

Feb 25, 2025 – 06:05 pm GMT

PDB ID 9GI0 : EMDB ID EMD-51366 : Title Truncated MmpL4 in detergent : Authors : Earp, J.C.; Garaeva, A.A.; Seeger, M.A. Deposited on 2024-08-16 : 3.00 Å(reported) Resolution : .

Based on initial model :

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

> The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

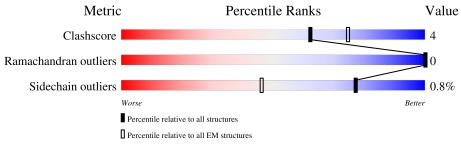
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${ m EM~structures}\ (\#{ m Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	78	78%	19%	
2	В	783	85%	7%	8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12388 atoms, of which 6294 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 Acyl carrier protein.

Mol	Chain	Residues	Atoms			AltConf	Trace			
1	А	77	Total 1170	C 368	Н 573	N 93	0 135	S 1	0	0

• Molecule 2 is a protein called Siderophore exporter MmpL4.

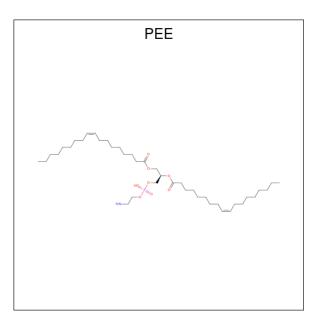
Mol	Chain	Residues	Atoms			AltConf	Trace			
2	В	722	Total 11089	C 3524	Н 5643	N 932	O 963	S 27	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1	VAL	MET	conflict	UNP P9WJV2
В	682	GLY	-	linker	UNP P9WJV2
В	683	GLY	-	linker	UNP P9WJV2
В	684	SER	-	linker	UNP P9WJV2
В	685	SER	-	linker	UNP P9WJV2
В	686	SER	-	linker	UNP P9WJV2
В	968	ALA	-	expression tag	UNP P9WJV2
В	969	LEU	-	expression tag	UNP P9WJV2
В	970	GLU	-	expression tag	UNP P9WJV2
В	971	VAL	-	expression tag	UNP P9WJV2
В	972	LEU	-	expression tag	UNP P9WJV2
В	973	PHE	-	expression tag	UNP P9WJV2
В	974	GLN	-	expression tag	UNP P9WJV2

• Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P).





Mol	Chain	Residues	Atoms			AltConf			
9	D	1	Total	С	Η	Ν	Ο	Р	0
J	D	1	129	41	78	1	8	1	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Chain A:
 78%
 19%
 ...

 Image: Bit of Bit
- Molecule 1: Acyl carrier protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	316324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	64.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEE

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		lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/601	0.52	0/812
2	В	0.26	0/5558	0.47	0/7557
All	All	0.26	0/6159	0.48	0/8369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	597	573	571	15	0
2	В	5446	5643	5638	37	0
3	В	51	78	82	0	0
All	All	6094	6294	6291	51	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 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:B:880:GLY:HA3	2:B:913:THR:HG21	1.73	0.70
1:A:51:PHE:CG	1:A:73:ILE:HD11	2.28	0.67
1:A:49:GLU:OE2	2:B:862:LYS:N	2.30	0.64
2:B:310:GLY:HA3	2:B:343:VAL:HG21	1.81	0.62
2:B:877:THR:OG1	2:B:917:ARG:NH2	2.33	0.61
2:B:211:ILE:HD11	2:B:886:THR:OG1	2.03	0.59
2:B:290:ASP:OD2	2:B:291:LYS:N	2.38	0.56
2:B:128:ASP:OD2	2:B:130:LEU:N	2.38	0.56
1:A:15:GLN:NE2	1:A:39:ASP:OD1	2.39	0.56
1:A:62:LYS:N	1:A:62:LYS:HD2	2.22	0.54
1:A:19:LYS:N	1:A:19:LYS:HE2	2.22	0.54
1:A:63:ILE:HD12	1:A:63:ILE:H	1.74	0.52
1:A:67:GLN:O	1:A:71:ASP:OD1	2.29	0.51
2:B:203:ILE:HD11	2:B:893:SER:HB2	1.93	0.51
2:B:853:PHE:O	2:B:857:ILE:HD13	2.10	0.51
2:B:58:VAL:HG11	2:B:330:THR:HG21	1.92	0.50
2:B:234:VAL:HG11	2:B:349:LEU:HD22	1.93	0.49
2:B:99:ASP:OD1	2:B:100:ALA:N	2.46	0.48
2:B:770:ASP:C	2:B:770:ASP:OD1	2.51	0.48
2:B:60:LEU:HD22	2:B:327:TYR:CE1	2.49	0.47
2:B:418:ASP:O	2:B:418:ASP:OD1	2.32	0.47
2:B:473:ILE:C	2:B:473:ILE:HD12	2.34	0.47
1:A:10:LYS:O	1:A:10:LYS:HD2	2.15	0.47
2:B:467:ILE:HD11	2:B:733:ILE:HG23	1.97	0.47
2:B:467:ILE:HD13	2:B:715:ILE:HD11	1.96	0.46
1:A:63:ILE:HD12	1:A:63:ILE:N	2.31	0.46
2:B:202:ARG:NH2	2:B:894:ASP:OD1	2.49	0.46
2:B:468:PHE:O	2:B:473:ILE:HD11	2.15	0.45
2:B:473:ILE:HD12	2:B:473:ILE:O	2.16	0.45
1:A:10:LYS:HD2	1:A:10:LYS:C	2.37	0.45
2:B:134:GLY:O	2:B:437:ARG:NH2	2.45	0.45
2:B:794:ILE:O	2:B:798:VAL:HG23	2.16	0.45
2:B:892:VAL:HG12	2:B:892:VAL:O	2.16	0.45
1:A:77:GLN:HA	1:A:77:GLN:OE1	2.17	0.45
2:B:841:VAL:HG21	2:B:883:PHE:CZ	2.52	0.45
2:B:845:TYR:CD1	2:B:913:THR:HG22	2.52	0.44
2:B:122:VAL:HG13	2:B:147:LEU:HD23	1.98	0.44
2:B:880:GLY:CA	2:B:913:THR:HG21	2.47	0.43
2:B:257:PHE:HD1	2:B:898:ILE:HD13	1.83	0.43
1:A:15:GLN:OE1	1:A:15:GLN:C	2.57	0.43
T.U.TO.ODU.ODI	1.11.10.0LIN.0		
2:B:755:GLY:O	2:B:759:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:N	1:A:20:GLN:CD	2.73	0.43
1:A:67:GLN:O	1:A:70:ILE:N	2.52	0.42
2:B:122:VAL:HG22	2:B:147:LEU:HD22	2.00	0.42
2:B:128:ASP:OD2	2:B:128:ASP:C	2.59	0.42
2:B:386:LEU:HB3	2:B:387:PRO:HD3	2.03	0.41
2:B:39:CYS:SG	2:B:234:VAL:HG13	2.62	0.40
2:B:909:LEU:O	2:B:913:THR:HG23	2.21	0.40
2:B:202:ARG:HE	2:B:892:VAL:HG12	1.87	0.40
2:B:890:MET:CE	2:B:898:ILE:HG13	2.52	0.40

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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	Perce	ntiles
1	А	75/78~(96%)	74 (99%)	1 (1%)	0	100	100
2	В	718/783~(92%)	710 (99%)	8 (1%)	0	100	100
All	All	793/861~(92%)	784 (99%)	9(1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	d Rotameric Outlier		Percentiles		
1	А	66/67~(98%)	65~(98%)	1 (2%)	60 83		
2	В	570/621~(92%)	566~(99%)	4 (1%)	81 91		
All	All	636/688~(92%)	631~(99%)	5(1%)	77 90		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	71	ASP
2	В	76	MET
2	В	693	ASN
2	В	696	PHE
2	В	770	ASP

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

Mol	Chain	Res	Type	
1	А	25	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link Bond lengths		Bond angles				
10101	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	PEE	В	1001	-	$50,\!50,\!50$	0.31	0	$53,\!55,\!55$	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	В	1001	-	-	15/54/54/54	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	1001	PEE	C1-O3P-P-O1P
3	В	1001	PEE	C4-O4P-P-O3P
3	В	1001	PEE	O5-C30-O3-C3
3	В	1001	PEE	C31-C30-O3-C3
3	В	1001	PEE	C33-C34-C35-C36
3	В	1001	PEE	C41-C42-C43-C44
3	В	1001	PEE	C31-C32-C33-C34
3	В	1001	PEE	C1-O3P-P-O4P
3	В	1001	PEE	C16-C17-C18-C19
3	В	1001	PEE	O3P-C1-C2-C3
3	В	1001	PEE	C2-C1-O3P-P
3	В	1001	PEE	O3P-C1-C2-O2
3	В	1001	PEE	C1-C2-C3-O3
3	В	1001	PEE	C4-O4P-P-O2P
3	В	1001	PEE	C18-C19-C20-C21

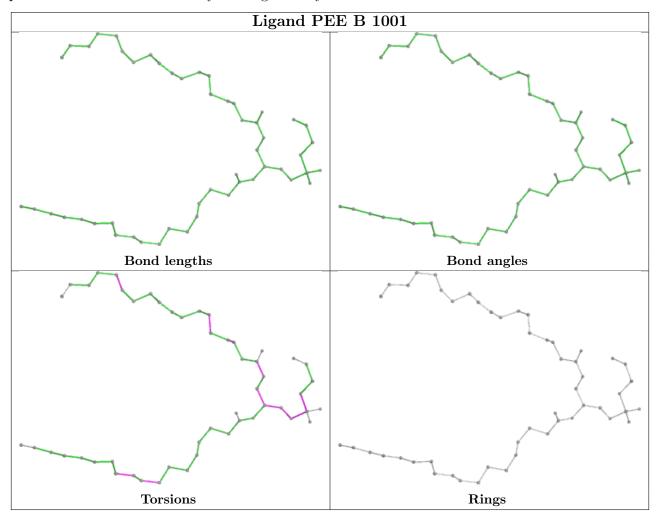
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

