



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 7, 2019 – 04:52 PM EDT

PDB ID : 6RAP
EMDB ID: : EMD-4784
Title : Cryo-EM structure of the anti-feeding prophage cap (AFP tube terminating cap)
Authors : Desfosses, A.
Deposited on : 2019-04-07
Resolution : 3.30 Å(reported)

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

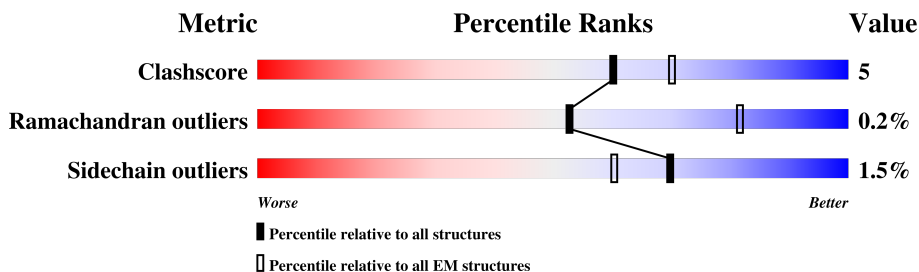
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	149	83% 16% .
1	B	149	89% 10% .
2	C	354	91% 7% ..
3	D	451	72% 7% 21%
4	E	295	73% 20% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9879 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 Afp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	148	Total	C	N	O	S	0	0
			1148	729	187	228	4		
1	A	149	Total	C	N	O	S	0	0
			1156	734	188	229	5		

- Molecule 2 is a protein called Afp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	349	Total	C	N	O	S	0	0
			2704	1732	447	519	6		

- Molecule 3 is a protein called Afp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	358	Total	C	N	O	S	0	0
			2747	1753	462	525	7		

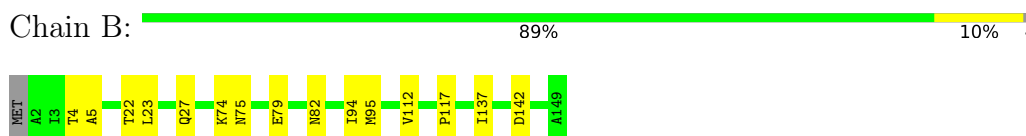
- Molecule 4 is a protein called Afp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	275	Total	C	N	O	S	0	0
			2124	1334	362	417	11		

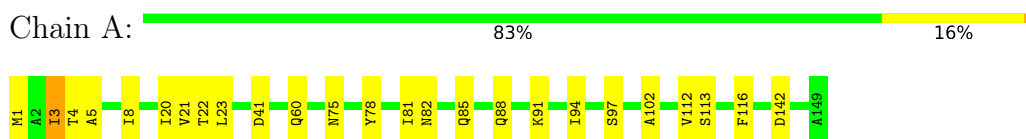
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

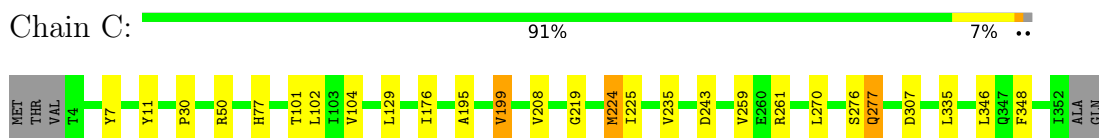
- Molecule 1: Afp1



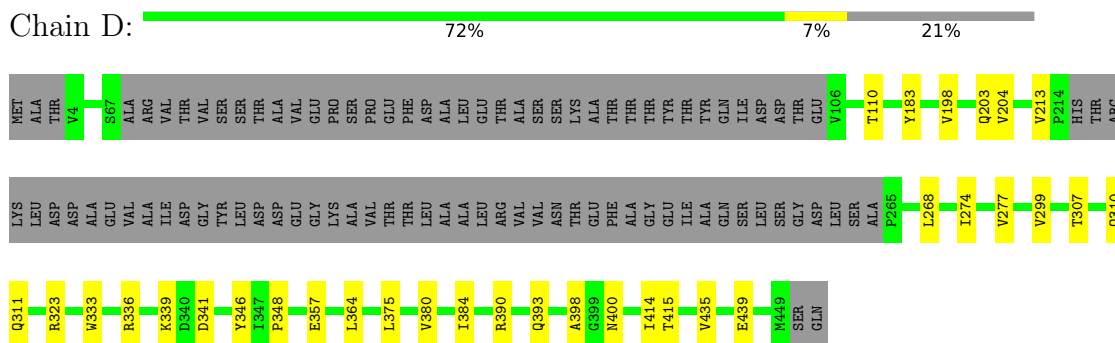
- Molecule 1: Afp1



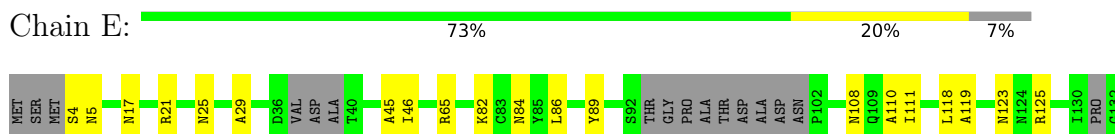
- Molecule 2: Afp2



- Molecule 3: Afp3



- Molecule 4: Afp16



A133	A134	T135	Q136	V137	L154	R157	V166	T167	L185	S196	V199	R205	E206	Q207	L208	R209	V210	A211	L212	GLY	GLY	ASP	TYR	D217	A218	C219	L220	A221	N222	V225	R226	L227	I242	V248	M251	N261	F264	R265	E266	N267	E268	K269	S270	V275	T276	Y280	R281	V282	N285	A286	V287	D288	K289	L292	T293	C294	I295
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	23797	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 ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.46	0/1180	0.66	0/1611
1	B	0.34	0/1172	0.60	1/1601 (0.1%)
2	C	0.46	0/2775	0.66	1/3793 (0.0%)
3	D	0.32	0/2809	0.56	0/3833
4	E	0.38	0/2162	0.72	3/2948 (0.1%)
All	All	0.39	0/10098	0.64	5/13786 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	E	227	LEU	CA-CB-CG	8.22	134.20	115.30
2	C	270	LEU	CA-CB-CG	6.29	129.76	115.30
4	E	86	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	23	LEU	CA-CB-CG	5.19	127.23	115.30
4	E	220	LEU	CA-CB-CG	5.13	127.10	115.30

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	1156	0	1135	18	0
1	B	1148	0	1123	6	0
2	C	2704	0	2617	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2747	0	2721	21	0
4	E	2124	0	2095	46	0
All	All	9879	0	9691	99	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.

The worst 5 of 99 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)
4:E:266:GLU:O	4:E:270:SER:OG	1.68	1.12
4:E:261:ASN:OD1	4:E:289:LYS:CE	2.11	0.98
4:E:261:ASN:OD1	4:E:289:LYS:HE3	1.65	0.94
4:E:207:GLN:HG2	4:E:275:VAL:HB	1.55	0.86
4:E:276:THR:OG1	4:E:281:ARG:N	2.13	0.81

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	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
1	B	146/149 (98%)	136 (93%)	8 (6%)	2 (1%)	12	43
2	C	347/354 (98%)	308 (89%)	39 (11%)	0	100	100
3	D	352/451 (78%)	328 (93%)	24 (7%)	0	100	100
4	E	267/295 (90%)	225 (84%)	42 (16%)	0	100	100
All	All	1259/1398 (90%)	1134 (90%)	123 (10%)	2 (0%)	53	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	ALA
1	B	4	THR

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	128/128 (100%)	122 (95%)	6 (5%)	29	62
1	B	127/128 (99%)	125 (98%)	2 (2%)	65	83
2	C	283/287 (99%)	279 (99%)	4 (1%)	69	85
3	D	293/368 (80%)	292 (100%)	1 (0%)	93	97
4	E	235/249 (94%)	232 (99%)	3 (1%)	71	85
All	All	1066/1160 (92%)	1050 (98%)	16 (2%)	70	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
2	C	50	ARG
3	D	400	ASN
1	A	75	ASN
4	E	17	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	325	ASN
3	D	310	GLN
4	E	116	GLN
2	C	277	GLN
4	E	54	HIS

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.