



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 2NOQ  
EMDB ID: : EMD-1285  
Title : Structure of ribosome-bound cricket paralysis virus IRES RNA  
Authors : Schuler, M.; Connell, S.R.; Lescoute, A.; Giesebrecht, J.; Dabrowski, M.; Schroeer, B.; Mielke, T.; Penczek, P.A.; Westhof, E.; Spahn, C.M.T.  
Deposited on : 2006-10-26  
Resolution : 7.30 Å(reported)  
Based on PDB ID : 1s1i, 1s1h

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

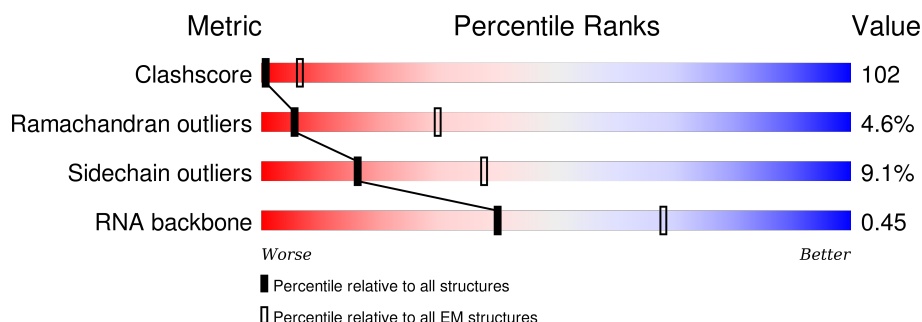
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.30 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  $\geq 3$ , 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	190	9% 54% 37%
2	B	46	28% 57% 13% .
3	C	13	15% 69% 15%
4	D	15	27% 53% 20%
5	E	53	28% 49% 19% .
6	F	150	27% 65% 8%
7	G	213	23% 71% 6%
8	H	165	13% 61% 22% .

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10909 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 CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	190	Total	C	N	O	P	0	0
			4023	1803	692	1338	190		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	46	Total	C	N	O	P	0	0
			986	439	184	318	45		

- Molecule 3 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	13	Total	C	N	O	P	0	0
			276	123	48	93	12		

- Molecule 4 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	15	Total	C	N	O	P	0	0
			319	142	55	107	15		

- Molecule 5 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	53	Total	C	N	O	P	0	0
			1142	508	213	368	53		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	150	Total	C	N	O	S	0	0
			1161	714	229	215	3		

- Molecule 7 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1683	1074	294	306	9		

- Molecule 8 is a protein called 60S ribosomal protein L11-B.

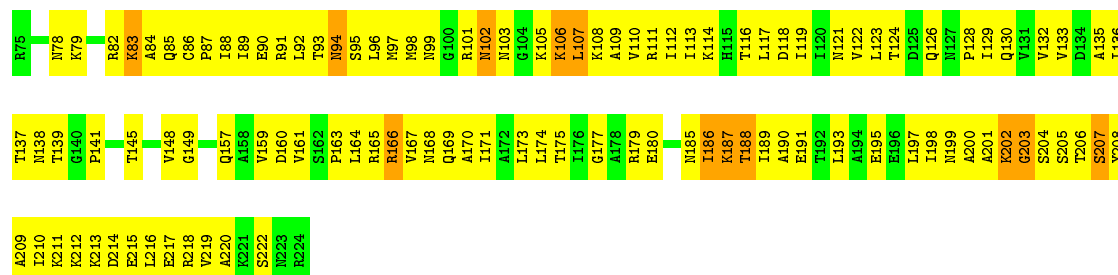
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	165	Total	C	N	O	S	0	0
			1319	826	247	242	4		





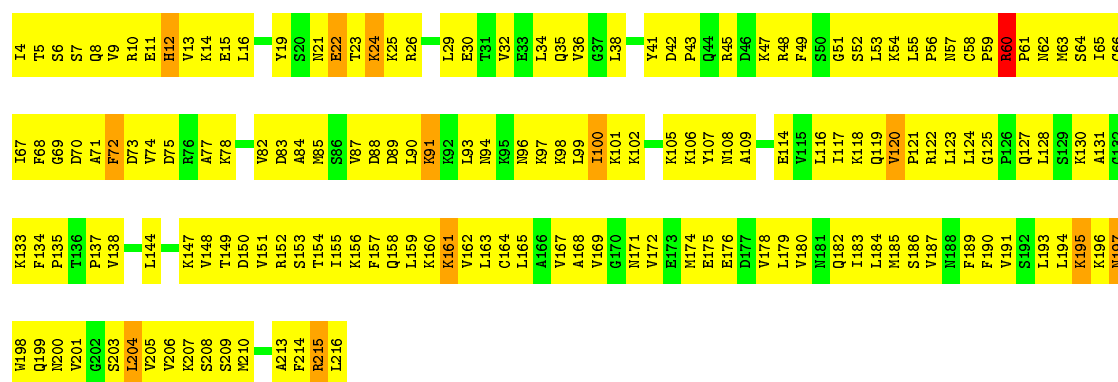
• Molecule 6: 40S ribosomal protein S5

Chain F: 27% 65% 8%



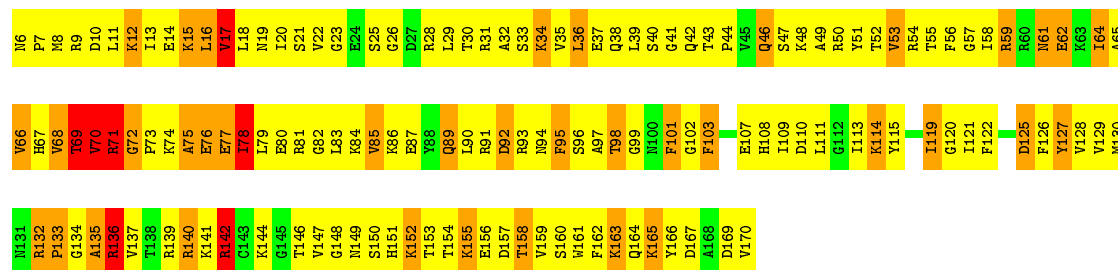
• Molecule 7: 60S ribosomal protein L1

Chain G: 23% 71% 6%



• Molecule 8: 60S ribosomal protein L11-B

Chain H: 13% 61% 22%



## 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	Not provided	Depositor
Microscope	FEI-POLARA G2	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	1.02	2/4495 (0.0%)	2.56	597/6995 (8.5%)
2	B	0.54	0/1100	0.78	3/1715 (0.2%)
3	C	0.51	0/305	0.79	0/474
4	D	0.47	0/355	0.83	0/551
5	E	1.08	3/1278 (0.2%)	0.94	6/1991 (0.3%)
6	F	1.05	0/1169	1.14	2/1570 (0.1%)
7	G	0.91	0/1707	1.11	1/2289 (0.0%)
8	H	1.20	1/1340 (0.1%)	1.89	20/1797 (1.1%)
All	All	0.98	6/11749 (0.1%)	1.87	629/17382 (3.6%)

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
2	B	0	2
5	E	0	3
8	H	0	1
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2160	G	O3'-P	-32.03	1.22	1.61
5	E	2166	G	O3'-P	-11.77	1.47	1.61
1	A	75	U	P-O5'	10.93	1.70	1.59
5	E	2138	G	OP3-P	-6.97	1.52	1.61
1	A	124	C	O3'-P	-5.62	1.54	1.61

The worst 5 of 629 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	46	GLN	CG-CD-OE1	-38.67	44.25	121.60
1	A	111	A	P-O3'-C3'	24.02	148.53	119.70
1	A	101	C	P-O3'-C3'	19.03	142.54	119.70
1	A	124	C	P-O3'-C3'	17.04	140.15	119.70
1	A	93	U	P-O3'-C3'	15.66	138.49	119.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	528	C	Sidechain
2	B	529	G	Sidechain
5	E	2150	A	Sidechain
5	E	2162	G	Sidechain
5	E	2174	G	Sidechain

## 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	4023	0	2022	648	0
2	B	986	0	500	69	0
3	C	276	0	142	46	0
4	D	319	0	161	21	0
5	E	1142	0	573	137	0
6	F	1161	0	1230	226	0
7	G	1683	0	1750	551	0
8	H	1319	0	1347	459	0
All	All	10909	0	7725	1899	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 102.

The worst 5 of 1899 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)
5:E:2154:G:H2'	7:G:160:LYS:CD	1.18	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2185:C:P	7:G:163:LEU:HD12	1.46	1.52
1:A:87:U:O4	6:F:218:ARG:CG	1.65	1.43
1:A:189:C:C4	3:C:1054:C:N4	1.88	1.42
7:G:151:VAL:C	7:G:154:THR:H	1.22	1.40

There are no symmetry-related clashes.

## 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	
6	F	148/150 (99%)	136 (92%)	10 (7%)	2 (1%)	14	58
7	G	207/213 (97%)	195 (94%)	8 (4%)	4 (2%)	10	52
8	H	163/165 (99%)	113 (69%)	32 (20%)	18 (11%)	0	11
All	All	518/528 (98%)	444 (86%)	50 (10%)	24 (5%)	5	32

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	186	ILE
7	G	60	ARG
8	H	64	ILE
8	H	66	VAL
8	H	68	VAL

### 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	
6	F	123/123 (100%)	115 (94%)	8 (6%)	21	58
7	G	194/194 (100%)	184 (95%)	10 (5%)	29	65
8	H	143/143 (100%)	119 (83%)	24 (17%)	2	19
All	All	460/460 (100%)	418 (91%)	42 (9%)	16	43

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	12	LYS
8	H	36	LEU
8	H	152	LYS
8	H	15	LYS
8	H	17	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	57	ASN
7	G	182	GLN
8	H	61	ASN
7	G	8	GLN
8	H	46	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	189/190 (99%)	65 (34%)	16 (8%)
2	B	45/46 (97%)	8 (17%)	3 (6%)
3	C	12/13 (92%)	2 (16%)	0
4	D	14/15 (93%)	4 (28%)	2 (14%)
5	E	52/53 (98%)	9 (17%)	7 (13%)
All	All	312/317 (98%)	88 (28%)	28 (8%)

5 of 88 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	G
1	A	13	A

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Mol	Chain	Res	Type
1	A	17	U
1	A	18	G
1	A	30	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	150	U
1	A	182	A
5	E	2159	A
1	A	156	A
1	A	177	U

#### 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 [i](#)

There are no chain breaks in this entry.