



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 02:08 PM BST

PDB ID : 5A5U
EMDB ID: : EMD-3057
Title : Structure of mammalian eIF3 in the context of the 43S preinitiation complex
Authors : des-Georges, A.; Dhote, V.; Kuhn, L.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.; Hashem, Y.
Deposited on : 2015-06-21
Resolution : 9.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

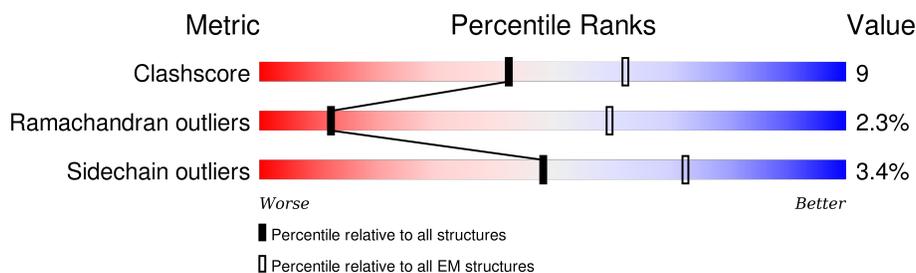
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	A	54	98% .
2	B	1121	46% 8% 45%
3	I	347	83% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8124 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 protein called EUKARYOTIC INITIATION FACTOR 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	54	397	246	74	77	0	0

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	613	5034	3228	871	915	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLU	ASP	CONFLICT	UNP G1SZ03
B	124	PHE	TYR	CONFLICT	UNP G1SZ03

- Molecule 3 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	342	2693	1711	443	530	9	0	0

4 Experimental information

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	EACH PARTICLE	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (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
2	B	0.73	1/5168 (0.0%)	1.18	26/6985 (0.4%)
3	I	1.14	3/2757 (0.1%)	0.96	6/3733 (0.2%)
All	All	0.89	4/7925 (0.1%)	1.11	32/10718 (0.3%)

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	B	3	22

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	648	GLU	N-CA	-13.23	1.19	1.46
3	I	67	CYS	CB-SG	-8.40	1.68	1.82
3	I	196	GLU	CG-CD	6.87	1.62	1.51
3	I	196	GLU	CB-CG	5.60	1.62	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	LYS	C-N-CA	17.02	164.26	121.70
2	B	215	SER	N-CA-CB	8.95	123.92	110.50
2	B	648	GLU	CA-C-O	-8.70	101.83	120.10
2	B	435	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	B	453	ARG	NE-CZ-NH1	8.54	124.57	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	211	VAL	CA
2	B	213	PHE	CA
2	B	214	GLU	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	ARG	Sidechain
2	B	156	TYR	Peptide
2	B	165	ARG	Sidechain
2	B	204	GLU	Peptide
2	B	79	ARG	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	397	0	156	1	0
2	B	5034	0	4952	120	0
3	I	2693	0	2609	112	0
All	All	8124	0	7717	137	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 9.

The worst 5 of 137 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)
2:B:646:SER:CB	2:B:654:ARG:HH12	1.05	1.61
2:B:675:LYS:HZ3	3:I:166:LYS:CG	1.30	1.44
2:B:218:ARG:NH1	3:I:2:LYS:HD2	1.12	1.43
2:B:682:ARG:NH1	3:I:248:LEU:HD12	1.26	1.41
2:B:646:SER:HB2	2:B:654:ARG:CZ	1.55	1.34

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	B	611/1121 (54%)	534 (87%)	56 (9%)	21 (3%)	5	40
3	I	340/347 (98%)	323 (95%)	16 (5%)	1 (0%)	46	83
All	All	951/1468 (65%)	857 (90%)	72 (8%)	22 (2%)	12	48

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	208	GLN
2	B	211	VAL
2	B	214	GLU
2	B	215	SER
2	B	323	CYS

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	B	547/928 (59%)	526 (96%)	21 (4%)	40	73
3	I	297/301 (99%)	289 (97%)	8 (3%)	52	79
All	All	844/1229 (69%)	815 (97%)	29 (3%)	48	75

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	408	ARG

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Mol	Chain	Res	Type
2	B	500	ASN
3	I	233	LYS
2	B	465	LYS
2	B	510	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	414	ASN
3	I	269	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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.