Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Aug 7, 2019 – 04:58 PM EDT

PDB ID	:	6RBK
EMDB ID:	:	EMD-4800
Title	:	Cryo-EM structure of the anti-feeding prophage (AFP) baseplate in extended state, 3-fold symmetrised
Authors	:	Desfosses, A.
Deposited on	:	2019-04-10
Resolution	:	3.40 Å(reported)

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

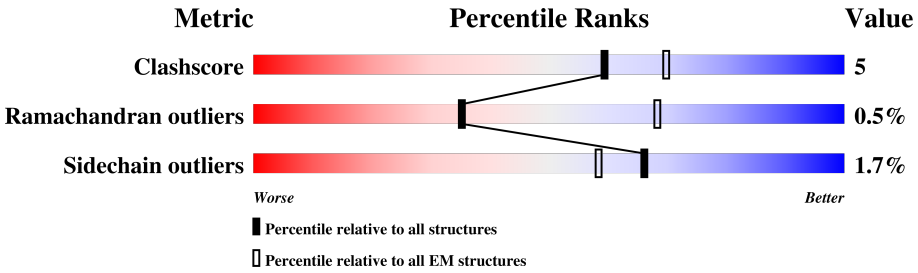
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 3.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	229	83% 14% •
1	B	229	81% 15% ••
2	C	529	79% 15% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7378 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 Afp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1728	1090	290	342	6		
1	B	224	Total	C	N	O	S	0	0
			1737	1096	292	343	6		

- Molecule 2 is a protein called Afp8.

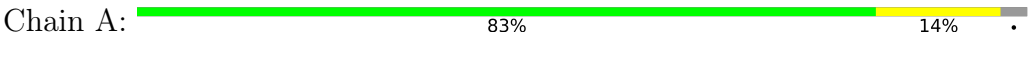
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	504	Total	C	N	O	S	0	0
			3913	2468	696	736	13		

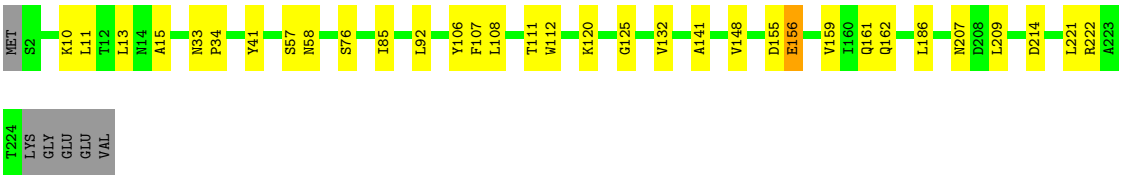
3 Residue-property plots (i)

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: Afp7

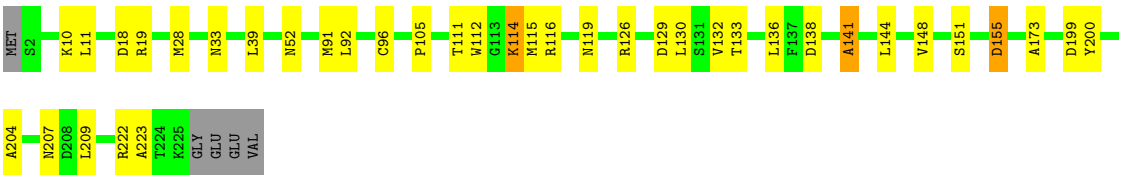
Chain A:





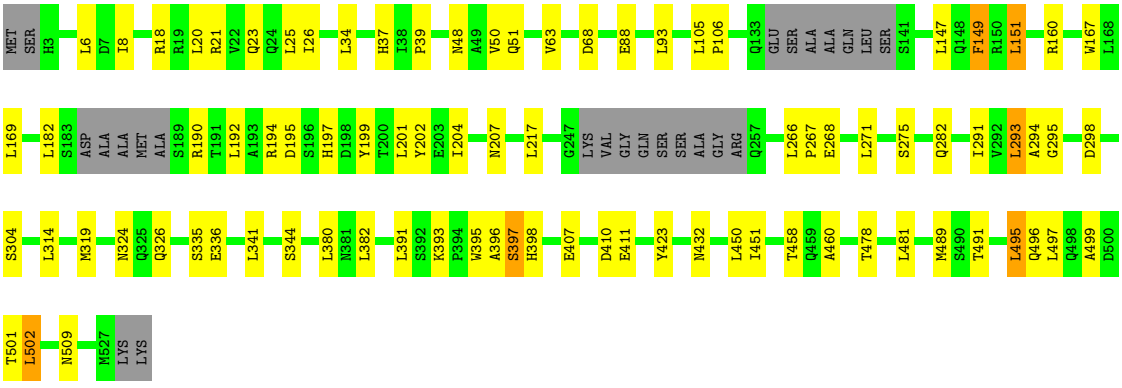
- Molecule 1: Afp7

Chain B:



- Molecule 2: Afp8

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	46991	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 ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	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	0.40	0/1761	0.72	1/2399 (0.0%)
1	B	0.40	0/1770	0.75	4/2410 (0.2%)
2	C	0.39	0/3995	0.74	10/5427 (0.2%)
All	All	0.40	0/7526	0.74	15/10236 (0.1%)

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	2
1	B	0	1
2	C	0	1
All	All	0	4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	144	LEU	CA-CB-CG	8.25	134.27	115.30
2	C	169	LEU	CA-CB-CG	7.45	132.43	115.30
1	A	11	LEU	CA-CB-CG	6.62	130.53	115.30
2	C	6	LEU	CA-CB-CG	6.57	130.41	115.30
2	C	314	LEU	CA-CB-CG	6.54	130.35	115.30
2	C	481	LEU	CA-CB-CG	6.33	129.87	115.30
1	B	199	ASP	CB-CG-OD1	6.32	123.98	118.30
2	C	397	SER	N-CA-CB	6.16	119.74	110.50
2	C	502	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	11	LEU	CA-CB-CG	6.01	129.13	115.30
2	C	495	LEU	CA-CB-CG	5.84	128.73	115.30
2	C	293	LEU	CA-CB-CG	5.82	128.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	105	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	39	LEU	CA-CB-CG	5.53	128.01	115.30
2	C	68	ASP	CB-CG-OD1	5.28	123.05	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	A	141	ALA	Peptide
1	B	141	ALA	Peptide
2	C	395	TRP	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	1728	0	1707	19	0
1	B	1737	0	1720	19	0
2	C	3913	0	3896	43	0
All	All	7378	0	7323	77	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 5.

All (77) 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)
2:C:106:PRO:HA	2:C:151:LEU:O	1.87	0.73
2:C:496:GLN:C	2:C:497:LEU:HD12	2.10	0.71
1:B:129:ASP:HB3	1:B:151:SER:HB3	1.76	0.66
1:A:207:ASN:HD21	1:A:222:ARG:H	1.42	0.65
1:A:10:LYS:HA	1:A:33:ASN:HD21	1.62	0.64
2:C:199:TYR:HB3	2:C:293:LEU:HD11	1.81	0.62
2:C:266:LEU:H	2:C:423:TYR:HE2	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:OD1	1:B:155:ASP:OD2	2.16	0.61
2:C:34:LEU:HB2	2:C:93:LEU:HB2	1.82	0.61
2:C:499:ALA:HB3	2:C:502:LEU:HB3	1.83	0.61
2:C:202:TYR:HE2	2:C:294:ALA:HB2	1.65	0.60
2:C:491:THR:HG22	2:C:495:LEU:HD23	1.84	0.60
1:A:125:GLY:HA2	1:A:155:ASP:HB2	1.82	0.60
2:C:282:GLN:NE2	2:C:344:SER:OG	2.35	0.60
2:C:190:ARG:NH2	2:C:298:ASP:O	2.34	0.59
2:C:326:GLN:NE2	2:C:336:GLU:OE1	2.36	0.58
1:B:132:VAL:HG12	1:B:148:VAL:HG22	1.85	0.58
2:C:496:GLN:O	2:C:497:LEU:HD12	2.02	0.58
2:C:495:LEU:HD13	2:C:497:LEU:HD11	1.86	0.57
1:B:52:ASN:HB2	2:C:194:ARG:O	2.06	0.56
2:C:411:GLU:OE1	2:C:432:ASN:ND2	2.36	0.56
1:A:132:VAL:HG12	1:A:148:VAL:HG22	1.89	0.55
1:A:156:GLU:OE2	1:A:156:GLU:HA	2.06	0.55
2:C:478:THR:O	2:C:489:MET:O	2.24	0.55
2:C:204:ILE:HG23	2:C:291:ILE:HG12	1.89	0.54
2:C:491:THR:CG2	2:C:495:LEU:HD23	2.37	0.54
2:C:304:SER:HA	2:C:319:MET:HA	1.87	0.54
2:C:23:GLN:HA	2:C:324:ASN:HD22	1.73	0.54
1:A:15:ALA:HB1	1:A:106:TYR:HB3	1.89	0.53
2:C:192:LEU:HD13	2:C:201:LEU:HD21	1.90	0.53
2:C:501:THR:OG1	2:C:501:THR:O	2.25	0.53
1:A:34:PRO:HD2	1:A:112:TRP:CH2	2.44	0.52
2:C:8:ILE:HG12	2:C:63:VAL:HG22	1.91	0.52
2:C:18:ARG:NH1	2:C:88:GLU:OE2	2.43	0.52
2:C:267:PRO:HD2	2:C:271:LEU:HD21	1.93	0.51
1:A:76:SER:HB3	1:A:85:ILE:HG23	1.93	0.50
1:A:57:SER:HB2	1:B:19:ARG:HH22	1.76	0.50
2:C:48:ASN:HA	2:C:51:GLN:HG2	1.94	0.50
1:A:92:LEU:HD13	1:A:148:VAL:HG11	1.93	0.50
1:A:186:LEU:HD13	1:A:221:LEU:HD21	1.94	0.49
2:C:167:TRP:CE3	2:C:182:LEU:HG	2.47	0.49
1:A:209:LEU:HB2	1:A:214:ASP:HB3	1.94	0.49
1:B:207:ASN:HD21	1:B:222:ARG:H	1.61	0.49
2:C:190:ARG:NH1	2:C:199:TYR:OH	2.45	0.49
1:A:156:GLU:HB3	1:A:161:GLN:HE21	1.77	0.49
1:B:10:LYS:HA	1:B:33:ASN:HD21	1.78	0.48
2:C:20:LEU:HD23	2:C:34:LEU:HD13	1.96	0.48
1:A:13:LEU:HD11	1:A:108:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:TRP:HE3	2:C:182:LEU:HG	1.79	0.47
2:C:39:PRO:HD2	2:C:50:VAL:HG21	1.96	0.47
1:A:120:LYS:HE3	1:A:156:GLU:OE1	2.15	0.46
2:C:18:ARG:HH11	2:C:37:HIS:HB2	1.80	0.46
1:B:28:MET:HB3	1:B:91:MET:HG2	1.98	0.45
2:C:451:ILE:HG23	2:C:458:THR:HG23	1.97	0.45
1:B:105:PRO:HB2	1:B:126:ARG:HD2	1.98	0.45
1:B:116:ARG:NH1	1:B:119:ASN:O	2.49	0.45
2:C:147:LEU:HD22	2:C:149:PHE:HD1	1.82	0.45
1:B:204:ALA:HA	1:B:209:LEU:HD13	1.98	0.44
2:C:407:GLU:N	2:C:410:ASP:OD2	2.50	0.44
2:C:151:LEU:HD12	2:C:151:LEU:HA	1.71	0.44
1:A:156:GLU:HB3	1:A:161:GLN:NE2	2.33	0.44
1:B:18:ASP:N	1:B:18:ASP:OD1	2.48	0.44
1:B:114:LYS:HA	1:B:114:LYS:HD2	1.68	0.43
2:C:160:ARG:NH2	2:C:268:GLU:OE2	2.50	0.43
1:A:41:TYR:HB2	1:B:130:LEU:HB3	2.01	0.43
2:C:380:LEU:HB3	2:C:382:LEU:HD23	2.02	0.42
1:B:173:ALA:HB3	1:B:223:ALA:HB3	2.02	0.42
1:B:138:ASP:H	1:B:141:ALA:HA	1.84	0.42
1:B:92:LEU:HD13	1:B:148:VAL:HG11	2.02	0.41
1:A:159:VAL:O	1:A:162:GLN:HB3	2.20	0.41
2:C:391:LEU:HD23	2:C:393:LYS:HE3	2.03	0.41
2:C:295:GLY:H	2:C:335:SER:H	1.69	0.41
1:B:96:CYS:HB2	1:B:130:LEU:HD22	2.03	0.41
1:B:112:TRP:HB3	1:B:115:MET:HB3	2.02	0.41
2:C:26:ILE:HG21	2:C:341:LEU:HD11	2.03	0.41
2:C:450:LEU:HG	2:C:460:ALA:HB1	2.02	0.40
2:C:217:LEU:O	2:C:275:SER:OG	2.34	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	221/229 (96%)	189 (86%)	32 (14%)	0	100 100
1	B	222/229 (97%)	186 (84%)	34 (15%)	2 (1%)	19 58
2	C	496/529 (94%)	418 (84%)	75 (15%)	3 (1%)	27 66
All	All	939/987 (95%)	793 (84%)	141 (15%)	5 (0%)	35 69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	396	ALA
2	C	397	SER
1	B	155	ASP
1	B	200	TYR
2	C	398	HIS

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	190/195 (97%)	188 (99%)	2 (1%)	76 89
1	B	191/195 (98%)	187 (98%)	4 (2%)	56 82
2	C	424/441 (96%)	416 (98%)	8 (2%)	60 83
All	All	805/831 (97%)	791 (98%)	14 (2%)	66 84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	156	GLU
1	B	111	THR
1	B	114	LYS
1	B	133	THR
1	B	136	LEU
2	C	21	ARG
2	C	25	LEU

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Mol	Chain	Res	Type
2	C	149	PHE
2	C	151	LEU
2	C	195	ASP
2	C	197	HIS
2	C	207	ASN
2	C	509	ASN

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	33	ASN
1	A	161	GLN
1	A	207	ASN
1	B	33	ASN
1	B	149	GLN
1	B	207	ASN
2	C	83	GLN
2	C	148	GLN
2	C	207	ASN
2	C	282	GLN
2	C	324	ASN
2	C	477	ASN
2	C	505	GLN
2	C	509	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

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.