



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 03:05 PM EDT

PDB ID : 4V3N
EMDB ID: : EMD-2796
Title : Membrane bound pleurotolysin prepore (TMH2 strand lock) trapped with engineered disulphide cross-link
Authors : Lukyanova, N.; Kondos, S.C.; Farabella, I.; Law, R.H.P.; Reboul, C.F.; Caradoc-Davies, T.T.; Spicer, B.A.; Kleifeld, O.; Perugini, M.; Ekkel, S.; Hatfaludi, T.; Oliver, K.; Hotze, E.M.; Tweten, R.K.; Whisstock, J.C.; Topf, M.; Dunstone, M.A.; Saibil, H.R.
Deposited on : unknown
Resolution : 14.00 Å(reported)
Based on PDB ID : 4OEB

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

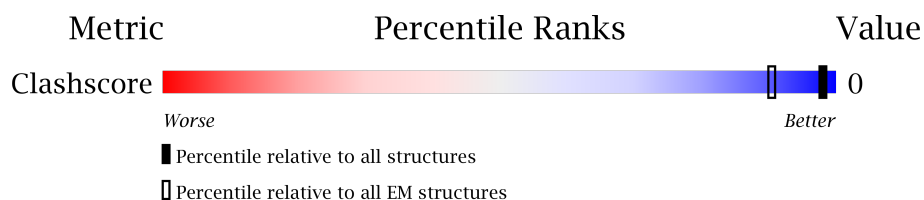
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

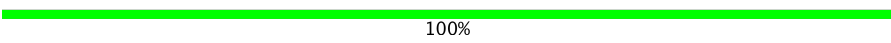




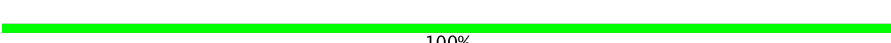





The reported resolution of this entry is 14.00 Å.

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.



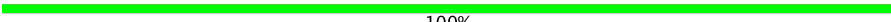
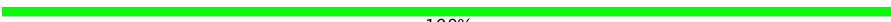







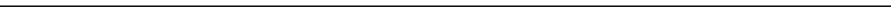
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336

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	1-A	135	 100%
1	1-B	135	 100%
1	10-A	135	 100%
1	10-B	135	 100%
1	11-A	135	 100%
1	11-B	135	 100%
1	12-A	135	 100%
1	12-B	135	 100%
1	2-A	135	 100%
1	2-B	135	 100%
1	3-A	135	 100%

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Mol	Chain	Length	Quality of chain
1	3-B	135	 100%
1	4-A	135	 100%
1	4-B	135	 100%
1	5-A	135	 100%
1	5-B	135	 100%
1	6-A	135	 100%
1	6-B	135	 100%
1	7-A	135	 100%
1	7-B	135	 100%
1	8-A	135	 100%
1	8-B	135	 100%
1	9-A	135	 100%
1	9-B	135	 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13160 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 PLEUROTOLYSIN A.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	1-A	135	Total C 135 135	0	135
1	2-A	135	Total C 135 135	0	135
1	3-A	135	Total C 135 135	0	135
1	4-A	135	Total C 135 135	0	135
1	5-A	135	Total C 135 135	0	135
1	6-A	135	Total C 135 135	0	135
1	7-A	135	Total C 135 135	0	135
1	8-A	135	Total C 135 135	0	135
1	9-A	135	Total C 135 135	0	135
1	10-A	135	Total C 135 135	0	135
1	11-A	135	Total C 135 135	0	135
1	12-A	135	Total C 135 135	0	135
1	13-A	135	Total C 135 135	0	135
1	14-A	135	Total C 135 135	0	135
1	15-A	135	Total C 135 135	0	135
1	16-A	135	Total C 135 135	0	135
1	17-A	135	Total C 135 135	0	135

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Mol	Chain	Residues	Atoms		AltConf	Trace
1	18-A	135	Total 135	C 135	0	135
1	19-A	135	Total 135	C 135	0	135
1	20-A	135	Total 135	C 135	0	135
1	1-B	135	Total 135	C 135	0	135
1	2-B	135	Total 135	C 135	0	135
1	3-B	135	Total 135	C 135	0	135
1	4-B	135	Total 135	C 135	0	135
1	5-B	135	Total 135	C 135	0	135
1	6-B	135	Total 135	C 135	0	135
1	7-B	135	Total 135	C 135	0	135
1	8-B	135	Total 135	C 135	0	135
1	9-B	135	Total 135	C 135	0	135
1	10-B	135	Total 135	C 135	0	135
1	11-B	135	Total 135	C 135	0	135
1	12-B	135	Total 135	C 135	0	135
1	13-B	135	Total 135	C 135	0	135
1	14-B	135	Total 135	C 135	0	135
1	15-B	135	Total 135	C 135	0	135
1	16-B	135	Total 135	C 135	0	135
1	17-B	135	Total 135	C 135	0	135
1	18-B	135	Total 135	C 135	0	135

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Mol	Chain	Residues	Atoms		AltConf	Trace
1	19-B	135	Total 135	C 135	0	135
1	20-B	135	Total 135	C 135	0	135

- Molecule 2 is a protein called PLEUROTOLYSIN B.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	1-C	388	Total 388	C 388	0	388
2	2-C	388	Total 388	C 388	0	388
2	3-C	388	Total 388	C 388	0	388
2	4-C	388	Total 388	C 388	0	388
2	5-C	388	Total 388	C 388	0	388
2	6-C	388	Total 388	C 388	0	388
2	7-C	388	Total 388	C 388	0	388
2	8-C	388	Total 388	C 388	0	388
2	9-C	388	Total 388	C 388	0	388
2	10-C	388	Total 388	C 388	0	388
2	11-C	388	Total 388	C 388	0	388
2	12-C	388	Total 388	C 388	0	388
2	13-C	388	Total 388	C 388	0	388
2	14-C	388	Total 388	C 388	0	388
2	15-C	388	Total 388	C 388	0	388
2	16-C	388	Total 388	C 388	0	388
2	17-C	388	Total 388	C 388	0	388

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	18-C	388	Total C 388 388	0	388
2	19-C	388	Total C 388 388	0	388
2	20-C	388	Total C 388 388	0	388

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	PHE	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	LEU	deletion	UNP Q5W9E8
C	?	-	MET	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	TYR	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	VAL	deletion	UNP Q5W9E8
C	?	-	LYS	deletion	UNP Q5W9E8
C	?	-	VAL	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	PRO	deletion	UNP Q5W9E8
C	?	-	PHE	deletion	UNP Q5W9E8
C	?	-	ILE	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	TYR	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	PHE	deletion	UNP Q5W9E8
C	?	-	LYS	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	ARG	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	VAL	deletion	UNP Q5W9E8
C	?	-	LYS	deletion	UNP Q5W9E8
C	?	-	GLN	deletion	UNP Q5W9E8
C	?	-	ASP	deletion	UNP Q5W9E8
C	?	-	VAL	deletion	UNP Q5W9E8
C	?	-	LYS	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	LEU	deletion	UNP Q5W9E8
C	?	-	GLU	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	VAL	deletion	UNP Q5W9E8
C	?	-	LYS	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	TRP	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	ALA	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	HIS	deletion	UNP Q5W9E8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	GLN	deletion	UNP Q5W9E8
C	?	-	GLY	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	ILE	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	THR	deletion	UNP Q5W9E8
C	?	-	SER	deletion	UNP Q5W9E8
C	?	-	GLN	deletion	UNP Q5W9E8
C	?	-	ASN	deletion	UNP Q5W9E8
C	?	-	ARG	deletion	UNP Q5W9E8

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	1110	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	ESTIMATED WITH CTFFIND3, THEN PHASES FLIPPED FOR EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	76148	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

4 Model quality [i](#)

4.1 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1-A	135	0	0	0	0
1	1-B	135	0	0	0	0
1	2-A	135	0	0	0	0
1	2-B	135	0	0	0	0
1	3-A	135	0	0	0	0
1	3-B	135	0	0	0	0
1	4-A	135	0	0	0	0
1	4-B	135	0	0	0	0
1	5-A	135	0	0	0	0
1	5-B	135	0	0	0	0
1	6-A	135	0	0	0	0
1	6-B	135	0	0	0	0
1	7-A	135	0	0	0	0
1	7-B	135	0	0	0	0
1	8-A	135	0	0	0	0
1	8-B	135	0	0	0	0
1	9-A	135	0	0	0	0
1	9-B	135	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-A	135	0	0	0	0
1	10-B	135	0	0	0	0
1	11-A	135	0	0	0	0
1	11-B	135	0	0	0	0
1	12-A	135	0	0	0	0
1	12-B	135	0	0	0	0
1	13-A	135	0	0	0	0
1	13-B	135	0	0	0	0
1	14-A	135	0	0	0	0
1	14-B	135	0	0	0	0
1	15-A	135	0	0	0	0
1	15-B	135	0	0	0	0
1	16-A	135	0	0	0	0
1	16-B	135	0	0	0	0
1	17-A	135	0	0	0	0
1	17-B	135	0	0	0	0
1	18-A	135	0	0	0	0
1	18-B	135	0	0	0	0
1	19-A	135	0	0	0	0
1	19-B	135	0	0	0	0
1	20-A	135	0	0	0	0
1	20-B	135	0	0	0	0
2	1-C	388	0	0	0	0
2	2-C	388	0	0	0	0
2	3-C	388	0	0	1	0
2	4-C	388	0	0	2	0
2	5-C	388	0	0	0	0
2	6-C	388	0	0	1	0
2	7-C	388	0	0	0	0
2	8-C	388	0	0	1	0
2	9-C	388	0	0	0	0
2	10-C	388	0	0	0	0
2	11-C	388	0	0	0	0
2	12-C	388	0	0	0	0
2	13-C	388	0	0	0	0
2	14-C	388	0	0	0	0
2	15-C	388	0	0	0	0
2	16-C	388	0	0	0	0
2	17-C	388	0	0	0	0
2	18-C	388	0	0	0	0
2	19-C	388	0	0	0	0
2	20-C	388	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13160	0	0	5	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 0.

All (5) 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:181:ILE:CA	2:C:182:GLY:CA	2.92	0.48
2:C:183:GLY:CA	2:C:248:GLY:CA	2.94	0.46
2:C:181:ILE:CA	2:C:182:GLY:CA	2.95	0.45
2:C:183:GLY:CA	2:C:248:GLY:CA	2.96	0.44
2:C:181:ILE:CA	2:C:182:GLY:CA	2.98	0.41

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.