



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3J2V
EMDB ID: : EMD-2278
Title : CryoEM structure of HBV core
Authors : Yu, X.; Jin, L.; Jih, J.; Shih, C.; Zhou, Z.H.
Deposited on : 2013-01-11
Resolution : 3.50 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>

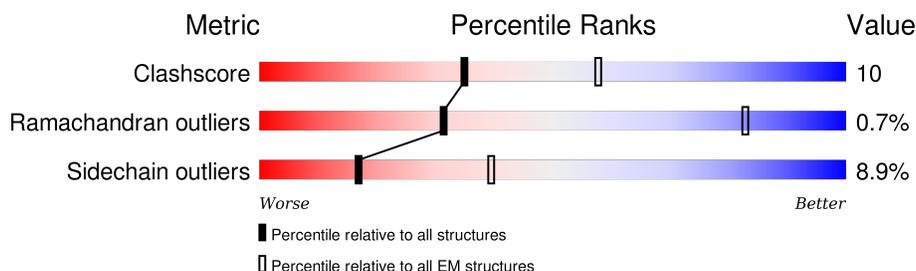
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 3.50 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	185	
1	B	185	
1	C	185	
1	D	185	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4629 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.

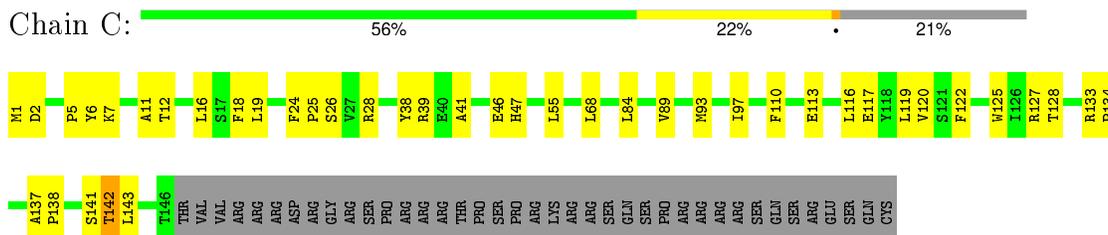
- Molecule 1 is a protein called PreC/core protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	146	1167	755	192	214	6	0	0
1	D	144	1151	746	190	209	6	0	0
1	B	146	1167	755	192	214	6	0	0
1	A	143	1144	741	189	208	6	0	0

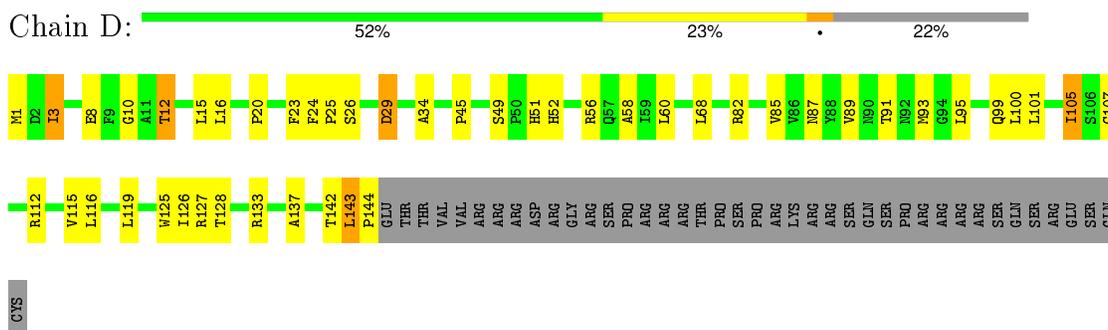
3 Residue-property plots [i](#)

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.

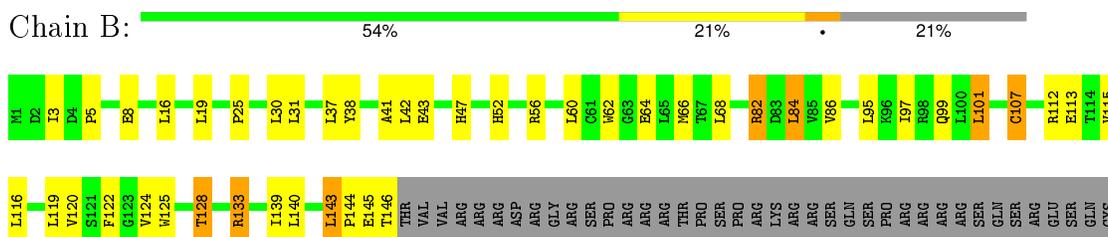
- Molecule 1: PreC/core protein



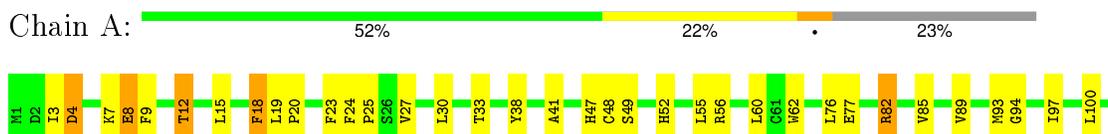
- Molecule 1: PreC/core protein



- Molecule 1: PreC/core protein



- Molecule 1: PreC/core protein



I105	S106	R112	F122	W125	R127	R133	P134	L140	S141	T142	L143	PRO	GLU	THR	THR	VAL	VAL	ARG	ARG	ARG	ASP	ARG	GLY	ARG	SER	PRO	ARG	ARG	THR	PRO	SER	PRO	PRO	ARG	LYS	ARG	ARG	SER	GLN	SER	PRO	ARG	ARG	ARG	SER	GLN	SER	ARG	GLU	SER	GLN
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	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	Not provided	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	0.36	0/1178	0.64	2/1613 (0.1%)
1	B	0.36	0/1202	0.56	0/1647
1	C	0.37	0/1202	0.59	0/1647
1	D	0.38	0/1186	0.55	0/1625
All	All	0.37	0/4768	0.59	2/6532 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ASP	C-N-CD	-6.89	105.44	120.60
1	A	4	ASP	C-N-CA	5.27	144.15	122.00

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	A	1144	0	1127	30	0
1	B	1167	0	1147	31	0
1	C	1167	0	1147	24	0
1	D	1151	0	1134	27	0
All	All	4629	0	4555	96	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 10.

The worst 5 of 96 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:B:47:HIS:ND1	1:A:8:GLU:OE2	2.17	0.77
1:D:51:HIS:NE2	1:D:107:CYS:SG	2.62	0.71
1:C:38:TYR:HB3	1:C:41:ALA:HB3	1.73	0.70
1:A:20:PRO:HG2	1:A:23:PHE:HB2	1.76	0.68
1:B:8:GLU:OE1	1:A:56:ARG:NH1	2.27	0.67

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	141/185 (76%)	136 (96%)	4 (3%)	1 (1%)	26	72
1	B	144/185 (78%)	137 (95%)	6 (4%)	1 (1%)	26	72
1	C	144/185 (78%)	138 (96%)	6 (4%)	0	100	100
1	D	142/185 (77%)	134 (94%)	6 (4%)	2 (1%)	14	58
All	All	571/740 (77%)	545 (95%)	22 (4%)	4 (1%)	31	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	ILE
1	D	143	LEU
1	B	143	LEU
1	A	3	ILE

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	127/168 (76%)	116 (91%)	11 (9%)	13	48
1	B	130/168 (77%)	119 (92%)	11 (8%)	13	49
1	C	130/168 (77%)	117 (90%)	13 (10%)	9	41
1	D	128/168 (76%)	117 (91%)	11 (9%)	13	49
All	All	515/672 (77%)	469 (91%)	46 (9%)	17	47

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	112	ARG
1	B	43	GLU
1	A	112	ARG
1	D	126	ILE
1	D	142	THR

Some 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 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.