wwPDB EM Map/Model Validation Report (i)

May 11, 2016 – 01:27 PM EDT

PDB ID	:	3J7L
EMDB ID:	:	EMD-6000
Title	:	Full virus map of brome mosaic virus
Authors	:	Wang, Z.; Hryc, C.; Bammes, B.; Afonine, P.V.; Jakana, J.; Chen, D.H.; Liu, X.; Baker, M.L.; Kao, C.; Ludtke, S.J.; Schmid, M.F.; Adams, P.D.; Chiu, W.
Deposited on	:	2014-07-18
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

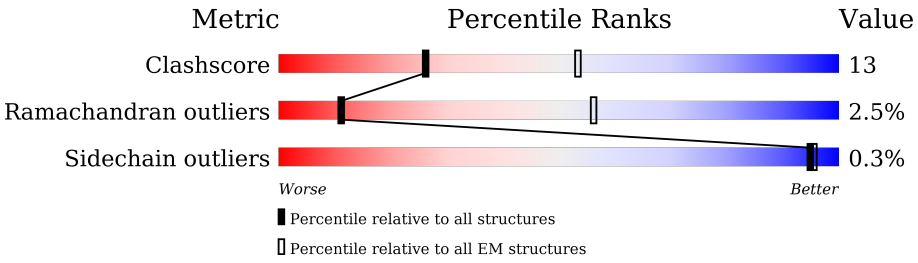
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 3.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	189	53% 25% • 21%
1	B	189	59% 26% • 13%
1	C	189	61% 24% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3613 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.

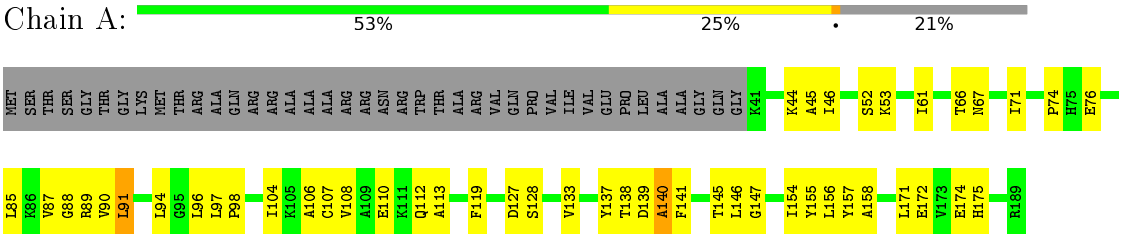
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	149	Total	C	N	O	S	0	0
			1133	728	190	212	3		
1	B	164	Total	C	N	O	S	0	0
			1240	796	210	231	3		
1	C	164	Total	C	N	O	S	0	0
			1240	796	210	231	3		

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.

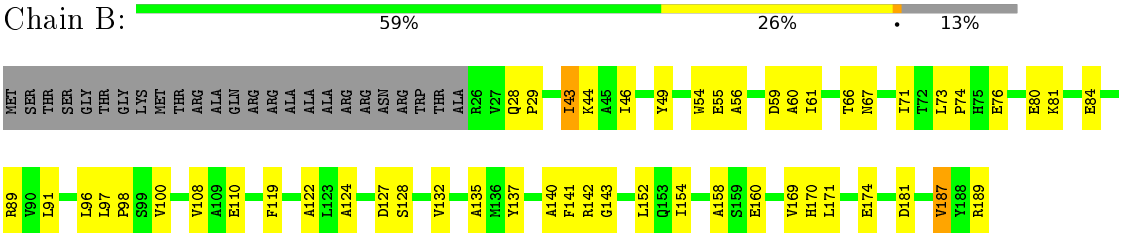
- Molecule 1: Capsid protein

Chain A:



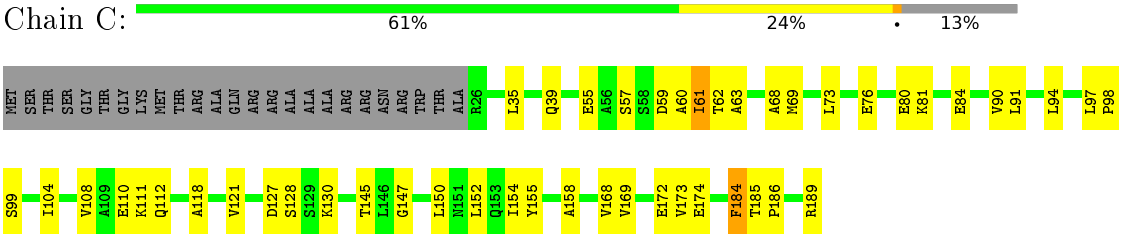
- Molecule 1: Capsid protein

Chain B:



- Molecule 1: Capsid protein

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	30000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	50000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	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	0.44	0/1154	0.57	0/1566
1	B	0.48	0/1263	0.58	0/1716
1	C	0.46	0/1263	0.54	0/1716
All	All	0.46	0/3680	0.56	0/4998

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

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	1133	0	1159	34	0
1	B	1240	0	1273	37	0
1	C	1240	0	1273	31	0
All	All	3613	0	3705	97	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 13.

All (97) 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:97:LEU:HD12	1:B:98:PRO:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HG22	1:A:147:GLY:H	1.42	0.81
1:C:145:THR:HG22	1:C:147:GLY:H	1.46	0.80
1:B:96:LEU:HD22	1:B:100:VAL:HG21	1.63	0.79
1:B:43:ILE:HG22	1:B:44:LYS:H	1.55	0.71
1:A:139:ASP:O	1:A:141:PHE:N	2.26	0.69
1:A:71:ILE:HD11	1:A:154:ILE:HG23	1.78	0.65
1:B:73:LEU:HG	1:B:74:PRO:HD2	1.80	0.64
1:B:56:ALA:HB3	1:B:169:VAL:HG23	1.78	0.64
1:A:61:ILE:HA	1:A:67:ASN:HD22	1.64	0.63
1:A:108:VAL:HG12	1:A:154:ILE:HG22	1.80	0.61
1:C:57:SER:HA	1:C:168:VAL:HG12	1.82	0.61
1:A:71:ILE:HD12	1:A:171:LEU:HD11	1.82	0.60
1:A:127:ASP:OD1	1:A:128:SER:N	2.35	0.60
1:A:53:LYS:HG2	1:A:172:GLU:HG2	1.83	0.60
1:C:104:ILE:HG22	1:C:158:ALA:HA	1.83	0.60
1:B:124:ALA:HA	1:C:189:ARG:HG3	1.84	0.59
1:A:97:LEU:HD12	1:A:98:PRO:HD2	1.83	0.59
1:A:96:LEU:HD11	1:A:104:ILE:HD11	1.83	0.59
1:C:97:LEU:HD23	1:C:99:SER:H	1.69	0.57
1:B:187:VAL:N	1:B:189:ARG:H	2.04	0.56
1:B:54:TRP:CE2	1:B:171:LEU:HD11	2.40	0.55
1:C:80:GLU:OE1	1:C:80:GLU:N	2.40	0.55
1:C:108:VAL:HG22	1:C:154:ILE:HG22	1.89	0.54
1:A:66:THR:HG22	1:A:157:TYR:HD1	1.72	0.54
1:B:43:ILE:HG22	1:B:44:LYS:N	2.23	0.54
1:C:94:LEU:HB3	1:C:169:VAL:HG12	1.90	0.53
1:A:96:LEU:HD21	1:A:104:ILE:HG12	1.89	0.53
1:B:46:ILE:HG23	1:B:49:TYR:CD2	2.43	0.53
1:B:55:GLU:OE1	1:B:170:HIS:ND1	2.42	0.53
1:C:55:GLU:OE1	1:C:55:GLU:N	2.42	0.53
1:C:108:VAL:HG13	1:C:152:LEU:HD21	1.92	0.52
1:C:84:GLU:N	1:C:84:GLU:OE1	2.44	0.51
1:A:127:ASP:O	1:A:133:VAL:HA	2.11	0.51
1:B:119:PHE:O	1:C:189:ARG:NH2	2.43	0.51
1:C:127:ASP:OD2	1:C:130:LYS:N	2.40	0.51
1:B:108:VAL:HG22	1:B:137:TYR:CZ	2.46	0.51
1:B:59:ASP:OD1	1:B:60:ALA:N	2.44	0.51
1:C:172:GLU:OE1	1:C:172:GLU:N	2.44	0.50
1:B:46:ILE:HG23	1:B:49:TYR:HD2	1.76	0.50
1:C:73:LEU:HD13	1:C:150:LEU:HD23	1.94	0.50
1:B:122:ALA:O	1:C:189:ARG:NE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:O	1:C:112:GLN:N	2.45	0.49
1:A:112:GLN:OE1	1:A:112:GLN:N	2.46	0.49
1:C:76:GLU:N	1:C:76:GLU:OE1	2.45	0.48
1:B:160:GLU:N	1:B:160:GLU:OE1	2.46	0.48
1:C:90:VAL:HG23	1:C:173:VAL:HG12	1.95	0.48
1:C:35:LEU:HG	1:C:39:GLN:HG2	1.95	0.48
1:B:81:LYS:NZ	1:B:181:ASP:OD1	2.24	0.48
1:C:104:ILE:HG13	1:C:128:SER:OG	2.13	0.48
1:B:110:GLU:N	1:B:110:GLU:OE1	2.45	0.47
1:A:85:LEU:HB2	1:A:146:LEU:HD12	1.96	0.47
1:A:46:ILE:HG13	1:A:89:ARG:HH12	1.79	0.47
1:B:137:TYR:HB3	1:B:140:ALA:HB3	1.96	0.47
1:C:97:LEU:HG	1:C:98:PRO:HD2	1.97	0.47
1:B:97:LEU:O	1:B:100:VAL:HG22	2.15	0.46
1:B:89:ARG:N	1:B:174:GLU:OE2	2.42	0.46
1:C:69:MET:HB3	1:C:154:ILE:HG13	1.98	0.46
1:A:74:PRO:HB2	1:A:76:GLU:HG2	1.98	0.46
1:A:87:VAL:HG12	1:A:88:GLY:O	2.16	0.46
1:B:91:LEU:HD12	1:B:135:ALA:O	2.16	0.46
1:B:55:GLU:CD	1:B:170:HIS:HD1	2.20	0.45
1:A:107:CYS:HG	1:A:119:PHE:HD1	1.65	0.45
1:A:110:GLU:OE2	1:B:80:GLU:HG2	2.16	0.45
1:B:71:ILE:HD11	1:B:171:LEU:HD21	1.97	0.45
1:B:84:GLU:N	1:B:84:GLU:OE1	2.49	0.45
1:A:44:LYS:HG3	1:A:45:ALA:O	2.16	0.45
1:A:52:SER:HB3	1:A:175:HIS:HE1	1.82	0.45
1:B:127:ASP:OD1	1:B:128:SER:N	2.50	0.45
1:A:137:TYR:HB3	1:A:140:ALA:HB3	1.99	0.45
1:C:68:ALA:HB2	1:C:155:TYR:HE1	1.81	0.44
1:A:104:ILE:HG22	1:A:158:ALA:HB2	1.99	0.44
1:B:66:THR:O	1:B:67:ASN:ND2	2.51	0.44
1:B:142:ARG:HA	1:B:143:GLY:HA2	1.62	0.44
1:B:141:PHE:CZ	1:B:152:LEU:HD21	2.53	0.43
1:B:154:ILE:HD12	1:B:169:VAL:HG21	2.00	0.43
1:B:76:GLU:N	1:B:76:GLU:OE1	2.52	0.43
1:C:108:VAL:CG1	1:C:152:LEU:HD21	2.49	0.43
1:B:28:GLN:HA	1:B:29:PRO:HD3	1.86	0.43
1:C:174:GLU:OE1	1:C:174:GLU:N	2.52	0.42
1:B:142:ARG:O	1:C:81:LYS:HD2	2.19	0.42
1:C:59:ASP:O	1:C:61:ILE:N	2.48	0.42
1:B:54:TRP:CZ2	1:B:171:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:PHE:HB3	1:C:185:THR:H	1.62	0.42
1:A:137:TYR:HB3	1:A:140:ALA:CB	2.50	0.42
1:A:106:ALA:HA	1:A:155:TYR:O	2.19	0.42
1:A:94:LEU:HD13	1:A:96:LEU:HD11	2.01	0.41
1:A:106:ALA:HB2	1:A:156:LEU:HD23	2.01	0.41
1:A:94:LEU:O	1:A:94:LEU:HD12	2.21	0.41
1:A:89:ARG:HB2	1:A:138:THR:HA	2.03	0.41
1:A:91:LEU:HD13	1:A:172:GLU:HB2	2.03	0.41
1:A:90:VAL:HG11	1:A:141:PHE:CD2	2.56	0.41
1:C:118:ALA:HA	1:C:121:VAL:HG12	2.02	0.40
1:C:91:LEU:HB3	1:C:172:GLU:OE2	2.20	0.40
1:B:61:ILE:HD13	1:B:158:ALA:HB3	2.03	0.40
1:A:46:ILE:N	1:A:174:GLU:OE2	2.53	0.40
1:A:71:ILE:HD11	1:A:154:ILE:CG2	2.49	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	147/189 (78%)	138 (94%)	7 (5%)	2 (1%)	14 59
1	B	162/189 (86%)	149 (92%)	10 (6%)	3 (2%)	10 54
1	C	162/189 (86%)	147 (91%)	8 (5%)	7 (4%)	3 35
All	All	471/567 (83%)	434 (92%)	25 (5%)	12 (2%)	11 49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ALA
1	B	43	ILE
1	B	187	VAL

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Mol	Chain	Res	Type
1	C	61	ILE
1	A	113	ALA
1	B	132	VAL
1	C	62	THR
1	C	111	LYS
1	C	63	ALA
1	C	60	ALA
1	C	184	PHE
1	C	186	PRO

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	117/146 (80%)	116 (99%)	1 (1%)	84 93
1	B	128/146 (88%)	128 (100%)	0	100 100
1	C	128/146 (88%)	128 (100%)	0	100 100
All	All	373/438 (85%)	372 (100%)	1 (0%)	95 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	175	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

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.