13 (8%)	6 (4%)	3	22
23	W	166/203 (82%)	152 (92%)	13 (8%)	1 (1%)	25	64
24	X	95/139 (68%)	86 (90%)	6 (6%)	3 (3%)	4	26
25	Y	99/190 (52%)	93 (94%)	6 (6%)	0	100	100
26	Z	119/126 (94%)	102 (86%)	14 (12%)	3 (2%)	5	32
27	0	60/162 (37%)	55 (92%)	3 (5%)	2 (3%)	4	25
28	1	136/146 (93%)	125 (92%)	10 (7%)	1 (1%)	22	61
29	2	96/127 (76%)	85 (88%)	9 (9%)	2 (2%)	7	37
30	3	117/124 (94%)	104 (89%)	10 (8%)	3 (3%)	5	31
31	4	64/67 (96%)	56 (88%)	5 (8%)	3 (5%)	2	17
32	5	221/257 (86%)	197 (89%)	20 (9%)	4 (2%)	8	41
33	6	96/108 (89%)	92 (96%)	2 (2%)	2 (2%)	7	37
34	7	92/120 (77%)	88 (96%)	4 (4%)	0	100	100
35	8	123/131 (94%)	109 (89%)	10 (8%)	4 (3%)	4	25
36	9	101/140 (72%)	86 (85%)	12 (12%)	3 (3%)	4	28
37	a	104/150 (69%)	98 (94%)	4 (4%)	2 (2%)	8	39
38	b	91/112 (81%)	86 (94%)	3 (3%)	2 (2%)	6	35
39	c	87/92 (95%)	68 (78%)	15 (17%)	4 (5%)	2	18
40	d	68/87 (78%)	65 (96%)	3 (4%)	0	100	100
41	e	39/51 (76%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	f	49/128 (38%)	45 (92%)	4 (8%)	0	100	100
43	g	35/39 (90%)	31 (89%)	4 (11%)	0	100	100
44	h	83/96 (86%)	74 (89%)	8 (10%)	1 (1%)	13	49
45	i	93/104 (89%)	82 (88%)	7 (8%)	4 (4%)	2	20
All	All	6124/7124 (86%)	5538 (90%)	438 (7%)	148 (2%)	9	34

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	PRO
5	E	18	PRO
6	F	102	PHE
7	G	130	HIS
7	G	143	ARG

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	
4	D	191/202 (95%)	174 (91%)	17 (9%)	9	35
5	E	335/340 (98%)	311 (93%)	24 (7%)	14	47
6	F	336/352 (96%)	306 (91%)	30 (9%)	9	35
7	G	110/155 (71%)	94 (86%)	16 (14%)	3	15
8	H	164/173 (95%)	139 (85%)	25 (15%)	3	13
9	I	189/203 (93%)	169 (89%)	20 (11%)	6	27
10	J	211/260 (81%)	189 (90%)	22 (10%)	7	28
11	K	181/182 (100%)	163 (90%)	18 (10%)	8	30
12	L	190/194 (98%)	168 (88%)	22 (12%)	5	24
13	M	106/110 (96%)	88 (83%)	18 (17%)	2	10
14	N	134/152 (88%)	112 (84%)	22 (16%)	2	11
15	O	121/122 (99%)	114 (94%)	7 (6%)	20	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	179/180 (99%)	162 (90%)	17 (10%)	8	32
17	Q	165/190 (87%)	156 (94%)	9 (6%)	21	57
18	R	214/254 (84%)	185 (86%)	29 (14%)	3	17
19	S	158/159 (99%)	141 (89%)	17 (11%)	6	27
20	T	161/163 (99%)	144 (89%)	17 (11%)	6	27
21	U	162/166 (98%)	148 (91%)	14 (9%)	10	38
22	V	140/144 (97%)	134 (96%)	6 (4%)	29	64
23	W	128/178 (72%)	113 (88%)	15 (12%)	5	23
24	X	92/131 (70%)	88 (96%)	4 (4%)	29	64
25	Y	90/177 (51%)	84 (93%)	6 (7%)	16	50
26	Z	111/115 (96%)	94 (85%)	17 (15%)	2	13
27	0	53/146 (36%)	47 (89%)	6 (11%)	6	25
28	1	127/132 (96%)	115 (91%)	12 (9%)	8	33
29	2	97/118 (82%)	91 (94%)	6 (6%)	18	53
30	3	110/115 (96%)	94 (86%)	16 (14%)	3	15
31	4	60/61 (98%)	54 (90%)	6 (10%)	7	30
32	5	201/231 (87%)	180 (90%)	21 (10%)	7	28
33	6	83/92 (90%)	69 (83%)	14 (17%)	2	10
34	7	90/112 (80%)	71 (79%)	19 (21%)	1	6
35	8	114/120 (95%)	97 (85%)	17 (15%)	3	14
36	9	90/127 (71%)	73 (81%)	17 (19%)	1	8
37	a	89/128 (70%)	79 (89%)	10 (11%)	6	25
38	b	82/97 (84%)	76 (93%)	6 (7%)	14	46
39	c	73/77 (95%)	65 (89%)	8 (11%)	6	26
40	d	69/83 (83%)	62 (90%)	7 (10%)	7	29
41	e	40/48 (83%)	33 (82%)	7 (18%)	2	9
42	f	45/114 (40%)	40 (89%)	5 (11%)	6	25
43	g	34/35 (97%)	32 (94%)	2 (6%)	19	54
44	h	70/80 (88%)	66 (94%)	4 (6%)	20	56
45	i	87/93 (94%)	80 (92%)	7 (8%)	12	42
All	All	5482/6311 (87%)	4900 (89%)	582 (11%)	10	27

5 of 582 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	6	33	CYS
44	h	17	ARG
34	7	36	LYS
33	6	28	PHE
36	9	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
29	2	37	ASN
37	a	6	HIS
30	3	43	ASN
32	5	250	ASN
38	b	98	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3163/3788 (83%)	934 (29%)	167 (5%)
2	B	117/119 (98%)	23 (19%)	1 (0%)
3	C	148/159 (93%)	43 (29%)	8 (5%)
All	All	3428/4066 (84%)	1000 (29%)	176 (5%)

5 of 1000 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	13	G
1	A	14	U
1	A	16	A
1	A	18	G

5 of 176 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2437	A
1	A	3381	A
1	A	2523	U
1	A	2886	A

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Mol	Chain	Res	Type
1	A	3477	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 168 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2660. 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 surface views

This section was not generated.

6.5 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

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

9 Map-model fit

This section was not generated.