



## wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 10:09 AM EST

PDB ID : 6ODJ  
EMDB ID : EMD-20021  
Title : PolyAla Model of the PRC from the Type 4 Secretion System of *H. pylori*  
Authors : Chung, J.M.; Sheedlo, M.J.; Campbell, A.; Sawhney, N.; Frick-Cheng, A.E.;  
Lacy, D.B.; Cover, T.L.; Ohi, M.D.  
Deposited on : 2019-03-26  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
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) : 2.41.4

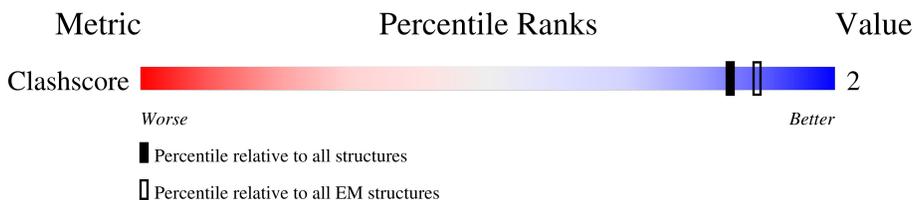
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

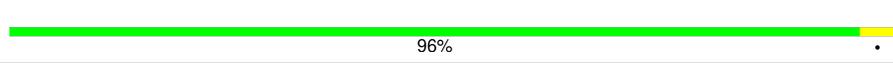
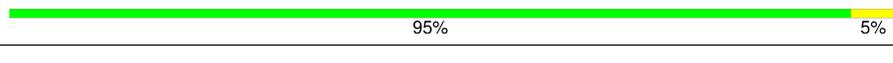
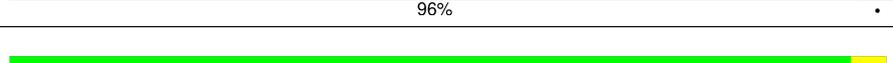
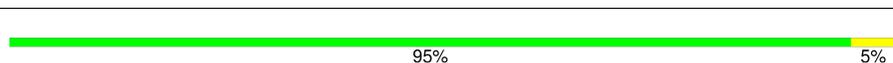
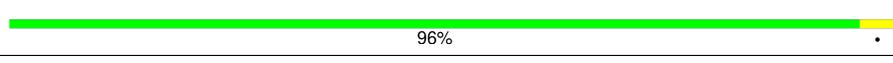
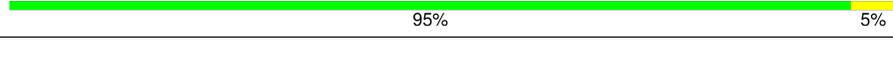
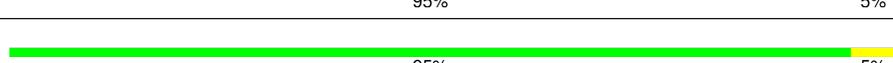
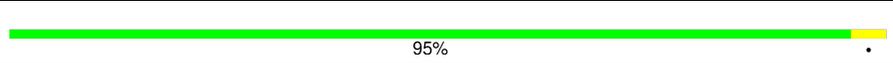
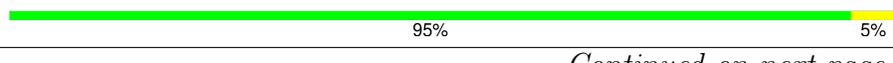
The reported resolution of this entry is 3.50 Å.

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.



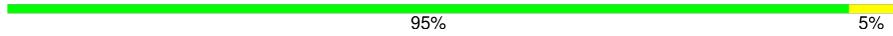
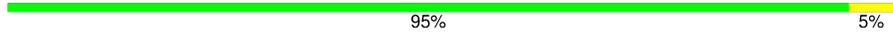
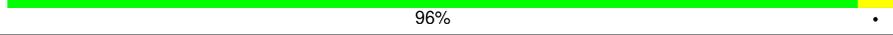
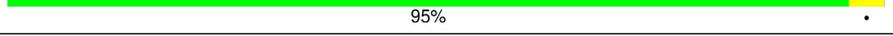
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	300	 96% .
1	B	300	 95% 5%
1	C	300	 96% .
1	D	300	 95% .
1	E	300	 95% 5%
1	F	300	 96% .
1	G	300	 95% 5%
1	H	300	 95% 5%
1	I	300	 95% 5%
1	J	300	 95% .
1	K	300	 95% 5%

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Mol	Chain	Length	Quality of chain
1	L	300	 95% 5%
1	M	300	 95% 5%
1	N	300	 95% 5%
1	O	300	 95% 5%
1	P	300	 96% .
1	Q	300	 95% .

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 25415 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.

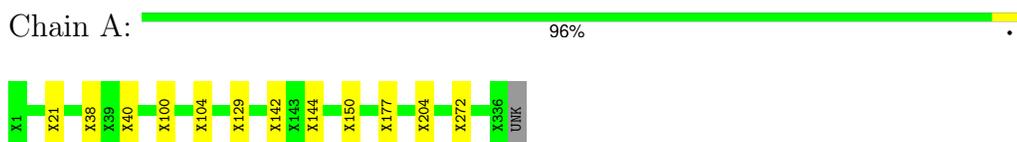
- Molecule 1 is a protein called PolyAla Model of PRC from H.pylori.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	299	1495	897	299	299	0	0
1	B	299	1495	897	299	299	0	0
1	C	299	1495	897	299	299	0	0
1	D	299	1495	897	299	299	0	0
1	E	299	1495	897	299	299	0	0
1	F	299	1495	897	299	299	0	0
1	G	299	1495	897	299	299	0	0
1	H	299	1495	897	299	299	0	0
1	I	299	1495	897	299	299	0	0
1	J	299	1495	897	299	299	0	0
1	K	299	1495	897	299	299	0	0
1	L	299	1495	897	299	299	0	0
1	M	299	1495	897	299	299	0	0
1	N	299	1495	897	299	299	0	0
1	O	299	1495	897	299	299	0	0
1	P	299	1495	897	299	299	0	0
1	Q	299	1495	897	299	299	0	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.

- Molecule 1: PolyAla Model of PRC from H.pylori





- Molecule 1: PolyAla Model of PRC from H.pylori

Chain G: 95% 5%



- Molecule 1: PolyAla Model of PRC from H.pylori

Chain H: 95% 5%





- Molecule 1: PolyAla Model of PRC from H.pylori

Chain N: 95% 5%



- Molecule 1: PolyAla Model of PRC from H.pylori

Chain O: 95% 5%



- Molecule 1: PolyAla Model of PRC from H.pylori

Chain P: 96% 4%



- Molecule 1: PolyAla Model of PRC from H.pylori

Chain Q: 95% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C17	Depositor
Number of particles used	20929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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.

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	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
1	G	0	6
1	H	0	6
1	I	0	6
1	J	0	6
1	K	0	6
1	L	0	6
1	M	0	6
1	N	0	6
1	O	0	6
1	P	0	6
1	Q	0	6
All	All	0	102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 102 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	A	177	UNK	Peptide
1	A	204	UNK	Peptide
1	A	38	UNK	Peptide
1	A	40	UNK	Peptide

## 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	1495	0	329	3	0
1	B	1495	0	329	4	0
1	C	1495	0	329	3	0
1	D	1495	0	329	4	0
1	E	1495	0	329	5	0
1	F	1495	0	329	3	0
1	G	1495	0	329	4	0
1	H	1495	0	329	5	0
1	I	1495	0	329	5	0
1	J	1495	0	329	4	0
1	K	1495	0	329	4	0
1	L	1495	0	329	4	0
1	M	1495	0	329	4	0
1	N	1495	0	329	4	0
1	O	1495	0	329	4	0
1	P	1495	0	329	3	0
1	Q	1495	0	329	4	0
All	All	25415	0	5593	64	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 2.

The worst 5 of 64 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:M:100:UNK:O	1:M:104:UNK:N	2.44	0.51
1:G:100:UNK:O	1:G:104:UNK:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:UNK:O	1:H:104:UNK:N	2.44	0.51
1:N:100:UNK:O	1:N:104:UNK:N	2.44	0.51
1:I:100:UNK:O	1:I:104:UNK:N	2.44	0.51

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 oligosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2
1	C	2
1	D	2
1	E	2
1	F	2
1	G	2
1	H	2
1	I	2
1	J	2
1	K	2
1	L	2
1	M	2
1	N	2
1	O	2
1	P	2
1	Q	2

The worst 5 of 34 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	67:UNK	C	100:UNK	N	92.23
1	B	67:UNK	C	100:UNK	N	92.23
1	C	67:UNK	C	100:UNK	N	92.23
1	D	67:UNK	C	100:UNK	N	92.23
1	E	67:UNK	C	100:UNK	N	92.23

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20021. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.