



wwPDB EM Map/Model Validation Report ⓘ

Jul 26, 2016 – 08:49 AM EDT

PDB ID : 5K1H
EMDB ID: : EMD-8195
Title : eIF3b relocated to the intersubunit face to interact with eIF1 and below the eIF2 ternary-complex. from the structure of a partial yeast 48S preinitiation complex in closed conformation.
Authors : Simonetti, A.; Brito Querido, J.; Myasnikov, A.G.; Mancera-Martinez, E.; Renaud, A.; Kuhn, L.; Hashem, Y.
Deposited on : 2016-05-18
Resolution : 4.90 Å(reported)
Based on PDB ID : 5A5U

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) : rb-20027939

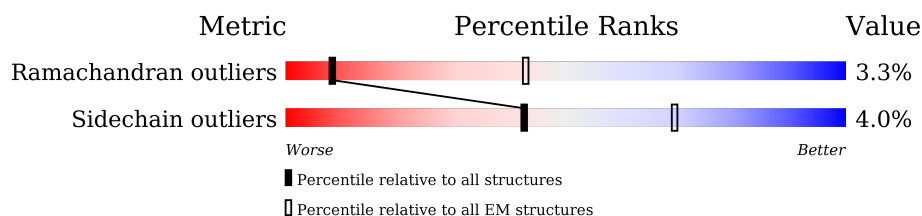
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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)
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	B	554	
2	A	54	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4760 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 translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	554	Total	C	N	O	S	0	0
			4545	2919	779	829	18		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	403	SER	THR	conflict	UNP P55884
B	499	SER	ASN	conflict	UNP P55884
B	506	SER	ILE	conflict	UNP P55884
B	?	-	PRO	deletion	UNP P55884
B	?	-	PRO	deletion	UNP P55884
B	?	-	THR	deletion	UNP P55884
B	?	-	LEU	deletion	UNP P55884
B	?	-	LEU	deletion	UNP P55884
B	?	-	SER	deletion	UNP P55884
B	?	-	GLN	deletion	UNP P55884
B	?	-	GLU	deletion	UNP P55884
B	?	-	GLN	deletion	UNP P55884
B	?	-	ILE	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884
B	?	-	GLN	deletion	UNP P55884
B	?	-	ILE	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884
B	?	-	ASP	deletion	UNP P55884
B	?	-	LEU	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884
B	?	-	TYR	deletion	UNP P55884
B	?	-	SER	deletion	UNP P55884
B	?	-	LYS	deletion	UNP P55884

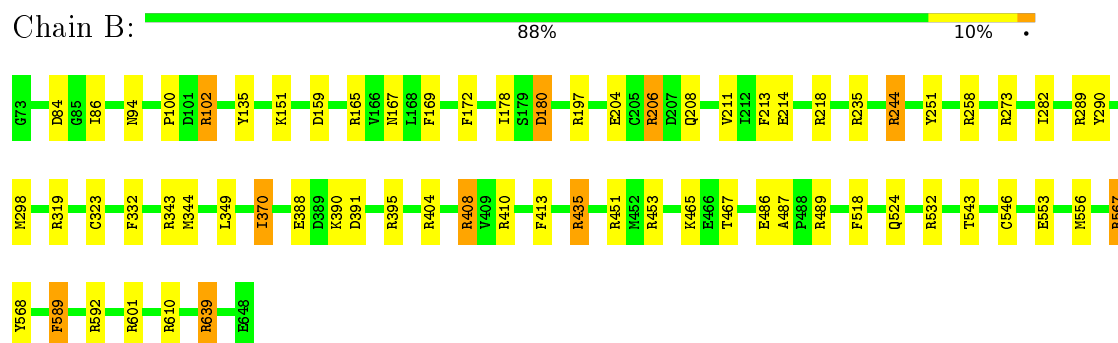
- Molecule 2 is a protein called eIF3a C-terminal tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	54	Total	C	N	O	0	0
			215	108	54	53		

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: Eukaryotic translation initiation factor 3 subunit B



- Molecule 2: eIF3a C-terminal tail



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	254957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	B	0.70	0/4672	1.16	30/6324 (0.5%)

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	B	3	18

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	244	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	B	435	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	404	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	B	453	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	610	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	197	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	408	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	410	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	610	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	451	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	592	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	343	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	206	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	B	532	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	489	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	451	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	235	ARG	NE-CZ-NH1	6.11	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	273	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	404	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	319	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	258	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	273	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	567	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	206	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	235	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	543	THR	C-N-CA	5.24	134.80	121.70
1	B	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	102	ARG	NE-CZ-NH1	5.08	122.84	120.30

All (3) chirality outliers are listed below:

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

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	ARG	Sidechain
1	B	135	TYR	Sidechain
1	B	165	ARG	Sidechain
1	B	180	ASP	Peptide
1	B	204	GLU	Peptide
1	B	244	ARG	Sidechain
1	B	251	TYR	Sidechain
1	B	289	ARG	Sidechain
1	B	290	TYR	Sidechain
1	B	344	MET	Peptide
1	B	395	ARG	Sidechain
1	B	408	ARG	Sidechain
1	B	435	ARG	Sidechain
1	B	553	GLU	Peptide
1	B	567	ARG	Sidechain
1	B	568	TYR	Sidechain
1	B	601	ARG	Sidechain
1	B	639	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	B	4545	0	4434	0	0
2	A	215	0	2	0	0
All	All	4760	0	4436	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	B	550/554 (99%)	483 (88%)	49 (9%)	18 (3%)	5	42

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	ASP
1	B	211	VAL
1	B	214	GLU
1	B	546	CYS
1	B	86	ILE
1	B	208	GLN
1	B	323	CYS
1	B	467	THR
1	B	84	ASP

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Mol	Chain	Res	Type
1	B	169	PHE
1	B	178	ILE
1	B	282	ILE
1	B	589	PHE
1	B	100	PRO
1	B	206	ARG
1	B	413	PHE
1	B	487	ALA
1	B	370	ILE

5.3.2 Protein sidechains ⓘ

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	B	495/495 (100%)	475 (96%)	20 (4%)	38 72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	151	LYS
1	B	159	ASP
1	B	167	ASN
1	B	172	PHE
1	B	213	PHE
1	B	298	MET
1	B	332	PHE
1	B	349	LEU
1	B	370	ILE
1	B	388	GLU
1	B	390	LYS
1	B	391	ASP
1	B	465	LYS
1	B	486	GLU
1	B	518	PHE
1	B	524	GLN

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Mol	Chain	Res	Type
1	B	556	MET
1	B	589	PHE
1	B	639	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	610:ARG	C	633:ILE	N	23.27