



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 3, 2016 – 04:34 PM EDT

PDB ID : 3NB3
EMDB ID: : EMD-5201
Title : The host outer membrane proteins OmpA and OmpC are packed at specific sites in the Shigella phage Sf6 virion as structural components
Authors : Zhao, H.; Sequeira, R.D.; Galeva, N.A.; Tang, L.
Deposited on : 2010-06-02
Resolution : 19.00 Å(reported)
Based on PDB ID : 1QJP, 2J1N

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

<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

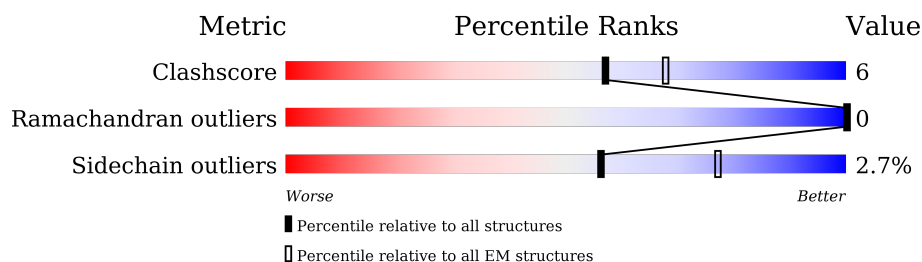
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 19.00 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	346	
1	B	346	
1	C	346	
2	D	346	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5945 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 A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	137	Total	C	N	O	S	0	0
			1077	695	178	200	4		
1	B	137	Total	C	N	O	S	0	0
			1077	695	178	200	4		
1	C	137	Total	C	N	O	S	0	0
			1077	695	178	200	4		

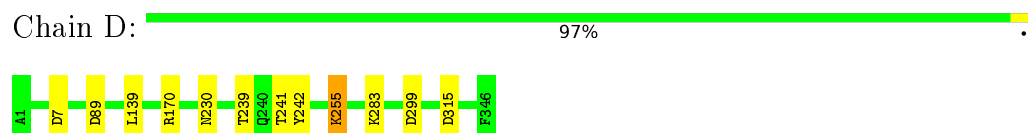
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLN	SEE REMARK 999	UNP P0A910
A	107	TYR	LYS	SEE REMARK 999	UNP P0A910
B	34	LYS	GLN	SEE REMARK 999	UNP P0A910
B	107	TYR	LYS	SEE REMARK 999	UNP P0A910
C	34	LYS	GLN	SEE REMARK 999	UNP P0A910
C	107	TYR	LYS	SEE REMARK 999	UNP P0A910

- Molecule 2 is a protein called Outer membrane protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	346	Total	C	N	O	S	0	0
			2714	1699	458	554	3		

- Molecule 2: Outer membrane protein C



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3232	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	1060	Depositor
Maximum defocus (nm)	471	Depositor
Magnification	39000	Depositor
Image detector	2Kx2K CCD	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	0.55	0/1108	1.55	17/1503 (1.1%)
1	B	0.55	0/1108	1.55	16/1503 (1.1%)
1	C	0.55	0/1108	1.55	16/1503 (1.1%)
2	D	0.53	3/2773 (0.1%)	0.65	2/3753 (0.1%)
All	All	0.54	3/6097 (0.0%)	1.23	51/8262 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	139	LEU	CB-CG	-13.65	1.12	1.52
2	D	255	LYS	CB-CG	-6.18	1.35	1.52
2	D	230	ASN	CB-CG	5.78	1.64	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	LEU	CA-CB-CG	12.13	143.21	115.30
1	B	90	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	C	90	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	90	ASP	CB-CG-OD2	-7.37	111.66	118.30
1	C	85	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	B	85	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	A	85	TYR	CB-CG-CD2	-7.26	116.65	121.00
1	B	60	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	A	60	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	60	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	96	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	139	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	139	LEU	CA-CB-CG	6.43	130.08	115.30
1	A	96	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	139	LEU	CA-CB-CG	6.42	130.06	115.30
1	B	96	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	89	ASP	CB-CG-OD2	-6.41	112.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	89	ASP	CB-CG-OD2	-6.34	112.60	118.30
2	D	139	LEU	CB-CG-CD2	6.32	121.74	111.00
1	B	91	LEU	CA-CB-CG	6.20	129.57	115.30
1	C	91	LEU	CA-CB-CG	6.19	129.55	115.30
1	A	91	LEU	CA-CB-CG	6.18	129.50	115.30
1	C	48	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	B	111	TYR	CB-CG-CD1	5.99	124.59	121.00
1	B	48	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	A	48	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	C	111	TYR	CB-CG-CD1	5.92	124.55	121.00
1	A	111	TYR	CB-CG-CD1	5.91	124.55	121.00
1	B	92	ASP	CA-CB-CG	5.80	126.16	113.40
1	A	92	ASP	CA-CB-CG	5.77	126.10	113.40
1	C	92	ASP	CA-CB-CG	5.77	126.10	113.40
1	B	71	ALA	N-CA-CB	5.75	118.15	110.10
1	C	71	ALA	N-CA-CB	5.74	118.13	110.10
1	A	71	ALA	N-CA-CB	5.71	118.09	110.10
1	C	116	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	94	TYR	CB-CG-CD1	5.20	124.12	121.00
1	A	116	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	72	TYR	N-CA-CB	5.18	119.93	110.60
1	A	72	TYR	N-CA-CB	5.18	119.93	110.60
1	C	72	TYR	N-CA-CB	5.18	119.92	110.60
1	A	94	TYR	CB-CG-CD1	5.16	124.09	121.00
1	B	94	TYR	CB-CG-CD1	5.15	124.09	121.00
1	B	116	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	8	TYR	CB-CG-CD2	5.12	124.07	121.00
1	C	8	TYR	CB-CG-CD2	5.09	124.05	121.00
1	A	8	TYR	CB-CG-CD2	5.08	124.05	121.00
1	B	8	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	A	8	TYR	CG-CD1-CE1	5.05	125.34	121.30
1	C	8	TYR	CG-CD1-CE1	5.05	125.34	121.30
1	A	116	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1077	0	1016	20	0
1	B	1077	0	1016	19	0
1	C	1077	0	1016	20	0
2	D	2714	0	2491	12	0
All	All	5945	0	5539	71	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 6.

All (71) 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:D:242:TYR:CE1	2:D:255:LYS:HE2	1.66	1.30
2:D:242:TYR:HE1	2:D:255:LYS:CE	1.51	1.24
1:A:93:ILE:CD1	1:A:127:VAL:HG12	1.76	1.16
1:C:93:ILE:CD1	1:C:127:VAL:HG12	1.76	1.14
1:B:93:ILE:CD1	1:B:127:VAL:HG12	1.76	1.14
1:C:93:ILE:HD13	1:C:127:VAL:HG12	1.09	1.07
1:A:93:ILE:HD13	1:A:127:VAL:HG12	1.09	1.06
1:B:93:ILE:HD13	1:B:127:VAL:HG12	1.09	1.05
1:A:93:ILE:HD13	1:A:127:VAL:CG1	1.89	1.02
1:C:93:ILE:HD13	1:C:127:VAL:CG1	1.89	1.02
1:B:93:ILE:HD13	1:B:127:VAL:CG1	1.89	1.02
1:B:35:LEU:HB2	1:B:61:MET:HE2	1.42	1.01
1:B:93:ILE:CD1	1:B:127:VAL:CG1	2.40	1.00
1:A:93:ILE:CD1	1:A:127:VAL:CG1	2.40	1.00
1:C:93:ILE:CD1	1:C:127:VAL:CG1	2.40	0.99
1:C:35:LEU:HB2	1:C:61:MET:HE2	1.47	0.94
2:D:242:TYR:HE1	2:D:255:LYS:HE2	0.77	0.93
1:A:35:LEU:HB2	1:A:61:MET:HE2	1.48	0.92
1:A:35:LEU:HB2	1:A:61:MET:CE	2.05	0.87
1:B:35:LEU:HB2	1:B:61:MET:CE	2.05	0.87
1:C:35:LEU:HB2	1:C:61:MET:CE	2.05	0.86
2:D:242:TYR:CE1	2:D:255:LYS:CE	2.42	0.83
1:B:60:ARG:NH2	1:B:72:TYR:CD1	2.56	0.74
1:A:60:ARG:NH2	1:A:72:TYR:CD1	2.56	0.73
1:C:60:ARG:NH2	1:C:72:TYR:CD1	2.56	0.72
2:D:242:TYR:CD1	2:D:255:LYS:HG2	2.24	0.72
2:D:242:TYR:CE1	2:D:255:LYS:CD	2.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:TYR:HE1	2:D:255:LYS:CD	2.07	0.65
1:A:93:ILE:HD11	1:A:127:VAL:CG1	2.29	0.63
1:A:101:VAL:HG12	1:A:119:VAL:HG22	1.83	0.61
1:B:101:VAL:HG12	1:B:119:VAL:HG22	1.83	0.61
1:C:93:ILE:HD11	1:C:127:VAL:CG1	2.29	0.61
1:C:101:VAL:HG12	1:C:119:VAL:HG22	1.83	0.60
1:A:60:ARG:NH2	1:A:72:TYR:CE1	2.71	0.59
1:C:60:ARG:NH2	1:C:72:TYR:CE1	2.71	0.58
1:B:60:ARG:NH2	1:B:72:TYR:CE1	2.71	0.58
1:B:93:ILE:HD11	1:B:127:VAL:CG1	2.29	0.58
1:B:93:ILE:HD11	1:B:127:VAL:HG12	1.81	0.57
1:A:35:LEU:HB2	1:A:61:MET:HE3	1.91	0.52
2:D:299:ASP:OD1	2:D:315:ASP:OD1	2.28	0.51
1:C:83:LEU:N	1:C:83:LEU:HD12	2.26	0.51
1:B:83:LEU:HD12	1:B:83:LEU:N	2.26	0.51
1:A:83:LEU:HD12	1:A:83:LEU:N	2.26	0.50
1:A:87:ILE:HG12	1:A:93:ILE:HG12	1.93	0.49
1:B:87:ILE:HG12	1:B:93:ILE:HG12	1.93	0.49
1:C:87:ILE:HG12	1:C:93:ILE:HG12	1.93	0.49
1:C:93:ILE:HD11	1:C:127:VAL:HG12	1.81	0.47
1:C:93:ILE:CD1	1:C:127:VAL:HG13	2.40	0.47
1:A:93:ILE:CD1	1:A:127:VAL:HG13	2.41	0.47
2:D:242:TYR:CE1	2:D:255:LYS:HD3	2.50	0.47
1:B:93:ILE:CD1	1:B:127:VAL:HG13	2.40	0.47
1:C:60:ARG:NH2	1:C:72:TYR:CG	2.84	0.45
1:B:60:ARG:NH2	1:B:72:TYR:CG	2.84	0.45
1:A:60:ARG:NH2	1:A:72:TYR:CG	2.84	0.45
2:D:242:TYR:CE1	2:D:255:LYS:HG2	2.51	0.45
2:D:239:THR:HG22	2:D:241:THR:HG23	1.99	0.45
1:A:71:ALA:HB3	1:A:107:TYR:HD2	1.82	0.44
1:C:35:LEU:HB2	1:C:61:MET:HE3	1.92	0.44
1:A:93:ILE:HD11	1:A:127:VAL:HG12	1.81	0.44
1:C:71:ALA:HB3	1:C:107:TYR:HD2	1.82	0.43
1:B:71:ALA:HB3	1:B:107:TYR:HD2	1.82	0.43
1:C:60:ARG:CZ	1:C:72:TYR:CG	3.02	0.43
1:A:60:ARG:CZ	1:A:72:TYR:CG	3.02	0.43
1:B:60:ARG:CZ	1:B:72:TYR:CG	3.02	0.43
1:A:87:ILE:CG1	1:A:93:ILE:HG12	2.49	0.42
1:B:87:ILE:CG1	1:B:93:ILE:HG12	2.49	0.42
1:C:87:ILE:CG1	1:C:93:ILE:HG12	2.49	0.41
1:A:60:ARG:NH1	1:A:72:TYR:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:NH1	1:B:72:TYR:CD2	2.89	0.41
1:C:60:ARG:NH1	1:C:72:TYR:CD2	2.89	0.41
2:D:242:TYR:CE1	2:D:255:LYS:CG	3.04	0.41

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	129/346 (37%)	128 (99%)	1 (1%)	0	100	100
1	B	129/346 (37%)	128 (99%)	1 (1%)	0	100	100
1	C	129/346 (37%)	128 (99%)	1 (1%)	0	100	100
2	D	344/346 (99%)	327 (95%)	17 (5%)	0	100	100
All	All	731/1384 (53%)	711 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	106/271 (39%)	102 (96%)	4 (4%)	40	73
1	B	106/271 (39%)	102 (96%)	4 (4%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	106/271 (39%)	102 (96%)	4 (4%)	40	73
2	D	275/275 (100%)	271 (98%)	4 (2%)	72	88
All	All	593/1088 (54%)	577 (97%)	16 (3%)	56	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	107	TYR
1	A	139	LEU
1	A	145	ASN
1	B	91	LEU
1	B	107	TYR
1	B	139	LEU
1	B	145	ASN
1	C	91	LEU
1	C	107	TYR
1	C	139	LEU
1	C	145	ASN
2	D	7	ASP
2	D	89	ASP
2	D	170	ARG
2	D	283	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	B	145	ASN
1	C	145	ASN
2	D	9	ASN
2	D	214	ASN
2	D	240	GLN

5.3.3 RNA ⓘ

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.