



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:39 PM EDT

PDB ID : 3JB2
EMDB ID: : EMD-6376
Title : Atomic model of cytoplasmic polyhedrosis virus with SAM and GTP
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

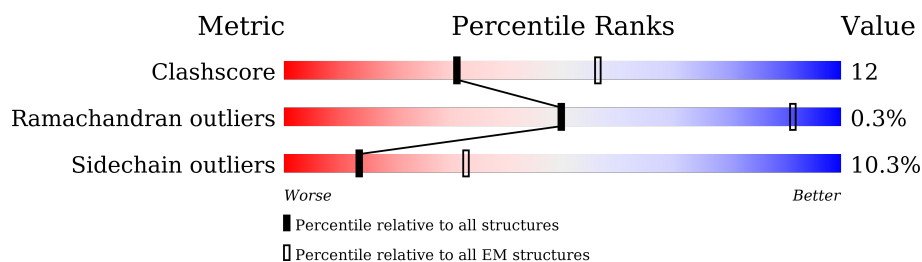
1 Overall quality at a glance

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	68% 29% .
2	B	1333	59% 26% . 11%
2	C	1333	63% 27% . 6%
3	D	448	45% 17% . 35%
3	E	448	45% 18% . 35%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32369 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	1251	Total	C	N	O	S	0	0
			9857	6222	1713	1884	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).



- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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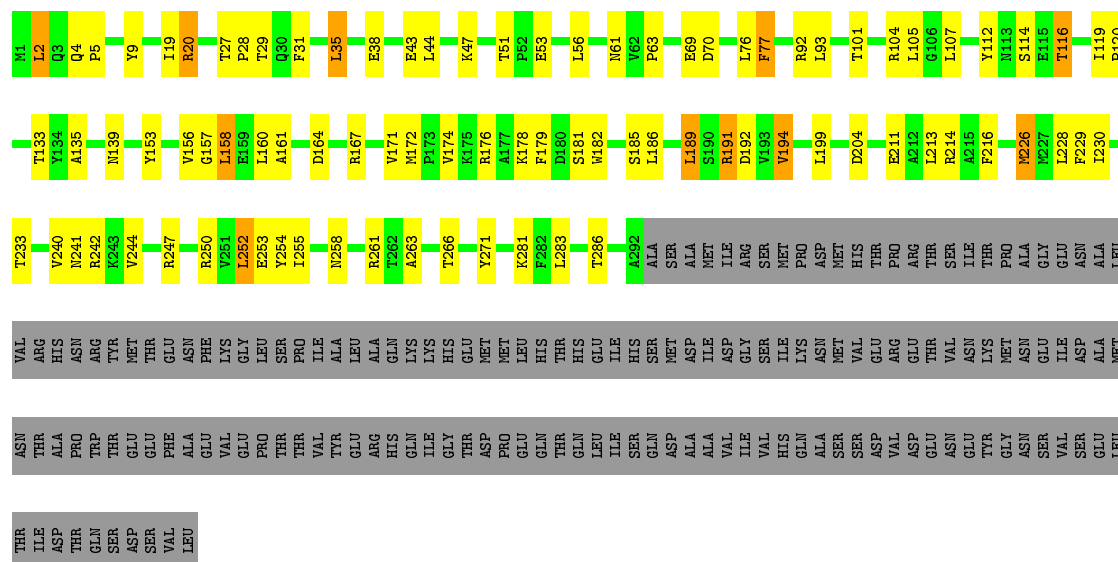
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			64	20	10	28	6	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

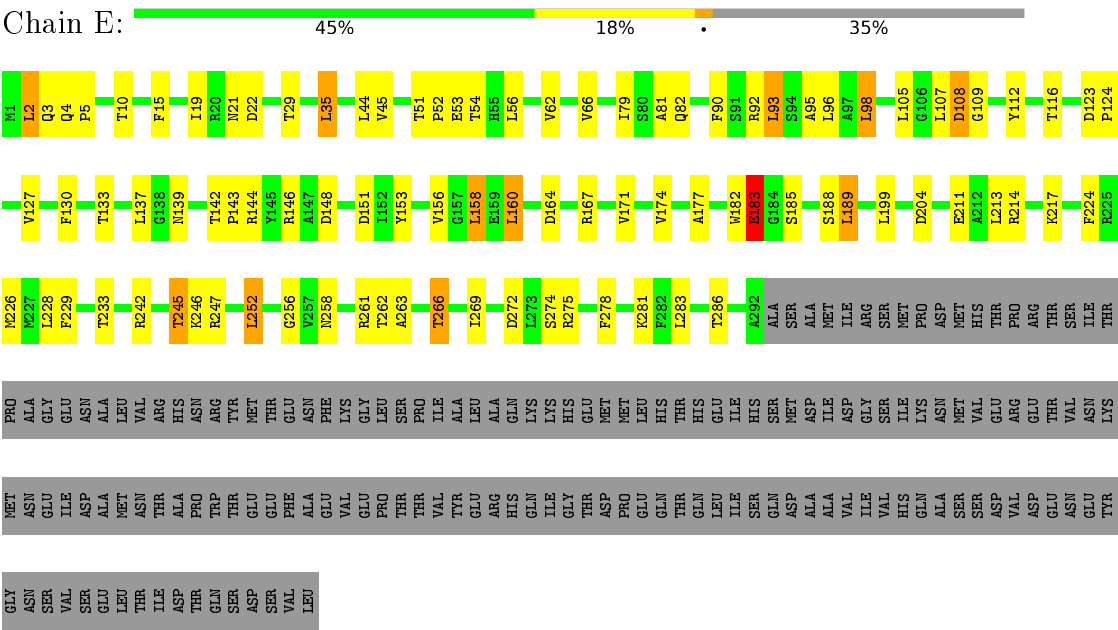
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	



	K161	L164	V168	K169	Y170	E171	D172	Q173	D178	D186	V190	T193	L196	A202	V203	V204	L208	N209	R210	D214	T215	A216	T217	L221	T222	K223	G224	I225	V228	Q229	D230	L231	L232	V233	P234	V237	T238	A239	Y247	G250	L251	V254	C155			
MET	HIS	SER	THR	ASN	ASN	SER	LYS	ASN	ASN	GLU	GLU	LYS	HIS	LYS	GLN	PRO	GLU	ILE	ASP	SER	SER	ALA	ASN	ASN	GLY	GLY	GLY	THR	SER	GLY	THR	ALA	ALA	THR	GLU	GLY	VAL	ARG	ASN	THR	GLU	GLY	ALA	SER	THR	ARG



● Molecule 3: Viral structural protein 5



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	46147	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: GTP, MG, 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	0.27	0/8619	0.49	0/11737
2	B	0.33	0/9590	0.55	0/13056
2	C	0.34	0/10058	0.56	0/13695
3	D	0.31	0/2327	0.54	0/3163
3	E	0.31	0/2327	0.53	0/3163
All	All	0.32	0/32921	0.54	0/44814

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 [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	192	0
2	B	9397	0	9315	244	0
2	C	9857	0	9767	235	0
3	D	2281	0	2282	57	0
3	E	2281	0	2282	52	0
4	A	54	0	44	4	0
5	A	64	0	24	2	0
6	A	1	0	0	0	0
All	All	32369	0	32113	749	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 749 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:383:SER:HB3	2:C:796:PRO:HG3	1.51	0.93
1:A:857:GLN:NE2	1:A:914:GLU:OE1	2.03	0.91
2:C:360:ILE:HD11	2:C:1054:ARG:HG2	1.54	0.89
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.58	0.84
2:B:383:SER:HB3	2:B:796:PRO:HG3	1.57	0.84

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%)	1006 (95%)	48 (4%)	1 (0%)	56	88
2	B	1187/1333 (89%)	1128 (95%)	55 (5%)	4 (0%)	46	80
2	C	1247/1333 (94%)	1183 (95%)	58 (5%)	6 (0%)	34	72
3	D	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	46	80
3	E	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	26	65
All	All	4069/4620 (88%)	3882 (95%)	173 (4%)	14 (0%)	50	80

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	229	GLN
2	B	1007	THR
2	B	1310	ARG
2	C	275	SER
3	E	183	GLU

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	942/943 (100%)	850 (90%)	92 (10%)	10	36
2	B	1038/1153 (90%)	933 (90%)	105 (10%)	9	33
2	C	1090/1153 (94%)	973 (89%)	117 (11%)	8	31
3	D	240/379 (63%)	218 (91%)	22 (9%)	11	40
3	E	240/379 (63%)	212 (88%)	28 (12%)	7	26
All	All	3550/4007 (89%)	3186 (90%)	364 (10%)	13	32

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1079	LEU
2	C	115	GLN
3	E	2	LEU
2	B	1110	LEU
2	B	1233	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1138	HIS
2	C	1308	ASN
2	C	291	HIS
2	B	935	GLN
2	B	1247	ASN

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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	1.09	2 (8%)	15,42,42	3.07	2 (13%)
4	SAM	A	1102	-	23,29,29	1.06	2 (8%)	15,42,42	2.97	1 (6%)
5	GTP	A	1103	-	26,34,34	0.91	1 (3%)	29,54,54	1.51	4 (13%)
5	GTP	A	1104	6	26,34,34	0.99	1 (3%)	29,54,54	1.51	4 (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
4	SAM	A	1102	-	-	0/8/33/33	0/3/3/3
5	GTP	A	1103	-	-	0/18/38/38	0/3/3/3
5	GTP	A	1104	6	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	SAM	C2-N1	2.36	1.38	1.33
4	A	1101	SAM	C2-N1	2.39	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1103	GTP	C6-N1	2.97	1.38	1.33
5	A	1104	GTP	C6-N1	3.43	1.39	1.33
4	A	1102	SAM	C2-N3	3.57	1.38	1.32

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-11.13	120.13	128.87
4	A	1102	SAM	N3-C2-N1	-11.07	120.18	128.87
5	A	1104	GTP	N3-C2-N1	-5.42	120.18	127.56
5	A	1103	GTP	N3-C2-N1	-4.96	120.81	127.56
5	A	1103	GTP	C5-C6-N1	-3.21	119.33	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	1	0
4	A	1102	SAM	3	0
5	A	1104	GTP	2	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.