



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J8B
EMDB ID: : EMD-2451
Title : Model of the human eIF3 PCI-MPN octamer docked into the 43S-HCV IRES
EM map
Authors : Erzberger, J.P.; Ban, N.
Deposited on : 2014-10-08
Resolution : unknown (reported)
Based on PDB ID : 3CHM, 4LCT, 3J47, 4U1C, 4B4T, 1RZ4, 4U1D, 4O8X

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

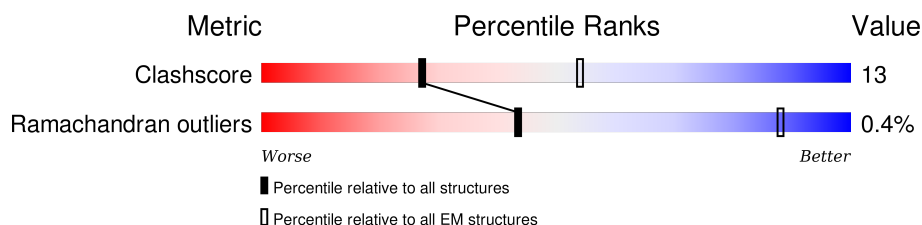
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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

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	529	85% 7% 8%
2	C	547	92% 8%
3	E	422	78% 13% 9%
4	F	327	67% 29%
5	H	343	68% 6% 26%
6	K	208	95% . .
7	L	540	41% 7% 52%
8	M	364	44% 5% 52%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12633 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 A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	488	Total	C	N	O	0	0
			2432	1456	488	488		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	546	Total	C	N	O	0	0
			2711	1619	546	546		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	384	Total	C	N	O	0	0
			1911	1143	384	384		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	232	Total	C	N	O	0	0
			1149	685	232	232		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	254	Total	C	N	O	0	0
			1262	754	254	254		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit K.

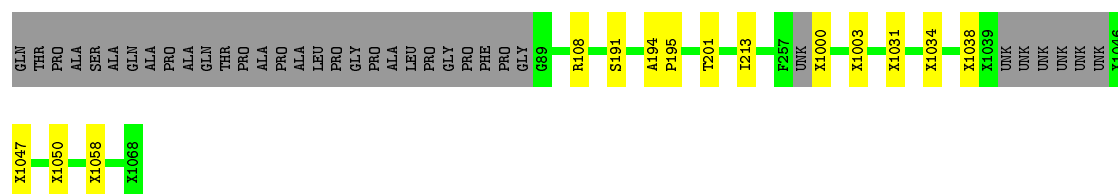
Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	204	Total	C	N	O	0	0
			1012	604	204	204		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	258	Total	C	N	O	0	0
			1281	765	258	258		

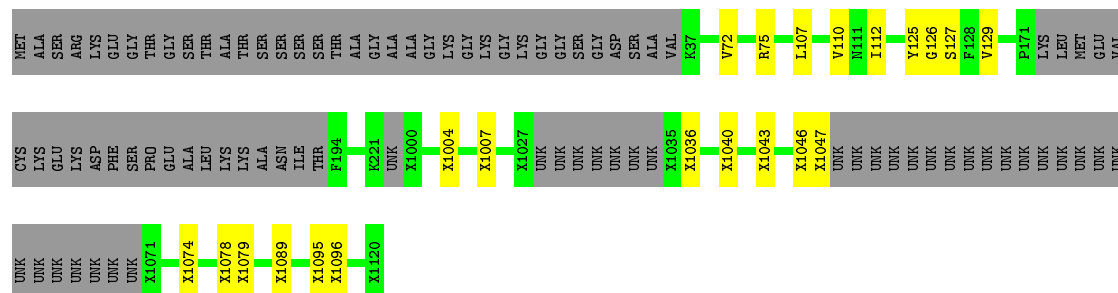
- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	176	Total	C	N	O	0	0
			875	523	176	176		



- Molecule 5: Eukaryotic translation initiation factor 3 subunit H

Chain H: 68% 6% 26%



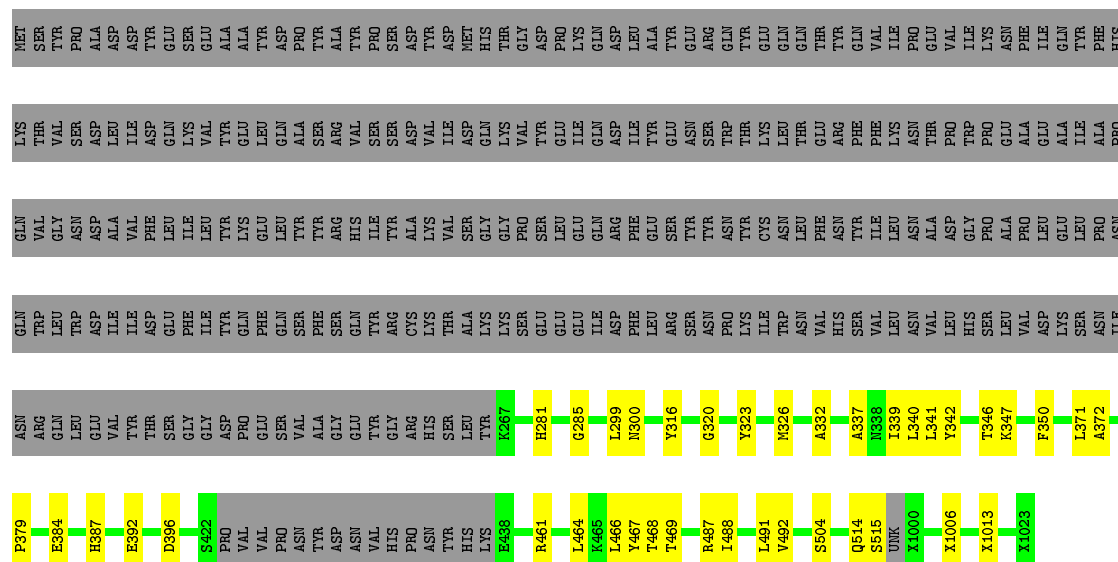
- Molecule 6: Eukaryotic translation initiation factor 3 subunit K

Chain K: 95% . .



- Molecule 7: Eukaryotic translation initiation factor 3 subunit L

Chain L: 41% 7% 52%



- Molecule 8: Eukaryotic translation initiation factor 3 subunit M

Chain M: 44% 5% 52%




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	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	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 ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/2260	0.57	6/3156 (0.2%)
2	C	0.28	0/2585	0.53	4/3606 (0.1%)
3	E	0.37	0/1778	0.57	1/2479 (0.0%)
4	F	0.47	0/833	0.61	0/1158
5	H	0.48	0/805	0.59	0/1119
6	K	0.23	0/925	0.56	0/1287
7	L	0.49	0/1159	0.61	0/1614
8	M	0.39	0/734	0.62	0/1023
All	All	0.37	0/11079	0.57	11/15442 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	PRO	N-CA-CB	6.42	111.00	103.30
2	C	606	PRO	N-CA-CB	6.28	110.83	103.30
1	A	400	PRO	N-CA-CB	6.26	110.82	103.30
2	C	628	PRO	N-CA-CB	5.91	110.39	103.30
1	A	266	PRO	N-CA-CB	5.66	110.09	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2432	0	1010	29	0
2	C	2711	0	1169	41	0
3	E	1911	0	807	65	0
4	F	1149	0	435	17	0
5	H	1262	0	439	27	0
6	K	1012	0	439	16	0
7	L	1281	0	526	57	0
8	M	875	0	364	18	0
All	All	12633	0	5189	230	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 13.

The worst 5 of 230 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:C:484:GLU:CB	2:C:502:LYS:CB	1.75	1.57
1:A:45:LYS:CB	1:A:82:ASN:CB	1.88	1.48
2:C:628:PRO:CB	3:E:352:SER:CB	1.93	1.45
7:L:467:TYR:O	7:L:515:SER:CB	1.65	1.44
3:E:1019:UNK:CB	7:L:347:LYS:CB	1.95	1.44

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	A	450/529 (85%)	440 (98%)	8 (2%)	2 (0%)	39	39
2	C	519/547 (95%)	492 (95%)	24 (5%)	3 (1%)	30	30
3	E	352/422 (83%)	332 (94%)	19 (5%)	1 (0%)	46	46
4	F	167/327 (51%)	162 (97%)	4 (2%)	1 (1%)	30	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	159/343 (46%)	153 (96%)	6 (4%)	0	100	100
6	K	183/208 (88%)	178 (97%)	5 (3%)	0	100	100
7	L	230/540 (43%)	218 (95%)	11 (5%)	1 (0%)	39	39
8	M	146/364 (40%)	143 (98%)	3 (2%)	0	100	100
All	All	2206/3280 (67%)	2118 (96%)	80 (4%)	8 (0%)	43	39

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	206	PRO
2	C	392	ASP
2	C	393	PRO
4	F	195	PRO
7	L	379	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.