



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 23, 2017 – 08:57 PM EDT

PDB ID : 4C4Q
EMDB ID: : EMD-2450
Title : Cryo-EM map of the CSFV IRES in complex with the small ribosomal 40S subunit and DHX29
Authors : Hashem, Y.; desGeorges, A.; Dhote, V.; Langlois, R.; Liao, H.Y.; Grassucci, R.A.; Pestova, T.V.; Hellen, C.U.T.; Frank, J.
Deposited on : unknown
Resolution : 8.50 Å(reported)
Based on PDB ID : 2XZM

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

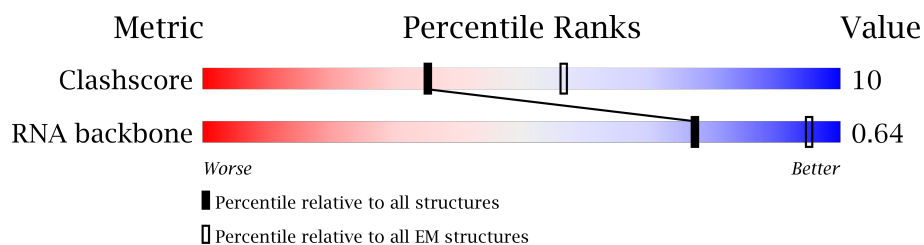
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

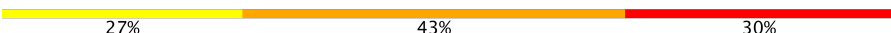
The reported resolution of this entry is 8.50 Å.

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	125131	1336
RNA backbone	3398	335

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	N	233	 27% 43% 30%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4986 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.

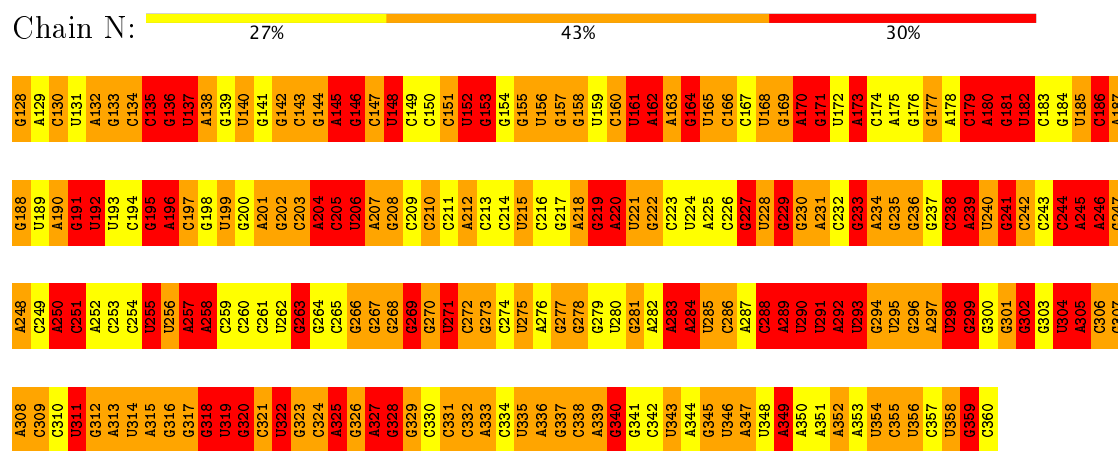
- Molecule 1 is a RNA chain called INTERNAL RIBOSOMAL ENTRY SITE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	233	Total	C	N	O	P	0	0
			4986	2225	908	1621	232		

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 the various outlier classes 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: INTERNAL RIBOSOMAL ENTRY SITE



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72900	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	12	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51570	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	N	3.32	735/5579 (13.2%)	3.44	1129/8700 (13.0%)

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	N	0	122

The worst 5 of 735 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	283	A	N9-C4	17.10	1.48	1.37
1	N	307	G	O3'-P	-15.46	1.42	1.61
1	N	323	G	N9-C8	-15.46	1.27	1.37
1	N	151	C	N1-C6	14.29	1.45	1.37
1	N	183	C	N1-C6	13.73	1.45	1.37

The worst 5 of 1129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	307	G	P-O3'-C3'	30.70	156.54	119.70
1	N	135	C	P-O3'-C3'	30.11	155.83	119.70
1	N	195	G	P-O3'-C3'	26.18	151.12	119.70
1	N	191	G	P-O3'-C3'	24.78	149.43	119.70
1	N	142	G	P-O3'-C3'	23.54	147.95	119.70

There are no chirality outliers.

5 of 122 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	128	G	Sidechain
1	N	130	C	Sidechain
1	N	132	A	Sidechain
1	N	135	C	Sidechain
1	N	136	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	N	4986	0	2463	72	0
All	All	4986	0	2463	72	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 72 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)
1:N:283:A:H3'	1:N:284:A:H5'	1.38	1.05
1:N:283:A:C3'	1:N:284:A:H5'	1.94	0.96
1:N:283:A:H3'	1:N:284:A:C5'	2.10	0.79
1:N:263:G:H1	1:N:275:U:H3	1.35	0.72
1:N:319:U:H2'	1:N:320:G:C5'	2.20	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	232/233 (99%)	63 (27%)	21 (9%)

5 of 63 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	136	G
1	N	137	U
1	N	143	C
1	N	145	A
1	N	146	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	195	G
1	N	234	A
1	N	304	U
1	N	191	G
1	N	307	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.