wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:35 PM BST

PDB ID	:	1ZO1
EMDB ID:	:	EMD-1248
Title	:	IF2, IF1, and tRNA fitted to cryo-EM data OF E. COLI 70S initiation complex
Authors	:	Allen, G.S.; Zavialov, A.; Gursky, R.; Ehrenberg, M.; Frank, J.
Deposited on	:	2005-05-12
Resolution	:	13.80 Å(reported)

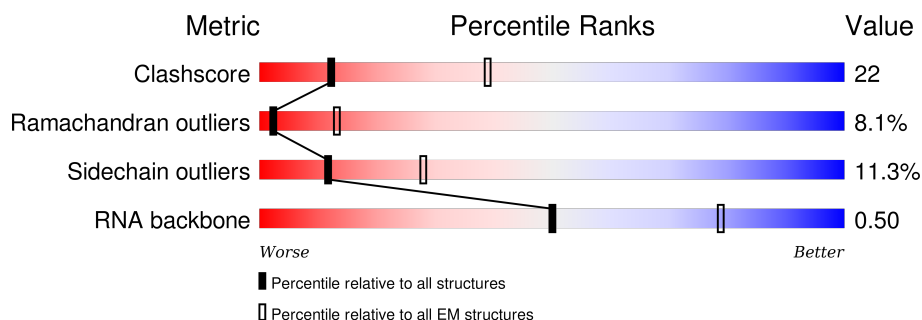|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 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		22
Ramachandran outliers		8.1%
Sidechain outliers		11.3%
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
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 >=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	F	76	87% 12%
2	I	501	68% 25% 6%
3	W	71	79% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5992 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 P/I-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 2 is a protein called translation initiation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	501	Total	C	N	O	S	0	0
			3800	2382	667	736	15		

- Molecule 3 is a protein called translation Initiation Factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

3 Residue-property plots (i)

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.
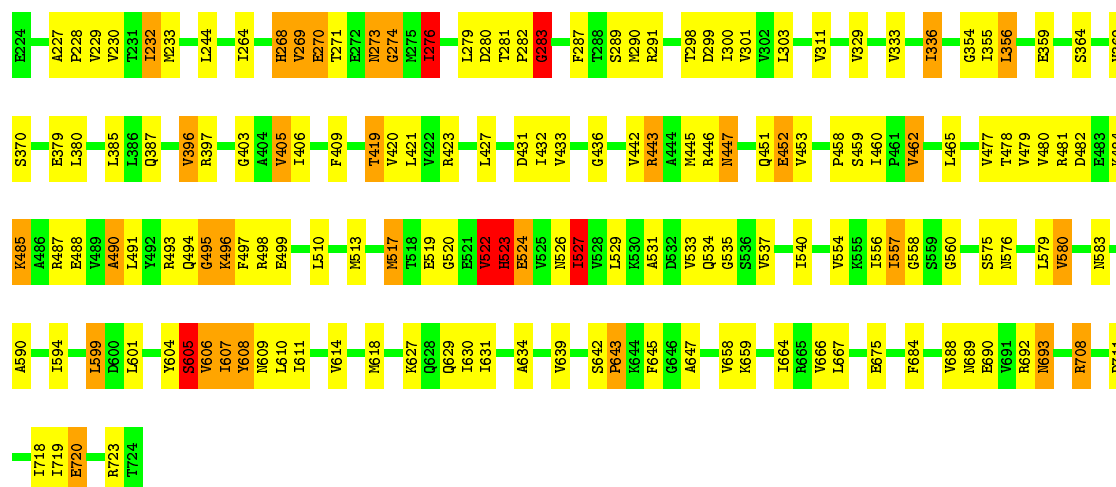
• Molecule 1: P/I-site tRNA

Chain F:
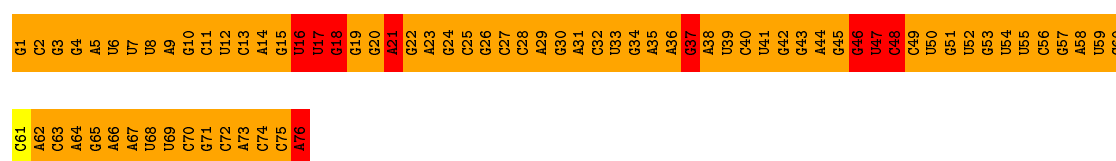
• Molecule 2: translation initiation factor 2

Chain I:

• Molecule 3: translation Initiation Factor 1

Chain W:
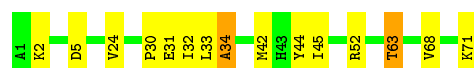
4 Experimental information (i)

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	F	5.60	277/1814 (15.3%)	6.11	700/2827 (24.8%)
2	I	0.66	0/3848	0.94	14/5200 (0.3%)
3	W	0.67	0/580	0.79	1/782 (0.1%)
All	All	3.07	277/6242 (4.4%)	3.54	715/8809 (8.1%)

The worst 5 of 277 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	39	U	C1'-N1	148.95	3.72	1.48
1	F	55	U	C1'-N1	91.84	2.86	1.48
1	F	75	C	O3'-P	29.95	1.97	1.61
1	F	19	G	N3-C4	13.35	1.44	1.35
1	F	22	G	N3-C4	13.34	1.44	1.35

The worst 5 of 715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	55	U	C6-N1-C1'	-83.91	3.73	121.20
1	F	39	U	C6-N1-C1'	-73.66	18.07	121.20
1	F	55	U	C5-C6-N1	-50.74	97.33	122.70
1	F	55	U	C6-N1-C2	28.91	138.35	121.00
1	F	10	G	C4-C5-N7	-24.56	100.98	110.80

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	F	1622	0	821	149	0
2	I	3800	0	3868	101	0
3	W	570	0	599	1	0
All	All	5992	0	5288	248	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 22.

The worst 5 of 248 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:F:75:C:O3'	1:F:76:A:P	1.97	1.23
1:F:36:A:H2'	1:F:37:G:H5"	1.15	1.09
1:F:74:C:H2'	1:F:75:C:C6	1.95	1.01
1:F:18:G:N2	1:F:57:G:H2'	1.78	0.99
2:I:432:ILE:HD12	2:I:445:MET:HG2	1.48	0.94

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	
2	I	499/501 (100%)	399 (80%)	60 (12%)	40 (8%)	1	19
3	W	69/71 (97%)	57 (83%)	6 (9%)	6 (9%)	1	17
All	All	568/572 (99%)	456 (80%)	66 (12%)	46 (8%)	2	19

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	270	GLU
2	I	283	GLY

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Mol	Chain	Res	Type
2	I	287	PHE
2	I	396	VAL
2	I	459	SER

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	
2	I	406/406 (100%)	361 (89%)	45 (11%)	8	34
3	W	62/62 (100%)	54 (87%)	8 (13%)	5	28
All	All	468/468 (100%)	415 (89%)	53 (11%)	12	33

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	499	GLU
2	I	556	ILE
3	W	42	MET
2	I	517	MET
2	I	527	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	334	ASN
2	I	365	GLN
2	I	447	ASN
2	I	534	GLN
2	I	689	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	F	75/76 (98%)	9 (12%)	4 (5%)

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	F	16	U
1	F	17	U
1	F	18	G
1	F	21	A
1	F	37	G

All (4) RNA pucker outliers are listed below:

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