



wwPDB EM Map/Model Validation Report ⓘ

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PDB ID : 4BX4
EMDB ID: : EMD-1300
Title : Fitting of the bacteriophage Phi8 P1 capsid protein into cryo-EM density
Authors : El Omari, K.; Sutton, G.; Ravantti, J.J.; Zhang, H.; Walter, T.S.; Grimes, J.M.; Bamford, D.H.; Stuart, D.I.; Mancini, E.J.
Deposited on : 2013-07-08
Resolution : 8.70 Å(reported)
Based on PDB ID : 4BTP

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

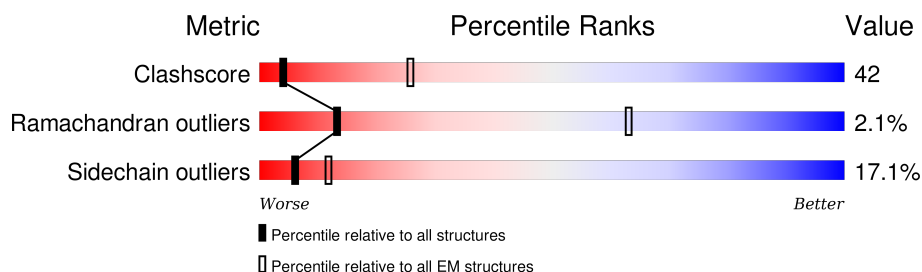
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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	792	
1	B	792	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11384 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 P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	738	Total	C	N	O	S	0	0
			5692	3588	984	1096	24		
1	B	738	Total	C	N	O	S	0	0
			5692	3588	984	1096	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	ASP	GLU	CONFLICT	UNP Q9MC13
B	691	ASP	GLU	CONFLICT	UNP Q9MC13




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided, Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	50000	Depositor
Image detector	E.G. KODAK SO163 FILM	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	3.90	1/5791 (0.0%)	0.94	4/7850 (0.1%)
1	B	0.58	0/5790	0.84	2/7847 (0.0%)
All	All	2.79	1/11581 (0.0%)	0.89	6/15697 (0.0%)

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	1	3
1	B	0	3
All	All	1	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	SER	N-CA	293.68	7.33	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	SER	N-CA-CB	33.33	160.49	110.50
1	A	370	SER	N-CA-C	-17.18	64.62	111.00
1	A	567	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	567	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	485	LEU	CA-CB-CG	5.47	127.88	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	370	SER	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	GLY	Peptide
1	A	595	ARG	Peptide
1	A	631	ALA	Peptide
1	B	263	GLY	Peptide
1	B	595	ARG	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	5692	0	5684	516	0
1	B	5692	0	5694	519	0
All	All	11384	0	11378	960	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 42.

The worst 5 of 960 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:A:39:TRP:CH2	1:A:515:TYR:CD2	1.78	1.69
1:A:289:ILE:HD13	1:A:515:TYR:CE2	1.22	1.63
1:A:39:TRP:CE3	1:A:515:TYR:CD2	1.87	1.63
1:A:39:TRP:HH2	1:A:515:TYR:CB	1.01	1.62
1:A:39:TRP:CZ3	1:A:515:TYR:CG	1.85	1.61

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	730/792 (92%)	640 (88%)	74 (10%)	16 (2%)	8	49
1	B	728/792 (92%)	641 (88%)	72 (10%)	15 (2%)	9	50
All	All	1458/1584 (92%)	1281 (88%)	146 (10%)	31 (2%)	13	50

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	SER
1	A	503	ILE
1	B	503	ILE
1	A	559	SER
1	A	643	GLY

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	617/663 (93%)	511 (83%)	106 (17%)	2	17
1	B	617/663 (93%)	512 (83%)	105 (17%)	2	18
All	All	1234/1326 (93%)	1023 (83%)	211 (17%)	6	17

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	703	THR
1	B	115	ASN
1	B	672	TYR
1	A	723	ILE
1	B	33	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	729	GLN
1	A	741	GLN
1	B	478	GLN
1	A	478	GLN
1	A	517	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.