Full wwPDB EM Validation Report (i)

Dec 13, 2022 – 12:02 AM EST

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 Full wwPDB EM Validation 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:

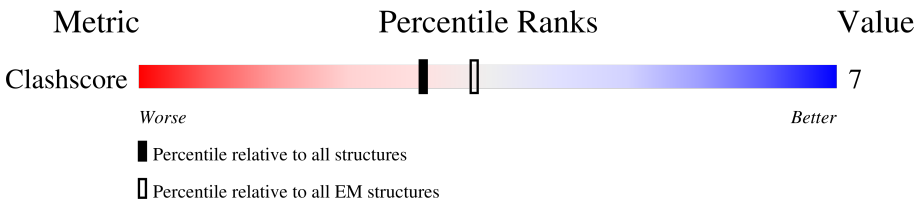
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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

2 Entry composition (i)

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
			Total	C		
1	R	120	120	120	0	120

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

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

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

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	2	256	256	256	0	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
			Total	C		
4	3	238	238	238	0	238

There is a discrepancy between the modelled and reference sequences:

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

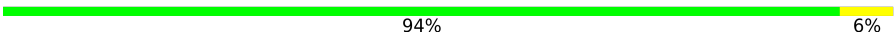
- Molecule 5 is a protein called COXSACKIEVIRUS CAPSID, COAT PROTEIN VP4.

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

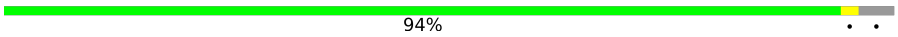
3 Residue-property plots (i)

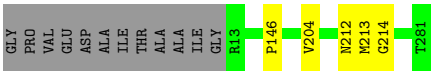
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

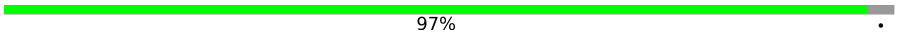
Chain R: 

• Molecule 2: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP1

Chain 1: 



• Molecule 3: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP2

Chain 2: 

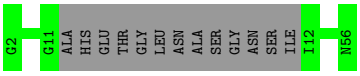
• Molecule 4: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP3

Chain 3:

There are no outlier residues recorded for this chain.

• Molecule 5: COXSACKIEVIRUS CAPSID, COAT PROTEIN VP4

Chain 4:



4 Data and refinement statistics (i)

Xtriage (Phenix) and 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) – 22.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-22.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	938	wwPDB-VP
Average B, all atoms ($Å^2$)	15.0	wwPDB-VP

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	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...

Continued from previous page...

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 monosaccharides 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.