



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 21, 2016 – 10:06 PM EST

PDB ID : 5KUA
EMDB ID: : EMD-8287
Title : Cryo-EM reconstruction of Neisseria meningitidis Type IV pilus
Authors : Kolappan, S.; Coureuil, M.; Yu, X.; Nassif, X.; Craig, L.; Egelman, E.H.
Deposited on : 2016-07-13
Resolution : 6.00 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

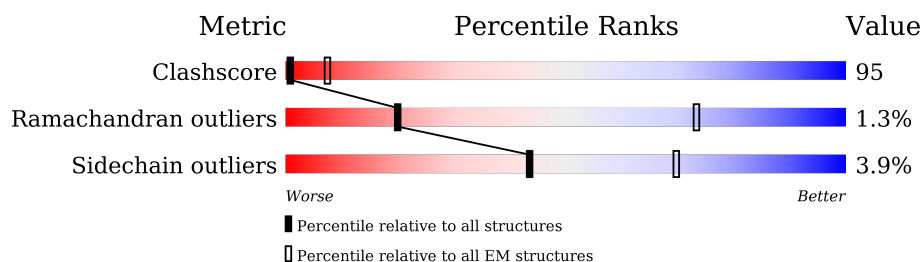
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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.



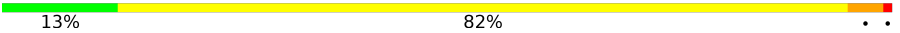
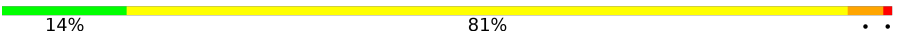
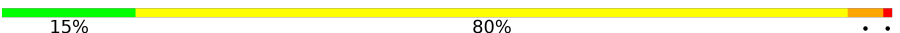


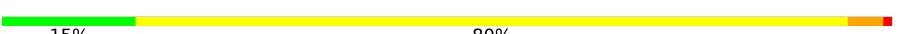
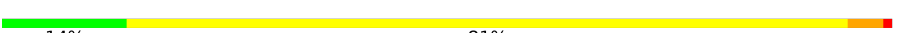




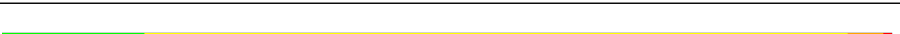





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	161	18% 77% . .
1	B	161	19% 76% . .
1	C	161	18% 78% . .
1	D	161	16% 80% . .
1	E	161	14% 81% . .
1	F	161	15% 80% . .
1	G	161	14% 81% . .
1	H	161	16% 80% . .
1	I	161	14% 81% . .

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Mol	Chain	Length	Quality of chain
1	J	161	 13%82%..
1	K	161	 14%81%..
1	L	161	 15%80%..
1	M	161	 14%81%..
1	N	161	 14%81%..
1	O	161	 15%80%..
1	P	161	 14%81%..
1	Q	161	 15%80%..
1	R	161	 14%81%..
1	S	161	 16%80%..
1	T	161	 14%81%..
1	U	161	 16%79%..
1	V	161	 14%81%..
1	W	161	 17%79%..
1	X	161	 16%79%..
1	Y	161	 17%78%..
1	Z	161	 17%79%..

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 31148 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 pilin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	B	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	C	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	D	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	E	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	F	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	G	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	H	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	I	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	J	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	K	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	L	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	M	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	N	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	O	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	P	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		
1	Q	161	Total	C	N	O	S	0	0
			1198	747	207	240	4		

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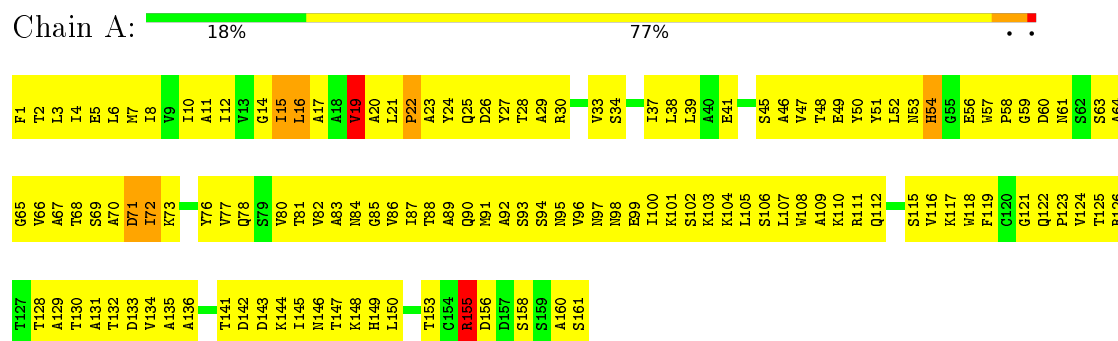
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	S	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	T	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	U	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	V	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	W	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	X	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	Y	161	Total 1198	C 747	N 207	O 240	S 4	0	0
1	Z	161	Total 1198	C 747	N 207	O 240	S 4	0	0

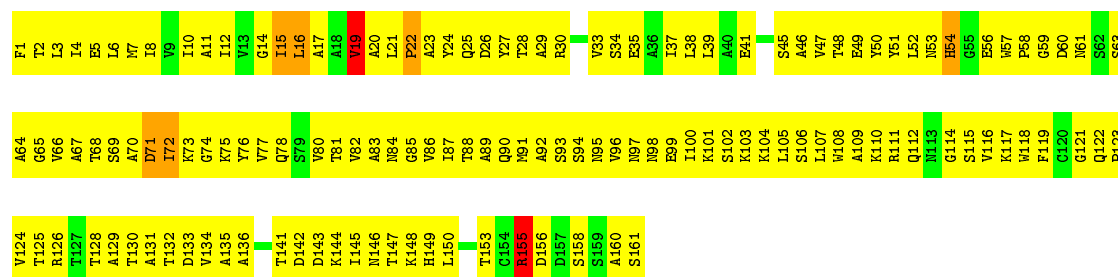
3 Residue-property plots

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: pilin



Chain D:  16% 80%



• Molecule 1: pilin

Chain E:  14% 81%

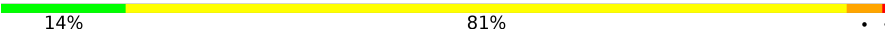


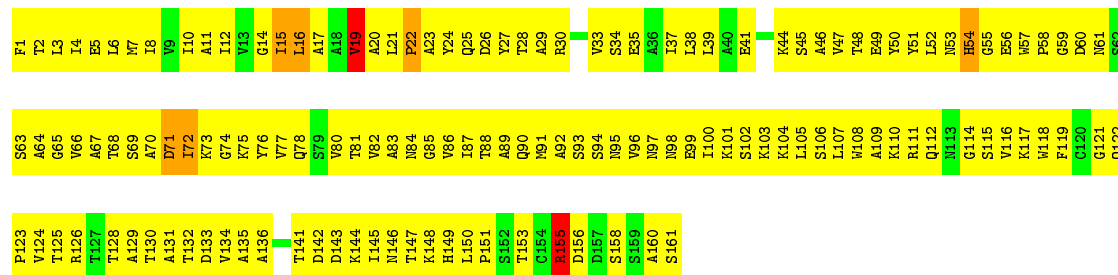
• Molecule 1: pilin

Chain F:  15% 80%

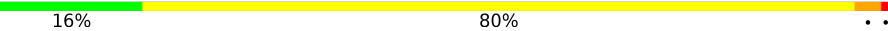


• Molecule 1: pilin

Chain G:  14% 81%



• Molecule 1: pilin

Chain H:  16% 80% ..



• Molecule 1: pilin

Chain I:  14% 81% ..

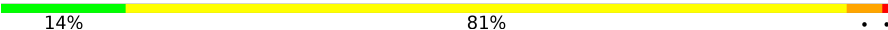


• Molecule 1: pilin

Chain J:  13% 82% ..

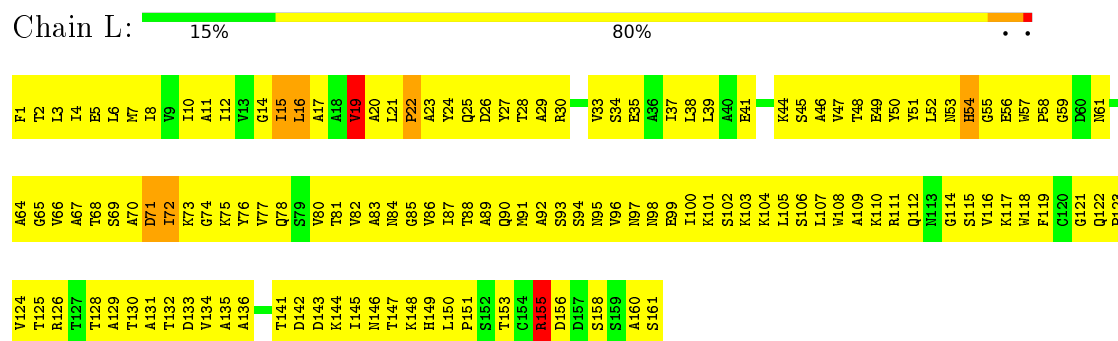


• Molecule 1: pilin

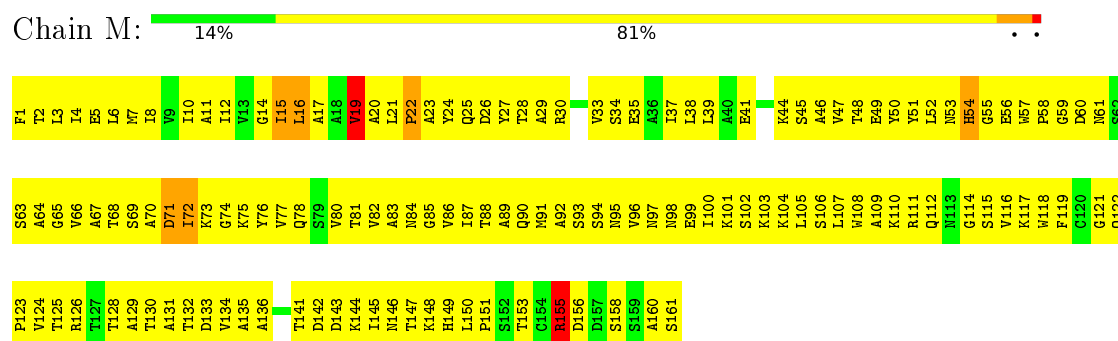
Chain K:  14% 81% ..



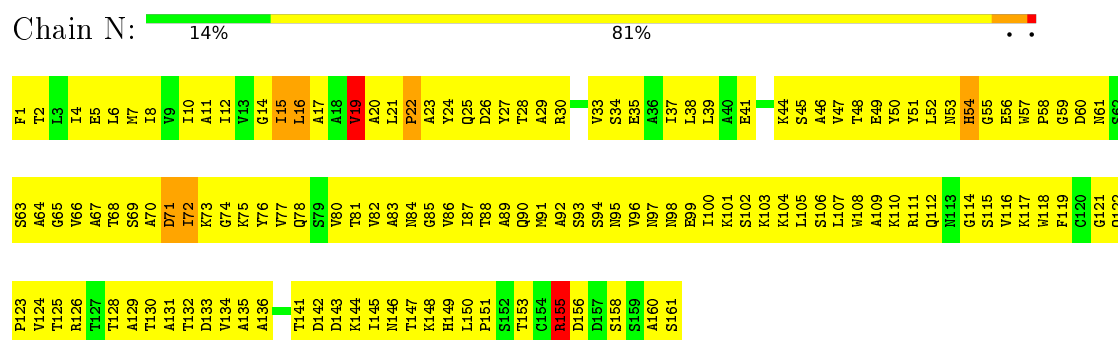
• Molecule 1: pilin



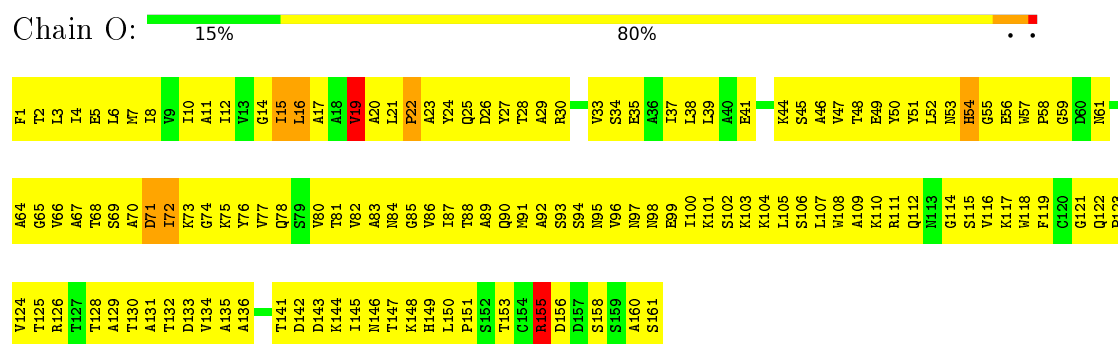
• Molecule 1: pilin



• Molecule 1: pilin



• Molecule 1: pilin



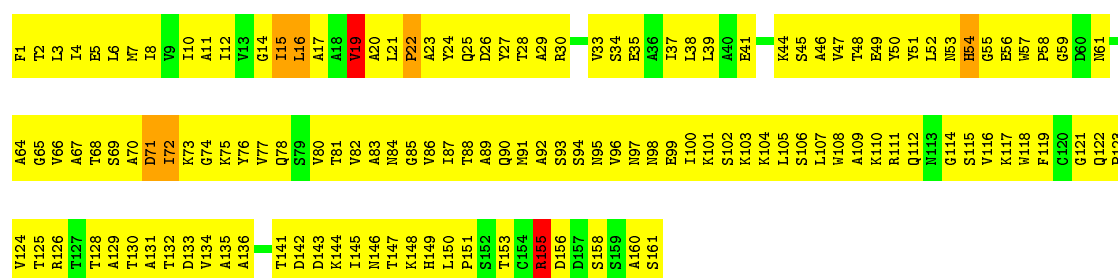
• Molecule 1: pilin

Chain P:  14% 81% .



- Molecule 1: pilin

Chain Q:  15% 80% .



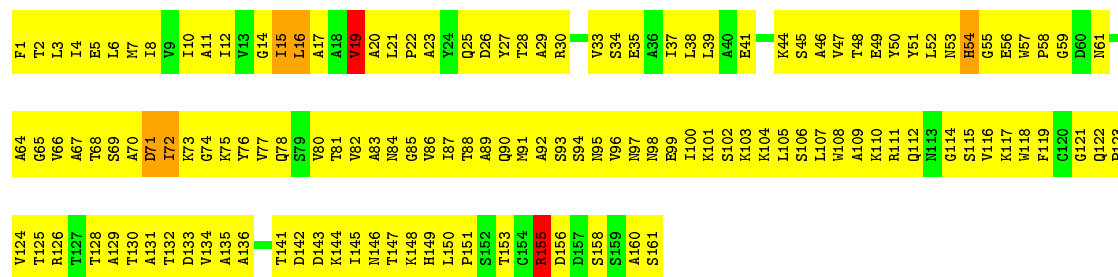
- Molecule 1: pilin

Chain R:  14% 81% .



- Molecule 1: pilin

Chain S:  16% 80% . .



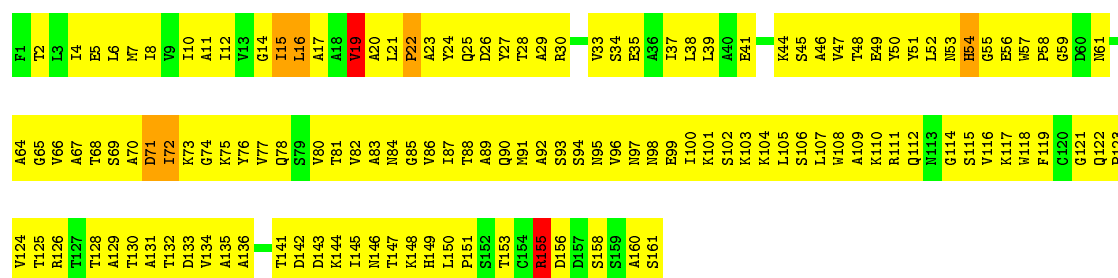
- Molecule 1: pilin

Chain T:  14% 81% ..



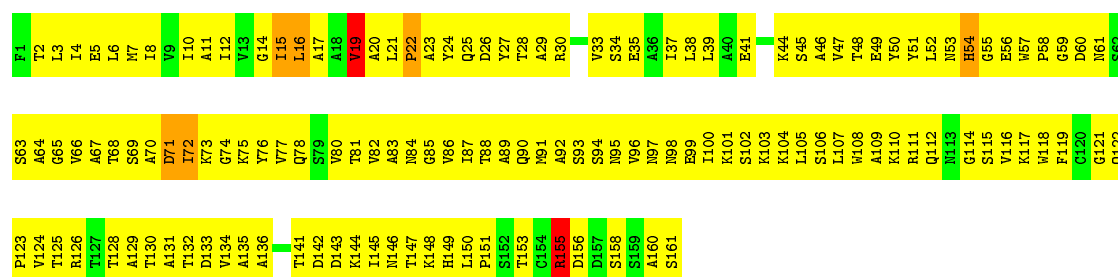
• Molecule 1: pilin

Chain U:  16% 79% ..



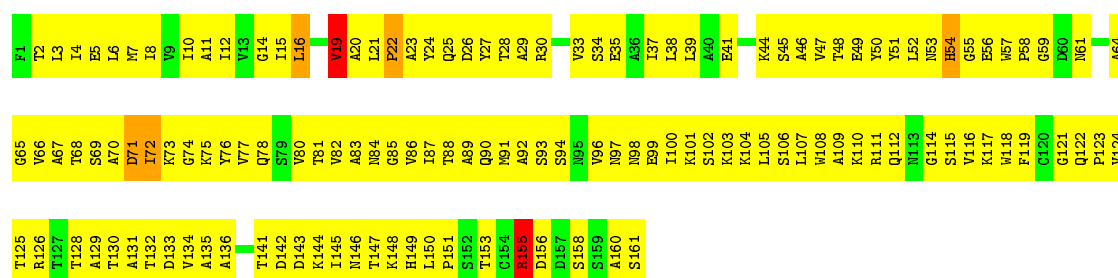
• Molecule 1: pilin

Chain V:  14% 81% ..

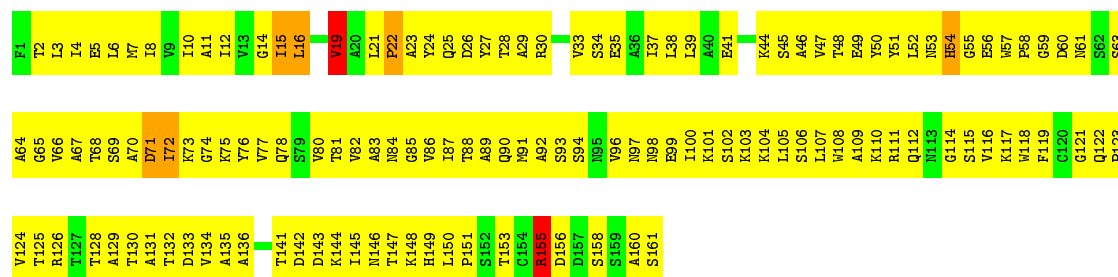


• Molecule 1: pilin

Chain W:  17% 79% ..



Chain X:  16% 79% ..



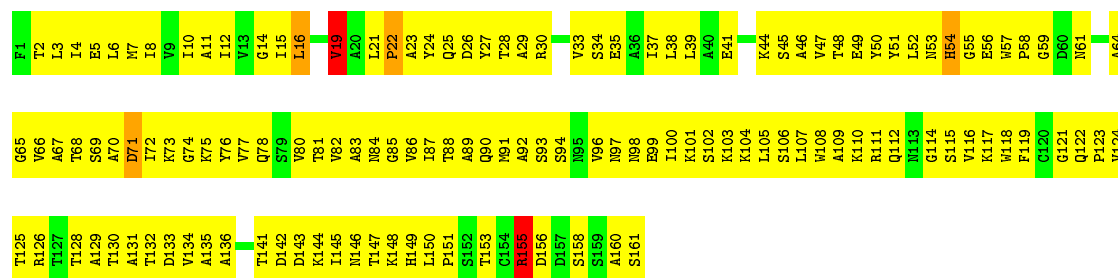
• Molecule 1: pilin

Chain Y:  17% 78% ..



• Molecule 1: pilin

Chain Z:  17% 79% ..



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	15586	Depositor
Resolution determination method	FSC 0.33 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.48	0/1216	0.59	0/1653
1	B	0.48	0/1216	0.59	0/1653
1	C	0.48	0/1216	0.59	0/1653
1	D	0.48	0/1216	0.59	0/1653
1	E	0.48	0/1216	0.59	0/1653
1	F	0.48	0/1216	0.59	0/1653
1	G	0.48	0/1216	0.59	0/1653
1	H	0.48	0/1216	0.59	0/1653
1	I	0.48	0/1216	0.59	0/1653
1	J	0.48	0/1216	0.59	0/1653
1	K	0.48	0/1216	0.59	0/1653
1	L	0.48	0/1216	0.59	0/1653
1	M	0.48	0/1216	0.59	0/1653
1	N	0.48	0/1216	0.59	0/1653
1	O	0.48	0/1216	0.59	0/1653
1	P	0.48	0/1216	0.59	0/1653
1	Q	0.48	0/1216	0.59	0/1653
1	R	0.48	0/1216	0.59	0/1653
1	S	0.48	0/1216	0.59	0/1653
1	T	0.48	0/1216	0.59	0/1653
1	U	0.48	0/1216	0.59	0/1653
1	V	0.48	0/1216	0.59	0/1653
1	W	0.49	0/1216	0.59	0/1653
1	X	0.49	0/1216	0.59	0/1653
1	Y	0.49	0/1216	0.59	0/1653
1	Z	0.49	0/1216	0.59	0/1653
All	All	0.48	0/31616	0.59	0/42978

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
1	Q	0	3
1	R	0	3
1	S	0	3
1	T	0	3
1	U	0	3
1	V	0	3
1	W	0	3
1	X	0	3
1	Y	0	3
1	Z	0	3
All	All	0	78

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ARG	Sidechain
1	A	22	PRO	Peptide
1	A	71	ASP	Peptide
1	B	22	PRO	Peptide
1	B	71	ASP	Peptide

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	1198	0	1200	234	0
1	B	1198	0	1200	235	0
1	C	1198	0	1200	237	0
1	D	1198	0	1200	248	0
1	E	1198	0	1200	272	0
1	F	1198	0	1200	264	0
1	G	1198	0	1200	270	0
1	H	1198	0	1200	278	0
1	I	1198	0	1200	275	0
1	J	1198	0	1200	275	0
1	K	1198	0	1200	276	0
1	L	1198	0	1200	282	0
1	M	1198	0	1200	272	0
1	N	1198	0	1200	277	0
1	O	1198	0	1200	275	0
1	P	1198	0	1200	279	0
1	Q	1198	0	1200	276	0
1	R	1198	0	1200	283	0
1	S	1198	0	1200	275	0
1	T	1198	0	1200	273	0
1	U	1198	0	1200	274	0
1	V	1198	0	1200	271	0
1	W	1198	0	1200	249	0
1	X	1198	0	1200	236	0
1	Y	1198	0	1200	238	0
1	Z	1198	0	1200	232	0
All	All	31148	0	31200	5933	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 95.

The worst 5 of 5933 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:K:19:VAL:HG23	1:O:112:GLN:HG3	1.17	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG23	1:E:112:GLN:HG3	1.17	1.17
1:L:19:VAL:HG23	1:P:112:GLN:HG3	1.17	1.17
1:V:19:VAL:HG23	1:Z:112:GLN:HG3	1.17	1.16
1:S:19:VAL:HG23	1:W:112:GLN:HG3	1.17	1.14

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	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	B	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	C	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	D	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	E	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	F	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	G	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	H	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	I	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	J	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	K	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	L	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	M	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	N	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	O	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	P	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	R	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	S	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	T	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	U	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	V	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	W	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	X	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	Y	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
1	Z	159/161 (99%)	120 (76%)	37 (23%)	2 (1%)	15	59
All	All	4134/4186 (99%)	3120 (76%)	962 (23%)	52 (1%)	20	59

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	72	ILE
1	G	72	ILE
1	H	72	ILE
1	A	72	ILE
1	B	72	ILE

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	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	B	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	C	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	D	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	E	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	F	128/128 (100%)	123 (96%)	5 (4%)	39	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	H	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	I	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	J	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	K	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	L	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	M	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	N	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	O	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	P	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	Q	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	R	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	S	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	T	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	U	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	V	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	W	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	X	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	Y	128/128 (100%)	123 (96%)	5 (4%)	39	72
1	Z	128/128 (100%)	123 (96%)	5 (4%)	39	72
All	All	3328/3328 (100%)	3198 (96%)	130 (4%)	43	72

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	54	HIS
1	O	19	VAL
1	Y	15	ILE
1	M	15	ILE
1	N	16	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	53	ASN
1	P	43	GLN
1	Y	53	ASN
1	M	78	GLN
1	N	90	GLN

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.