



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:08 PM BST

PDB ID : 5A79  
EMDB ID: : EMD-3073  
Title : Novel inter-subunit contacts in Barley Stripe Mosaic Virus revealed by cryo-EM  
Authors : Clare, D.K.; Pechnikova, E.; Skurat, E.; Makarov, V.; Sokolova, O.S.; Solovyev, A.G.; V Orlova, E.  
Deposited on : 2015-07-03  
Resolution : 4.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

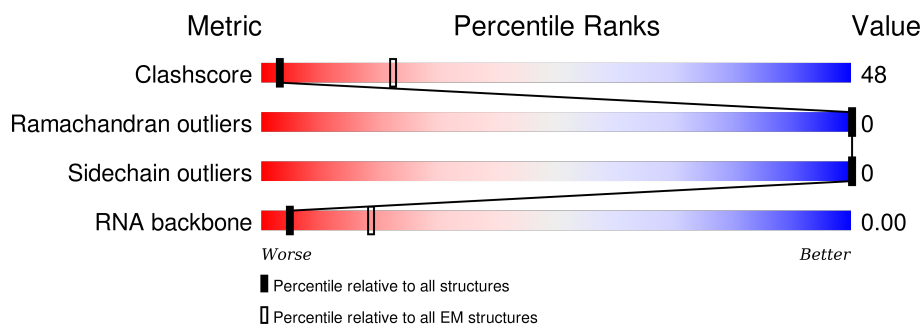
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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
RNA backbone	3027	244

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  $\geq 3$ , 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	198	 37% 49% 11%
2	R	3	 33% 67%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1515 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	177	Total	C	N	O	0	0
			1448	918	264	266		

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	3	Total	C	N	O	P	0	0
			67	30	15	19	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



#### • Molecule 2: RNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPED EACH PARTICLE, Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	150000	Depositor
Image detector	GATAN US4000 4K CCD	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	0.37	0/1481	0.75	4/2011 (0.2%)
2	R	0.16	0/75	0.57	0/115
All	All	0.37	0/1556	0.74	4/2126 (0.2%)

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	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	27	GLY	N-CA-C	5.55	126.98	113.10
1	A	81	GLY	N-CA-C	5.25	126.23	113.10
1	A	129	ALA	N-CA-C	5.19	125.01	111.00
1	A	104	THR	N-CA-C	5.12	124.81	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	PRO	Peptide
1	A	126	LEU	Mainchain
1	A	192	ILE	Peptide
1	A	44	ASP	Mainchain

## 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	1448	0	1423	142	0
2	R	67	0	34	19	0
All	All	1515	0	1457	144	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 48.

All (144) 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:28:VAL:O	1:A:31:ASP:HB3	1.46	1.13
1:A:72:PRO:HG2	1:A:79:PHE:CE1	1.97	0.98
1:A:160:LEU:HD22	2:R:1:G:N7	1.82	0.94
1:A:160:LEU:HD22	2:R:1:G:C5	2.03	0.93
1:A:42:PHE:HB2	1:A:67:LEU:HD11	1.51	0.92
1:A:121:ASN:O	1:A:124:ILE:HD12	1.72	0.89
1:A:35:HIS:HB3	1:A:38:ALA:HB3	1.56	0.87
1:A:117:GLN:HE22	2:R:3:A:N6	1.72	0.86
1:A:75:VAL:HA	1:A:77:ARG:H	1.38	0.86
1:A:72:PRO:HG2	1:A:79:PHE:CD1	2.13	0.84
1:A:29:PHE:O	1:A:30:ASP:HB2	1.76	0.83
1:A:7:THR:HG21	1:A:80:ALA:HA	1.60	0.83
1:A:123:ASP:OD1	1:A:124:ILE:HD12	1.77	0.83
1:A:23:VAL:HG21	1:A:188:LEU:HD11	1.62	0.81
1:A:160:LEU:HD22	2:R:1:G:C8	2.14	0.81
1:A:72:PRO:CG	1:A:79:PHE:CE1	2.63	0.81
1:A:13:HIS:O	1:A:191:ILE:HG22	1.82	0.80
1:A:124:ILE:HG23	1:A:128:ARG:NH2	1.97	0.79
1:A:72:PRO:CG	1:A:79:PHE:HE1	1.96	0.79
1:A:28:VAL:O	1:A:31:ASP:CB	2.29	0.78
1:A:42:PHE:CD1	1:A:67:LEU:HD13	2.19	0.78
1:A:148:THR:HG23	1:A:149:LEU:O	1.84	0.77
2:R:3:A:N3	2:R:3:A:H5"	2.01	0.75
1:A:29:PHE:HE1	1:A:71:LEU:HB3	1.52	0.75
1:A:160:LEU:CD2	2:R:1:G:N7	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HG2	1:A:79:PHE:HE1	1.48	0.73
1:A:95:PRO:HB2	1:A:97:PHE:CE2	2.24	0.71
1:A:160:LEU:HD13	2:R:1:G:C6	2.26	0.71
1:A:91:TYR:CE2	1:A:93:PRO:HB3	2.27	0.70
1:A:75:VAL:HA	1:A:77:ARG:N	2.07	0.69
1:A:67:LEU:N	1:A:68:ASP:HA	2.06	0.69
1:A:157:ASP:OD2	2:R:3:A:H1'	1.94	0.68
1:A:160:LEU:HD23	2:R:2:A:H5''	1.75	0.67
1:A:15:ILE:O	1:A:16:GLU:HB3	1.92	0.67
1:A:7:THR:HG21	1:A:80:ALA:CA	2.26	0.66
1:A:160:LEU:CD2	2:R:1:G:C8	2.79	0.66
1:A:160:LEU:HD13	2:R:1:G:O6	1.96	0.65
1:A:3:ASN:N	1:A:68:ASP:OD2	2.31	0.64
1:A:29:PHE:O	1:A:30:ASP:CB	2.46	0.64
1:A:42:PHE:CD1	1:A:67:LEU:CD1	2.81	0.64
1:A:42:PHE:CB	1:A:67:LEU:HD11	2.25	0.63
1:A:156:LYS:HE2	2:R:1:G:H21	1.62	0.63
1:A:117:GLN:HE22	2:R:3:A:H62	1.45	0.62
1:A:29:PHE:CE1	1:A:71:LEU:HD22	2.35	0.62
1:A:44:ASP:O	1:A:45:ASN:C	2.35	0.62
1:A:29:PHE:C	1:A:31:ASP:H	2.02	0.61
1:A:121:ASN:O	1:A:124:ILE:CD1	2.46	0.61
1:A:35:HIS:HB3	1:A:38:ALA:CB	2.30	0.61
1:A:7:THR:O	1:A:77:ARG:NH1	2.34	0.61
1:A:7:THR:HG21	1:A:80:ALA:CB	2.32	0.60
1:A:124:ILE:CG2	1:A:128:ARG:NH2	2.66	0.59
1:A:190:TRP:O	1:A:191:ILE:HG22	2.02	0.59
1:A:119:HIS:CE1	1:A:121:ASN:HB2	2.39	0.57
1:A:191:ILE:HG23	1:A:191:ILE:O	2.04	0.57
1:A:117:GLN:NE2	2:R:3:A:N6	2.50	0.57
1:A:157:ASP:OD2	2:R:3:A:C1'	2.53	0.56
1:A:29:PHE:CE1	1:A:71:LEU:HB3	2.38	0.56
1:A:7:THR:CG2	1:A:80:ALA:CB	2.84	0.56
1:A:47:ARG:N	1:A:48:GLY:HA3	2.21	0.56
1:A:92:LEU:HG	1:A:92:LEU:O	2.06	0.56
1:A:124:ILE:CG1	1:A:128:ARG:HH21	2.19	0.55
1:A:13:HIS:H	1:A:191:ILE:CG2	2.19	0.54
1:A:29:PHE:HE1	1:A:71:LEU:CB	2.20	0.54
1:A:123:ASP:OD1	1:A:124:ILE:N	2.40	0.54
1:A:28:VAL:CG1	1:A:71:LEU:CD1	2.85	0.54
1:A:122:ARG:HD3	1:A:125:GLU:CD	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:CG2	1:A:80:ALA:HB2	2.38	0.53
1:A:74:ASP:O	1:A:77:ARG:HG3	2.08	0.53
1:A:3:ASN:ND2	1:A:68:ASP:OD2	2.41	0.53
1:A:3:ASN:CA	1:A:68:ASP:OD2	2.57	0.52
1:A:13:HIS:H	1:A:191:ILE:HG22	1.73	0.52
1:A:16:GLU:HG3	1:A:16:GLU:O	2.10	0.52
1:A:52:SER:HB2	1:A:57:ARG:HH11	1.74	0.52
1:A:123:ASP:O	1:A:126:LEU:N	2.41	0.52
1:A:121:ASN:O	1:A:123:ASP:OD1	2.27	0.52
1:A:42:PHE:CG	1:A:67:LEU:HD11	2.45	0.52
1:A:13:HIS:O	1:A:191:ILE:CG2	2.55	0.52
1:A:15:ILE:HD11	1:A:189:GLU:HB3	1.92	0.52
1:A:44:ASP:O	1:A:46:LEU:N	2.44	0.51
1:A:3:ASN:O	1:A:5:SER:N	2.42	0.51
1:A:35:HIS:O	1:A:39:TRP:N	2.40	0.51
1:A:75:VAL:HG23	1:A:76:ASP:HA	1.92	0.51
1:A:74:ASP:H	1:A:77:ARG:HB2	1.74	0.51
1:A:7:THR:HG23	1:A:80:ALA:HB2	1.93	0.51
1:A:192:ILE:O	1:A:193:PRO:C	2.50	0.51
1:A:104:THR:O	1:A:107:GLU:N	2.39	0.50
1:A:36:VAL:O	1:A:37:GLU:HG2	2.12	0.50
1:A:28:VAL:HG11	1:A:71:LEU:CD1	2.42	0.50
1:A:29:PHE:C	1:A:31:ASP:N	2.64	0.49
1:A:15:ILE:O	1:A:16:GLU:CB	2.57	0.49
1:A:130:LYS:HG3	1:A:130:LYS:O	2.12	0.49
1:A:33:TRP:HB2	1:A:70:ASP:O	2.13	0.49
1:A:3:ASN:HA	1:A:68:ASP:OD2	2.13	0.49
2:R:3:A:N3	2:R:3:A:C5'	2.73	0.49
1:A:101:ASP:OD1	1:A:102:LYS:N	2.43	0.48
1:A:160:LEU:HD23	2:R:2:A:C5'	2.43	0.48
1:A:124:ILE:C	1:A:126:LEU:H	2.16	0.48
1:A:99:ARG:HB3	1:A:175:PRO:HG2	1.96	0.48
1:A:24:VAL:HG22	1:A:25:GLU:H	1.79	0.48
1:A:82:ALA:HB3	1:A:92:LEU:HG	1.96	0.47
1:A:193:PRO:O	1:A:194:ASP:C	2.52	0.47
1:A:122:ARG:HD3	1:A:125:GLU:OE1	2.13	0.47
1:A:28:VAL:HG11	1:A:71:LEU:HD11	1.96	0.47
1:A:185:GLU:HG3	1:A:186:LEU:N	2.30	0.46
1:A:153:GLN:NE2	1:A:157:ASP:OD1	2.48	0.46
1:A:65:ALA:O	1:A:66:ALA:HB3	2.16	0.46
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:C	1:A:38:ALA:H	2.19	0.45
1:A:19:TRP:O	1:A:24:VAL:HG12	2.16	0.45
1:A:29:PHE:HE1	1:A:71:LEU:HD22	1.80	0.45
1:A:84:GLY:HA3	1:A:91:TYR:HA	1.98	0.45
1:A:46:LEU:HA	1:A:49:ILE:HD12	1.97	0.45
1:A:160:LEU:HD22	2:R:1:G:C4	2.50	0.45
1:A:124:ILE:HD12	1:A:124:ILE:H	1.81	0.45
1:A:74:ASP:O	1:A:75:VAL:C	2.54	0.45
1:A:122:ARG:HA	1:A:125:GLU:OE1	2.16	0.44
1:A:57:ARG:O	1:A:115:THR:HG21	2.17	0.44
1:A:63:TYR:O	1:A:65:ALA:O	2.35	0.44
1:A:121:ASN:C	1:A:123:ASP:H	2.20	0.44
1:A:29:PHE:CE1	1:A:71:LEU:HD13	2.52	0.44
1:A:36:VAL:HG22	1:A:98:PHE:CE2	2.53	0.44
1:A:126:LEU:HD23	1:A:127:ASN:HA	1.99	0.44
1:A:126:LEU:HD23	1:A:127:ASN:N	2.33	0.44
1:A:101:ASP:O	1:A:102:LYS:C	2.55	0.43
1:A:121:ASN:O	1:A:123:ASP:N	2.52	0.43
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.60	0.43
1:A:91:TYR:CD2	1:A:93:PRO:HB3	2.54	0.42
1:A:185:GLU:HG3	1:A:186:LEU:CD1	2.50	0.42
1:A:113:ARG:NH1	1:A:116:ASP:OD1	2.50	0.42
1:A:51:PHE:HA	1:A:52:SER:HA	1.70	0.42
1:A:14:TYR:H	1:A:75:VAL:CG2	2.33	0.42
1:A:183:GLU:O	1:A:187:ALA:HA	2.19	0.42
1:A:153:GLN:HB3	1:A:154:PRO:HD3	2.02	0.42
1:A:126:LEU:HD23	1:A:127:ASN:CA	2.50	0.41
1:A:119:HIS:CD2	1:A:120:ASN:H	2.37	0.41
1:A:117:GLN:HA	1:A:118:PRO:HD3	1.87	0.41
1:A:98:PHE:CE1	1:A:176:VAL:HG12	2.55	0.41
1:A:117:GLN:NE2	2:R:3:A:H62	2.13	0.41
1:A:33:TRP:NE1	1:A:71:LEU:HD12	2.36	0.41
1:A:18:GLN:OE1	1:A:188:LEU:HA	2.20	0.41
1:A:123:ASP:OD1	1:A:124:ILE:CD1	2.60	0.40
1:A:54:ALA:C	1:A:56:SER:H	2.24	0.40
1:A:111:LEU:HD22	1:A:162:TYR:CE1	2.57	0.40
1:A:126:LEU:HD22	1:A:127:ASN:CG	2.42	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	173/198 (87%)	152 (88%)	21 (12%)	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 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	153/169 (90%)	153 (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	3	ASN
1	A	117	GLN
1	A	119	HIS
1	A	127	ASN
1	A	153	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	2/3 (66%)	2 (100%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	A
2	R	3	A

There are no RNA pucker outliers to report.

## 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.