



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 10:33 AM EDT

PDB ID : 4A8D
EMDB ID: : EMD-1505
Title : DegP dodecamer with bound OMP
Authors : Malet, H.; Krojer, T.; Sawa, J.; Schafer, E.; Saibil, H.R.; Ehrmann, M.; Clausen, T.
Deposited on : unknown
Resolution : 28.00 Å(reported)
Based on PDB ID : 3CS0

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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

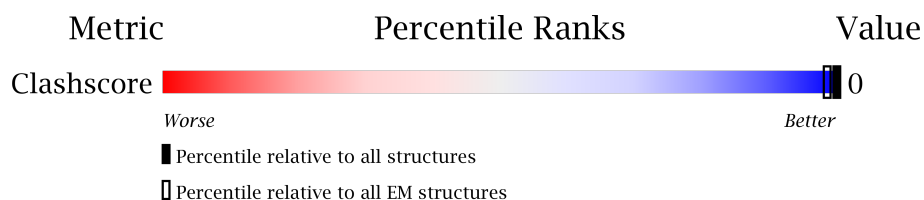
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY












The reported resolution of this entry is 28.00 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.




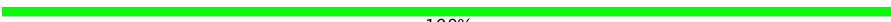
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336

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	A	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	
1	F	448	
1	G	448	
1	H	448	
1	I	448	
1	J	448	
1	K	448	

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Mol	Chain	Length	Quality of chain
1	L	448	 86%14%
2	M	346	 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4954 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 PERIPLASMIC SERINE ENDOPROTEASE DEGP.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	384	Total C 384 384	0	384
1	B	384	Total C 384 384	0	384
1	C	384	Total C 384 384	0	384
1	D	384	Total C 384 384	0	384
1	E	384	Total C 384 384	0	384
1	F	384	Total C 384 384	0	384
1	G	384	Total C 384 384	0	384
1	H	384	Total C 384 384	0	384
1	I	384	Total C 384 384	0	384
1	J	384	Total C 384 384	0	384
1	K	384	Total C 384 384	0	384
1	L	384	Total C 384 384	0	384

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	engineered mutation	UNP P0C0V0
B	210	ALA	SER	engineered mutation	UNP P0C0V0
C	210	ALA	SER	engineered mutation	UNP P0C0V0
D	210	ALA	SER	engineered mutation	UNP P0C0V0
E	210	ALA	SER	engineered mutation	UNP P0C0V0
F	210	ALA	SER	engineered mutation	UNP P0C0V0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	210	ALA	SER	engineered mutation	UNP P0C0V0
H	210	ALA	SER	engineered mutation	UNP P0C0V0
I	210	ALA	SER	engineered mutation	UNP P0C0V0
J	210	ALA	SER	engineered mutation	UNP P0C0V0
K	210	ALA	SER	engineered mutation	UNP P0C0V0
L	210	ALA	SER	engineered mutation	UNP P0C0V0


- Molecule 2 is a protein called OUTER MEMBRANE PROTEIN C.

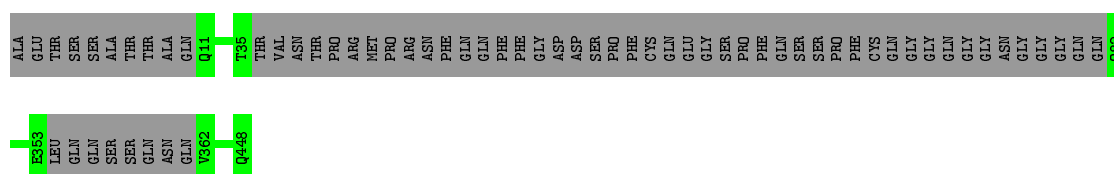
Mol	Chain	Residues	Atoms	AltConf	Trace
2	M	346	Total C 346 346	0	346

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain A: 




- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain B: 




- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain C: 




- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain D: 




- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain E:  86% 14%

ALA GLU THR SER SER ALA THR ALA ALA GLN Q11 T35 THR VAL ASN THR PRO ARG MET PRO ARG ASN PHE PHE GLN GLN PHE PHE GLY ASP ASP SER PRO PHE CYS GLN GLU GLY SER PRO PHE PHE GLN SER SER PRO PHE CYS GLN GLY GLN GLN GLY GLY GLN GLN GLN Q82

E353 LEU GLN GLN SER SER GLN ASN GLN V362 Q448

- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain F:  86% 14%

ALA GLU THR SER SER ALA THR ALA ALA GLN Q11 T35 THR VAL ASN THR PRO ARG MET PRO ARG ASN PHE PHE GLN GLN PHE PHE GLY ASP ASP SER PRO PHE CYS GLN GLU GLY SER PRO PHE PHE GLN SER SER PRO PHE CYS GLN GLY GLN GLN GLY GLY GLN GLN GLN Q82

E353 LEU GLN GLN SER SER GLN ASN GLN V362 Q448


- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain G:  86% 14%

ALA GLU THR SER SER ALA THR ALA ALA GLN Q11 T35 THR VAL ASN THR PRO ARG MET PRO ARG ASN PHE PHE GLN GLN PHE PHE GLY ASP ASP SER PRO PHE CYS GLN GLU GLY SER PRO PHE PHE GLN SER SER PRO PHE CYS GLN GLY GLN GLN GLY GLY GLN GLN GLN Q82

E353 LEU GLN GLN SER SER GLN ASN GLN V362 Q448


- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

Chain H:  86% 14%

ALA GLU THR SER SER ALA THR ALA ALA GLN Q11 T35 THR VAL ASN THR PRO ARG MET PRO ARG ASN PHE PHE GLN GLN PHE PHE GLY ASP ASP SER PRO PHE CYS GLN GLU GLY SER PRO PHE PHE GLN SER SER PRO PHE CYS GLN GLY GLN GLN GLY GLY GLN GLN GLN Q82

E353 LEU GLN GLN SER SER GLN ASN GLN V362 Q448

- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

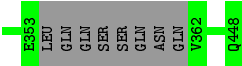
Chain I:  86% 14%

ALA GLU THR SER SER ALA THR ALA ALA GLN Q11 T35 THR VAL ASN THR PRO ARG MET PRO ARG ASN PHE PHE GLN GLN PHE PHE GLY ASP ASP SER PRO PHE CYS GLN GLU GLY SER PRO PHE PHE GLN SER SER PRO PHE CYS GLN GLY GLN GLN GLY GLY GLN GLN GLN Q82

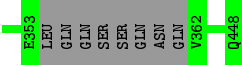
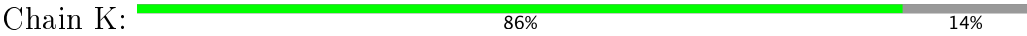
E353 LEU GLN GLN SER SER GLN ASN GLN V362 Q448

- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP

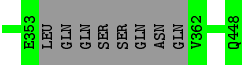
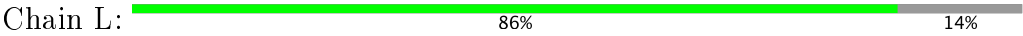
Chain J:  86% 14%



- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP



- Molecule 1: PERIPLASMIC SERINE ENDOPROTEASE DEGP



- Molecule 2: OUTER MEMBRANE PROTEIN C



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	6285	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	68100	Depositor
Image detector	GENERIC CCD	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).

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.

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	A	384	0	0	0	0
1	B	384	0	0	0	0
1	C	384	0	0	0	0
1	D	384	0	0	0	0
1	E	384	0	0	0	0
1	F	384	0	0	0	0
1	G	384	0	0	0	0
1	H	384	0	0	0	0
1	I	384	0	0	0	0
1	J	384	0	0	0	0
1	K	384	0	0	0	0
1	L	384	0	0	0	0
2	M	346	0	0	0	0
All	All	4954	0	0	0	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.

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](#)

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

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.