wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 01:45 AM EST

PDB ID	:	3JB0
EMDB ID	:	EMD-6374
Title	:	Atomic model of cytoplasmic polyhedrosis virus with GTP
Authors	:	Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on	:	2015-07-06
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

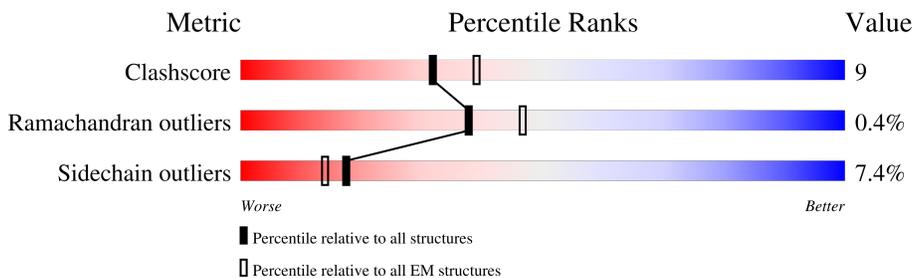|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.4%
Sidechain outliers		7.4%

Worse *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1058	69% 28% •
2	B	1333	66% 22% • 11%
2	C	1333	71% 21% • 6%
3	D	448	47% 16% • 35%
3	E	448	48% 16% • 35%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 32276 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 8434	C 5345	N 1457	O 1587	S 45	0	0

- Molecule 2 is a protein called Capsid protein VP1.

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

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

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP
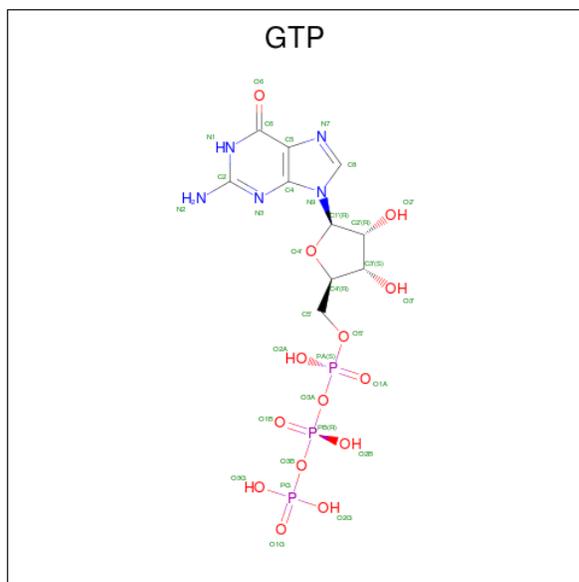
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	32	10	5	14	3	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

Chain A:

• Molecule 2: Capsid protein VP1

Chain B:

• Molecule 2: Capsid protein VP1

Chain C:

71% 21% • 6%

• Molecule 3: Viral structural protein 5

Chain D:

• Molecule 3: Viral structural protein 5

Chain E:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	71946	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	60535	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.28	0/8619	0.50	4/11737 (0.0%)
2	B	0.35	0/9590	0.55	0/13056
2	C	0.34	0/10052	0.56	1/13687 (0.0%)
3	D	0.33	0/2327	0.54	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.33	0/32915	0.54	5/44806 (0.0%)

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
2	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ALA	C-N-CD	-8.43	102.05	120.60
1	A	78	TYR	C-N-CD	-6.39	106.53	120.60
1	A	186	ALA	C-N-CA	5.95	147.00	122.00
2	C	1116	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	78	TYR	C-N-CA	5.08	143.36	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	384	MET	Peptide

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	8434	0	8399	183	0
2	B	9397	0	9315	180	0
2	C	9851	0	9762	180	0
3	D	2281	0	2282	44	0
3	E	2281	0	2282	45	0
4	A	32	0	12	2	0
All	All	32276	0	32052	608	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 9.

The worst 5 of 608 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:111:LEU:HD13	1:A:142:ASN:HB3	1.60	0.84
2:B:709:MET:O	2:B:715:ASN:ND2	2.13	0.82
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.44	0.82
2:B:461:ARG:HH21	2:B:504:ASP:HB2	1.48	0.79
1:A:255:ARG:NH2	4:A:1101:GTP:O2A	2.15	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	1012 (96%)	40 (4%)	3 (0%)	41	71
2	B	1187/1333 (89%)	1145 (96%)	39 (3%)	3 (0%)	41	71
2	C	1246/1333 (94%)	1197 (96%)	41 (3%)	8 (1%)	25	58
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	41	71
3	E	290/448 (65%)	284 (98%)	6 (2%)	0	100	100
All	All	4068/4620 (88%)	3919 (96%)	134 (3%)	15 (0%)	38	66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	C	288	THR
2	C	1267	THR
1	A	483	MET

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%)	849 (90%)	93 (10%)	8	24
2	B	1038/1153 (90%)	980 (94%)	58 (6%)	21	52
2	C	1089/1153 (94%)	1018 (94%)	71 (6%)	17	45
3	D	240/379 (63%)	219 (91%)	21 (9%)	10	30
3	E	240/379 (63%)	220 (92%)	20 (8%)	11	32
All	All	3549/4007 (89%)	3286 (93%)	263 (7%)	17	38

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	107	LEU

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Mol	Chain	Res	Type
3	D	191	ARG
3	E	252	LEU
2	B	264	LEU
2	B	147	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	981	HIS
2	C	1138	HIS
2	B	491	ASN
2	B	1138	HIS
2	B	1332	ASN

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 monosaccharides 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	GTP	A	1101	-	26,34,34	1.14	2 (7%)	32,54,54	1.55	6 (18%)

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	GTP	A	1101	-	-	6/18/38/38	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	GTP	C5-C6	-3.98	1.39	1.47
4	A	1101	GTP	C2-N3	2.26	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	GTP	PB-O3B-PG	-3.76	119.91	132.83
4	A	1101	GTP	C8-N7-C5	3.57	109.78	102.99
4	A	1101	GTP	C5-C6-N1	3.07	119.38	113.95
4	A	1101	GTP	C2-N1-C6	-2.93	119.69	125.10
4	A	1101	GTP	PA-O3A-PB	-2.07	125.72	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	GTP	C5'-O5'-PA-O3A
4	A	1101	GTP	C4'-C5'-O5'-PA
4	A	1101	GTP	C5'-O5'-PA-O2A
4	A	1101	GTP	O4'-C4'-C5'-O5'
4	A	1101	GTP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP A 1101

Bond lengths

Bond angles

Torsions

Rings
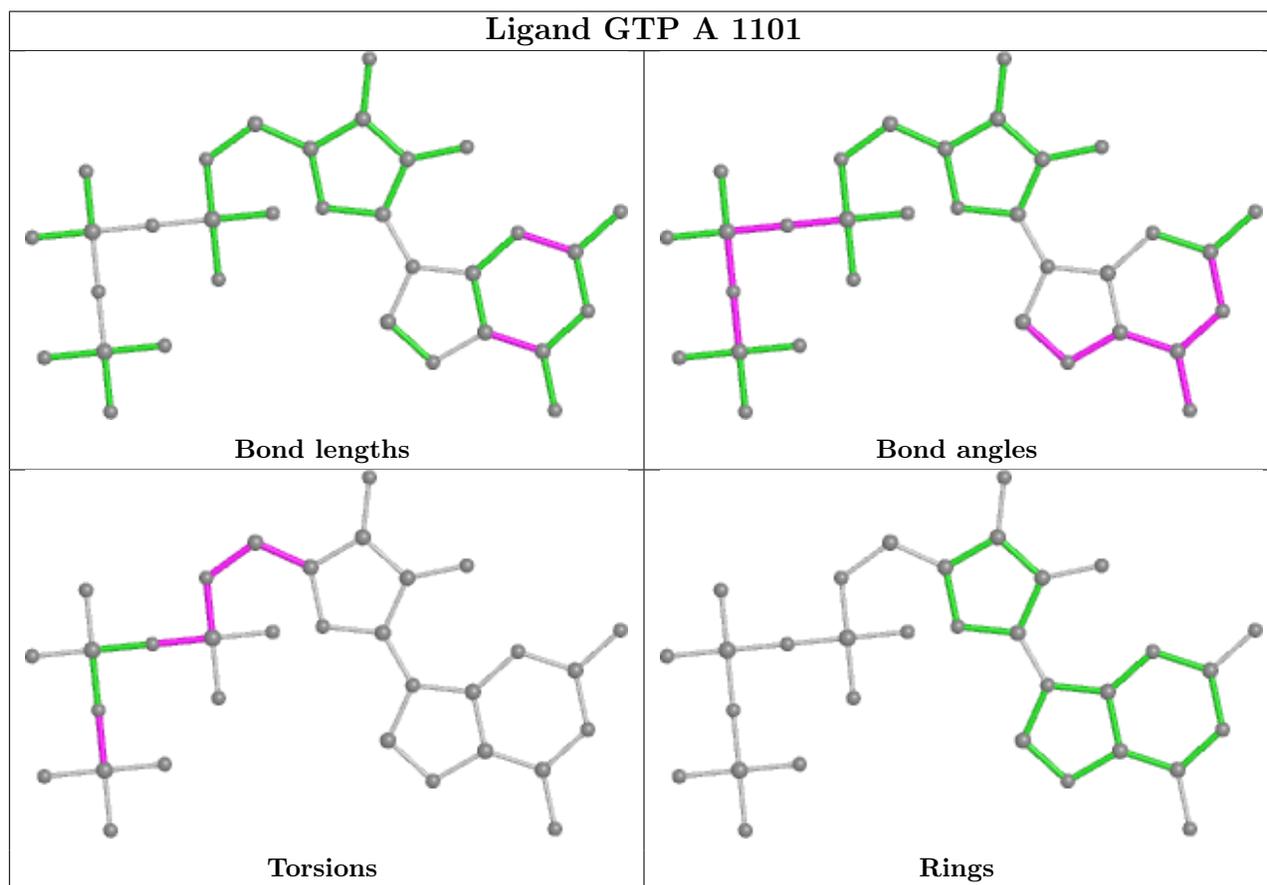
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-6374. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal surface views ⓘ

This section was not generated.

6.5 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7   Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1   Map-value distribution ⓘ

This section was not generated.

7.2   Volume estimate versus contour level ⓘ

This section was not generated.

7.3   Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.