![WORLDWIDE PDB PROTEIN DATA BANK / EMDataBank Unified Data Resource for 3DEM]

wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 01:04 PM EDT

PDB ID	:	4D5N
EMDB ID:	:	EMD-2810
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	:	unknown
Resolution	:	9.00 Å(reported)

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
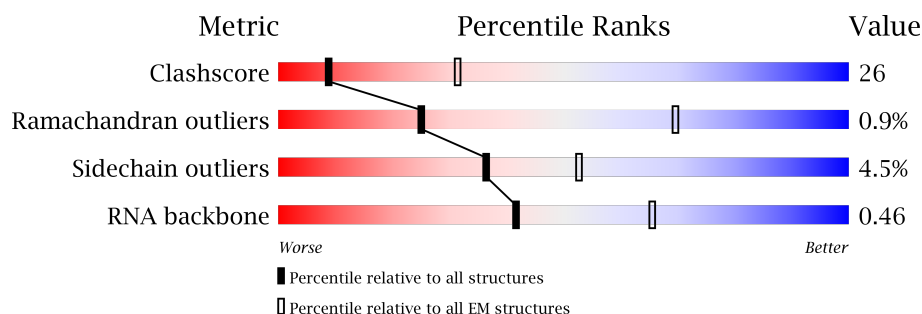with specific help available everywhere you see the ⓘ symbol.

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1 Overall quality at a glance ⓘ

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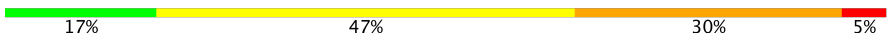*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		0.9%
Sidechain outliers		4.5%
RNA backbone		0.46

Worse ... *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
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 <=5%

Mol	Chain	Length	Quality of chain
1	A	436	61% ... 36% ... •
2	X	201	17% ... 47% ... 30% ... 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9841 atoms, of which 2134 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 EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	436	3450	2193	582	663	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	LEU	-	expression tag	UNP P62495
A	439	GLU	-	expression tag	UNP P62495
A	440	HIS	-	expression tag	UNP P62495

- Molecule 2 is a RNA chain called CRICKET PARALYSIS VIRUS IRES RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	X	201	6391	1908	2134	735	1413	201	0	0

There is a discrepancy between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
X	6178	A	U	conflict	GB 8895506

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: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1

Chain A:
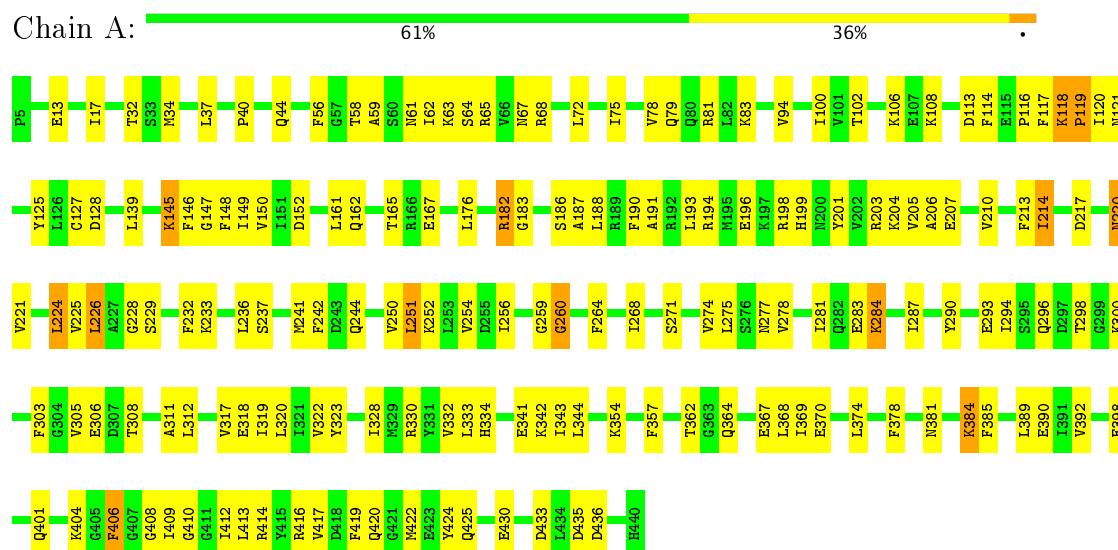
• Molecule 2: CRICKET PARALYSIS VIRUS IRES RNA

Chain X:
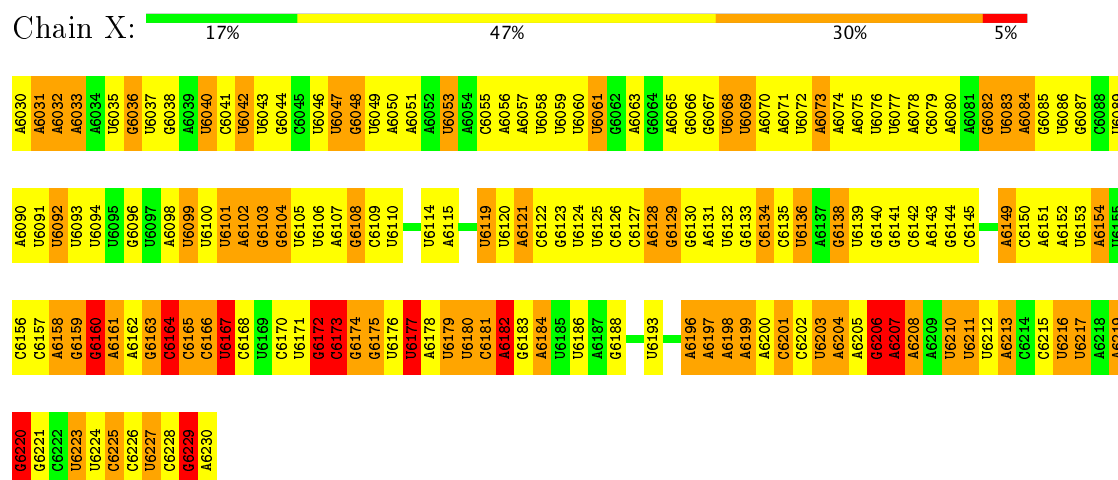
4   Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109596	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 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	0.38	0/3509	0.60	0/4718
2	X	1.44	87/4751 (1.8%)	1.76	216/7379 (2.9%)
All	All	1.12	87/8260 (1.1%)	1.43	216/12097 (1.8%)

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	X	0	1

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	6173	C	O3'-P	-20.25	1.36	1.61
2	X	6229	G	O3'-P	19.60	1.84	1.61
2	X	6079	C	N3-C4	19.11	1.47	1.33
2	X	6177	U	O3'-P	-18.38	1.39	1.61
2	X	6219	A	O3'-P	-15.94	1.42	1.61

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	6079	C	C5-C6-N1	19.33	130.66	121.00
2	X	6114	U	C4-C5-C6	-18.67	108.50	119.70
2	X	6114	U	N3-C4-C5	17.51	125.11	114.60
2	X	6077	U	C2-N3-C4	-15.01	118.00	127.00
2	X	6161	A	N1-C2-N3	-14.98	121.81	129.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	6160	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	3450	0	3456	188	0
2	X	4257	2134	2152	160	0
All	All	7707	2134	5608	345	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 26.

The worst 5 of 345 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:A:256:ILE:HD12	1:A:264:PHE:CD1	1.46	1.47
1:A:259:GLY:HA3	1:A:264:PHE:CZ	1.50	1.44
1:A:256:ILE:HD12	1:A:264:PHE:CE1	1.53	1.41
1:A:259:GLY:HA3	1:A:264:PHE:CE1	1.64	1.30
1:A:256:ILE:CD1	1:A:264:PHE:CD1	2.21	1.23

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	
1	A	434/436 (100%)	419 (96%)	11 (2%)	4 (1%)	20	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	260	GLY
1	A	187	ALA
1	A	119	PRO

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	376/376 (100%)	359 (96%)	17 (4%)	32	63

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ILE
1	A	220	ASN
1	A	317	VAL
1	A	188	LEU
1	A	357	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	425	GLN
1	A	282	GLN
1	A	121	ASN
1	A	266	GLN

5.3.3　RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	194/201 (96%)	49 (25%)	0

5 of 49 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	6032	A
2	X	6033	A
2	X	6036	G
2	X	6042	U
2	X	6043	U

There are no RNA pucker outliers to report.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	X	11

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	6150:C	O3'	6151:A	P	11.37
1	X	6065:A	O3'	6066:G	P	10.22
1	X	6106:U	O3'	6107:A	P	9.31
1	X	6136:U	O3'	6137:A	P	8.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	6073:A	O3'	6074:A	P	3.28