



## wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J1A  
EMDB ID: : EMD-5388  
Title : HK97-like fold fitted into 3D reconstruction of bacteriophage CW02  
Authors : Shen, P.S.; Domek, M.J.; Sanz-Garcia, E.; Makaju, A.; Taylor, R.; Culumber, M.; Breakwell, D.P.; Prince, J.T.; Belnap, D.M.  
Deposited on : 2012-01-31  
Resolution : 16.00 Å(reported)  
Based on PDB ID : 1OHG

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 898 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 capsid protein.

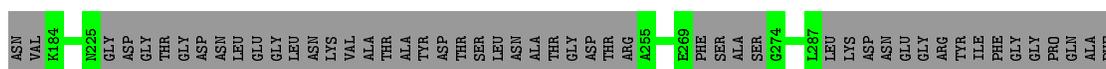
Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	128	Total C 128 128	0	128
1	B	128	Total C 128 128	0	128
1	C	128	Total C 128 128	0	128
1	D	128	Total C 128 128	0	128
1	E	128	Total C 128 128	0	128
1	F	128	Total C 128 128	0	128
1	G	130	Total C 130 130	0	130

### 3 Residue-property plots [i](#)

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.

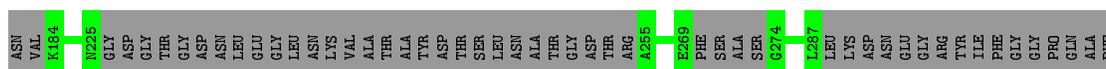
- Molecule 1: capsid protein

Chain A:  64% 36%



- Molecule 1: capsid protein

Chain B:  64% 36%



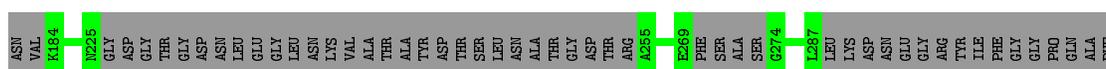
- Molecule 1: capsid protein

Chain C:  64% 36%



- Molecule 1: capsid protein

Chain D:  64% 36%



- Molecule 1: capsid protein

Chain E:  64% 36%

ASN VAL K184 N225 GLY ASP ASP GLY THR THR GLN GLY ASP ASP ASN LEU LEU LEU LEU ASN ASN LYS VAL VAL ALA THR THR TYR TYR ASP THR THR SER LEU LEU ASN ALA ALA THR THR GLY ASP ASP ARG A255 E269 PHE SER ALA ALA G274 L287 LEU LYS ASP ASP ASN ASN GLU GLY GLY TYR THR TYR ILE PHE PHE GLY PRO GLN ALA PHE

THR SER ASN I307 P315 THR LYS ALA THR GLN ALA ALA ASN GLY LEU T323 S346 ARG GLU ASP ARG ASP ASN PHE VAL LYS ASN M357 T380

- Molecule 1: capsid protein

Chain F:  64% 36%

ASN VAL K184 N225 GLY ASP ASP GLY THR THR GLN GLY ASP ASP ASN LEU LEU LEU LEU ASN ASN LYS VAL VAL ALA THR THR TYR TYR ASP THR THR SER LEU LEU ASN ALA ALA THR THR GLY ASP ASP ARG A255 E269 PHE SER ALA ALA G274 L287 LEU LYS ASP ASP ASN ASN GLU GLY GLY TYR THR TYR ILE PHE PHE GLY PRO GLN ALA PHE

THR SER ASN I307 P315 THR LYS ALA THR GLN ALA ALA ASN GLY LEU T323 S346 ARG GLU ASP ARG ASP ASN PHE VAL LYS ASN M357 T380

- Molecule 1: capsid protein

Chain G:  65% 35%

H182 G226 ASP THR THR GLY ASP ASN LEU G235 A242 TYR THR THR SER SER LEU LEU ASN ASN ALA THR TYR TYR ASP THR ARG A255 E269 PHE SER ALA SER G274 L287 LEU LYS ASP ASN ASN GLU GLY ARG TYR ILE PHE PHE GLY GLY PRO PRO GLN ALA PHE THR THR SER ASN ASN ILE MET TRP GLY L311

P315 THR LYS ALA GLN ALA ALA GLY T323 S346 ARG GLU ASP ARG ASP ASN ASN PHE VAL LYS M357 H370 THR ARG PRO THR ALA I376 T380

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	8695	Depositor
Resolution determination method	FSC at 0.5 cutoff	Depositor
CTF correction method	whole micrograph	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	39000	Depositor
Image detector	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	128	0	0	0	0
1	B	128	0	0	0	0
1	C	128	0	0	0	0
1	D	128	0	0	0	0
1	E	128	0	0	0	0
1	F	128	0	0	0	0
1	G	130	0	0	0	0
All	All	898	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.