



wwPDB EM Map/Model Validation Report ⓘ

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PDB ID : 3JB4
EMDB ID: : EMD-6394
Title : Structure of Ljungan virus: insight into picornavirus packaging
Authors : Zhu, L.; Wang, X.X.; Ren, J.S.; Porta, C.; Wenham, H.; Ekstrom, J.-O.; Panjwani, A.; Knowles, N.J.; Kotecha, A.; Siebert, A.; Lindberg, M.; Fry, E.E.; Rao, Z.H.; Tuthill, T.J.; Stuart, D.I.
Deposited on : 2015-07-21
Resolution : 3.80 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

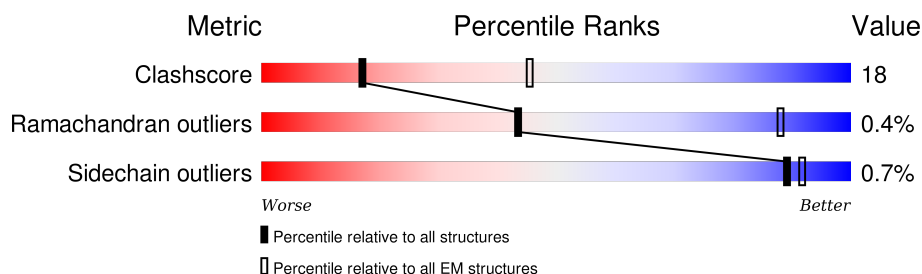
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	297	
2	B	259	
3	C	244	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5272 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	212	Total	C	N	O	S	0	0
			1648	1046	289	305	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	LEU	ALA	CONFLICT	UNP Q8JV21
A	80	THR	SER	CONFLICT	UNP Q8JV21
A	125	HIS	PHE	CONFLICT	UNP Q8JV21
A	242	ALA	ARG	CONFLICT	UNP Q8JV21

- Molecule 2 is a protein called VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	222	Total	C	N	O	S	0	0
			1713	1090	290	324	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	LEU	PRO	CONFLICT	UNP Q8JV21

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	241	Total	C	N	O	S	0	0
			1911	1213	334	349	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	161	ASP	GLU	CONFLICT	UNP Q8JV21
C	243	MET	TRP	CONFLICT	UNP Q8JV21

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	5558	Depositor
Resolution determination method	FSC 0.143	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)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4k x 4k)	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.37	0/1690	0.54	1/2298 (0.0%)
2	B	0.39	0/1765	0.52	0/2427
3	C	0.40	0/1958	0.55	0/2658
All	All	0.39	0/5413	0.54	1/7383 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	84	ASP	Peptide

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	1648	0	1602	59	0
2	B	1713	0	1632	63	0
3	C	1911	0	1871	95	0
All	All	5272	0	5105	187	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 18.

The worst 5 of 187 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:A:76:ILE:HD12	3:C:189:TRP:CZ3	1.45	1.48
1:A:76:ILE:CD1	3:C:189:TRP:HZ3	1.34	1.36
2:B:197:VAL:CG1	3:C:58:GLY:CA	2.21	1.19
2:B:197:VAL:HG12	3:C:58:GLY:CA	1.73	1.18
2:B:197:VAL:HG12	3:C:58:GLY:N	1.66	1.09

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	210/297 (71%)	204 (97%)	4 (2%)	2 (1%)	19	66
2	B	220/259 (85%)	211 (96%)	9 (4%)	0	100	100
3	C	239/244 (98%)	227 (95%)	11 (5%)	1 (0%)	39	80
All	All	669/800 (84%)	642 (96%)	24 (4%)	3 (0%)	43	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	16	VAL

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Mol	Chain	Res	Type
1	A	198	ASN
1	A	231	PHE

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	178/253 (70%)	176 (99%)	2 (1%)	80	92
2	B	186/220 (84%)	186 (100%)	0	100	100
3	C	207/210 (99%)	205 (99%)	2 (1%)	82	92
All	All	571/683 (84%)	567 (99%)	4 (1%)	89	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LEU
1	A	202	LEU
3	C	61	VAL
3	C	190	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	189	GLN
3	C	244	GLN
3	C	106	HIS
1	A	174	ASN
3	C	123	ASN

5.3.3 RNA ⓘ

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.