wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:37 PM BST

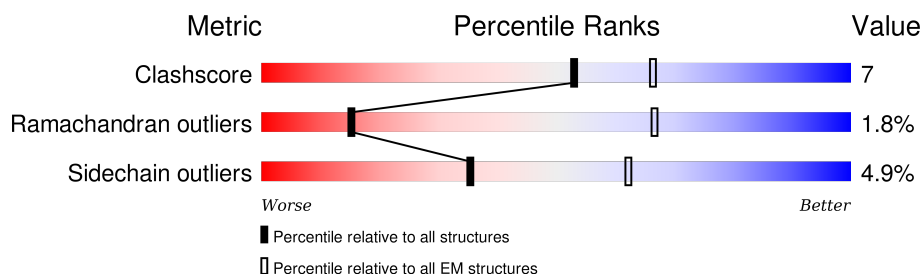|		
PDB ID	:	3CRE
EMDB ID:	:	EMD-1494
Title	:	Electron Microscopy model of the Saf Pilus- Type A
Authors	:	Salih, O.; Remaut, H.; Waksman, G.; Orlova, E.V.
Deposited on	:	2008-04-07
Resolution	:	17.00 Å(reported)

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 17.00 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		1.8%
Sidechain outliers		4.9%

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	123	84% · 13% ·
2	B	144	72% · 22% · 6%
3	C	19	68% · 32%

WORLDWIDE PDB
PROTEIN DATA BANK

EMDataBank
Unified Data Resource for 3DEM

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2135 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 Outer membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	123	Total	C	N	O	S	0	0
			914	570	158	185	1		

- Molecule 2 is a protein called Outer membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1075	671	184	219	1		

- Molecule 3 is a protein called Outer membrane protein.

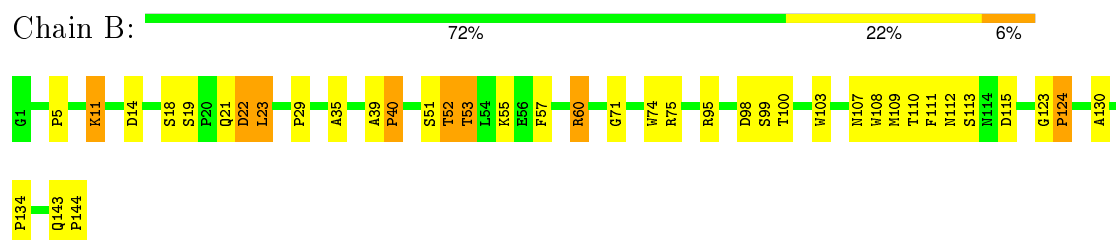| Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	19	Total	C	N	O	0	0
			146	91	23	32		

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: Outer membrane protein

Chain A:

84% 13% •

D22 P29 K55 E56 R60 G71 R75 K79 E84 R95 R96 W108 M109 D115 P124 A125 Q126 T129 A130 D131 T132 P144
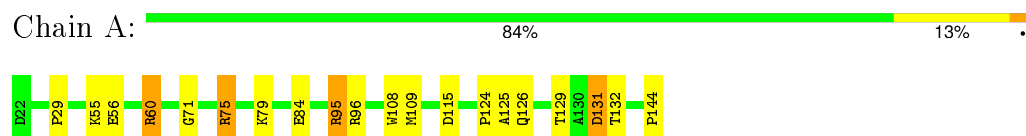
- Molecule 2: Outer membrane protein

Chain B:

72% 22% 6%

G1 P5 K11 D14 S18 S19 P20 Q21 D22 L23 P29 A35 A39 P40 S51 T52 T53 L54 K55 E56 F57 R60 G71 W74 R75 R95 D98 S99 T100 W103 N107 W108 M109 T110 F111 N112 S113 N114 D115 G123 P124 A130

P134 Q143 P144

- Molecule 3: Outer membrane protein

Chain C:

68% 32%

G1 S2 F3 N6 K11 S19
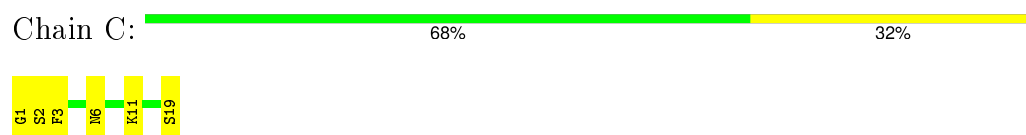
4   Experimental information (i)

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	n/a	Depositor
Microscope	Philips Tecnai 100 kV electron microscope	Depositor
Voltage (kV)	100	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	44000	Depositor
Image detector	Kodak SO163 film	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	0.81	0/928	1.57	10/1264 (0.8%)
2	B	0.93	0/1093	1.52	9/1488 (0.6%)
3	C	0.91	0/148	1.23	0/197
All	All	0.88	0/2169	1.52	19/2949 (0.6%)

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
2	B	0	3
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	NE-CZ-NH1	14.16	127.38	120.30
2	B	60	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	A	115	ASP	CB-CG-OD1	9.91	127.22	118.30
2	B	95	ARG	NE-CZ-NH2	9.72	125.16	120.30
2	B	75	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	95	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	A	96	ARG	NE-CZ-NH2	7.15	123.87	120.30
2	B	108	TRP	CE2-CD2-CG	-6.38	102.19	107.30
1	A	131	ASP	N-CA-CB	-6.29	99.28	110.60
1	A	75	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	109	MET	CG-SD-CE	6.22	110.14	100.20
2	B	103	TRP	CE2-CD2-CG	-6.14	102.39	107.30
2	B	11	LYS	CG-CD-CE	5.69	128.96	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LYS	CA-C-O	-5.45	108.65	120.10
2	B	40	PRO	CA-CB-CG	-5.42	93.70	104.00
2	B	124	PRO	CA-CB-CG	-5.36	93.81	104.00
2	B	74	TRP	CE2-CD2-CG	-5.34	103.03	107.30
1	A	108	TRP	CG-CD2-CE3	-5.28	129.14	133.90
1	A	71	GLY	CA-C-O	-5.11	111.40	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
1	A	95	ARG	Sidechain
2	B	123	GLY	Peptide
2	B	39	ALA	Peptide
2	B	57	PHE	Sidechain

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	914	0	920	7	0
2	B	1075	0	1076	22	0
3	C	146	0	139	10	0
All	All	2135	0	2135	29	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 7.

All (29) 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:B:130:ALA:CB	3:C:19:SER:OG	1.67	1.41
2:B:130:ALA:HB2	3:C:19:SER:OG	1.01	1.16
2:B:130:ALA:HB2	3:C:19:SER:CB	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ALA:HB3	3:C:19:SER:OG	1.82	0.76
1:A:79:LYS:NZ	2:B:14:ASP:OD1	2.19	0.74
2:B:53:THR:O	2:B:55:LYS:NZ	2.25	0.69
1:A:56:GLU:OE2	1:A:144:PRO:HG3	1.96	0.65
2:B:35:ALA:HB3	3:C:19:SER:HB3	1.80	0.63
2:B:71:GLY:O	2:B:109:MET:SD	2.61	0.58
2:B:35:ALA:CB	3:C:19:SER:HB3	2.34	0.58
1:A:56:GLU:CD	1:A:144:PRO:HG3	2.26	0.56
2:B:98:ASP:OD2	2:B:112:ASN:ND2	2.39	0.56
2:B:144:PRO:O	3:C:1:GLY:N	2.40	0.54
1:A:75:ARG:NH2	1:A:84:GLU:OE1	2.40	0.54
3:C:2:SER:OG	3:C:3:PHE:N	2.42	0.52
2:B:99:SER:OG	2:B:100:THR:N	2.43	0.52
1:A:124:PRO:O	1:A:126:GLN:N	2.45	0.48
2:B:22:ASP:OD1	2:B:23:LEU:N	2.47	0.48
2:B:19:SER:OG	3:C:1:GLY:N	2.47	0.48
2:B:60:ARG:NH2	2:B:107:ASN:O	2.46	0.47
2:B:144:PRO:OXT	3:C:1:GLY:N	2.46	0.47
1:A:131:ASP:OD2	1:A:132:THR:N	2.47	0.47
2:B:51:SER:OG	2:B:52:THR:N	2.50	0.45
2:B:98:ASP:OD1	2:B:112:ASN:N	2.50	0.45
2:B:21:GLN:N	2:B:143:GLN:OE1	2.50	0.44
2:B:51:SER:O	2:B:53:THR:N	2.50	0.44
1:A:75:ARG:NE	1:A:84:GLU:OE1	2.48	0.44
2:B:110:THR:C	2:B:111:PHE:CD1	2.92	0.43
2:B:115:ASP:C	2:B:115:ASP:OD2	2.59	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	121/123 (98%)	114 (94%)	5 (4%)	2 (2%)	11	55
2	B	142/144 (99%)	123 (87%)	16 (11%)	3 (2%)	9	50
3	C	17/19 (90%)	14 (82%)	3 (18%)	0	100	100
All	All	280/286 (98%)	251 (90%)	24 (9%)	5 (2%)	15	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ALA
1	A	129	THR
2	B	18	SER
2	B	52	THR
2	B	113	SER

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	103/103 (100%)	102 (99%)	1 (1%)	82	92
2	B	123/123 (100%)	114 (93%)	9 (7%)	17	54
3	C	18/18 (100%)	16 (89%)	2 (11%)	8	34
All	All	244/244 (100%)	232 (95%)	12 (5%)	35	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
2	B	5	PRO
2	B	11	LYS
2	B	22	ASP
2	B	23	LEU
2	B	29	PRO
2	B	40	PRO
2	B	53	THR

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Mol	Chain	Res	Type
2	B	124	PRO
2	B	134	PRO
3	C	6	ASN
3	C	11	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	112	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.