

Nov 29, 2022 - 01:51 AM EST

PDB ID 7UD4 : EMDB ID EMD-26453 : Cryo-EM structure of AAV-PHP.eB Title : Authors Jang, S.; Shen, H.K.; Ding, X.; Miles, T.F.; Gradinaru, V. : Deposited on 2022-03-18 : 2.24 Å(reported) Resolution : Based on initial model 3UX1 ·

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 (1)) were used in the production of this report:

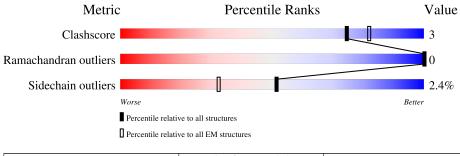
EMDB validation analysis	:	0.0.1. dev 43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.24 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	EM structures		
Metric	$(\# {\rm Entries})$	$(\# \mathbf{Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		

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	٨	749						
	A	743	63%	7%	30%			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4163 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	А	522	Total 4163	C 2630	N 722	O 797	S 14	0	0

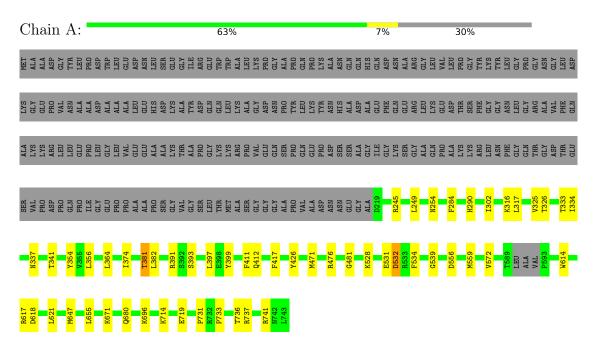
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	587	ASP	ALA	conflict	UNP Q6JC40
А	588	GLY	-	insertion	UNP Q6JC40
А	589	THR	-	insertion	UNP Q6JC40
А	590	LEU	-	insertion	UNP Q6JC40
А	591	ALA	-	insertion	UNP Q6JC40
А	592	VAL	-	insertion	UNP Q6JC40
A	593	PRO	-	insertion	UNP Q6JC40
А	594	PHE	-	insertion	UNP Q6JC40
А	595	LYS	GLN	conflict	UNP Q6JC40



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: Capsid protein VP1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/4289	0.48	0/5842	

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	А	4163	0	3915	26	0
All	All	4163	0	3915	26	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 (26) 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:381:THR:HG21	1:A:393:SER:H	1.46	0.81
1:A:618:ASP:OD1	1:A:736:THR:OG1	2.17	0.62
1:A:539:GLY:O	1:A:617:ARG:NH2	2.38	0.57
1:A:382:LEU:HD12	1:A:391:ARG:HB3	1.87	0.55
1:A:316:LYS:HG3	1:A:412:GLN:HG3	1.88	0.54

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EMD-26453,	7UD4
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Continued from prev	1.0	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:337:ASN:ND2	1:A:680:GLN:OE1	2.41	0.53
1:A:317:LEU:HB2	1:A:411:PHE:HB3	1.91	0.52
1:A:417:PHE:HD2	1:A:647:MET:HE1	1.76	0.51
1:A:471:MET:O	1:A:476:ARG:NH2	2.40	0.50
1:A:559:MET:HE3	1:A:733:PRO:HG3	1.93	0.50
1:A:302:ILE:HG22	1:A:736:THR:HG22	1.96	0.48
1:A:531:GLU:HB3	1:A:534:PHE:HD2	1.79	0.47
1:A:426:TYR:O	1:A:737:ARG:HG2	2.18	0.44
1:A:528:LYS:HG3	1:A:572:VAL:HG21	1.99	0.43
1:A:397:LEU:HD21	1:A:655:LEU:HD22	2.00	0.43
1:A:245:ARG:HG3	1:A:364:LEU:HB3	2.00	0.43
1:A:284:PHE:CZ	1:A:317:LEU:HD21	2.54	0.43
1:A:696:LYS:HA	1:A:696:LYS:HD3	1.78	0.42
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.92	0.42
1:A:532:ASP:OD2	1:A:532:ASP:N	2.52	0.42
1:A:290:HIS:N	1:A:621:LEU:O	2.53	0.41
1:A:325:VAL:HG22	1:A:334:ILE:HG12	2.02	0.41
1:A:249:LEU:HB2	1:A:374:ILE:HD12	2.02	0.41
1:A:719:GLU:HB3	1:A:731:PRO:HG3	2.02	0.41
1:A:354:TYR:CE2	1:A:356:LEU:HB2	2.56	0.41
1:A:481:GLY:HA3	1:A:614:TRP:HB3	2.03	0.40

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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	А	518/743~(70%)	509~(98%)	9~(2%)	0	100	100

There are no Ramachandran outliers to report.



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	457/621~(74%)	446 (98%)	11 (2%)	49 55

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	254	ASN
1	А	326	THR
1	А	333	THR
1	А	341	THR
1	А	381	THR
1	А	399	TYR
1	А	532	ASP
1	А	556	ASP
1	А	671	LYS
1	А	714	LYS
1	А	741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26453. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section was not generated.

