Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 30, 2017 – 08:42 PM EST

PDB ID	:	5WTF
EMDB ID:	:	EMD-6687
Title	:	Cryo-EM structure for Hepatitis A virus empty particle
Authors	:	Wang, X.; Zhu, L.; Dang, M.; Hu, Z.; Gao, Q.; Yuan, S.; Sun, Y.; Zhang, B.; Ren, J.; Walter, T.S.; Wang, J.; Fry, E.E.; Stuart, D.I.; Rao, Z.
Deposited on	:	2016-12-11
Resolution	:	3.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

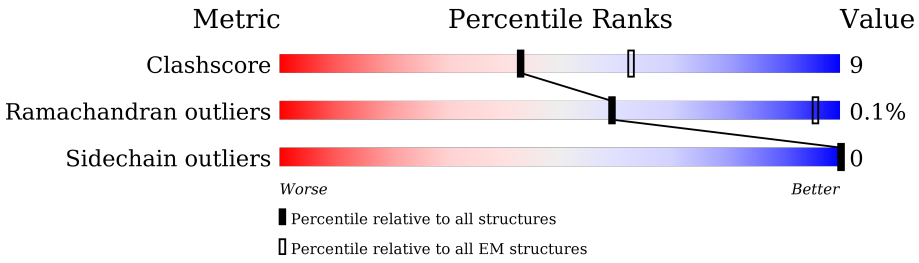
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.90 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	224	76% 24%
2	B	203	80% 20%
3	C	246	80% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5343 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
			Total	C	N	O	S		
1	A	224	1777	1146	289	336	6	0	0

- Molecule 2 is a protein called VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	203	1610	1040	273	294	3	0	0

- Molecule 3 is a protein called VP3.

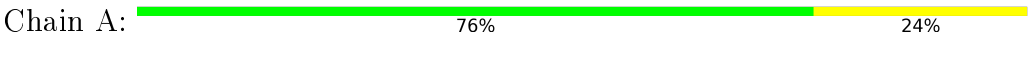
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	246	1956	1248	331	363	14	0	0

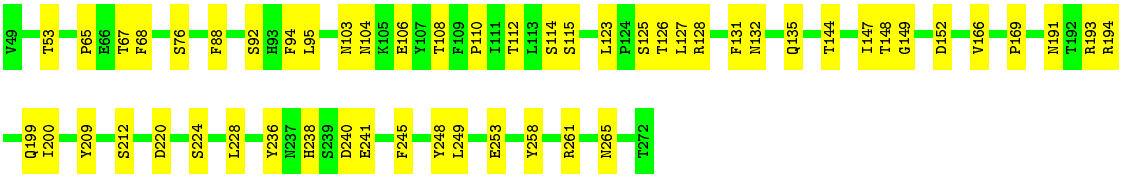
3 Residue-property plots (i)

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: VP1

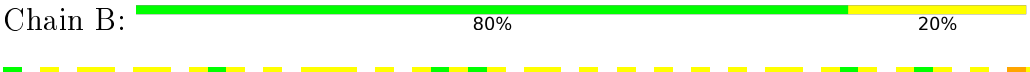
Chain A:

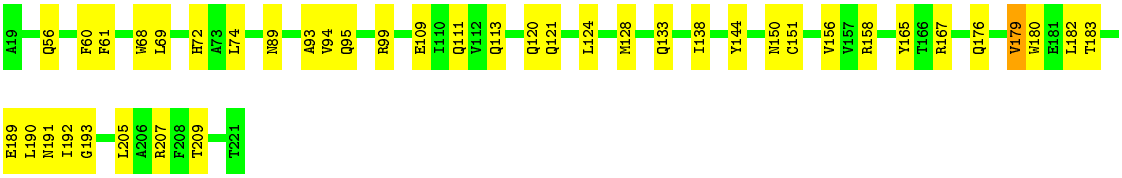




- Molecule 2: VP0

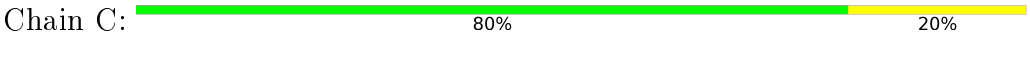
Chain B:

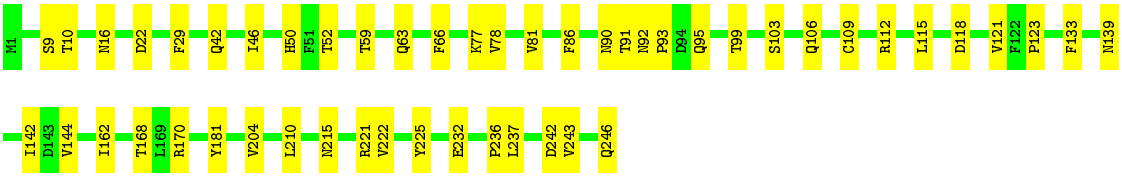




- Molecule 3: VP3

Chain C:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4000	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 ($e^-/Å^2$)	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	0.43	0/1829	0.50	0/2495
2	B	0.45	0/1654	0.52	0/2255
3	C	0.45	0/2007	0.50	0/2733
All	All	0.44	0/5490	0.51	0/7483

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	TYR	Peptide

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	1777	0	1722	38	0
2	B	1610	0	1595	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1956	0	1911	40	0
All	All	5343	0	5228	91	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 9.

All (91) 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:111:GLN:HB2	2:B:205:LEU:HB2	1.63	0.80
2:B:95:GLN:HE21	2:B:99:ARG:HB2	1.49	0.76
3:C:118:ASP:HB2	3:C:225:TYR:HB2	1.70	0.73
1:A:135:GLN:NE2	1:A:212:SER:OG	2.25	0.69
2:B:111:GLN:OE1	2:B:158:ARG:HG2	1.95	0.67
1:A:115:SER:OG	1:A:132:ASN:OD1	2.13	0.65
3:C:90:ASN:OD1	3:C:91:THR:N	2.30	0.65
2:B:167:ARG:HH12	2:B:176:GLN:HG2	1.62	0.64
1:A:110:PRO:HD3	1:A:169:PRO:HB3	1.80	0.63
1:A:106:GLU:OE2	1:A:108:THR:OG1	2.16	0.62
1:A:265:ASN:ND2	3:C:95:GLN:OE1	2.34	0.61
2:B:109:GLU:OE1	2:B:207:ARG:NE	2.33	0.58
2:B:69:LEU:H	2:B:72:HIS:CD2	2.20	0.58
2:B:113:GLN:HG2	2:B:156:VAL:HG22	1.85	0.57
1:A:88:PHE:HE1	3:C:236:PRO:HB3	1.69	0.57
2:B:69:LEU:H	2:B:72:HIS:HD2	1.51	0.56
1:A:112:THR:HG22	1:A:114:SER:H	1.71	0.56
1:A:238:HIS:NE2	1:A:241:GLU:OE1	2.40	0.54
3:C:50:HIS:CE1	3:C:52:THR:HG1	2.26	0.54
2:B:138:ILE:HG12	3:C:95:GLN:NE2	2.23	0.54
1:A:209:TYR:CE2	3:C:42:GLN:HB2	2.43	0.54
3:C:81:VAL:HG12	3:C:115:LEU:HD12	1.90	0.54
1:A:65:PRO:HB3	3:C:170:ARG:HD3	1.90	0.53
2:B:61:PHE:HE2	2:B:94:VAL:HB	1.74	0.53
3:C:78:VAL:HG21	3:C:144:VAL:HG11	1.90	0.53
3:C:16:ASN:ND2	3:C:22:ASP:OD2	2.32	0.53
1:A:265:ASN:HD22	3:C:95:GLN:HB2	1.72	0.53
1:A:147:ILE:HG23	1:A:245:PHE:HE1	1.74	0.53
1:A:166:VAL:HG11	1:A:228:LEU:HD22	1.91	0.52
3:C:112:ARG:HD2	3:C:181:TYR:CE1	2.45	0.52
2:B:138:ILE:HG12	3:C:95:GLN:HE22	1.75	0.52
1:A:261:ARG:HA	2:B:144:TYR:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:ASP:OD1	3:C:243:VAL:N	2.44	0.51
2:B:133:GLN:HE21	2:B:183:THR:HG21	1.76	0.51
2:B:74:LEU:HB2	2:B:189:GLU:OE2	2.11	0.50
3:C:133:PHE:HD1	3:C:204:VAL:HG22	1.77	0.50
1:A:144:THR:HG1	1:A:248:TYR:HB2	1.77	0.49
3:C:63:GLN:HE21	3:C:221:ARG:HD3	1.77	0.49
1:A:88:PHE:CE1	3:C:236:PRO:HB3	2.48	0.48
1:A:94:PHE:HA	1:A:248:TYR:HD1	1.77	0.48
3:C:139:ASN:OD1	3:C:142:ILE:HG23	2.13	0.48
3:C:66:PHE:CE2	3:C:210:LEU:HB2	2.49	0.48
1:A:240:ASP:OD1	1:A:241:GLU:N	2.43	0.48
1:A:127:LEU:HD22	1:A:131:PHE:HE2	1.79	0.47
2:B:165:TYR:CD1	2:B:179:VAL:HG22	2.49	0.47
3:C:109:CYS:SG	3:C:237:LEU:HD23	2.53	0.47
1:A:53:THR:O	3:C:168:THR:HB	2.15	0.47
1:A:94:PHE:HA	1:A:248:TYR:CD1	2.49	0.47
2:B:179:VAL:HG12	2:B:180:TRP:CD1	2.50	0.46
2:B:193:GLY:HA3	3:C:215:ASN:O	2.16	0.46
1:A:67:THR:HG22	1:A:68:PHE:CD1	2.50	0.46
3:C:9:SER:OG	3:C:10:THR:N	2.49	0.46
3:C:77:LYS:HE3	3:C:246:GLN:NE2	2.31	0.46
1:A:123:LEU:O	1:A:128:ARG:HB2	2.15	0.46
1:A:191:ASN:HD22	1:A:194:ARG:HH12	1.63	0.46
3:C:121:VAL:HG12	3:C:222:VAL:HG22	1.98	0.46
2:B:191:ASN:OD1	3:C:221:ARG:NH2	2.49	0.46
1:A:92:SER:OG	1:A:248:TYR:HB3	2.16	0.45
2:B:182:LEU:HD23	2:B:183:THR:N	2.31	0.45
2:B:60:PHE:CE1	2:B:207:ARG:HD3	2.51	0.45
2:B:120:GLN:HG2	2:B:192:ILE:HG22	1.98	0.45
1:A:220:ASP:O	1:A:224:SER:OG	2.27	0.44
3:C:118:ASP:OD1	3:C:170:ARG:HG2	2.17	0.44
2:B:207:ARG:NH2	2:B:209:THR:HG22	2.33	0.44
1:A:265:ASN:HD22	3:C:95:GLN:CB	2.31	0.44
2:B:150:ASN:OD1	2:B:151:CYS:N	2.50	0.44
2:B:56:GLN:NE2	2:B:93:ALA:O	2.40	0.44
1:A:253:GLU:N	1:A:253:GLU:OE1	2.51	0.43
1:A:103:ASN:ND2	1:A:104:ASN:OD1	2.52	0.43
3:C:133:PHE:CD1	3:C:204:VAL:HG22	2.54	0.43
3:C:121:VAL:HG23	3:C:123:PRO:HD3	2.01	0.42
3:C:92:ASN:HA	3:C:93:PRO:HA	1.95	0.42
1:A:95:LEU:HD22	1:A:249:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:MET:SD	2:B:182:LEU:HD12	2.59	0.42
3:C:63:GLN:NE2	3:C:221:ARG:HD3	2.34	0.42
1:A:148:THR:HG22	1:A:149:GLY:N	2.34	0.42
2:B:95:GLN:NE2	2:B:99:ARG:HB2	2.26	0.42
1:A:125:SER:OG	1:A:126:THR:N	2.53	0.42
1:A:144:THR:HG22	1:A:199:GLN:HG2	2.02	0.42
2:B:68:TRP:CE2	2:B:124:LEU:HD21	2.55	0.41
2:B:89:ASN:O	2:B:95:GLN:HB2	2.20	0.41
1:A:152:ASP:OD1	1:A:193:ARG:HD2	2.20	0.41
3:C:103:SER:HA	3:C:106:GLN:HG2	2.02	0.41
1:A:76:SER:OG	3:C:232:GLU:OE2	2.24	0.41
1:A:200:ILE:HD13	3:C:29:PHE:CZ	2.55	0.41
1:A:258:TYR:HD1	3:C:46:ILE:O	2.04	0.41
3:C:121:VAL:HG11	3:C:162:ILE:HD12	2.02	0.41
3:C:86:PHE:CE1	3:C:243:VAL:HG22	2.55	0.41
2:B:121:GLN:O	2:B:190:LEU:HD12	2.21	0.41
1:A:144:THR:OG1	1:A:248:TYR:HB2	2.21	0.40
3:C:59:THR:OG1	3:C:99:THR:HB	2.20	0.40

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	222/224 (99%)	210 (95%)	12 (5%)	0	100 100
2	B	201/203 (99%)	188 (94%)	12 (6%)	1 (0%)	34 76
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100 100
All	All	667/673 (99%)	631 (95%)	35 (5%)	1 (0%)	59 89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	179	VAL

5.3.2 Protein sidechains (i)

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	197/197 (100%)	197 (100%)	0	100	100
2	B	177/177 (100%)	177 (100%)	0	100	100
3	C	217/217 (100%)	217 (100%)	0	100	100
All	All	591/591 (100%)	591 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	135	GLN
2	B	72	HIS
2	B	76	HIS
2	B	133	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.