



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 16, 2018 – 10:52 pm GMT

PDB ID : 5H0S
EMDB ID: : EMD-9565
Title : EM Structure of VP1A and VP1B
Authors : Li, X.; Zhou, N.; Xu, B.; Chen, W.; Zhu, B.; Wang, X.; Wang, J.; Liu, H.;
Cheng, L.
Deposited on : 2016-10-06
Resolution : 3.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary 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 ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

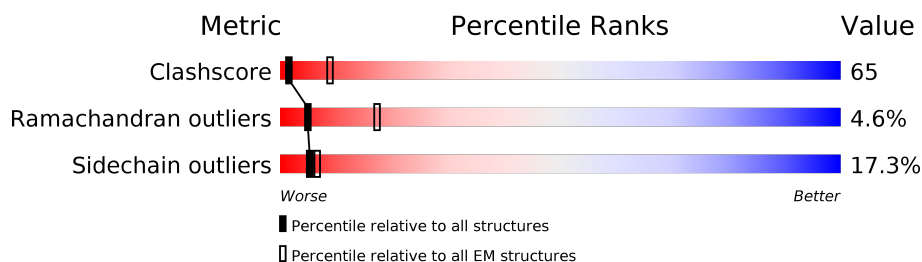
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	B	1333	
1	C	1333	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18885 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.

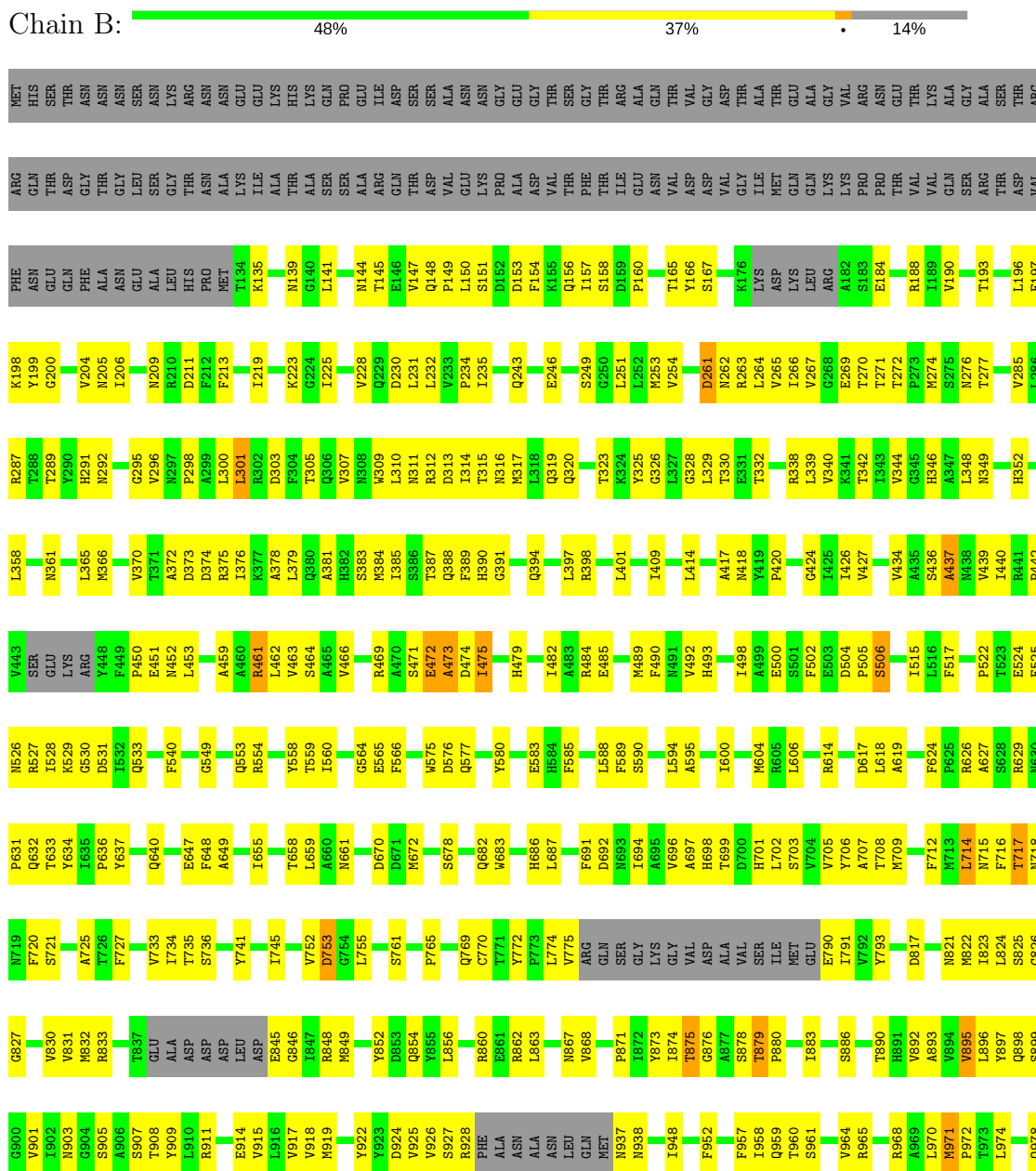
- Molecule 1 is a protein called VP1.

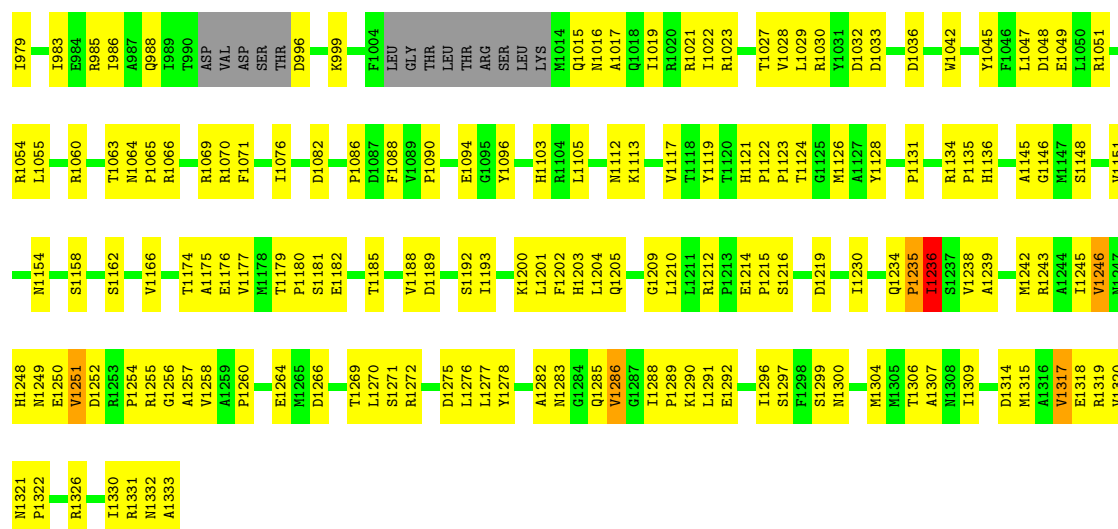
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1148	Total	C	N	O	S	0	0
			9058	5731	1574	1718	35		
1	C	1247	Total	C	N	O	S	0	0
			9827	6202	1709	1878	38		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

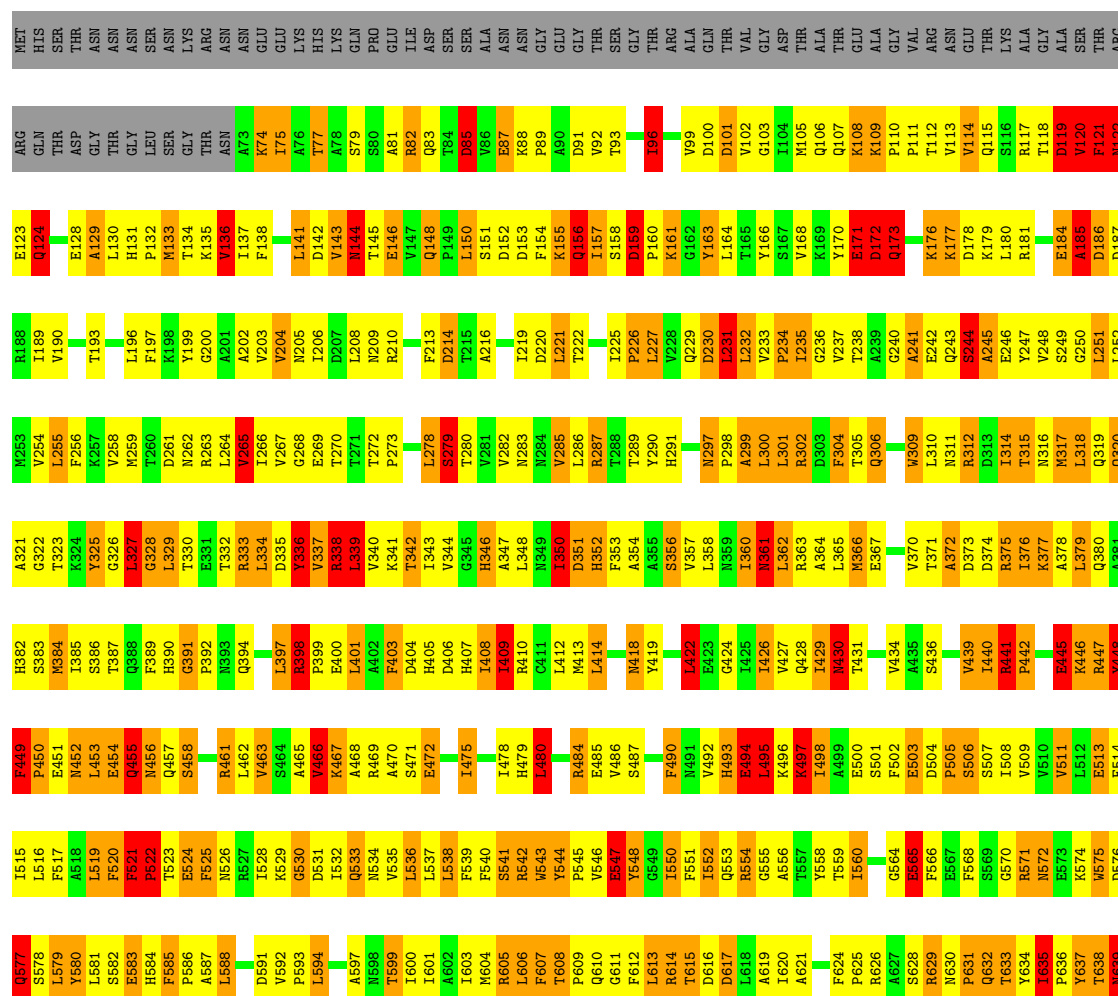
• Molecule 1: VP1





• Molecule 1: VP1

Chain C: 19% 39% 27% 8% 6%






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	27000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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	B	0.47	1/9244 (0.0%)	0.65	4/12582 (0.0%)
1	C	1.88	114/10028 (1.1%)	1.75	273/13653 (2.0%)
All	All	1.39	115/19272 (0.6%)	1.34	277/26235 (1.1%)

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	B	0	9
1	C	0	30
All	All	0	39

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	543	TRP	CB-CG	-12.16	1.28	1.50
1	C	683	TRP	CB-CG	-11.34	1.29	1.50
1	C	278	LEU	C-N	10.07	1.57	1.34
1	C	449	PHE	C-N	9.81	1.52	1.34
1	C	1167	ASP	CB-CG	-9.25	1.32	1.51

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	772	TYR	C-N-CD	-26.11	63.15	120.60
1	C	1121	HIS	C-N-CD	-19.15	78.48	120.60
1	C	870	ASP	C-N-CD	-18.50	79.91	120.60
1	C	285	VAL	O-C-N	17.98	151.47	122.70
1	C	173	GLN	O-C-N	-17.55	94.62	122.70

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	ASP	Peptide
1	B	506	SER	Peptide
1	B	717	THR	Peptide
1	B	825	SER	Peptide
1	B	875	THR	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	B	9058	0	8964	531	0
1	C	9827	0	9719	1974	0
All	All	18885	0	18683	2459	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 65.

The worst 5 of 2459 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:C:835:TYR:CE1	1:C:942:HIS:HB3	1.27	1.68
1:C:1278:TYR:CD2	1:C:1288:ILE:HG13	1.23	1.64
1:C:910:LEU:HD23	1:C:915:VAL:CG2	1.27	1.63
1:C:233:VAL:CG2	1:C:234:PRO:HD2	1.28	1.62
1:C:1093:PRO:HG2	1:C:1096:TYR:CE1	1.30	1.61

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	B	1132/1333 (85%)	999 (88%)	121 (11%)	12 (1%)	16	50
1	C	1243/1333 (93%)	937 (75%)	209 (17%)	97 (8%)	1	7
All	All	2375/2666 (89%)	1936 (82%)	330 (14%)	109 (5%)	5	17

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	VAL
1	C	121	PHE
1	C	122	ASN
1	C	129	ALA
1	C	144	ASN

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	B	1000/1155 (87%)	993 (99%)	7 (1%)	85	91
1	C	1087/1155 (94%)	733 (67%)	354 (33%)	0	1
All	All	2087/2310 (90%)	1726 (83%)	361 (17%)	5	10

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	685	ARG
1	C	849	MET
1	C	1253	ARG
1	C	720	PHE
1	C	797	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN
1	C	311	ASN
1	C	1203	HIS
1	C	229	GLN
1	C	369	ASN

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 [i](#)

There are no chain breaks in this entry.