wwPDB EM Validation Summary Report (i)

Dec 17, 2023 – 04:42 PM EST

PDB ID	:	1C2X
Title	:	5S RRNA STRUCTURE FITTED TO A CRYO-ELECTRON MICROSCOPIC MAP AT 7.5 ANGSTROMS RESOLUTION
Authors	:	Brimacombe, R.; Mueller, F.
Deposited on	:	1999-07-28
Resolution	:	7.50 Å(reported)
Based on initial models	:	1CSW, 1CSV

This is a wwPDB EM 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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

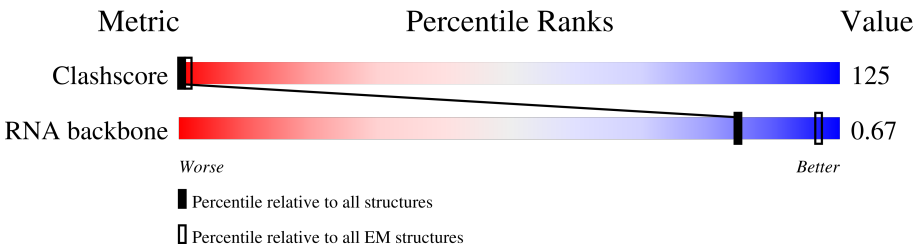
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.50 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	158937	4297
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	C	120	9% 42% 12% 37%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2576 atoms, of which 6 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 5S RIBOSOMAL RNA.

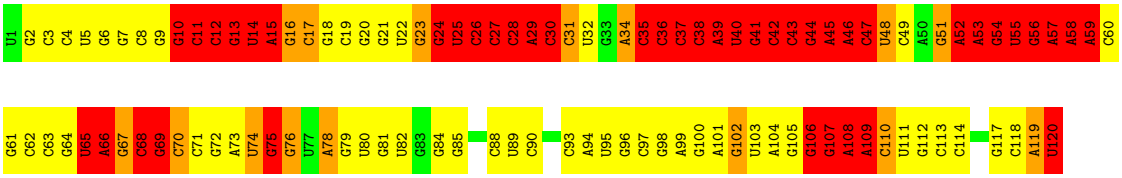
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	C	120	2576	1144	6	468	838	120	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 5S RIBOSOMAL RNA

Chain C: 9% 42% 12% 37%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	ERNA-3D	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2576	wwPDB-VP
Average B, all atoms ($Å^2$)	0.0	wwPDB-VP

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	4.71	208/2873 (7.2%)	2.59	153/4478 (3.4%)

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	C	12	3

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	G	O3'-P	37.73	2.06	1.61
1	C	75	G	C3'-O3'	33.41	1.89	1.42
1	C	75	G	C5'-C4'	29.32	1.86	1.51
1	C	57	A	P-O5'	28.89	1.88	1.59
1	C	52	A	P-O5'	27.90	1.87	1.59

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	G	C5'-C4'-O4'	39.12	156.05	109.10
1	C	43	C	P-O5'-C5'	35.96	178.43	120.90
1	C	46	A	P-O5'-C5'	34.16	175.56	120.90
1	C	40	U	P-O5'-C5'	32.52	172.93	120.90
1	C	44	G	P-O5'-C5'	31.89	171.92	120.90

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	11	C	C4'

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Mol	Chain	Res	Type	Atom
1	C	12	C	C4'
1	C	15	A	C4'
1	C	24	G	C4'
1	C	39	A	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	A	Sidechain
1	C	59	A	Sidechain
1	C	75	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	C	2570	6	1302	483	0
All	All	2570	6	1302	483	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 125.

The worst 5 of 483 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:C:15:A:C1'	1:C:15:A:N9	1.68	1.56
1:C:69:G:N9	1:C:69:G:C1'	1.70	1.55
1:C:38:C:N1	1:C:38:C:C1'	1.68	1.55
1:C:58:A:N9	1:C:58:A:C1'	1.69	1.55
1:C:36:C:N1	1:C:36:C:C1'	1.69	1.55

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 (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	119/120 (99%)	53 (44%)	38 (31%)

5 of 53 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	11	C
1	C	12	C
1	C	13	G
1	C	14	U
1	C	15	A

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	59	A
1	C	108	A
1	C	65	U
1	C	69	G
1	C	119	A

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 monosaccharides 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
1	C	48

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	75:G	O3'	76:G	P	2.06
1	C	47:C	O3'	48:U	P	1.93
1	C	69:G	O3'	70:C	P	1.90
1	C	56:G	O3'	57:A	P	1.89
1	C	59:A	O3'	60:C	P	1.89