



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:23 am GMT

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 Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

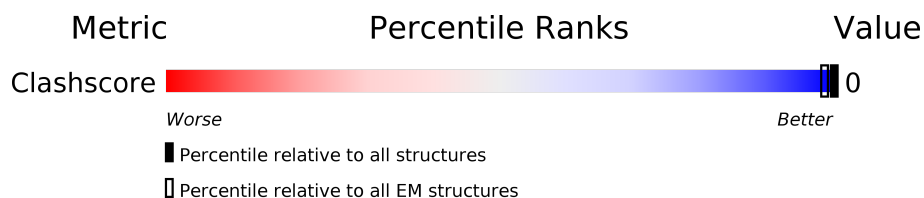
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*








The reported resolution of this entry is 16.00 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	125131	1336

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  $\geq 3$ , 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	199	 64% 36%
1	B	199	 64% 36%
1	C	199	 64% 36%
1	D	199	 64% 36%
1	E	199	 64% 36%
1	F	199	 64% 36%
1	G	199	 65% 35%

## 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.

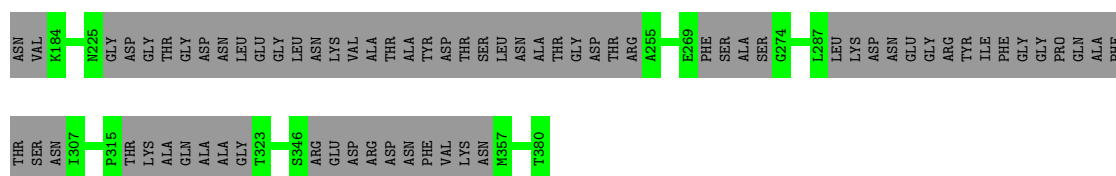
Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	128	Total 128	C 128	0	128
1	B	128	Total 128	C 128	0	128
1	C	128	Total 128	C 128	0	128
1	D	128	Total 128	C 128	0	128
1	E	128	Total 128	C 128	0	128
1	F	128	Total 128	C 128	0	128
1	G	130	Total 130	C 130	0	130

### 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 the various outlier classes 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.

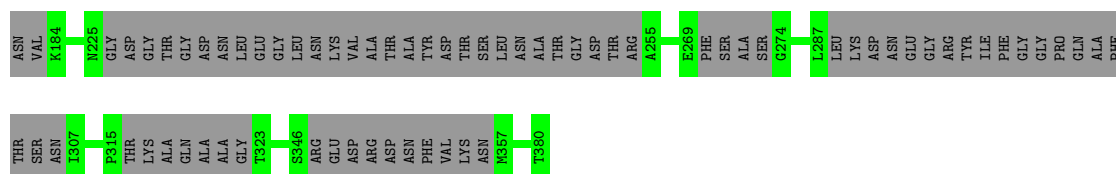
- Molecule 1: capsid protein

Chain A: 



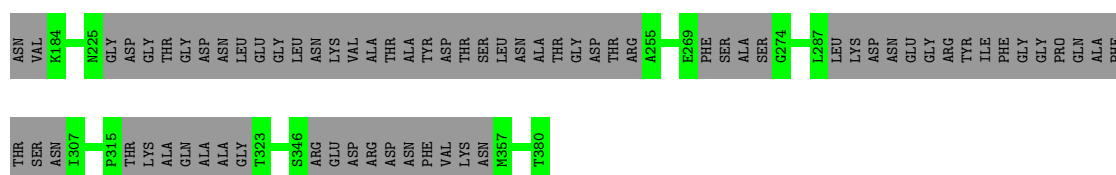
- Molecule 1: capsid protein

Chain B: 



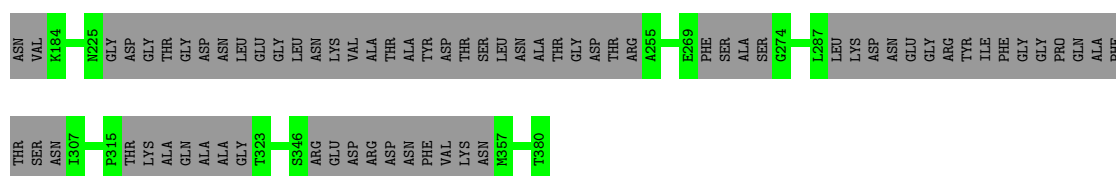
- Molecule 1: capsid protein

Chain C: 



- Molecule 1: capsid protein

Chain D: 



- Molecule 1: capsid protein

THR	SER	ASN	I307	F315	THR	LYS	ALA	GLN	ALA	ALA	T323	S346	ARG	GLU	ASP	ARG	ASP	ASN	PHE	VAL	LYS	ASN	THR	THR	THR	THR	LEU	ASN	ALA	ALA	THR	GLY	ASP	THR	ARG	A255	E269	PHE	SER	ALA	SER	G274	L287	LEU	LYS	ASP	ASN	GLU	GLY	ARG	TYR	ILE	PHE	GLY	PRO	GLN	ALA	PHE
ASN	VAL	K184	V225	GLY	ASP	GLY	THR	GLY	ASP	ASN	LEU	GLU	GLY	LEU	ASN	LYS	VAL	ALA	THR	ALA	ALA	TYR	ASP	THR	THR	THR	LEU	ASN	ALA	THR	GLY	ASP	THR	ARG	A255	E269	PHE	SER	ALA	SER	G274	L287	LEU	LYS	ASP	ASN	GLU	GLY	ARG	TYR	ILE	PHE	GLY	PRO	GLN	ALA	PHE	

- Chain F:  64% 36%

THR	SER	ASN	I307	P315	THR	LYS	ALA	GLN	ALA	ALA	T323	S346	ARG	GLU	ASP	ARG	ASP	ASN	PHE	VAL	LYS	PHE	M357	T380																						
ASV	VAL	K184	V275	GLY	ASP	GLY	THR	GLY	ASP	ASN	LEU	GLU	GLY	LEU	ASN	LYS	VAL	ALA	THR	TYR	ASP	SER	THR	ARG	E269	PHE	SER	ALA	SER	G274	L287	LEU	LYS	ASP	ASN	GLU	GLY	ARG	TYR	ILE	PHE	GLY	PRO	GLN	ALA	PHE

- Chain G:  65% 35%

P315 THR LYS ALA GLN ALA ALA ASP ASP ASP ASN PHE VAL LYS ASN M357 H370 THR ARG PRO THR ALA T376 T380  
 N182 G226 ASP GLY THR GLY ASP ASN LEU GLU G235 A242 THR ASP THR SER LEU ASN ALA THR GLY ASP THR ARG A255 F269 PHE SER SER ALA ALA G274 L287 LEU LYS LYS ASP ASN ASN GLU GLY ARG ASP TYR ILE PHE GLY GLY PRO GLN ALA PHE THR SER ASN ILE MET TRP GLY T381

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	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	37564	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).

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 [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	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.