



wwPDB EM Map/Model Validation Report ⓘ

Sep 14, 2016 – 11:16 AM EDT

PDB ID : 5GKA
EMDB ID: : EMD-9517
Title : cryo-EM structure of human Aichi virus
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Deposited on : 2016-07-04
Resolution : 3.70 Å(reported)

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) : rb-20027939

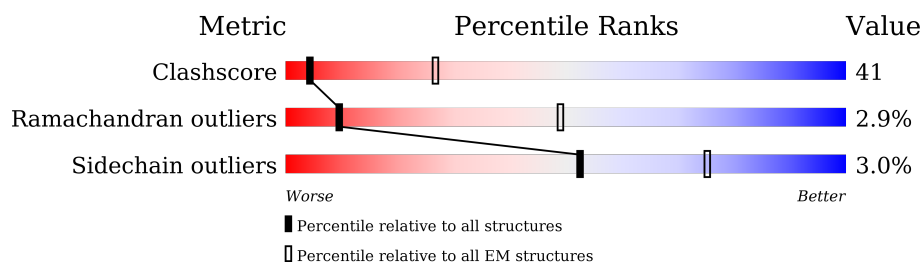
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	253	
2	B	367	
3	C	222	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6087 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	253	Total	C	N	O	S	0	0
			1911	1236	304	362	9		

- Molecule 2 is a protein called capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	333	Total	C	N	O	S	0	0
			2492	1595	409	481	7		

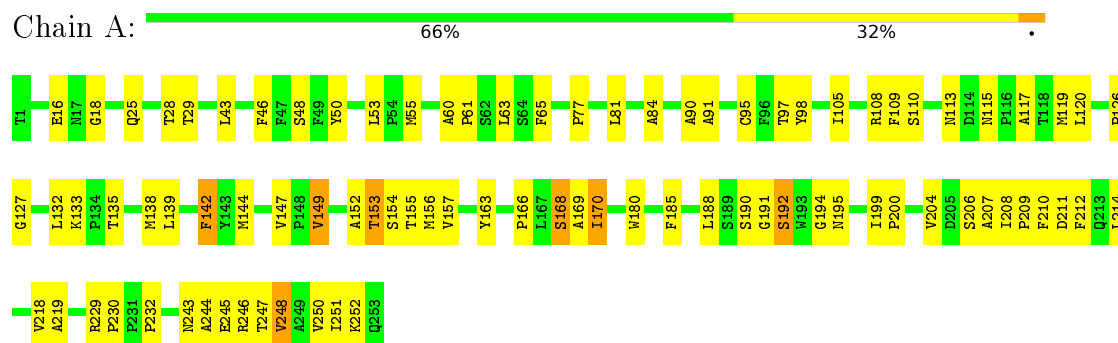
- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	222	Total	C	N	O	S	0	0
			1684	1088	285	304	7		

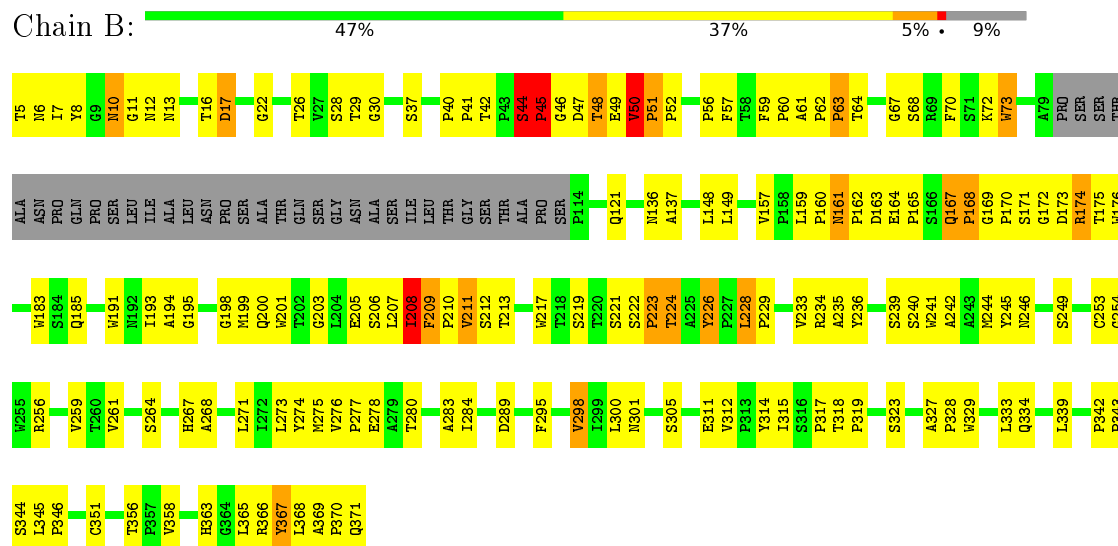
3 Residue-property plots

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.

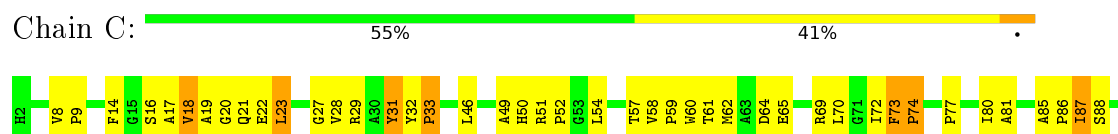
• Molecule 1: capsid protein VP1



• Molecule 2: capsid protein VP0



• Molecule 3: capsid protein VP3






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.49	0/1976	0.63	0/2720
2	B	0.61	0/2587	0.76	7/3586 (0.2%)
3	C	0.58	0/1741	0.68	1/2397 (0.0%)
All	All	0.56	0/6304	0.70	8/8703 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	44	SER	C-N-CD	5.87	140.72	128.40
2	B	169	GLY	N-CA-C	-5.51	99.33	113.10
2	B	167	GLN	C-N-CD	5.46	139.87	128.40
2	B	161	ASN	C-N-CD	5.40	139.74	128.40
3	C	73	PHE	C-N-CD	5.26	139.45	128.40

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	1911	0	1854	141	0
2	B	2492	0	2350	260	0
3	C	1684	0	1636	126	0
All	All	6087	0	5840	486	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 41.

The worst 5 of 486 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:B:217:TRP:CZ3	2:B:234:ARG:HD2	1.30	1.67
2:B:45:PRO:CB	2:B:61:ALA:HB3	1.26	1.64
2:B:367:TYR:CE2	3:C:122:THR:HG21	1.42	1.54
2:B:45:PRO:HB3	2:B:61:ALA:CB	1.35	1.50
2:B:233:VAL:HG21	2:B:371:GLN:NE2	1.22	1.48

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	251/253 (99%)	228 (91%)	19 (8%)	4 (2%)	12	58
2	B	329/367 (90%)	277 (84%)	36 (11%)	16 (5%)	3	32
3	C	220/222 (99%)	195 (89%)	22 (10%)	3 (1%)	14	60
All	All	800/842 (95%)	700 (88%)	77 (10%)	23 (3%)	9	46

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	THR
1	A	192	SER
2	B	44	SER
2	B	174	ARG
2	B	208	ILE

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	210/212 (99%)	207 (99%)	3 (1%)	74	91
2	B	276/310 (89%)	266 (96%)	10 (4%)	42	78
3	C	175/177 (99%)	168 (96%)	7 (4%)	38	76
All	All	661/699 (95%)	641 (97%)	20 (3%)	52	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	226	TYR
2	B	228	LEU
3	C	132	MET
2	B	209	PHE
2	B	224	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
2	B	371	GLN
2	B	200	GLN
1	A	35	ASN
2	B	167	GLN

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 [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.