



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:21 PM EDT

PDB ID : 3JB1
EMDB ID: : EMD-6375
Title : Atomic model of cytoplasmic polyhedrosis virus with SAM
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 3.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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-20027939

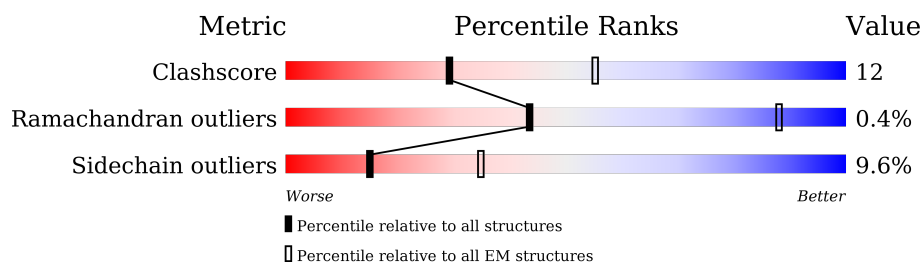
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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

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	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32271 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

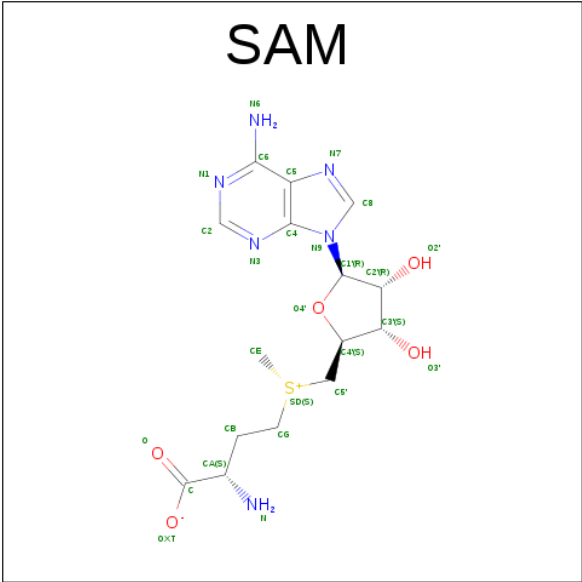
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

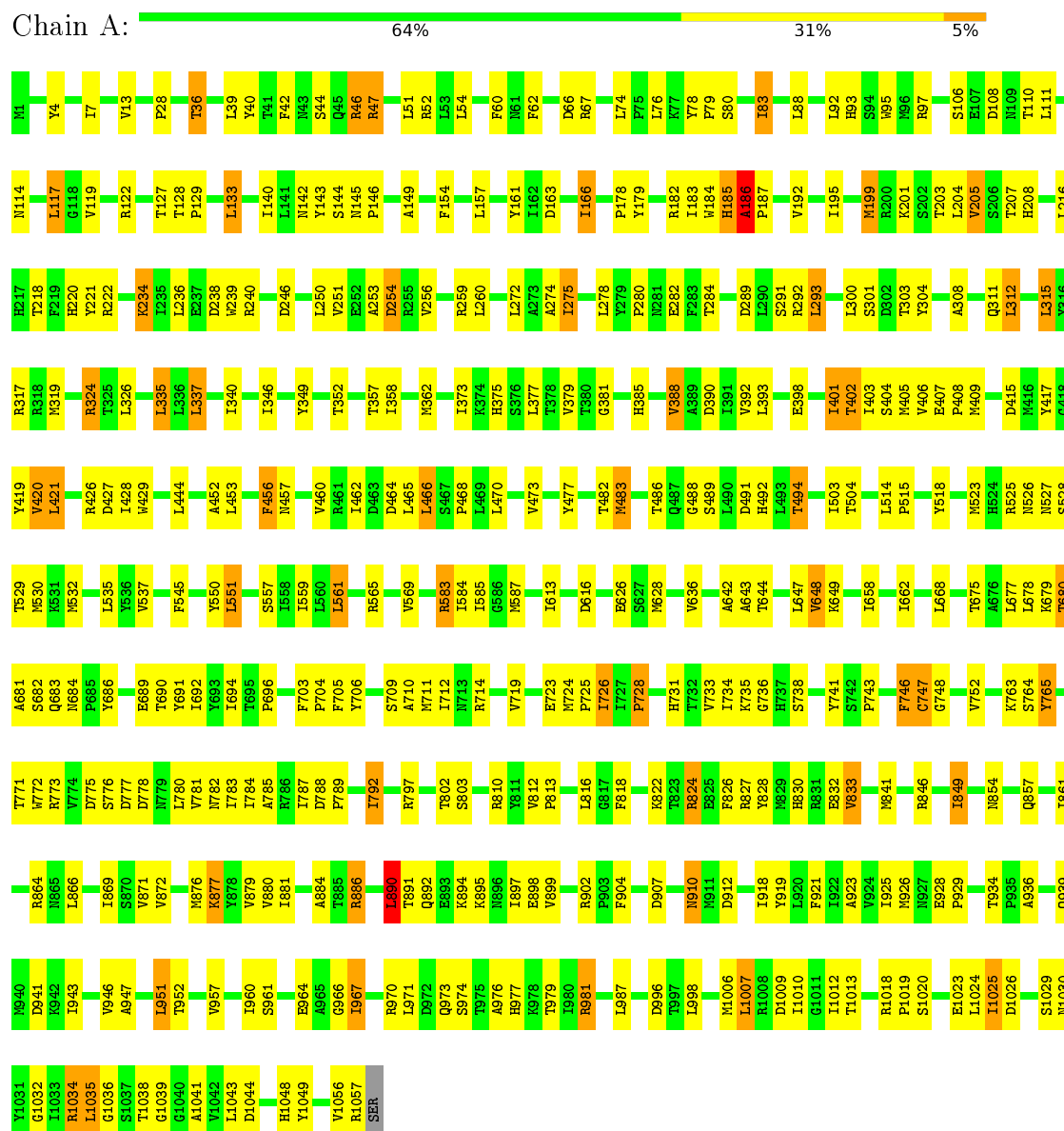


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			27	15	6	5	1	

3 Residue-property plots

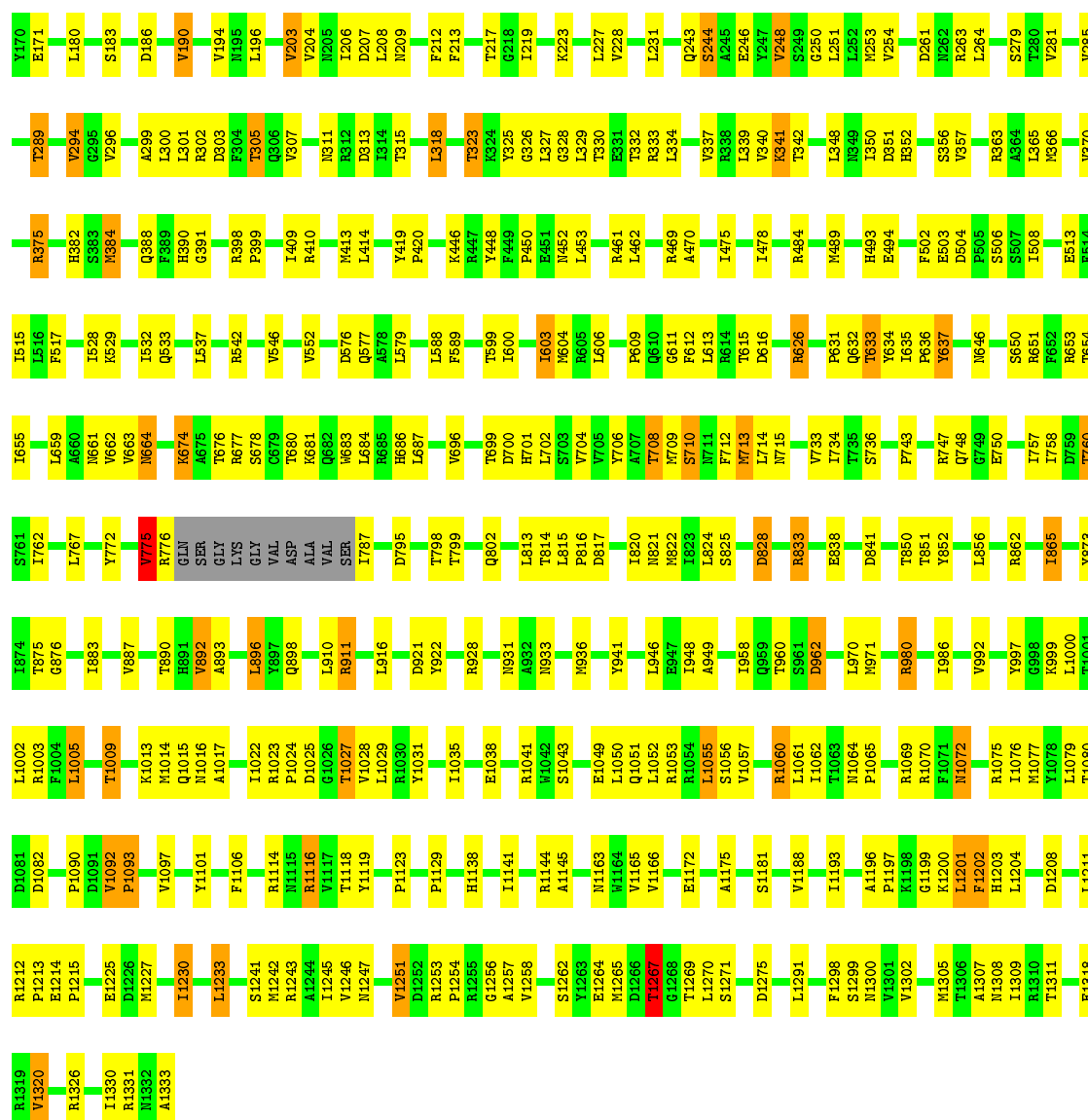
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Structural protein VP3



• Molecule 2: Capsid protein VP1





ARG
GLU
THR
VAL
ASN
LYS
MET
ASN
GLU
ILE
ASP
ALA
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ILE
ASP
THR
GLN
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ASP
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VAL
LEU

- Molecule 3: Viral structural protein 5



M1
L2
Q3
Q4
I19
D22
T29
Q30
F31
L35
A39
L44
V45
T48
E53
T54
H55
L56
V66
D70
Q74
A81
F90
S91
R92
L93
L96
T101
L105
I111
Y112
M113
T116
D123
P124
T133
Y134
A135
K136
L137

G138
H139
D148
D151
H152
Y153
A154
H155
V156
E159
L160
D164
R167
V171
H172
P173
A177
D180
S181
W182
S185
L186
L189
S190
V193
W196
L199
D204
L213
R225
M226
K227
L228
F229
I230
T233
V240
R247
R250
V251

L252
E253
Y254
G256
V257
T262
T266
D272
L273
S274
R275
K281
F282
L283
T286
A292
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	44908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	0.28	0/8619	0.52	3/11737 (0.0%)
2	B	0.33	0/9590	0.54	0/13056
2	C	0.34	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.54	0/3163
3	E	0.30	0/2327	0.52	0/3163
All	All	0.32	0/32915	0.54	3/44806 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.20	102.57	120.60
1	A	186	ALA	C-N-CA	5.69	145.91	122.00
1	A	890	LEU	CA-CB-CG	5.39	127.70	115.30

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	8434	0	8399	219	0
2	B	9397	0	9315	255	0
2	C	9851	0	9762	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2281	0	2282	62	0
3	E	2281	0	2282	47	0
4	A	27	0	22	5	0
All	All	32271	0	32062	785	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 12.

The worst 5 of 785 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:C:709:MET:O	2:C:715:ASN:ND2	2.09	0.85
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.60	0.83
3:D:44:LEU:HG	3:D:174:VAL:HG22	1.64	0.79
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.65	0.78
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.64	0.78

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	1055/1058 (100%)	1004 (95%)	45 (4%)	6 (1%)	30	68
2	B	1187/1333 (89%)	1135 (96%)	49 (4%)	3 (0%)	46	80
2	C	1246/1333 (94%)	1181 (95%)	60 (5%)	5 (0%)	39	75
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	46	80
3	E	290/448 (65%)	281 (97%)	9 (3%)	0	100	100
All	All	4068/4620 (88%)	3882 (95%)	171 (4%)	15 (0%)	43	75

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	C	1145	ALA
2	C	1251	VAL
2	B	1123	PRO
3	D	244	VAL

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	A	942/943 (100%)	829 (88%)	113 (12%)	6	24
2	B	1038/1153 (90%)	963 (93%)	75 (7%)	18	53
2	C	1089/1153 (94%)	980 (90%)	109 (10%)	9	34
3	D	240/379 (63%)	215 (90%)	25 (10%)	9	32
3	E	240/379 (63%)	222 (92%)	18 (8%)	17	51
All	All	3549/4007 (89%)	3209 (90%)	340 (10%)	15	37

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	797	SER
2	C	98	ASN
3	D	160	LEU
2	B	851	THR
2	B	1092	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1138	HIS
2	C	156	GLN
2	C	981	HIS
2	B	858	HIS
2	C	1138	HIS

5.3.3 RNA ⓘ

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	SAM	A	1101	-	23,29,29	1.06	2 (8%)	15,42,42	2.92	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	A	1101	-	-	0/8/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N1	2.53	1.38	1.33
4	A	1101	SAM	C2-N3	3.47	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1101	SAM	N3-C2-N1	-10.65	120.51	128.87
4	A	1101	SAM	C4'-O4'-C1'	2.14	111.91	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	5	0

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.