



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:37 PM BST

PDB ID : 3A69
EMDB ID: : EMD-1647
Title : Atomic model of the bacterial flagellar hook based on docking an X-ray derived structure and terminal two alpha-helices into an 7.1 angstrom resolution cryoEM map
Authors : Fujii, T.; Kato, T.; Namba, K.
Deposited on : 2009-08-26
Resolution : 7.10 Å(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>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

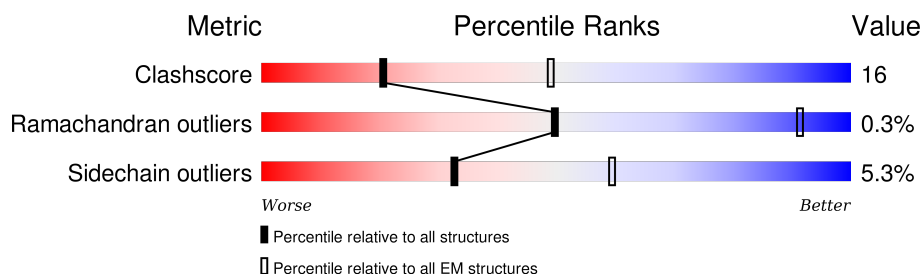
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.10 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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	402	 70% 14% • 14%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2573 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 Flagellar hook protein flgE.

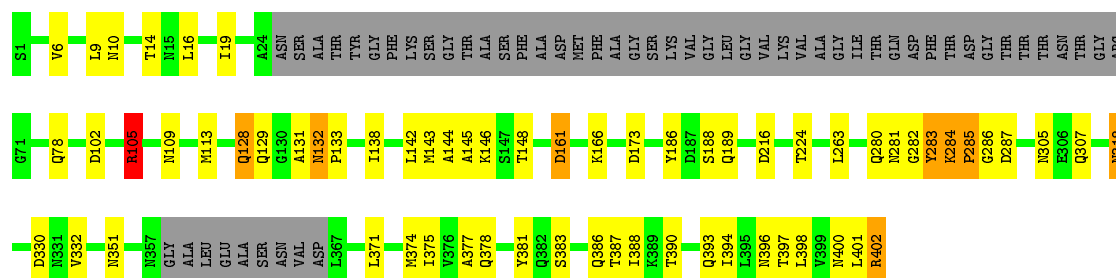
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	347	Total	C	N	O	S	0	0
			2573	1584	446	536	7		

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 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: Flagellar hook protein flgE

Chain A: 



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	each images	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	50000	Depositor
Image detector	16 megapixels slow-scan CCD camera, TemCam-F415MP	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.59	0/2610	0.79	8/3557 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	105	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	330	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	161	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	102	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	173	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	216	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	144	ALA	N-CA-CB	5.12	117.27	110.10

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	2573	0	2487	80	0
All	All	2573	0	2487	80	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 16.

All (80) 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:A:19:ILE:HG21	1:A:374:MET:SD	1.66	1.34
1:A:19:ILE:CG2	1:A:374:MET:SD	2.21	1.29
1:A:19:ILE:CB	1:A:374:MET:SD	2.34	1.15
1:A:398:LEU:HA	1:A:401:LEU:HD12	1.24	1.13
1:A:6:VAL:O	1:A:9:LEU:HG	1.48	1.11
1:A:16:LEU:HD21	1:A:377:ALA:HB3	1.28	1.08
1:A:19:ILE:HB	1:A:374:MET:SD	1.94	1.05
1:A:401:LEU:O	1:A:402:ARG:HD2	1.61	0.98
1:A:19:ILE:CD1	1:A:374:MET:SD	2.53	0.97
1:A:16:LEU:HD21	1:A:377:ALA:CB	1.98	0.93
1:A:283:TYR:CE2	1:A:307:GLN:HG3	2.10	0.86
1:A:142:LEU:HG	1:A:143:MET:H	1.41	0.84
1:A:143:MET:HB2	1:A:285:PRO:HB3	1.62	0.81
1:A:6:VAL:HA	1:A:9:LEU:CD2	2.11	0.80
1:A:16:LEU:CD2	1:A:377:ALA:HB3	2.10	0.80
1:A:397:THR:O	1:A:401:LEU:HG	1.82	0.78
1:A:19:ILE:HD13	1:A:374:MET:SD	2.22	0.78
1:A:283:TYR:CD2	1:A:307:GLN:HG3	2.19	0.78
1:A:9:LEU:HD12	1:A:10:ASN:N	1.99	0.77
1:A:19:ILE:HG21	1:A:374:MET:CG	2.16	0.76
1:A:401:LEU:O	1:A:402:ARG:CD	2.33	0.75
1:A:128:GLN:H	1:A:128:GLN:HE21	1.35	0.75
1:A:283:TYR:O	1:A:283:TYR:HD1	1.68	0.74
1:A:19:ILE:HD12	1:A:374:MET:SD	2.29	0.72
1:A:105:ARG:HD3	1:A:138:ILE:O	1.91	0.70
1:A:401:LEU:O	1:A:402:ARG:CB	2.41	0.69
1:A:9:LEU:CD1	1:A:10:ASN:OD1	2.40	0.69
1:A:386:GLN:O	1:A:390:THR:HG23	1.92	0.69
1:A:401:LEU:O	1:A:402:ARG:HB2	1.95	0.66
1:A:6:VAL:O	1:A:9:LEU:CG	2.37	0.65
1:A:398:LEU:HA	1:A:401:LEU:CD1	2.15	0.65
1:A:318:ASN:OD1	1:A:351:ASN:ND2	2.30	0.64
1:A:143:MET:CE	1:A:305:ASN:HD21	2.11	0.63
1:A:145:ALA:HA	1:A:285:PRO:CD	2.28	0.63
1:A:9:LEU:HD11	1:A:10:ASN:OD1	1.98	0.62
1:A:9:LEU:HD23	1:A:388:ILE:HD11	1.82	0.61
1:A:19:ILE:HB	1:A:374:MET:CE	2.31	0.61
1:A:6:VAL:HA	1:A:9:LEU:HD21	1.84	0.59
1:A:19:ILE:CG1	1:A:374:MET:SD	2.90	0.59
1:A:9:LEU:HB2	1:A:381:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TYR:HE2	1:A:307:GLN:HG3	1.65	0.58
1:A:9:LEU:HD23	1:A:388:ILE:CD1	2.34	0.57
1:A:393:GLN:O	1:A:397:THR:HG23	2.04	0.56
1:A:9:LEU:HD12	1:A:10:ASN:OD1	2.05	0.55
1:A:283:TYR:CD1	1:A:283:TYR:C	2.81	0.54
1:A:6:VAL:HA	1:A:9:LEU:HD23	1.90	0.54
1:A:142:LEU:HG	1:A:143:MET:N	2.17	0.53
1:A:186:TYR:CE2	1:A:284:LYS:HE3	2.44	0.53
1:A:401:LEU:O	1:A:402:ARG:CG	2.56	0.53
1:A:283:TYR:HD1	1:A:283:TYR:C	2.12	0.51
1:A:6:VAL:C	1:A:9:LEU:HG	2.26	0.51
1:A:132:ASN:HD22	1:A:133:PRO:HD2	1.75	0.51
1:A:128:GLN:CG	1:A:131:ALA:HB2	2.40	0.51
1:A:145:ALA:HA	1:A:285:PRO:HD3	1.92	0.50
1:A:10:ASN:O	1:A:14:THR:HG23	2.12	0.50
1:A:128:GLN:HG2	1:A:128:GLN:O	2.12	0.50
1:A:145:ALA:HA	1:A:285:PRO:HD2	1.94	0.49
1:A:383:SER:O	1:A:387:THR:HG23	2.12	0.48
1:A:186:TYR:HE2	1:A:284:LYS:HE3	1.78	0.48
1:A:132:ASN:HD22	1:A:133:PRO:CD	2.26	0.47
1:A:113:MET:HE1	1:A:332:VAL:HG21	1.96	0.47
1:A:109:ASN:HD21	1:A:113:MET:CE	2.26	0.47
1:A:9:LEU:HD12	1:A:9:LEU:C	2.35	0.47
1:A:286:GLY:O	1:A:287:ASP:OD2	2.33	0.46
1:A:16:LEU:O	1:A:374:MET:HE1	2.15	0.46
1:A:148:THR:OG1	1:A:282:GLY:HA3	2.16	0.45
1:A:16:LEU:CD2	1:A:377:ALA:CB	2.81	0.45
1:A:19:ILE:HB	1:A:374:MET:HE1	1.99	0.45
1:A:396:ASN:O	1:A:400:ASN:ND2	2.49	0.45
1:A:280:GLN:N	1:A:280:GLN:OE1	2.50	0.45
1:A:143:MET:HE2	1:A:305:ASN:HD21	1.83	0.45
1:A:128:GLN:NE2	1:A:128:GLN:H	2.11	0.44
1:A:284:LYS:O	1:A:284:LYS:HG3	2.18	0.44
1:A:374:MET:O	1:A:378:GLN:HG3	2.18	0.44
1:A:394:ILE:O	1:A:398:LEU:HG	2.18	0.44
1:A:283:TYR:O	1:A:283:TYR:CD1	2.58	0.44
1:A:143:MET:O	1:A:285:PRO:HG2	2.20	0.42
1:A:371:LEU:O	1:A:375:ILE:HG13	2.20	0.41
1:A:283:TYR:HD2	1:A:307:GLN:HG3	1.82	0.41
1:A:146:LYS:HD3	1:A:281:ASN:O	2.21	0.40

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	341/402 (85%)	336 (98%)	4 (1%)	1 (0%)	46 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	PRO

5.3.2 Protein sidechains [i](#)

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	283/322 (88%)	268 (95%)	15 (5%)	28 64

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	105	ARG
1	A	128	GLN
1	A	129	GLN
1	A	132	ASN
1	A	161	ASP
1	A	166	LYS
1	A	188	SER
1	A	189	GLN
1	A	224	THR

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Mol	Chain	Res	Type
1	A	263	LEU
1	A	283	TYR
1	A	284	LYS
1	A	318	ASN
1	A	402	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	88	ASN
1	A	98	GLN
1	A	109	ASN
1	A	111	GLN
1	A	128	GLN
1	A	132	ASN
1	A	196	ASN
1	A	244	ASN
1	A	305	ASN
1	A	318	ASN
1	A	322	ASN
1	A	351	ASN
1	A	400	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.