wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:45 PM BST

PDB ID	:	3J1V
EMDB ID:	:	EMD-1875
Title	:	A refined model of the prototypical Salmonella typhimurium T3SS basal body reveals the molecular basis for its assembly
Authors	:	Sgourakis, N.G.; Bergeron, J.R.C.; Strynadka, N.J.C.; Baker, D.
Deposited on	:	2012-07-08
Resolution	:	unknown (reported)

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

For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
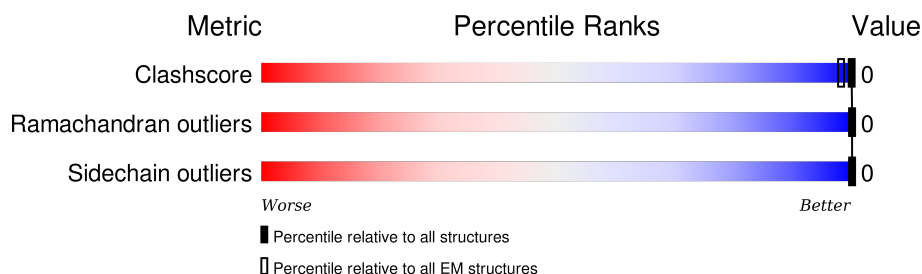http://wwpdb.org/validation/2016/EMValidationReportHelp

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 unknown.

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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		0
Sidechain outliers		0
	Worse *Better*	

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	157	89% 11%
1	B	157	89% 11%
1	C	157	89% 11%
1	D	157	89% 11%
1	E	157	89% 11%
1	F	157	89% 11%
1	G	157	89% 11%
1	H	157	89% 11%
1	I	157	89% 11%

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Mol	Chain	Length	Quality of chain
1	J	157	89% 11%
1	K	157	89% 11%
1	L	157	89% 11%
1	M	157	89% 11%
1	N	157	89% 11%
1	O	157	89% 11%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 16650 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 Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	B	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	C	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	D	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	E	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	F	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	G	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	H	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	I	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	J	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	K	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	L	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	M	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	N	139	Total 1110	C 711	N 189	O 204	S 6	0	0
1	O	139	Total 1110	C 711	N 189	O 204	S 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
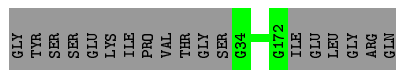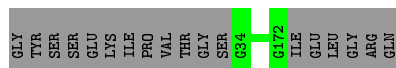
• Molecule 1: Protein InvG

Chain A:
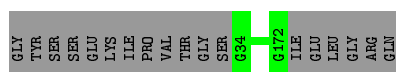
• Molecule 1: Protein InvG

Chain B:

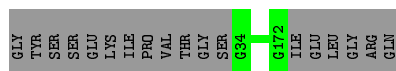• Molecule 1: Protein InvG

Chain C:

• Molecule 1: Protein InvG

Chain D:

• Molecule 1: Protein InvG

Chain E:
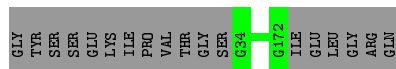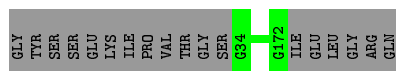

• Molecule 1: Protein InvG

Chain F:

• Molecule 1: Protein InvG

Chain G: 89% 11%

GLY TYR SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain H: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain I: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain J: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain K: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain L: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain M: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain N: 89% 11%

GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

• Molecule 1: Protein InvG

Chain O:

89%11%
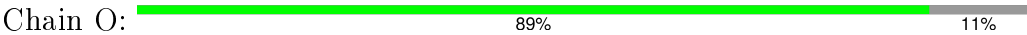
GLY TYR SER SER GLU LYS ILE PRO VAL THR GLY SER G34 G172 ILE GLU LEU GLY ARG GLN

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	0.83	0/1133	0.72	0/1528
1	B	0.83	0/1133	0.72	0/1528
1	C	0.83	0/1133	0.72	0/1528
1	D	0.83	0/1133	0.72	0/1528
1	E	0.83	0/1133	0.72	0/1528
1	F	0.83	0/1133	0.72	0/1528
1	G	0.83	0/1133	0.72	0/1528
1	H	0.83	0/1133	0.72	0/1528
1	I	0.83	0/1133	0.72	0/1528
1	J	0.83	0/1133	0.72	0/1528
1	K	0.83	0/1133	0.72	0/1528
1	L	0.83	0/1133	0.72	0/1528
1	M	0.83	0/1133	0.72	0/1528
1	N	0.83	0/1133	0.72	0/1528
1	O	0.83	0/1133	0.72	0/1528
All	All	0.83	0/16995	0.72	0/22920

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 ⓘ

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	1110	0	1102	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1110	0	1102	0	0
1	C	1110	0	1102	0	0
1	D	1110	0	1102	0	0
1	E	1110	0	1102	0	0
1	F	1110	0	1102	0	0
1	G	1110	0	1102	0	0
1	H	1110	0	1102	0	0
1	I	1110	0	1102	0	0
1	J	1110	0	1102	0	0
1	K	1110	0	1102	0	0
1	L	1110	0	1102	0	0
1	M	1110	0	1102	0	0
1	N	1110	0	1102	0	0
1	O	1110	0	1102	0	0
All	All	16650	0	16530	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)

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	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	B	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	C	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	D	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	E	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	F	137/157 (87%)	135 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	H	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	I	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	J	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	K	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	L	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	M	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	N	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
1	O	137/157 (87%)	135 (98%)	2 (2%)	0	100	100
All	All	2055/2355 (87%)	2025 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	119/134 (89%)	119 (100%)	0	100	100
1	B	119/134 (89%)	119 (100%)	0	100	100
1	C	119/134 (89%)	119 (100%)	0	100	100
1	D	119/134 (89%)	119 (100%)	0	100	100
1	E	119/134 (89%)	119 (100%)	0	100	100
1	F	119/134 (89%)	119 (100%)	0	100	100
1	G	119/134 (89%)	119 (100%)	0	100	100
1	H	119/134 (89%)	119 (100%)	0	100	100
1	I	119/134 (89%)	119 (100%)	0	100	100
1	J	119/134 (89%)	119 (100%)	0	100	100
1	K	119/134 (89%)	119 (100%)	0	100	100
1	L	119/134 (89%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	119/134 (89%)	119 (100%)	0	100	100
1	N	119/134 (89%)	119 (100%)	0	100	100
1	O	119/134 (89%)	119 (100%)	0	100	100
All	All	1785/2010 (89%)	1785 (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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.