



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Dec 19, 2016 – 11:43 AM EST

PDB ID : 5M5H
EMDB ID: : EMD-4155
Title : RIBOSOME-BOUND YIDC INSERTASE
Authors : Kedrov, A.; Wickles, S.; Crevenna, A.H.; van der Sluis, E.; Buschauer, R.;
Berninghausen, O.; Lamb, D.C.; Beckmann, R.
Deposited on : 2016-10-21
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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-20028442

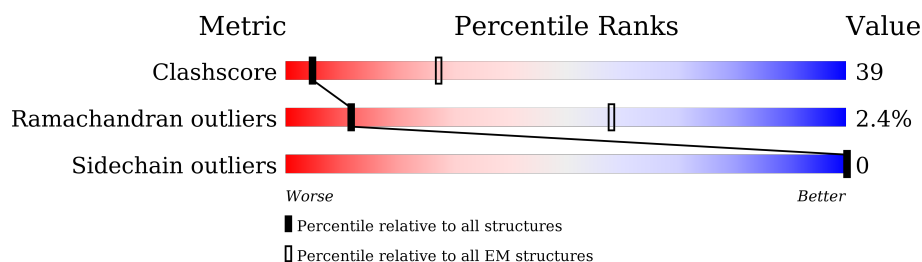
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 4.50 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	551	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1086 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 Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1086	757	157	164	8		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	LEU	-	expression tag	UNP B7MGC7
A	542	GLU	-	expression tag	UNP B7MGC7
A	543	SER	-	expression tag	UNP B7MGC7
A	544	SER	-	expression tag	UNP B7MGC7
A	545	GLY	-	expression tag	UNP B7MGC7
A	546	GLU	-	expression tag	UNP B7MGC7
A	547	ASN	-	expression tag	UNP B7MGC7
A	548	LEU	-	expression tag	UNP B7MGC7
A	549	TYR	-	expression tag	UNP B7MGC7
A	550	PHE	-	expression tag	UNP B7MGC7
A	551	GLN	-	expression tag	UNP B7MGC7

- Molecule 1: Membrane protein insertase YidC

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	42658	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

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	0.37	0/1126	0.76	1/1537 (0.1%)

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	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	513	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	VAL	Peptide
1	A	424	PHE	Peptide

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	1086	0	1095	84	0
All	All	1086	0	1095	84	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 39.

All (84) 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:432:ILE:O	1:A:436:LEU:HB2	1.59	1.02
1:A:361:ILE:O	1:A:365:VAL:HB	1.69	0.91
1:A:472:GLY:O	1:A:476:PHE:HB3	1.80	0.81
1:A:336:ILE:HD12	1:A:431:PRO:HD3	1.66	0.76
1:A:498:MET:O	1:A:501:ILE:N	2.19	0.76
1:A:462:ASP:HB2	1:A:511:SER:HB3	1.68	0.76
1:A:461:GLN:HA	1:A:510:PRO:HA	1.67	0.75
1:A:440:LEU:HD11	1:A:513:LEU:HB2	1.72	0.71
1:A:471:MET:O	1:A:475:MET:HB3	1.91	0.70
1:A:472:GLY:O	1:A:476:PHE:CB	2.40	0.69
1:A:447:ARG:HG2	1:A:448:GLN:HG3	1.75	0.68
1:A:436:LEU:O	1:A:439:MET:HB3	1.93	0.68
1:A:341:PHE:HE1	1:A:442:GLY:HA3	1.58	0.67
1:A:347:ILE:HD13	1:A:360:ILE:HG22	1.77	0.66
1:A:345:LYS:HA	1:A:348:HIS:CE1	2.32	0.63
1:A:430:MET:O	1:A:434:LEU:HB2	1.98	0.63
1:A:521:ASN:O	1:A:525:ILE:HG12	1.99	0.63
1:A:344:LEU:O	1:A:348:HIS:ND1	2.31	0.62
1:A:475:MET:SD	1:A:521:ASN:ND2	2.72	0.62
1:A:359:ILE:O	1:A:362:THR:HB	2.01	0.60
1:A:468:PRO:HB3	1:A:503:THR:HG23	1.84	0.60
1:A:518:ILE:O	1:A:522:LEU:HG	2.02	0.58
1:A:454:TRP:CD1	1:A:466:ILE:HD12	2.39	0.58
1:A:498:MET:HA	1:A:501:ILE:HB	1.86	0.58
1:A:436:LEU:HD21	1:A:516:TYR:CD2	2.39	0.57
1:A:433:PHE:CD1	1:A:513:LEU:HD21	2.40	0.57
1:A:364:ILE:O	1:A:367:GLY:N	2.38	0.56
1:A:455:ILE:H	1:A:455:ILE:HD12	1.71	0.56
1:A:337:SER:HA	1:A:435:ALA:HB2	1.89	0.55
1:A:471:MET:HE1	1:A:517:TYR:HB3	1.89	0.54
1:A:333:LEU:N	1:A:434:LEU:HD13	2.23	0.53
1:A:333:LEU:HD22	1:A:434:LEU:HD22	1.90	0.53
1:A:454:TRP:CD1	1:A:455:ILE:HG13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:HG21	1:A:439:MET:HG3	1.90	0.53
1:A:341:PHE:CE1	1:A:442:GLY:HA3	2.41	0.53
1:A:437:TYR:O	1:A:441:MET:HG2	2.09	0.52
1:A:431:PRO:O	1:A:435:ALA:HB3	2.10	0.52
1:A:461:GLN:OE1	1:A:461:GLN:N	2.42	0.52
1:A:522:LEU:HD23	1:A:525:ILE:HG13	1.92	0.51
1:A:506:PHE:CD1	1:A:514:VAL:HG22	2.45	0.51
1:A:364:ILE:C	1:A:367:GLY:H	2.14	0.50
1:A:494:ILE:O	1:A:498:MET:HG3	2.12	0.49
1:A:333:LEU:HD11	1:A:437:TYR:HB3	1.95	0.49
1:A:368:ILE:O	1:A:371:PRO:HD2	2.14	0.48
1:A:354:TRP:CD2	1:A:446:LEU:HD11	2.48	0.48
1:A:442:GLY:HA2	1:A:443:SER:HA	1.54	0.48
1:A:471:MET:O	1:A:475:MET:CB	2.60	0.48
1:A:338:GLN:HG2	1:A:342:LYS:HE3	1.96	0.48
1:A:344:LEU:HD22	1:A:361:ILE:HD12	1.96	0.48
1:A:351:VAL:O	1:A:353:ASN:N	2.47	0.47
1:A:465:TYR:O	1:A:468:PRO:HD2	2.14	0.47
1:A:351:VAL:HG12	1:A:351:VAL:O	2.14	0.47
1:A:503:THR:O	1:A:507:LEU:HG	2.15	0.47
1:A:358:ILE:HG23	1:A:439:MET:SD	2.56	0.46
1:A:433:PHE:CE1	1:A:513:LEU:HD21	2.51	0.46
1:A:436:LEU:HB3	1:A:513:LEU:HD12	1.98	0.46
1:A:356:PHE:CD1	1:A:359:ILE:HD12	2.52	0.45
1:A:436:LEU:HA	1:A:439:MET:HB3	1.98	0.45
1:A:462:ASP:HB3	1:A:465:TYR:HA	1.99	0.45
1:A:527:GLN:HG3	1:A:528:GLN:N	2.32	0.45
1:A:341:PHE:O	1:A:344:LEU:HB3	2.17	0.45
1:A:370:TYR:N	1:A:371:PRO:HD2	2.32	0.45
1:A:344:LEU:HB2	1:A:361:ILE:HD12	1.97	0.45
1:A:356:PHE:HD1	1:A:359:ILE:HD12	1.82	0.44
1:A:466:ILE:O	1:A:469:ILE:N	2.51	0.43
1:A:336:ILE:HG21	1:A:431:PRO:HB3	1.99	0.43
1:A:469:ILE:O	1:A:473:VAL:HG23	2.17	0.43
1:A:333:LEU:HD12	1:A:438:TYR:CD2	2.53	0.43
1:A:354:TRP:CE3	1:A:446:LEU:HD11	2.53	0.43
1:A:462:ASP:OD2	1:A:465:TYR:N	2.52	0.43
1:A:455:ILE:HD11	1:A:467:LEU:HD11	2.01	0.43
1:A:333:LEU:HB3	1:A:438:TYR:HE2	1.83	0.42
1:A:355:GLY:HA3	1:A:451:PHE:CD1	2.54	0.42
1:A:362:THR:HG21	1:A:519:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:CG	1:A:507:LEU:HD22	2.54	0.42
1:A:355:GLY:HA3	1:A:451:PHE:HD1	1.84	0.42
1:A:358:ILE:HA	1:A:361:ILE:HG22	2.01	0.42
1:A:468:PRO:HA	1:A:471:MET:HB3	2.02	0.41
1:A:465:TYR:CD1	1:A:507:LEU:HD22	2.56	0.41
1:A:498:MET:O	1:A:499:PRO:C	2.57	0.41
1:A:333:LEU:HD13	1:A:434:LEU:HB3	2.03	0.41
1:A:355:GLY:HA2	1:A:358:ILE:HD12	2.03	0.41
1:A:525:ILE:HG22	1:A:526:ILE:HD13	2.03	0.40
1:A:504:VAL:HA	1:A:507:LEU:HD12	2.04	0.40

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	126/551 (23%)	112 (89%)	11 (9%)	3 (2%)	7 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	VAL
1	A	352	GLY
1	A	425	PRO

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	
1	A	116/471 (25%)	116 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	521	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.