



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:34 PM BST

PDB ID : 1JEW
Title : CRYO-EM STRUCTURE OF COXSACKIEVIRUS B3(M STRAIN) WITH ITS CELLULAR RECEPTOR, COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR (CAR).
Authors : Rossmann, M.G.; He, Y.
Deposited on : 2001-06-19
Resolution : 22.00 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) : trunk27241

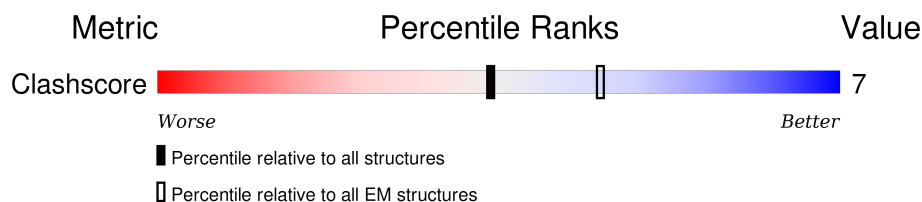
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

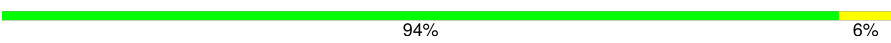
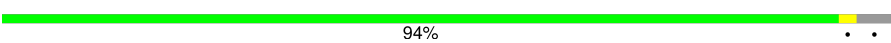
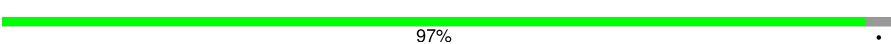
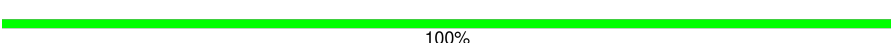

The reported resolution of this entry is 22.00 Å.

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	114402	924

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	R	120	 94% 6%
2	1	281	 94% . .
3	2	263	 97% .
4	3	238	 100%
5	4	68	 81% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 938 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	R	120	Total	C	0	120
			120	120		

- Molecule 2 is a protein called COXSACKIEVIRUS CAPSID, COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	1	269	Total	C	0	269
			269	269		

- Molecule 3 is a protein called COXSACKIEVIRUS CAPSID, COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	2	256	Total	C	0	256
			256	256		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	151	THR	SER	CONFLICT	UNP Q66282
2	245	VAL	ILE	CONFLICT	UNP Q66282

- Molecule 4 is a protein called COXSACKIEVIRUS CAPSID, COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	3	238	Total	C	0	238
			238	238		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	234	GLU	GLN	CONFLICT	UNP Q66282

- Molecule 5 is a protein called COXSACKIEVIRUS CAPSID, COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	4	55	Total	C	0	55
			55	55		

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.

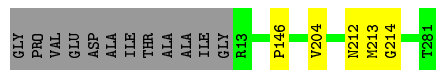
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain R: 



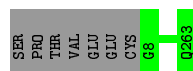
- Molecule 2: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP1

Chain 1: 



- Molecule 3: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP2

Chain 2: 




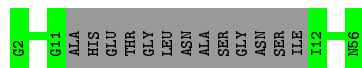
- Molecule 4: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP3

Chain 3: 

There are no outlier residues recorded for this chain.

- Molecule 5: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP4

Chain 4: 



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of images	Not provided	Depositor
Resolution determination method	THE RESOLUTION OF THE FINAL RECONSTRUCTED DENSITY WAS DETERMINED TO BE AT LEAST 22 ANGSTROMS, AS MEASURED BY RANDOMLY SPLITTING THE PARTICLES INTO TWO SETS AND COMPARING STRUCTURE FACTORS OBTAINED FROM SEPARATE RECONSTRUCTIONS (BAKER ET AL. 1991, BIOPHYS.J. 60, 1445-1456). THE EIGENVALUE SPECTRUM GAVE AN INDICATION OF THE RANDOMNESS OF THE DATA THAT WAS INCLUDED IN THE RECONSTRUCTION. THE COMPLETENESS OF THE DATA WAS VERIFIED IN THAT ALL EIGENVALUES EXCEEDED 1.0.	Depositor
CTF correction method	Not provided	Depositor
Microscope	PHILLIPS CM300 FEG	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4600	Depositor
Magnification	61000	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	R	120	0	0	7	0
2	1	269	0	0	6	0
3	2	256	0	0	0	0
4	3	238	0	0	0	0
5	4	55	0	0	0	0
All	All	938	0	0	7	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 7.

All (7) 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:R:50:GLU:CA	2:1:213:MET:CA	1.83	1.50
1:R:48:SER:CA	2:1:212:ASN:CA	2.10	1.27
1:R:49:PRO:CA	2:1:212:ASN:CA	2.14	1.24
1:R:50:GLU:CA	2:1:214:GLY:CA	2.40	0.99

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:25:THR:CA	2:1:204:VAL:CA	2.71	0.68
1:R:52:GLN:CA	2:1:146:PRO:CA	2.93	0.46
1:R:127:ALA:CA	1:R:128:PRO:CA	2.97	0.43

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 ⓘ

There are no chain breaks in this entry.