wwPDB EM Validation Summary Report (i)

Apr 11, 2024 – 04:00 PM EDT

PDB ID	:	1M0F
Title	:	Structural Studies of Bacteriophage alpha3 Assembly, Cryo-electron microscopy
Authors	:	Bernal, R.A.; Hafenstein, S.; Olson, N.H.; Bowman, V.D.; Chipman, P.R.; Baker, T.S.; Fane, B.A.; Rossmann, M.G.
Deposited on	:	2002-06-12
Resolution	:	16.00 Å(reported)
Based on initial models	:	1M06, 1CD3

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

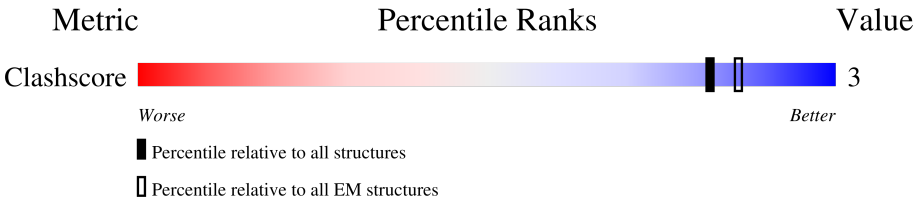
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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	158937	4297

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1	152	94% 6%
1	2	152	88% • 11%
1	3	152	91% • 8%
1	4	152	96% •
2	F	431	83% 16%
3	G	187	100%
4	B	68	97% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1179 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 Scaffolding protein D.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	1	143	Total C 143 143	0	143
1	2	135	Total C 135 135	0	135
1	3	140	Total C 140 140	0	140
1	4	146	Total C 146 146	0	146

- Molecule 2 is a protein called Capsid Protein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	F	360	Total C 360 360	0	360

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	160	GLY	ARG	SEE REMARK 999	UNP P08767

- Molecule 3 is a protein called Major Spike Protein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	G	187	Total C 187 187	0	187

- Molecule 4 is a protein called Scaffolding Protein B.

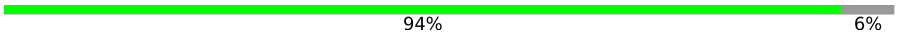
Mol	Chain	Residues	Atoms	AltConf	Trace
4	B	68	Total C 68 68	0	68

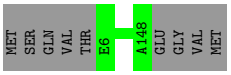
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Scaffolding protein D

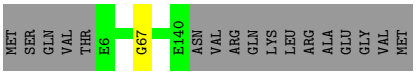
Chain 1:





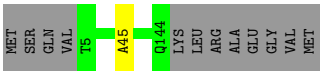
- Molecule 1: Scaffolding protein D

Chain 2:



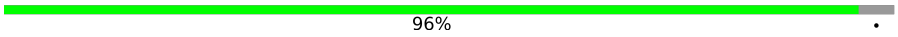
- Molecule 1: Scaffolding protein D

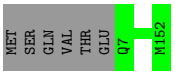
Chain 3:



- Molecule 1: Scaffolding protein D

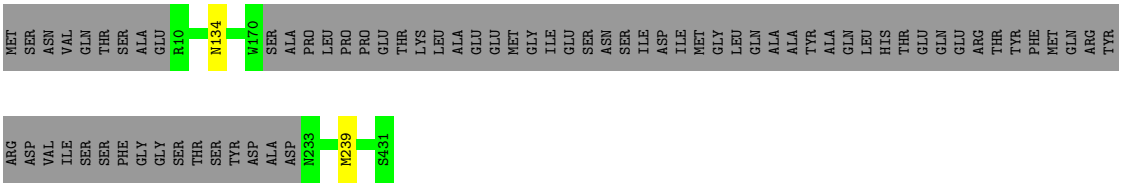
Chain 4:





- Molecule 2: Capsid Protein F

Chain F:



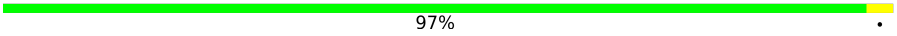
- Molecule 3: Major Spike Protein G

Chain G:

There are no outlier residues recorded for this chain.

• Molecule 4: Scaffolding Protein B

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 16.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-16.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1179	wwPDB-VP
Average B, all atoms (Å^2)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1	143	0	0	0	0
1	2	135	0	0	1	0
1	3	140	0	0	1	0
1	4	146	0	0	0	0
2	F	360	0	0	2	0
3	G	187	0	0	0	0
4	B	68	0	0	2	0
All	All	1179	0	0	3	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 3.

All (3) 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:F:134:ASN:CA	4:B:120:PHE:CA	2.24	1.14
2:F:239:MET:CA	4:B:80:GLY:CA	2.44	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:67:GLY:CA	1:3:45:ALA:CA	2.95	0.45

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.