wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:34 PM BST

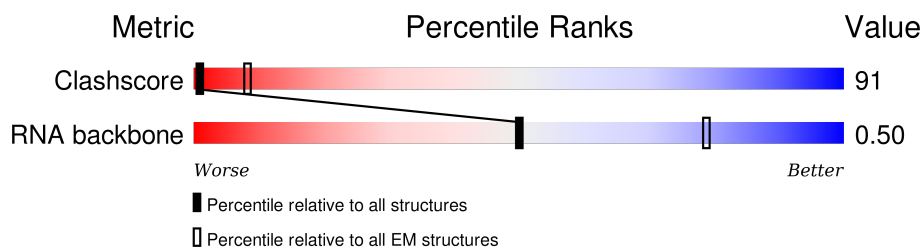|		
PDB ID	:	1ZO3
EMDB ID:	:	EMD-1248
Title	:	The P-site and P/E-site tRNA structures fitted to P/I site codon.
Authors	:	Allen, G.S.; Zavialov, A.; Gursky, R.; Ehrenberg, M.; Frank, J.
Deposited on	:	2005-05-12
Resolution	:	13.80 Å(reported)

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 13.80 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	Percentile Ranks	Value
Clashscore		91
RNA backbone		0.50

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
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	76	• 87% 12%
1	B	76	• 87% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3250 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 tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		
1	B	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		

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 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: tRNA

Chain A:

• Molecule 1: tRNA

Chain B:

4 Experimental information (i)

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	DEFOCUS GROUPS 0.93-3.93 UM	Depositor
Microscope	TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	-930.00	Depositor
Maximum defocus (nm)	-3930.00	Depositor
Magnification	Not provided	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	5.59	278/1817 (15.3%)	6.10	698/2831 (24.7%)
1	B	6.39	280/1817 (15.4%)	6.28	698/2831 (24.7%)
All	All	6.01	558/3634 (15.4%)	6.19	1396/5662 (24.7%)

The worst 5 of 558 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	U	C1'-N1	148.98	3.72	1.48
1	B	39	U	C1'-N1	148.94	3.72	1.48
1	B	1	G	P-OP2	106.09	3.29	1.49
1	A	55	U	C1'-N1	91.85	2.86	1.48
1	B	55	U	C1'-N1	91.80	2.86	1.48

The worst 5 of 1396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	39	U	C6-N1-C1'	-73.68	18.05	121.20
1	A	39	U	C6-N1-C1'	-73.67	18.06	121.20
1	A	55	U	C5-C6-N1	-50.83	97.29	122.70

There are no chirality outliers.

There are no planarity outliers.

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	1625	0	811	298	0
1	B	1625	0	814	296	0
All	All	3250	0	1625	438	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 91.

The worst 5 of 438 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:33:U:C4	1:B:34:G:H2'	1.18	1.64
1:A:37:G:C6	1:B:36:A:C2	2.04	1.45
1:A:33:U:C6	1:B:33:U:O2'	1.70	1.42
1:A:33:U:H1'	1:B:35:A:N6	1.41	1.36
1:A:32:C:C6	1:B:33:U:N3	1.70	1.35

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	A	75/76 (98%)	9 (12%)	4 (5%)
1	B	75/76 (98%)	9 (12%)	4 (5%)
All	All	150/152 (98%)	18 (12%)	8 (5%)

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	U

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Mol	Chain	Res	Type
1	A	17	U
1	A	18	G
1	A	21	A
1	A	37	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	47	U
1	B	47	U
1	B	17	U
1	A	46	G
1	B	16	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.