



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:45 PM BST

PDB ID : 4D67
EMDB ID: : EMD-2813
Title : Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors : Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on : 2014-11-08
Resolution : 9.00 Å(reported)
Based on PDB ID : 4CXD

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>

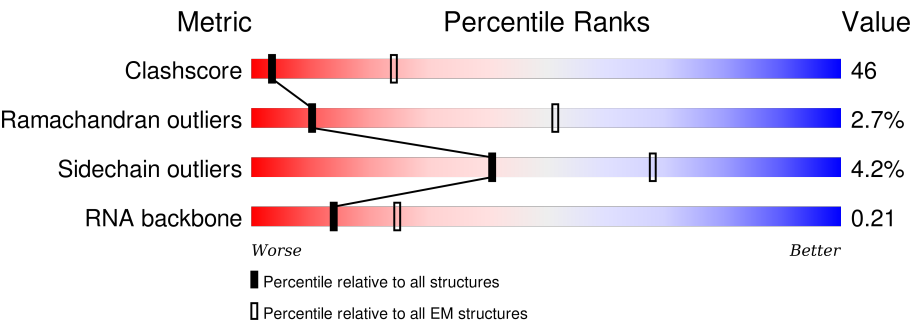
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.00 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.






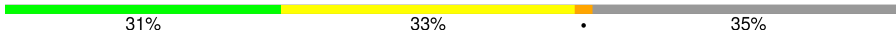


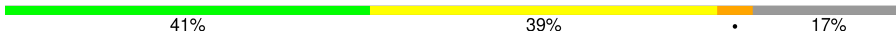










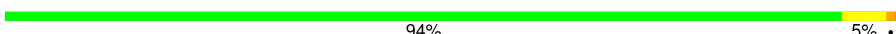







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	257	<div><div>57%</div><div>38%</div><div>• •</div></div>
2	B	403	<div><div>57%</div><div>36%</div><div>5% •</div></div>
3	C	427	<div><div>45%</div><div>35%</div><div>5% • 15%</div></div>
4	D	297	<div><div>55%</div><div>40%</div><div>• •</div></div>
5	E	288	<div><div>23%</div><div>28%</div><div>• 45%</div></div>
6	F	248	<div><div>52%</div><div>40%</div><div>• 6%</div></div>
7	G	266	<div><div>50%</div><div>35%</div><div>• • 12%</div></div>
8	H	192	<div><div>56%</div><div>41%</div><div>•</div></div>










Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	214	
10	J	178	
11	L	211	
12	M	215	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	159	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	105	 83%8% • 8%
35	j	97	 84% • 12%
36	k	70	 97% ••
37	l	51	 94% ••
38	m	128	 38% • 59%
39	n	25	 100%
40	o	106	 93%7%
41	p	92	 93%5% •
42	t	137	 86%7% • 5%
43	u	210	 92%8%
44	2	5025	 7%28%36% • 28%
45	3	194	 7%38%35% • 19%
46	4	121	 12%33%51% ••

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 136495 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 protein called 60S RIBOSOMAL PROTEIN L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	1
			1888	1183	388	311	6		

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	396	Total	C	N	O	S	0	1
			3190	2030	601	545	14		

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	364	Total	C	N	O	S	0	1
			2889	1817	578	480	14		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	290	Total	C	N	O	S	0	0
			2361	1489	431	427	14		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	158	Total	C	N	O	0	0
			1286	834	238	214		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	234	Total	C	N	O	S	0	0
			1949	1252	376	312	9		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	235	Total	C	N	O	S	0	1
			1881	1197	363	317	4		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1535	965	286	278	6		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	196	Total	C	N	O	S	0	0
			1604	1022	308	262	12		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	200	Total	C	N	O	S	0	1
			1617	1013	335	265	4		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	140	Total	C	N	O	S	0	1
			1139	730	219	183	7		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	204	Total	C	N	O	S	0	0
			1708	1077	360	266	5		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	196	Total	C	N	O	S	0	1
			1607	1034	316	252	5		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	1
			1234	771	241	213	9		

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	184	Total	C	N	O	S	0	0
			1493	933	311	244	5		

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	183	Total	C	N	O	S	0	1
			1526	943	331	242	10		

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	173	Total	C	N	O	S	0	0
			1438	916	280	232	10		

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	102	Total	C	N	O	S	0	1
			827	529	146	150	2		

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	128	Total	C	N	O	S	0	0
			963	610	181	167	5		

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	64	Total	C	N	O	S	0	1
			529	337	104	85	3		

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			975	624	183	167	1		

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	128	Total	C	N	O	S	0	1
			1065	668	217	177	3		

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	136	Total	C	N	O	S	0	0
			1114	719	209	182	4		

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1161	736	237	185	3		

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	69	Total	C	N	O	S	0	1
			560	344	123	90	3		

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	104	Total	C	N	O	S	0	1
			802	508	142	145	7		

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	109	Total	C	N	O	S	0	0
			904	570	174	158	2		

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	1
			1053	664	219	165	5		

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	107	Total	C	N	O	S	0	0
			865	550	172	140	3		

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	115	Total	C	N	O	S	0	1
			907	566	188	147	6		

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	97	Total	C	N	O	S	0	1
			783	488	168	122	5		

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	85	Total	C	N	O	S	0	1
			690	423	153	109	5		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 38 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			428	266	90	66	6		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	106	Total	C	N	O	S	0	0
			870	547	176	140	7		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			707	445	136	119	7		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	130	Total	C	N	O	S	0	1
			1043	646	220	172	5		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	210	Total	C	N	O	S	0	0
			1621	990	278	347	6		

- Molecule 44 is a RNA chain called 28S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	3616	Total	C	N	O	P	0	0
			77488	34508	14153	25212	3615		

- Molecule 45 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	157	Total	C	N	O	P	0	0
			3334	1489	587	1102	156		

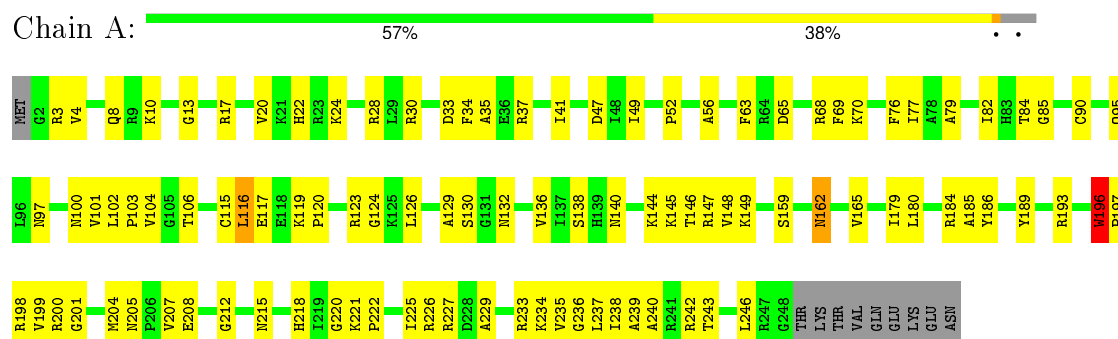
- Molecule 46 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

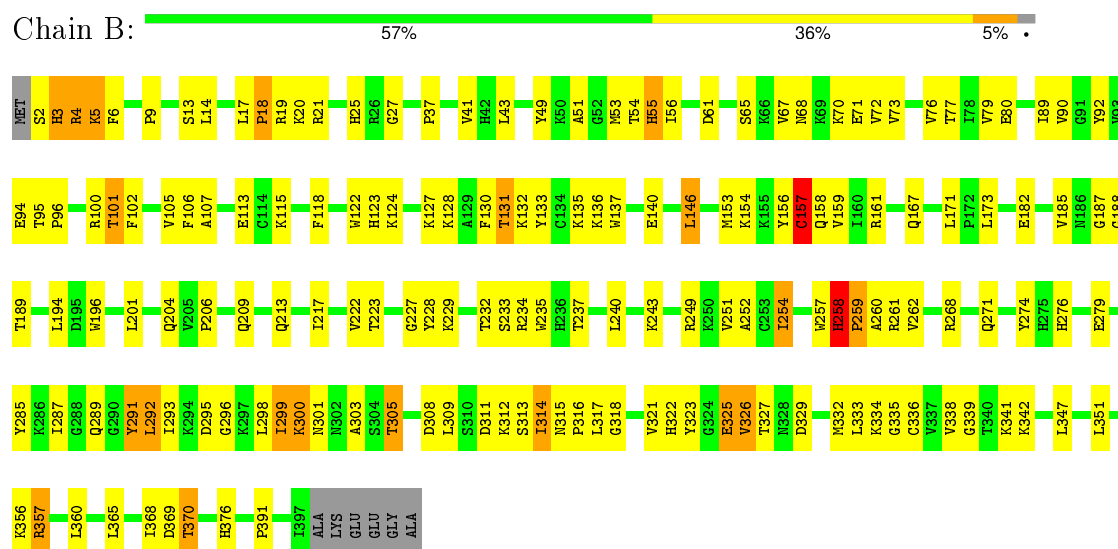
3 Residue-property plots

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.

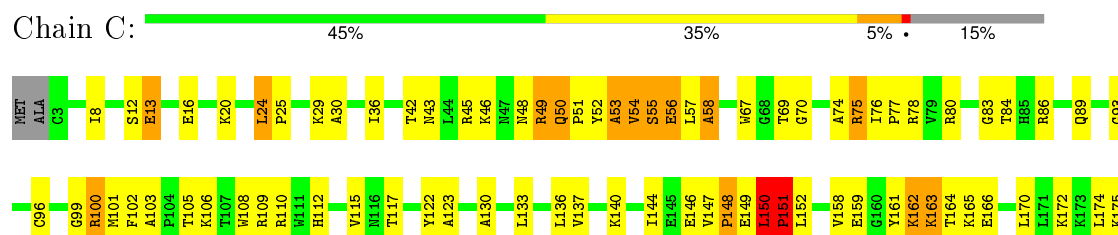
• Molecule 1: 60S RIBOSOMAL PROTEIN L8

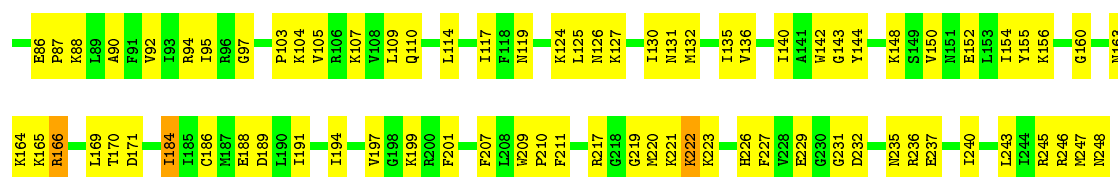


• Molecule 2: 60S RIBOSOMAL PROTEIN L3



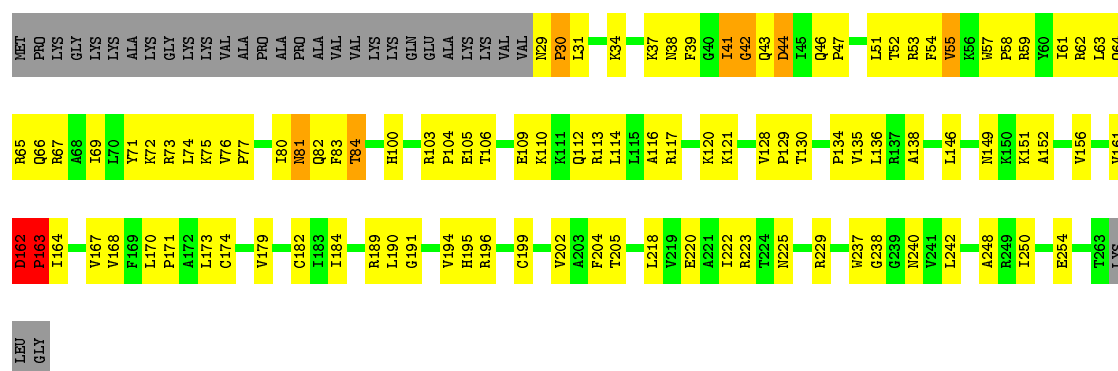
• Molecule 3: 60S RIBOSOMAL PROTEIN L4





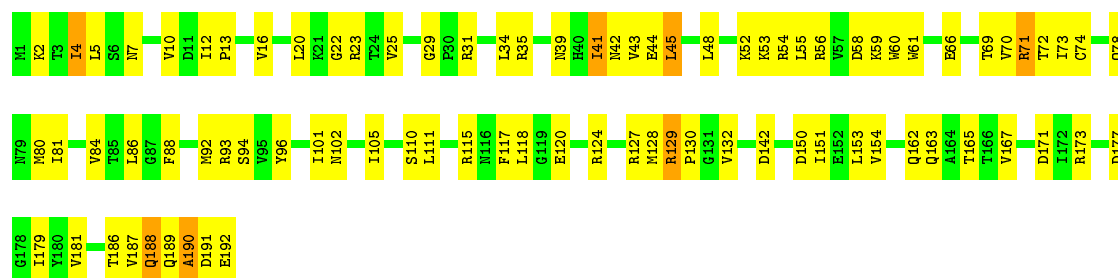
• Molecule 7: 60S RIBOSOMAL PROTEIN L7A

Chain G: 50% 35% 12%



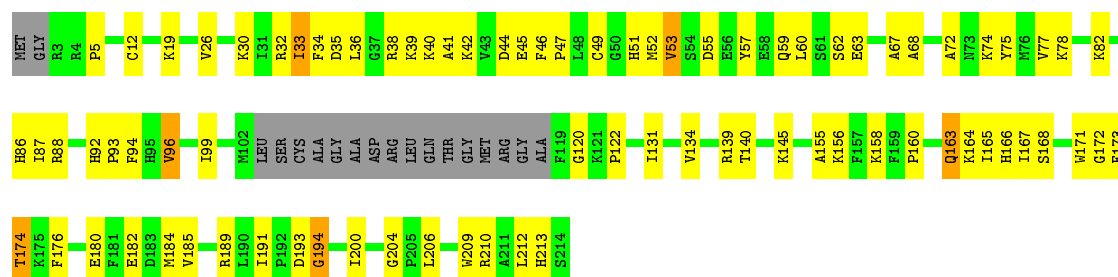
• Molecule 8: 60S RIBOSOMAL PROTEIN L9

Chain H: 56% 41%



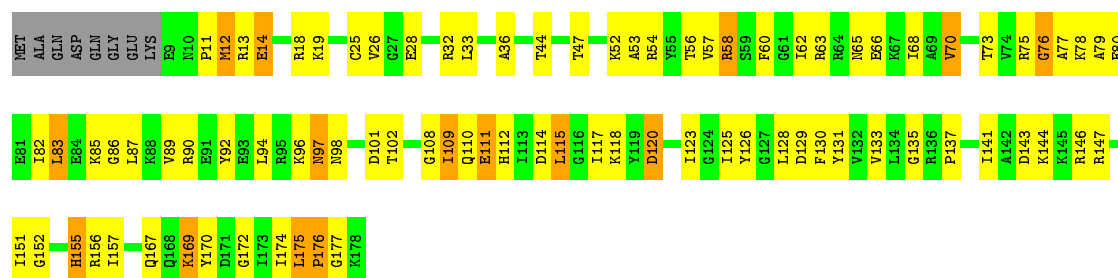
• Molecule 9: 60S RIBOSOMAL PROTEIN L10

Chain I: 53% 36% 8%



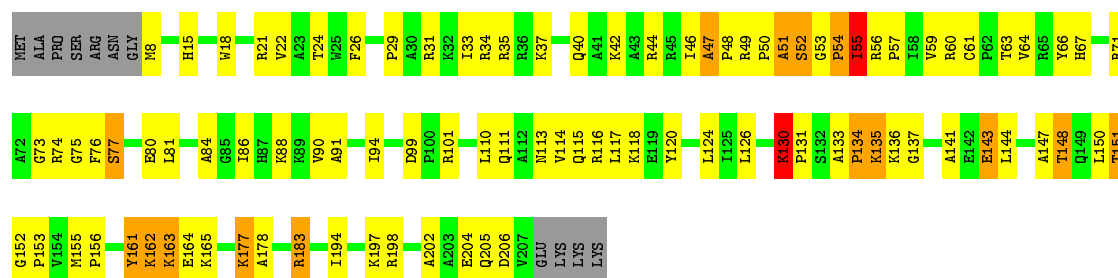
• Molecule 10: 60S RIBOSOMAL PROTEIN L11

Chain J: 47% 40% 8%



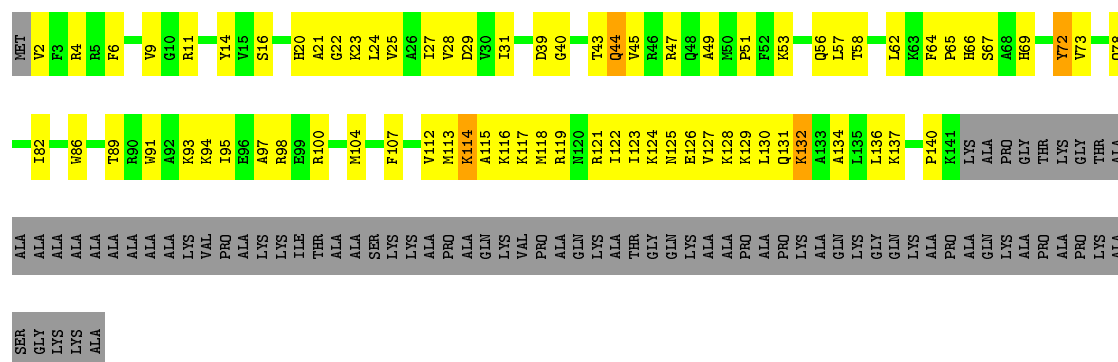
• Molecule 11: 60S RIBOSOMAL PROTEIN L13

Chain L: 50% 37% 7% 5%



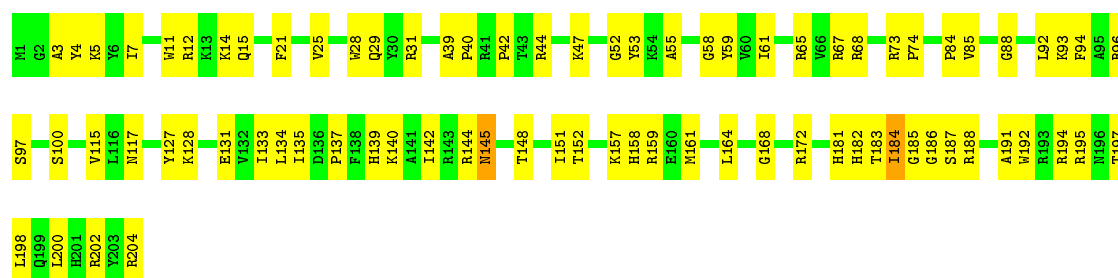
• Molecule 12: 60S RIBOSOMAL PROTEIN L14

Chain M: 31% 33% 35%



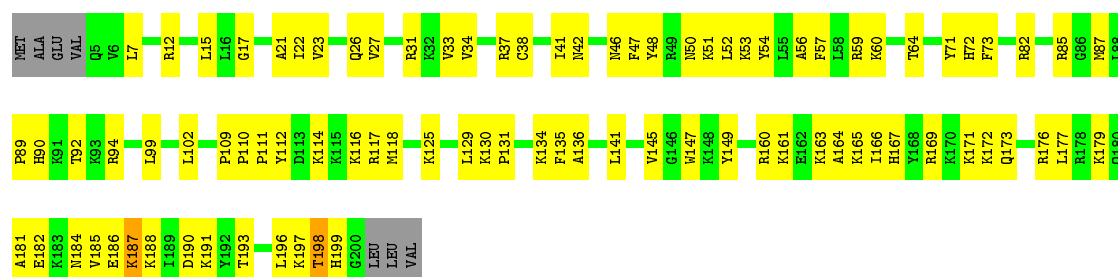
• Molecule 13: 60S RIBOSOMAL PROTEIN L15

Chain N: 61% 38%



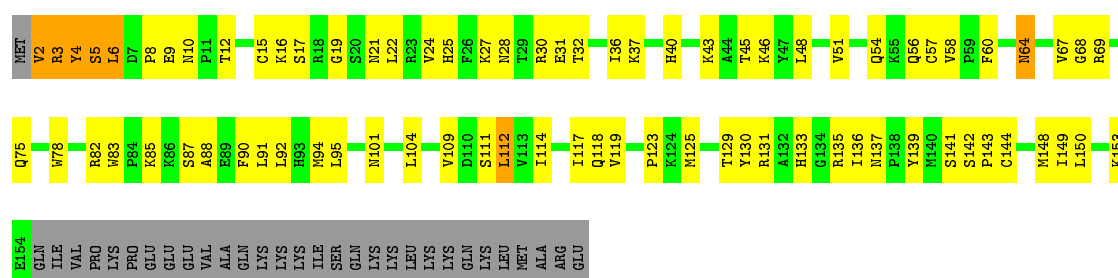
• Molecule 14: 60S RIBOSOMAL PROTEIN L13A

Chain O: 



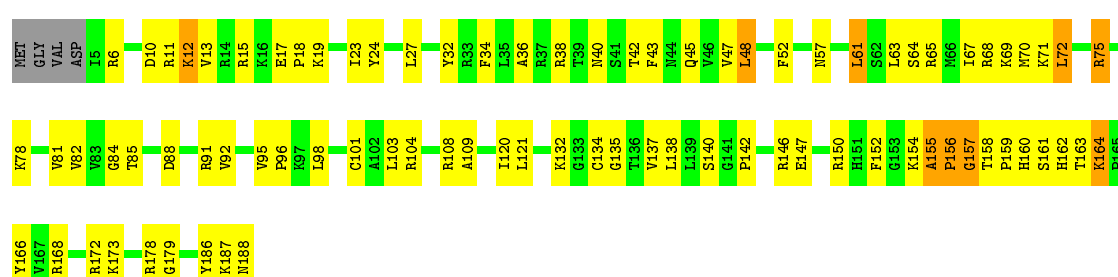
• Molecule 15: 60S RIBOSOMAL PROTEIN L17

Chain P: 



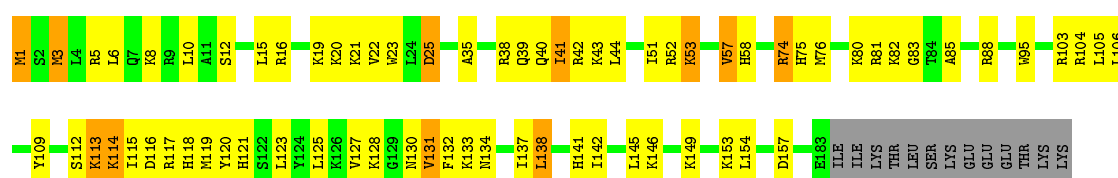
• Molecule 16: 60S RIBOSOMAL PROTEIN L18

Chain Q: 



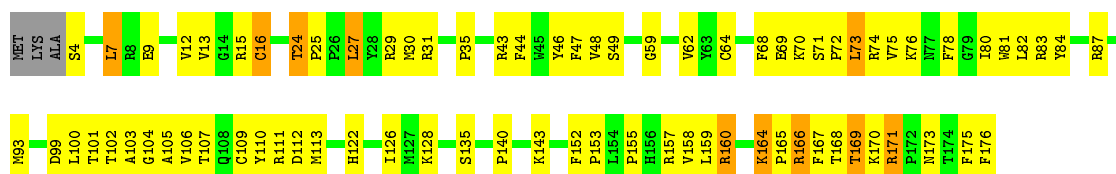
• Molecule 17: 60S RIBOSOMAL PROTEIN L19

Chain R: 



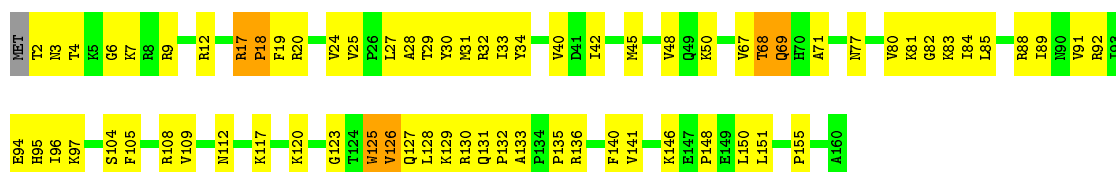
• Molecule 18: 60S RIBOSOMAL PROTEIN L18A

Chain S: 



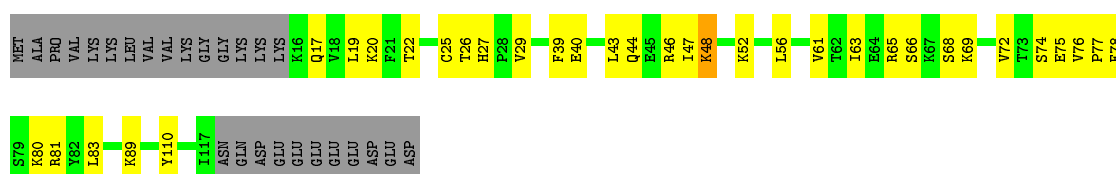
• Molecule 19: 60S RIBOSOMAL PROTEIN L21

Chain T: 55% 41% . .



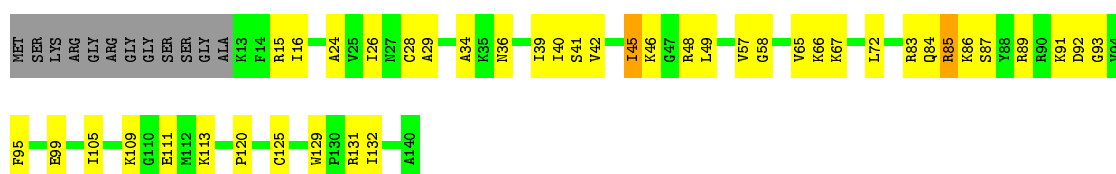
• Molecule 20: 60S RIBOSOMAL PROTEIN L22

Chain U: 53% 26% . 20%



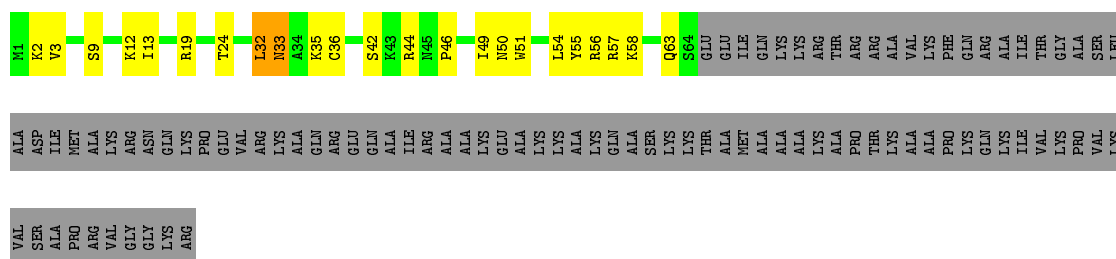
• Molecule 21: 60S RIBOSOMAL PROTEIN L23

Chain V: 61% 29% . 9%



• Molecule 22: 60S RIBOSOMAL PROTEIN L24

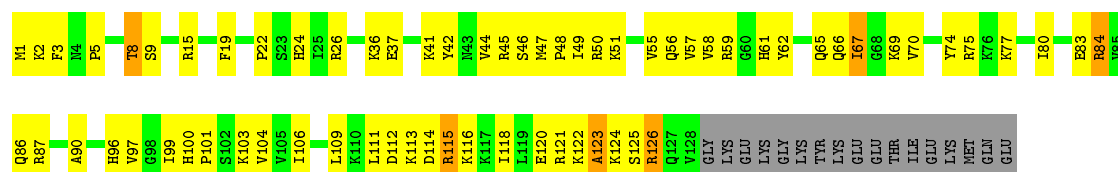
Chain W: 26% 13% . 59%



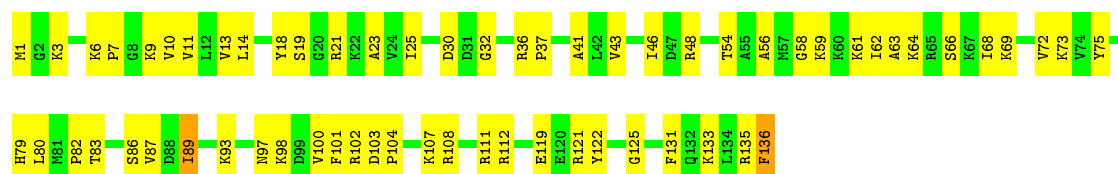
• Molecule 23: 60S RIBOSOMAL PROTEIN L23A

Chain X: 46% 30% 24%

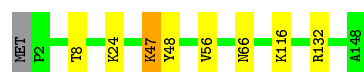
• Molecule 24: 60S RIBOSOMAL PROTEIN L26



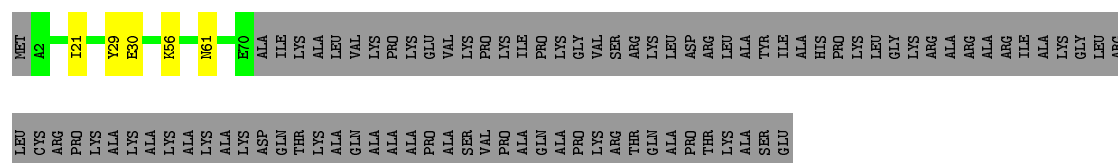
• Molecule 25: 60S RIBOSOMAL PROTEIN L27



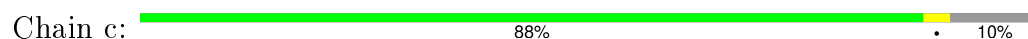
• Molecule 26: 60S RIBOSOMAL PROTEIN L27A



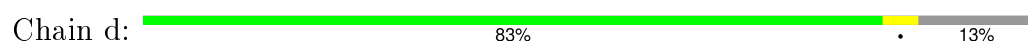
• Molecule 27: 60S RIBOSOMAL PROTEIN L29

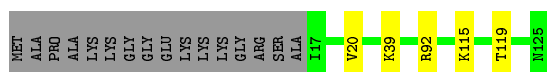


• Molecule 28: 60S RIBOSOMAL PROTEIN L30



• Molecule 29: 60S RIBOSOMAL PROTEIN L31





- Molecule 30: 60S RIBOSOMAL PROTEIN L32

Chain e: 90% 5%



- Molecule 31: 60S RIBOSOMAL PROTEIN L35A

Chain f: 86% 10% ..



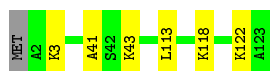
- Molecule 32: 60S RIBOSOMAL PROTEIN L34

Chain g: 87% 10% ..



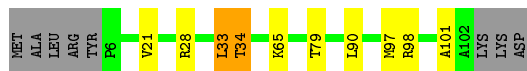
- Molecule 33: 60S RIBOSOMAL PROTEIN L35

Chain h: 94% 5% ..



- Molecule 34: 60S RIBOSOMAL PROTEIN L36

Chain i: 83% 8% 8%



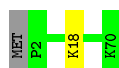
- Molecule 35: 60S RIBOSOMAL PROTEIN L37

Chain j: 84% 12%



- Molecule 36: 60S RIBOSOMAL PROTEIN L38

Chain k: 97% ..



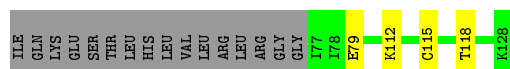
- Molecule 37: 60S RIBOSOMAL PROTEIN L39

Chain l:  94%



- Molecule 38: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain m:  38% 59%



- Molecule 39: 60S RIBOSOMAL PROTEIN L41

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 60S RIBOSOMAL PROTEIN L36A

Chain o:  93% 7%




- Molecule 41: 60S RIBOSOMAL PROTEIN L37A

Chain p:  93% 5%



- Molecule 42: 60S RIBOSOMAL PROTEIN L28

Chain t:  86% 7% 5%



- Molecule 43: 60S RIBOSOMAL PROTEIN L10A

Chain u:  92% 8%



- Molecule 44: 28S RRNA

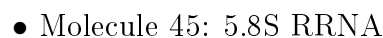




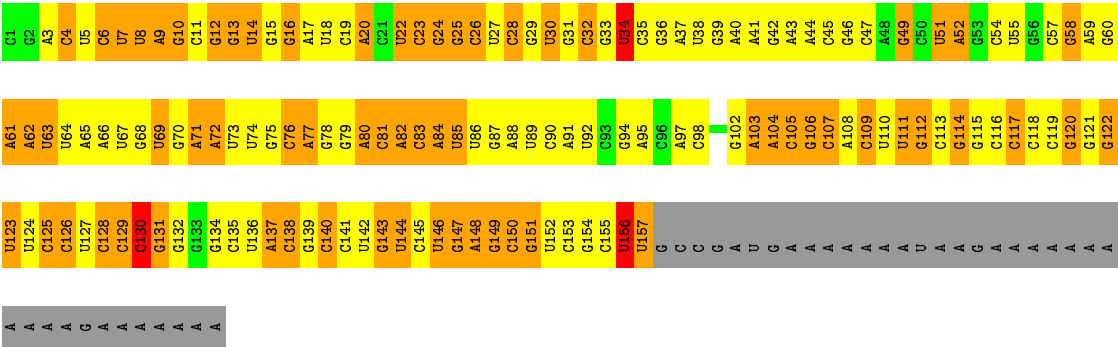






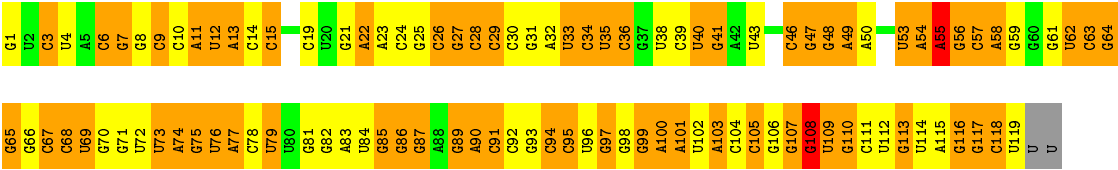



Chain 3:  7% 38% 35% • 19%



● Molecule 46: 5S rRNA

Chain 4: 12% 33% 51% . .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	115000	Depositor
Image detector	TVIPS TEMCAM F416	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.44	0/1926	0.67	0/2583
10	J	0.49	0/1385	0.71	0/1852
11	L	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
12	M	0.49	0/1162	0.70	0/1556
13	N	0.43	0/1753	0.65	0/2348
14	O	0.44	0/1639	0.69	0/2193
15	P	0.44	0/1260	0.70	0/1691
16	Q	0.45	0/1517	0.74	0/2026
17	R	0.41	0/1542	0.64	0/2037
18	S	0.45	0/1478	0.73	0/1985
19	T	0.46	0/1325	0.72	0/1770
2	B	0.45	0/3258	0.73	2/4361 (0.0%)
20	U	0.47	0/841	0.71	0/1128
21	V	0.43	0/977	0.63	0/1312
22	W	0.43	0/542	0.59	0/722
23	X	0.41	0/992	0.67	0/1334
24	Y	0.47	0/1082	0.72	1/1441 (0.1%)
25	Z	0.47	0/1137	0.79	0/1517
26	a	0.45	0/1190	0.71	0/1591
27	b	0.45	0/570	0.72	0/752
28	c	0.46	0/813	0.70	0/1091
29	d	0.45	0/919	0.67	0/1238
3	C	0.47	0/2943	0.73	1/3953 (0.0%)
30	e	0.45	0/1071	0.68	0/1428
31	f	0.50	0/884	0.81	0/1185
32	g	0.48	0/917	0.74	0/1222
33	h	0.38	0/1022	0.64	0/1351
34	i	0.43	0/793	0.75	0/1048
35	j	0.49	0/704	0.76	0/931
36	k	0.43	0/574	0.73	0/761
37	l	0.40	0/453	0.61	0/599
38	m	0.42	0/434	0.70	0/575
39	n	0.40	0/240	0.50	0/305
4	D	0.49	1/2406 (0.0%)	0.70	1/3221 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	o	0.46	0/884	0.74	0/1166
41	p	0.40	0/717	0.61	0/953
42	t	0.48	0/1058	0.75	0/1416
43	u	0.45	0/1638	0.69	1/2222 (0.0%)
44	2	0.41	22/86672 (0.0%)	0.81	41/135198 (0.0%)
45	3	0.36	0/3723	0.79	1/5800 (0.0%)
46	4	0.38	0/2836	0.82	3/4421 (0.1%)
5	E	0.52	0/1311	0.73	0/1763
6	F	0.45	0/1985	0.68	0/2644
7	G	0.46	0/1914	0.72	0/2578
8	H	0.43	0/1554	0.69	0/2089
9	I	0.42	0/1642	0.67	0/2194
All	All	0.43	25/147330 (0.0%)	0.77	54/217756 (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
44	2	0	34
45	3	0	2
All	All	0	36

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1701	C	C5'-C4'	18.32	1.73	1.51
44	2	1673	C	C3'-O3'	15.33	1.63	1.42
44	2	1701	C	O5'-C5'	14.40	1.67	1.44
44	2	1673	C	O3'-P	14.19	1.78	1.61
44	2	1701	C	P-O5'	13.52	1.73	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	1701	C	O4'-C4'-C3'	-15.18	88.82	104.00
2	B	258	HIS	C-N-CD	-13.98	89.84	120.60
44	2	1701	C	O4'-C1'-N1	12.32	118.06	108.20
44	2	1701	C	C4'-C3'-O3'	12.21	137.41	113.00
44	2	1701	C	C2'-C3'-O3'	-10.63	86.10	109.50

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	2	1	C	Sidechain
44	2	115	C	Sidechain
44	2	121	A	Sidechain
44	2	149	U	Sidechain
44	2	2	G	Sidechain

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	1888	0	1983	135	0
2	B	3190	0	3327	164	0
3	C	2889	0	3064	277	0
4	D	2361	0	2385	157	0
5	E	1286	0	1398	171	0
6	F	1949	0	2093	134	0
7	G	1881	0	2018	136	0
8	H	1535	0	1611	94	0
9	I	1604	0	1652	60	0
10	J	1362	0	1399	89	0
11	L	1617	0	1725	120	0
12	M	1139	0	1204	134	0
13	N	1708	0	1761	97	0
14	O	1607	0	1745	127	0
15	P	1234	0	1263	91	0
16	Q	1493	0	1612	119	0
17	R	1526	0	1682	75	0
18	S	1438	0	1472	85	0
19	T	1297	0	1366	115	0
20	U	827	0	852	29	0
21	V	963	0	1026	42	0
22	W	529	0	541	27	0
23	X	975	0	1053	64	0
24	Y	1065	0	1145	102	0
25	Z	1114	0	1194	62	0
26	a	1161	0	1213	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	560	0	590	0	0
28	c	802	0	845	0	0
29	d	904	0	947	0	0
30	e	1053	0	1144	0	0
31	f	865	0	904	0	0
32	g	907	0	1002	0	0
33	h	1014	0	1148	0	0
34	i	783	0	862	0	0
35	j	690	0	719	0	0
36	k	568	0	637	0	0
37	l	443	0	483	0	0
38	m	428	0	466	0	0
39	n	239	0	289	0	0
40	o	870	0	943	0	0
41	p	707	0	760	0	0
42	t	1043	0	1120	0	0
43	u	1621	0	1555	0	0
44	2	77488	0	39153	7461	0
45	3	3334	0	1693	313	0
46	4	2538	0	1286	273	0
All	All	136495	0	98330	9536	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 46.

The worst 5 of 9536 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)
44:2:1673:C:C3'	44:2:1673:C:O3'	1.63	1.46
44:2:1701:C:C5'	44:2:1701:C:O5'	1.67	1.39
44:2:3910:G:O2'	44:2:3911:A:H5'	1.22	1.34
1:A:196:TRP:HB3	1:A:197:PRO:CD	1.62	1.25
20:U:29:VAL:O	44:2:4022:C:O2'	186.30	1.23

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	
1	A	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	16	61
2	B	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	4	38
3	C	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	3	35
4	D	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	11	55
5	E	156/288 (54%)	141 (90%)	8 (5%)	7 (4%)	3	33
6	F	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	11	55
7	G	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	4	36
8	H	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	12	56
9	I	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	12	56
10	J	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	22
11	L	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	2	28
12	M	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	14	58
13	N	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	13	57
14	O	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	13	57
15	P	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	9	51
16	Q	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	5	40
17	R	181/196 (92%)	174 (96%)	4 (2%)	3 (2%)	11	55
18	S	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	4	39
19	T	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	10	52
20	U	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
21	V	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	12	56
22	W	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
23	X	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
24	Y	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	7	47
25	Z	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	5	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	5	40
27	b	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	2	26
28	c	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	9	51
29	d	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	21	67
30	e	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	7	47
31	f	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	3	32
32	g	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	4	39
33	h	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	7	46
34	i	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	2	25
35	j	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	7	47
36	k	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	13	57
37	l	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	9	50
38	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	51
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	10	52
41	p	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	5	40
42	t	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	2	29
43	u	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	14	58
All	All	6479/7422 (87%)	6102 (94%)	200 (3%)	177 (3%)	10	45

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	196	TRP
2	B	4	ARG
2	B	5	LYS
2	B	157	CYS

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	
1	A	189/199 (95%)	184 (97%)	5 (3%)	54	80
2	B	344/349 (99%)	326 (95%)	18 (5%)	29	65
3	C	302/348 (87%)	284 (94%)	18 (6%)	24	60
4	D	244/250 (98%)	237 (97%)	7 (3%)	50	78
5	E	143/252 (57%)	135 (94%)	8 (6%)	26	62
6	F	203/215 (94%)	196 (97%)	7 (3%)	44	75
7	G	199/223 (89%)	192 (96%)	7 (4%)	43	74
8	H	171/171 (100%)	164 (96%)	7 (4%)	37	71
9	I	170/181 (94%)	161 (95%)	9 (5%)	28	64
10	J	143/149 (96%)	137 (96%)	6 (4%)	36	70
11	L	167/177 (94%)	156 (93%)	11 (7%)	21	57
12	M	118/161 (73%)	114 (97%)	4 (3%)	44	75
13	N	172/172 (100%)	170 (99%)	2 (1%)	78	90
14	O	168/174 (97%)	166 (99%)	2 (1%)	78	90
15	P	133/163 (82%)	126 (95%)	7 (5%)	28	64
16	Q	162/165 (98%)	157 (97%)	5 (3%)	47	77
17	R	161/175 (92%)	150 (93%)	11 (7%)	20	57
18	S	155/157 (99%)	148 (96%)	7 (4%)	34	69
19	T	139/140 (99%)	134 (96%)	5 (4%)	42	74
20	U	91/115 (79%)	88 (97%)	3 (3%)	45	76
21	V	100/107 (94%)	99 (99%)	1 (1%)	82	92
22	W	55/126 (44%)	52 (94%)	3 (6%)	27	63
23	X	107/133 (80%)	105 (98%)	2 (2%)	65	86
24	Y	119/135 (88%)	115 (97%)	4 (3%)	44	75
25	Z	118/118 (100%)	112 (95%)	6 (5%)	29	66
26	a	120/121 (99%)	116 (97%)	4 (3%)	45	76
27	b	58/126 (46%)	57 (98%)	1 (2%)	68	87
28	c	88/97 (91%)	87 (99%)	1 (1%)	80	91
29	d	100/110 (91%)	96 (96%)	4 (4%)	38	71
30	e	115/121 (95%)	112 (97%)	3 (3%)	54	80
31	f	87/89 (98%)	79 (91%)	8 (9%)	11	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	98/100 (98%)	88 (90%)	10 (10%)	9	37
33	h	109/110 (99%)	106 (97%)	3 (3%)	51	78
34	i	82/89 (92%)	76 (93%)	6 (7%)	17	54
35	j	71/80 (89%)	69 (97%)	2 (3%)	51	78
36	k	64/65 (98%)	64 (100%)	0	100	100
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	84
38	m	48/116 (41%)	45 (94%)	3 (6%)	22	59
39	n	24/24 (100%)	24 (100%)	0	100	100
40	o	94/94 (100%)	89 (95%)	5 (5%)	28	64
41	p	74/75 (99%)	72 (97%)	2 (3%)	52	79
42	t	113/121 (93%)	106 (94%)	7 (6%)	23	60
43	u	177/177 (100%)	163 (92%)	14 (8%)	15	51
All	All	5642/6318 (89%)	5403 (96%)	239 (4%)	41	70

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	N	31	ARG
17	R	138	LEU
42	t	20	ARG
15	P	2	VAL
16	Q	75	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	180	GLN
18	S	117	HIS
38	m	87	GLN
15	P	54	GLN
16	Q	162	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	2	3605/5025 (71%)	2046 (56%)	325 (9%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	3	156/194 (80%)	81 (51%)	6 (3%)
46	4	118/121 (97%)	68 (57%)	9 (7%)
All	All	3879/5340 (72%)	2195 (56%)	340 (8%)

5 of 2195 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	2	2	G
44	2	3	C
44	2	5	A
44	2	6	C
44	2	8	U

5 of 340 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	2006	C
44	2	2561	G
44	2	4867	G
44	2	2034	G
44	2	2371	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.