wwPDB EM Map/Model Validation Report (i)

May 12, 2016 – 11:27 AM EDT

PDB ID	:	5IT9
EMDB ID:	:	EMD-8124
Title	:	Structure of the yeast Kluyveromyces lactis small ribosomal subunit in complex with the cricket paralysis virus IRES.
Authors	:	Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on	:	2016-03-16
Resolution	:	3.80 Å(reported)
Based on PDB ID	:	?

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

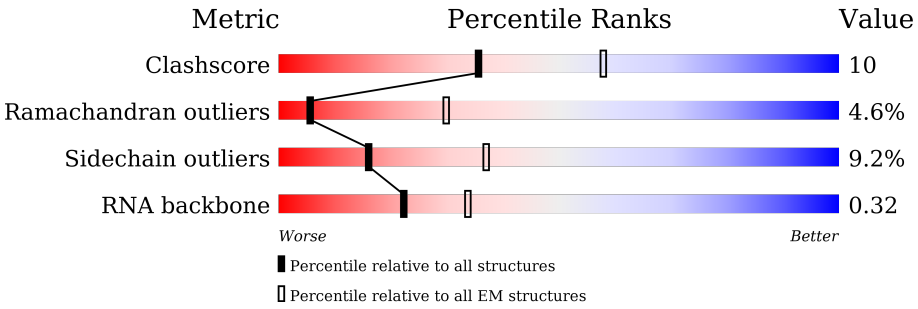
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 3.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	206	76% 22% •
2	B	214	89% 10% •
3	C	217	83% 15% •
4	D	223	87% 13%
5	E	260	88% 11% •
6	F	206	78% 20% •
7	G	226	80% 16% • •
8	H	184	82% 17% •

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Mol	Chain	Length	Quality of chain
9	I	200	71% 19% 6%
10	J	182	73% 19% 8%
11	K	96	80% 20%
12	L	155	88% 10%
13	M	122	82% 16%
14	N	150	86% 13%
15	O	127	86% 13%
16	P	123	77% 19%
17	Q	141	84% 13%
18	R	129	82% 16%
19	S	145	76% 21%
20	T	143	86% 12%
21	U	106	85% 14%
22	V	87	85% 15%
23	W	129	72% 24%
24	X	145	78% 19%
25	Y	134	75% 19% 5%
26	Z	70	56% 31% 11%
27	a	100	80% 16%
28	b	82	90% 10%
29	c	63	95% 5%
30	d	53	92% 8%
31	e	55	87% 13%
32	f	69	80% 17%
33	g	324	92% 6%

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Mol	Chain	Length	Quality of chain
34	2	1780	36% 47% 16%
35	i	192	44% 55%

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80144 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 Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 2 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 3 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 4 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 5 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 7 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 8 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 9 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 10 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 11 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 12 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 13 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	122	Total	C	N	O	0	0
			922	575	167	180		

- Molecule 14 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 15 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 16 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 17 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 18 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	129	Total	C	N	O	S	0	0
			1031	641	193	194	3		

- Molecule 19 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 20 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 21 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 22 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 23 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 24 is a protein called Ribosomal protein uS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	145	Total	C	N	O	S	0	0
			1127	713	219	192	3		

- Molecule 25 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 26 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 27 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	100	Total	C	N	O	S	0	0
			798	491	170	131	6		

- Molecule 28 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	82	Total	C	N	O	S	0	0
			617	384	113	114	6		

- Molecule 29 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 30 is a protein called Ribosomal protein eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 31 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	55	Total	C	N	O	S	0	0
			443	276	90	76	1		

- Molecule 32 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 33 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 35 is a RNA chain called Cricket paralysis virus IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	192	Total	C	N	O	P	0	0
			3968	1774	669	1333	192		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	6176	C	U	conflict	GB 8895506

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	X	1	Total	Mg	0
			1	1	
36	G	1	Total	Mg	0
			1	1	
36	2	76	Total	Mg	0
			76	76	
36	T	1	Total	Mg	0
			1	1	
36	N	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

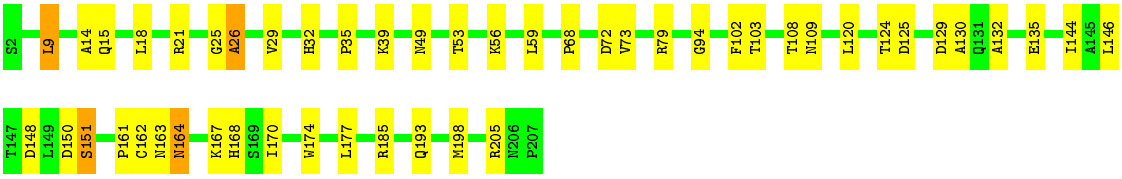
Mol	Chain	Residues	Atoms		AltConf
37	b	1	Total	Zn	0
			1	1	
37	a	1	Total	Zn	0
			1	1	
37	f	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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.

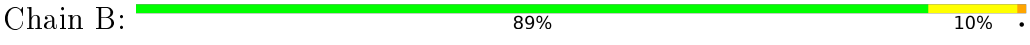
- Molecule 1: Ribosomal protein uS2

Chain A:



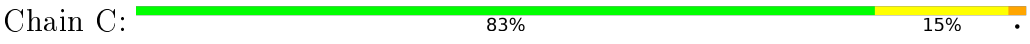
- Molecule 2: Ribosomal protein eS1

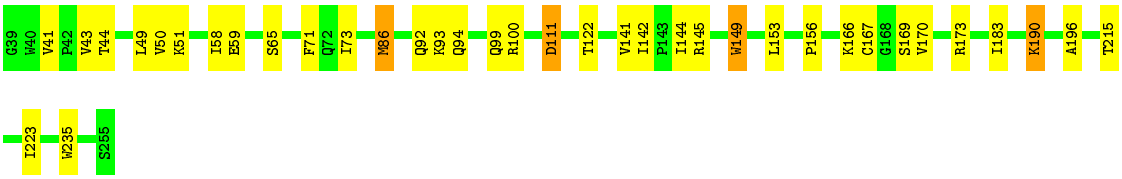
Chain B:



- Molecule 3: Ribosomal protein uS5

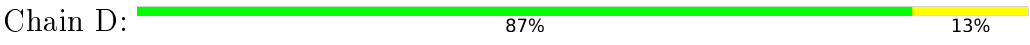
Chain C:

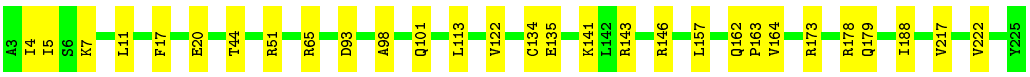




- Molecule 4: Ribosomal protein uS3

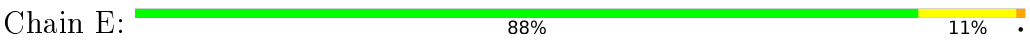
Chain D:





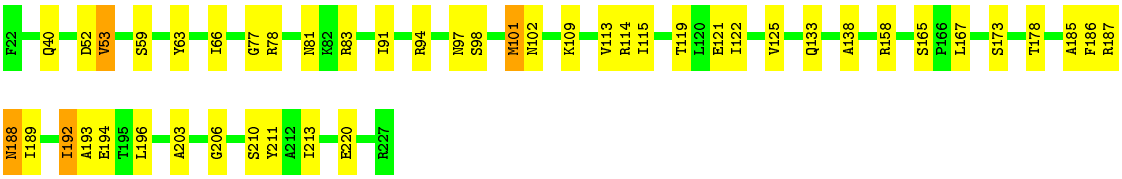
- Molecule 5: Ribosomal protein eS4

Chain E:



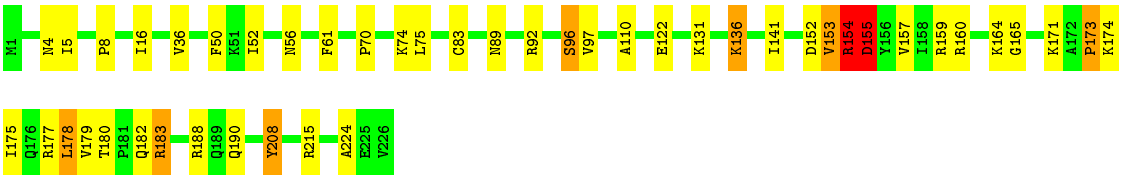
• Molecule 6: Ribosomal protein uS7

Chain F:



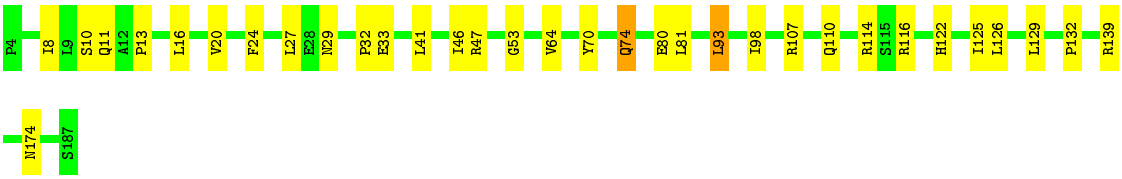
• Molecule 7: Ribosomal protein eS6

Chain G:



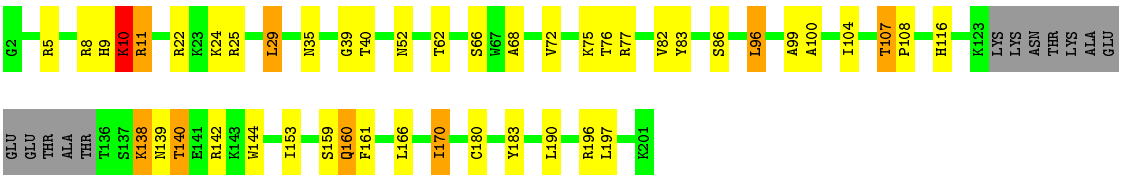
• Molecule 8: Ribosomal protein eS7

Chain H:



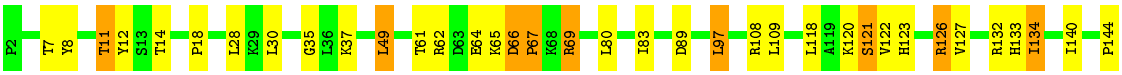
• Molecule 9: Ribosomal protein eS8

Chain I:



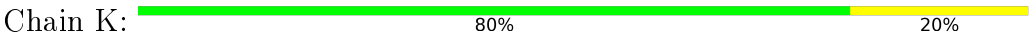
• Molecule 10: Ribosomal protein uS4

Chain J:



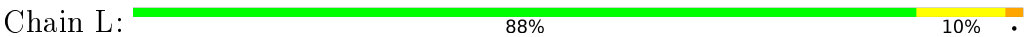
- Molecule 11: Ribosomal protein eS10

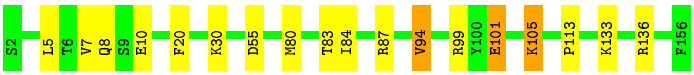
Chain K:



- Molecule 12: Ribosomal protein uS17

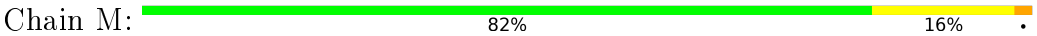
Chain L:

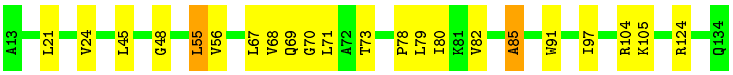




- Molecule 13: Ribosomal protein eS12

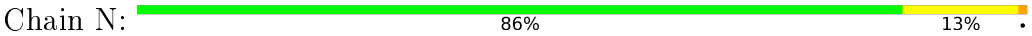
Chain M:

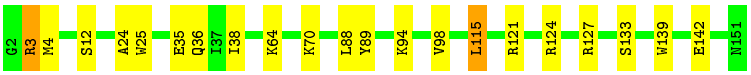




- Molecule 14: Ribosomal protein uS15

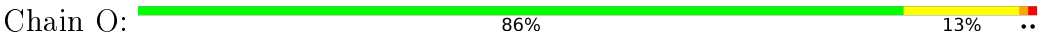
Chain N:





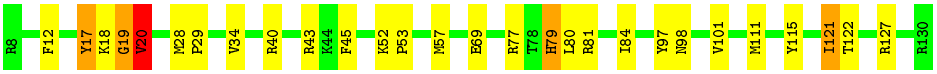
- Molecule 15: Ribosomal protein uS14

Chain O:



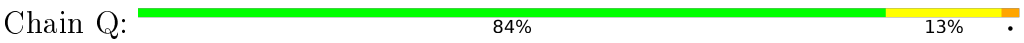
- Molecule 16: Ribosomal protein uS19

Chain P:



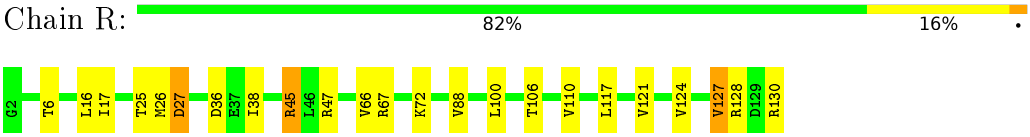
- Molecule 17: Ribosomal protein uS9

Chain Q:



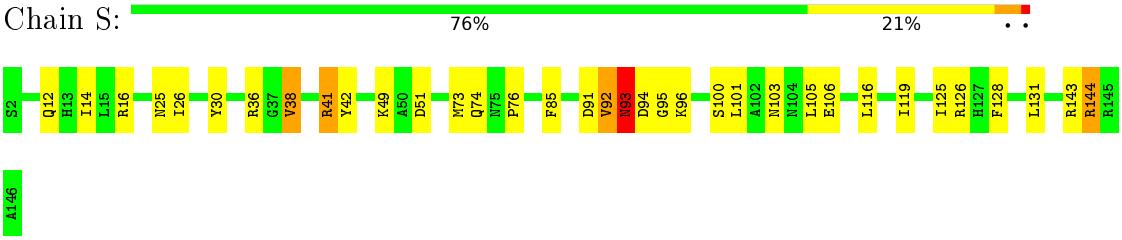
- Molecule 18: Ribosomal protein eS17

Chain R:



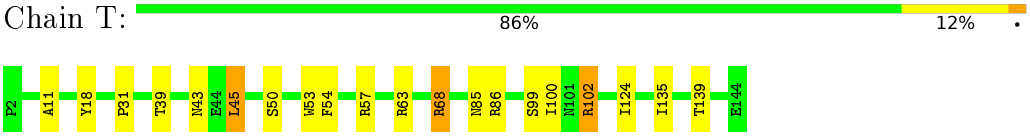
- Molecule 19: Ribosomal protein uS13

Chain S:



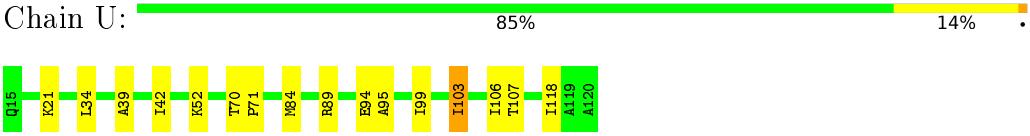
- Molecule 20: Ribosomal protein eS19

Chain T:



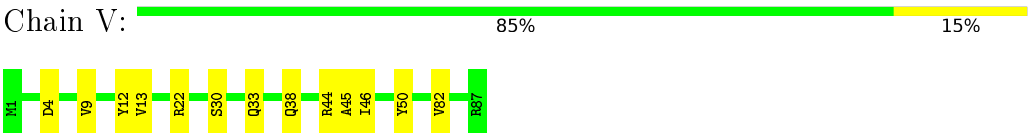
- Molecule 21: Ribosomal protein uS10

Chain U:



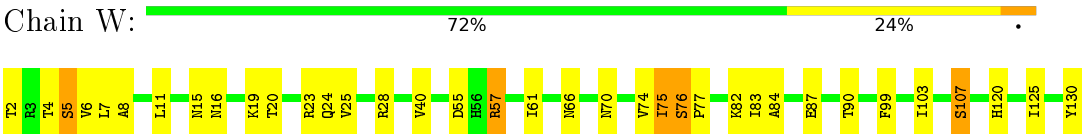
- Molecule 22: Ribosomal protein eS21

Chain V:



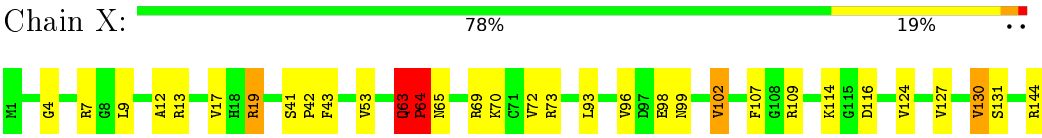
- Molecule 23: Ribosomal protein uS8

Chain W:



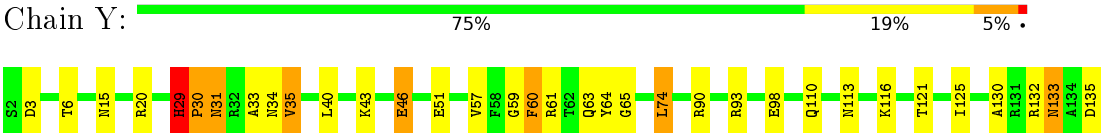
- Molecule 24: Ribosomal protein uS21

Chain X:



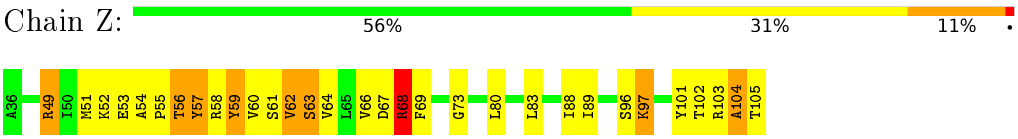
• Molecule 25: Ribosomal protein eS24

Chain Y:



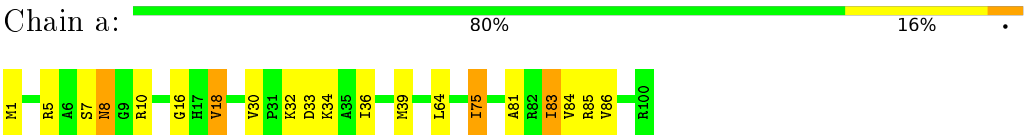
• Molecule 26: Ribosomal protein eS25

Chain Z:



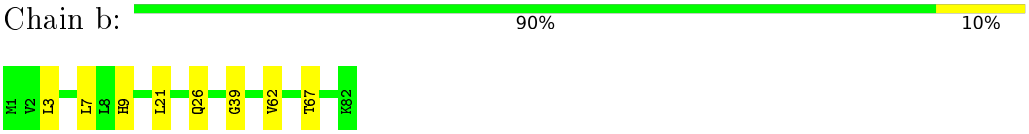
• Molecule 27: Ribosomal protein eS26

Chain a:



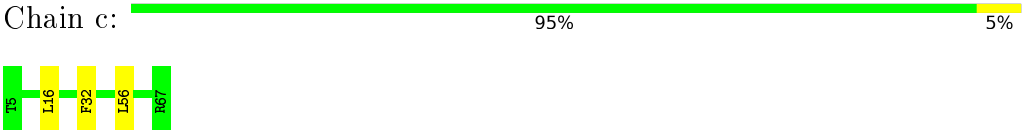
• Molecule 28: Ribosomal protein eS27

Chain b:



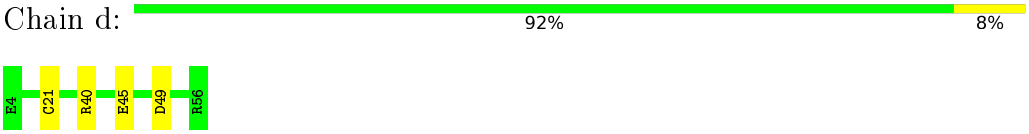
• Molecule 29: Ribosomal protein eS28

Chain c:



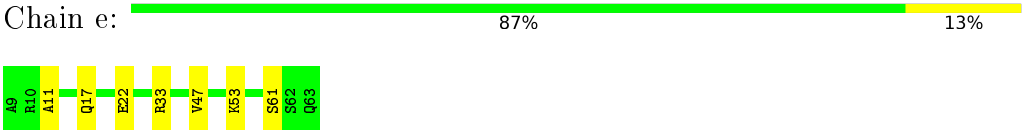
• Molecule 30: Ribosomal protein eS29

Chain d:



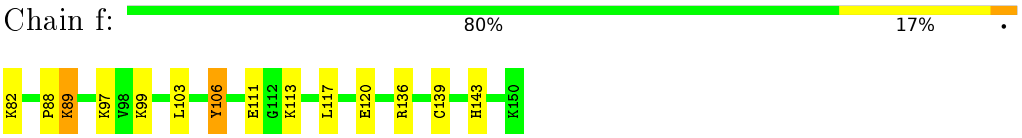
• Molecule 31: Ribosomal protein eS30

Chain e:



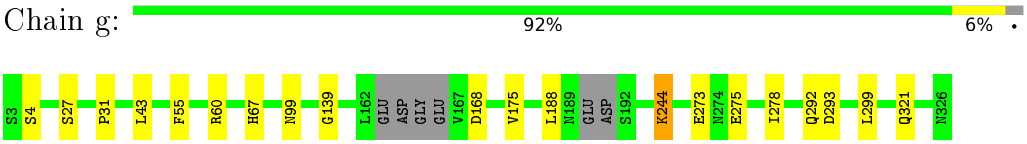
• Molecule 32: Ribosomal protein eS31

Chain f:



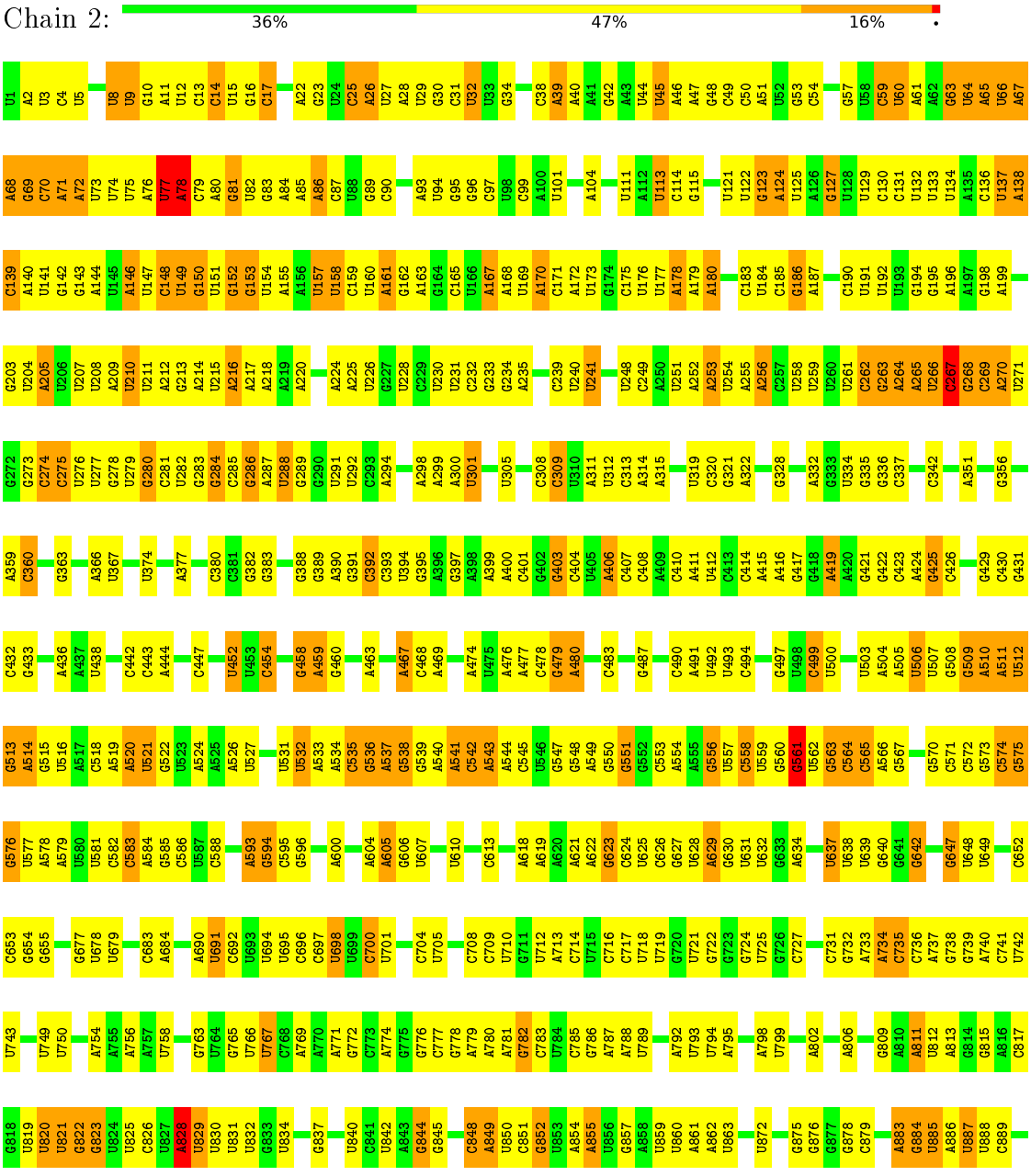
• Molecule 33: Ribosomal protein RACK1

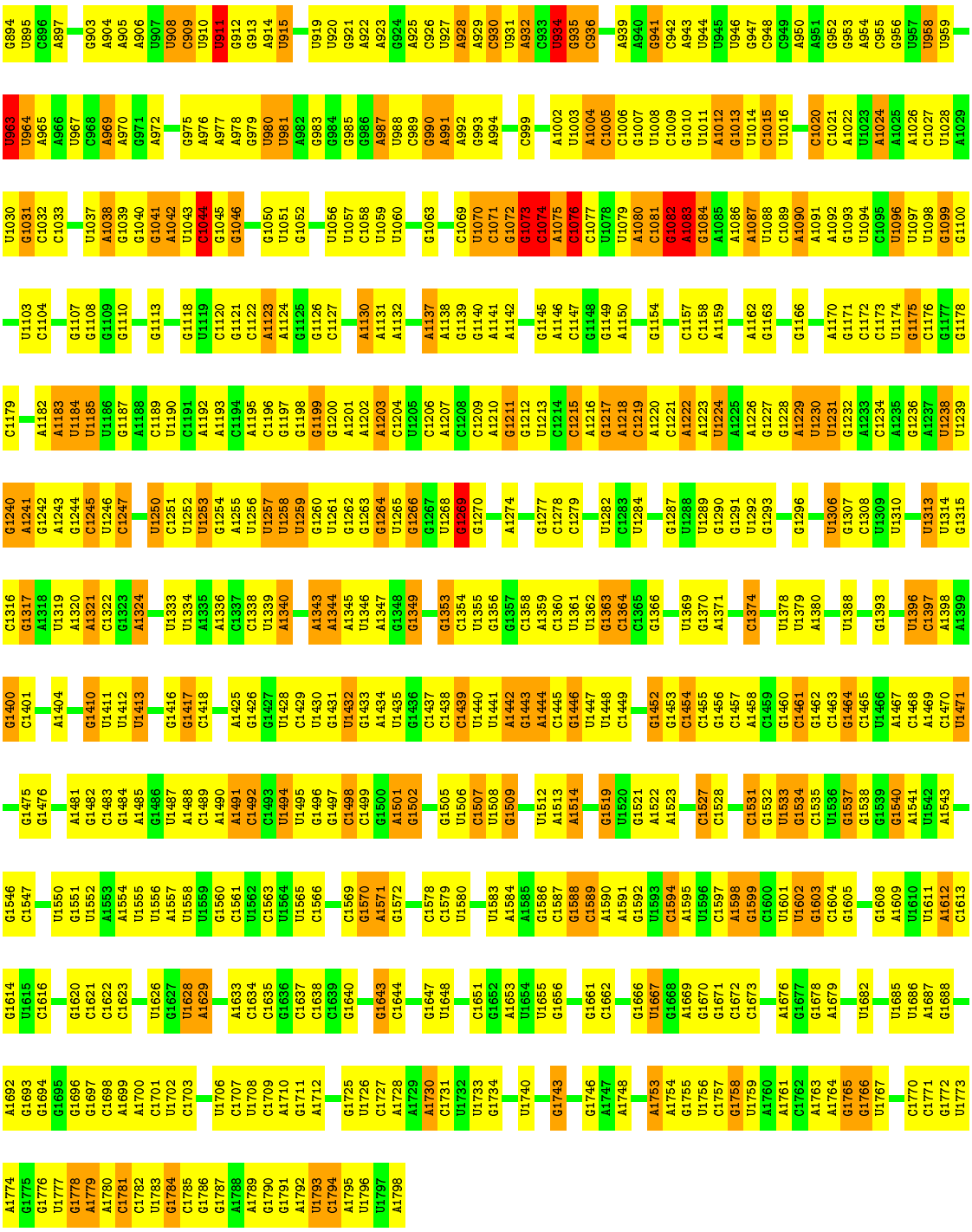
Chain g:



• Molecule 34: 18S ribosomal RNA

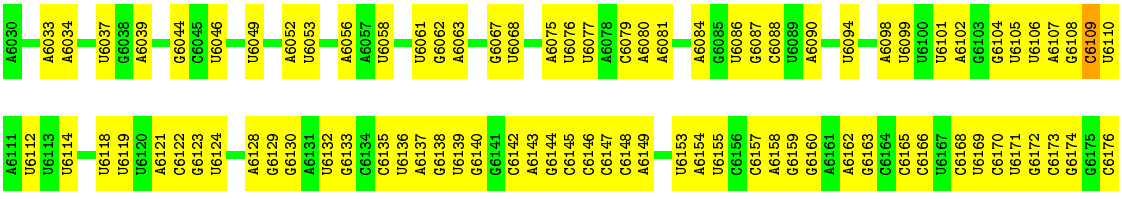
Chain 2:

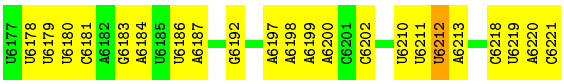




• Molecule 35: Cricket paralysis virus IRES RNA

Chain i:




U6177
U6178
U6179
U6180
C6181
A6182
G6183
A6184
U6185
U6186
A6187
G6192
A6197
A6198
A6199
A6200
C6201
C6202
U6210
U6211
U6212
A6213
C6218
U6219
A6220
C6221

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	54481	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.39	0/1656	0.77	0/2264
10	J	0.44	1/1495 (0.1%)	0.90	3/2001 (0.1%)
11	K	0.40	0/831	0.68	0/1123
12	L	0.36	0/1276	0.67	0/1718
13	M	0.40	0/929	0.76	0/1255
14	N	0.40	0/1210	0.84	0/1628
15	O	0.40	0/953	0.77	0/1279
16	P	0.53	1/1000 (0.1%)	0.80	1/1343 (0.1%)
17	Q	0.38	0/1125	0.75	1/1510 (0.1%)
18	R	0.40	0/1042	0.84	0/1399
19	S	0.45	1/1212 (0.1%)	0.81	2/1629 (0.1%)
2	B	0.38	0/1747	0.71	0/2353
20	T	0.36	0/1129	0.75	0/1520
21	U	0.35	0/857	0.69	0/1158
22	V	0.37	0/696	0.69	0/938
23	W	0.40	0/1039	0.81	0/1399
24	X	0.39	0/1145	0.81	1/1526 (0.1%)
25	Y	0.39	0/1075	0.77	0/1433
26	Z	0.42	0/567	0.81	1/762 (0.1%)
27	a	0.40	0/810	0.82	0/1084
28	b	0.34	0/627	0.67	0/847
29	c	0.37	0/496	0.73	0/666
3	C	0.37	0/1659	0.71	0/2252
30	d	0.38	0/457	0.64	0/607
31	e	0.36	0/450	0.68	0/599
32	f	0.42	0/562	0.67	0/751
33	g	0.35	0/2521	0.58	0/3431
34	2	0.34	14/42269 (0.0%)	0.78	26/65862 (0.0%)
35	i	0.34	1/4425 (0.0%)	0.72	1/6875 (0.0%)
4	D	0.36	0/1769	0.70	0/2378
5	E	0.36	0/2122	0.67	0/2861
6	F	0.38	0/1628	0.79	0/2198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
7	G	0.46	2/1835 (0.1%)	0.80	2/2451 (0.1%)
8	H	0.38	0/1507	0.73	0/2028
9	I	0.40	0/1519	0.79	0/2033
All	All	0.37	20/85640 (0.0%)	0.76	38/125161 (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
1	A	0	2
10	J	0	1
15	O	0	1
17	Q	0	2
22	V	0	1
23	W	0	1
26	Z	0	1
27	a	0	1
34	2	0	7
7	G	0	1
All	All	0	18

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	1073	G	C2-N2	-13.62	1.21	1.34
34	2	1074	C	C4-N4	11.59	1.44	1.33
34	2	1072	G	C2-N2	10.69	1.45	1.34
34	2	1073	G	N1-C2	-10.45	1.29	1.37
34	2	1073	G	C6-O6	-10.32	1.14	1.24

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	1073	G	N1-C2-N2	-16.67	101.20	116.20
34	2	1074	C	C2'-C3'-O3'	11.15	134.03	109.50
34	2	1074	C	N1-C1'-C2'	-9.84	101.17	112.00
26	Z	68	ARG	N-CA-C	-8.17	88.93	111.00
34	2	78	A	C4'-C3'-O3'	7.94	128.88	113.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ASN	Peptide
1	A	168	HIS	Peptide
7	G	155	ASP	Peptide
10	J	66	ASP	Peptide
15	O	122	PRO	Peptide

5.2 Too-close contacts (i)

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	1616	0	1636	18	0
2	B	1722	0	1795	3	0
3	C	1629	0	1710	8	0
4	D	1744	0	1825	2	0
5	E	2078	0	2157	4	0
6	F	1609	0	1679	25	0
7	G	1812	0	1911	56	0
8	H	1483	0	1579	6	0
9	I	1493	0	1515	19	0
10	J	1471	0	1554	37	0
11	K	809	0	810	4	0
12	L	1248	0	1311	5	0
13	M	922	0	953	7	0
14	N	1187	0	1251	5	0
15	O	942	0	979	8	0
16	P	980	0	1026	22	0
17	Q	1105	0	1170	6	0
18	R	1031	0	1082	6	0
19	S	1193	0	1217	21	0
20	T	1110	0	1124	4	0
21	U	845	0	913	5	0
22	V	687	0	682	2	0
23	W	1021	0	1056	12	0
24	X	1127	0	1210	22	0
25	Y	1061	0	1111	14	0
26	Z	558	0	585	74	0
27	a	798	0	855	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	617	0	642	0	0
29	c	494	0	534	0	0
30	d	446	0	436	0	0
31	e	443	0	481	0	0
32	f	549	0	564	0	0
33	g	2466	0	2406	0	0
34	2	37797	0	19010	942	0
35	i	3968	0	1986	0	0
36	2	76	0	0	0	0
36	G	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	X	1	0	0	0	0
37	a	1	0	0	0	0
37	b	1	0	0	0	0
37	f	1	0	0	0	0
All	All	80144	0	60755	1189	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 1189 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)
26:Z:52:LYS:HA	26:Z:53:GLU:CG	1.47	1.43
34:2:513:G:H1	34:2:542:C:N4	1.27	1.31
24:X:63:GLN:NE2	34:2:1753:A:OP1	1.64	1.29
34:2:480:A:N1	34:2:506:U:C4	2.04	1.26
26:Z:51:MET:O	26:Z:53:GLU:HA	1.13	1.26

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	204/206 (99%)	168 (82%)	25 (12%)	11 (5%)	2	30
2	B	212/214 (99%)	174 (82%)	32 (15%)	6 (3%)	6	47
3	C	215/217 (99%)	187 (87%)	21 (10%)	7 (3%)	5	43
4	D	221/223 (99%)	198 (90%)	17 (8%)	6 (3%)	6	48
5	E	258/260 (99%)	214 (83%)	36 (14%)	8 (3%)	5	45
6	F	204/206 (99%)	174 (85%)	21 (10%)	9 (4%)	3	35
7	G	224/226 (99%)	186 (83%)	29 (13%)	9 (4%)	4	38
8	H	182/184 (99%)	155 (85%)	16 (9%)	11 (6%)	2	27
9	I	184/200 (92%)	154 (84%)	22 (12%)	8 (4%)	3	35
10	J	180/182 (99%)	151 (84%)	17 (9%)	12 (7%)	1	25
11	K	94/96 (98%)	80 (85%)	7 (7%)	7 (7%)	1	21
12	L	153/155 (99%)	129 (84%)	17 (11%)	7 (5%)	3	34
13	M	120/122 (98%)	94 (78%)	21 (18%)	5 (4%)	3	36
14	N	148/150 (99%)	130 (88%)	14 (10%)	4 (3%)	6	48
15	O	125/127 (98%)	108 (86%)	11 (9%)	6 (5%)	3	32
16	P	121/123 (98%)	96 (79%)	16 (13%)	9 (7%)	1	21
17	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	4	41
18	R	127/129 (98%)	106 (84%)	14 (11%)	7 (6%)	2	29
19	S	143/145 (99%)	119 (83%)	17 (12%)	7 (5%)	3	32
20	T	141/143 (99%)	126 (89%)	10 (7%)	5 (4%)	4	42
21	U	104/106 (98%)	93 (89%)	7 (7%)	4 (4%)	4	39
22	V	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	23
23	W	127/129 (98%)	107 (84%)	14 (11%)	6 (5%)	3	33
24	X	143/145 (99%)	121 (85%)	15 (10%)	7 (5%)	3	32
25	Y	132/134 (98%)	113 (86%)	9 (7%)	10 (8%)	1	20
26	Z	68/70 (97%)	58 (85%)	5 (7%)	5 (7%)	1	21
27	a	98/100 (98%)	74 (76%)	13 (13%)	11 (11%)	0	10
28	b	80/82 (98%)	64 (80%)	12 (15%)	4 (5%)	3	31
29	c	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
30	d	51/53 (96%)	41 (80%)	10 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	e	53/55 (96%)	47 (89%)	3 (6%)	3 (6%)	2 28
32	f	67/69 (97%)	50 (75%)	11 (16%)	6 (9%)	1 16
33	g	312/324 (96%)	261 (84%)	44 (14%)	7 (2%)	8 52
All	All	4776/4866 (98%)	4024 (84%)	534 (11%)	218 (5%)	5 34

5 of 218 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ALA
2	B	100	PHE
3	C	149	TRP
4	D	164	VAL
6	F	59	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	174/174 (100%)	160 (92%)	14 (8%)	15 54
2	B	196/196 (100%)	182 (93%)	14 (7%)	18 59
3	C	176/176 (100%)	154 (88%)	22 (12%)	6 33
4	D	185/185 (100%)	165 (89%)	20 (11%)	8 41
5	E	223/223 (100%)	204 (92%)	19 (8%)	13 52
6	F	174/174 (100%)	158 (91%)	16 (9%)	11 48
7	G	192/192 (100%)	175 (91%)	17 (9%)	12 50
8	H	164/164 (100%)	149 (91%)	15 (9%)	12 48
9	I	148/158 (94%)	126 (85%)	22 (15%)	4 26
10	J	153/153 (100%)	135 (88%)	18 (12%)	6 35
11	K	88/88 (100%)	82 (93%)	6 (7%)	20 61
12	L	136/136 (100%)	126 (93%)	10 (7%)	17 57
13	M	97/97 (100%)	91 (94%)	6 (6%)	23 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	127/127 (100%)	116 (91%)	11 (9%)	13 50
15	O	96/96 (100%)	90 (94%)	6 (6%)	22 63
16	P	105/106 (99%)	96 (91%)	9 (9%)	13 51
17	Q	117/117 (100%)	109 (93%)	8 (7%)	20 61
18	R	117/117 (100%)	104 (89%)	13 (11%)	8 39
19	S	128/128 (100%)	111 (87%)	17 (13%)	5 31
20	T	117/117 (100%)	106 (91%)	11 (9%)	11 47
21	U	96/96 (100%)	92 (96%)	4 (4%)	36 74
22	V	73/73 (100%)	69 (94%)	4 (6%)	27 68
23	W	110/110 (100%)	97 (88%)	13 (12%)	6 35
24	X	120/120 (100%)	105 (88%)	15 (12%)	6 33
25	Y	108/108 (100%)	94 (87%)	14 (13%)	5 32
26	Z	60/60 (100%)	55 (92%)	5 (8%)	14 52
27	a	85/85 (100%)	73 (86%)	12 (14%)	4 29
28	b	72/72 (100%)	68 (94%)	4 (6%)	26 67
29	c	55/55 (100%)	52 (94%)	3 (6%)	27 68
30	d	46/46 (100%)	42 (91%)	4 (9%)	13 50
31	e	49/49 (100%)	45 (92%)	4 (8%)	14 53
32	f	58/60 (97%)	48 (83%)	10 (17%)	2 18
33	g	265/270 (98%)	251 (95%)	14 (5%)	28 69
All	All	4110/4128 (100%)	3730 (91%)	380 (9%)	16 48

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	132	ARG
15	O	71	CYS
30	d	49	ASP
10	J	176	ARG
12	L	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	79	HIS
17	Q	83	GLN
25	Y	34	ASN
16	P	98	ASN
19	S	89	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	2	1778/1780 (99%)	767 (43%)	111 (6%)
35	i	184/192 (95%)	107 (58%)	0
All	All	1962/1972 (99%)	874 (44%)	111 (5%)

5 of 874 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	2	2	A
34	2	3	U
34	2	4	C
34	2	5	U
34	2	9	U

5 of 111 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	2	605	A
34	2	792	A
34	2	1598	A
34	2	621	A
34	2	708	C

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

Of 83 ligands modelled in this entry, 83 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	657:C	O3'	676:G	P	17.80