



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3JB6
EMDB ID: : EMD-6408
Title : In situ structures of the segmented genome and RNA polymerase complex
inside a dsRNA virus
Authors : Zhang, X.; Ding, K.; Yu, X.K.; Chang, W.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-08-02
Resolution : 3.30 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) : trunk27241

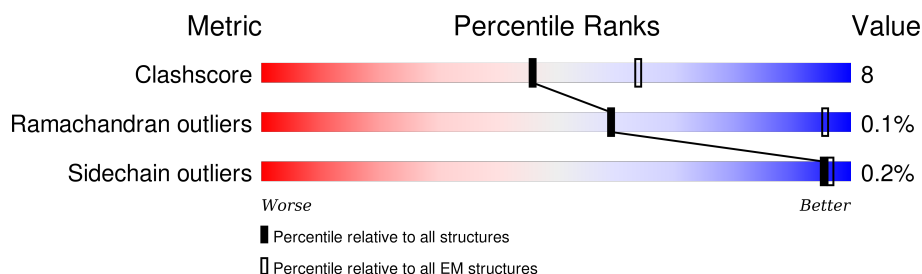
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	1225	80% 17% .
2	B	561	72% 17% 11%
3	C	24	13% 42% 33% 13%
3	D	24	25% 38% . 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13904 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1196	Total	C	N	O	S	0	0
			9556	6062	1651	1807	36		

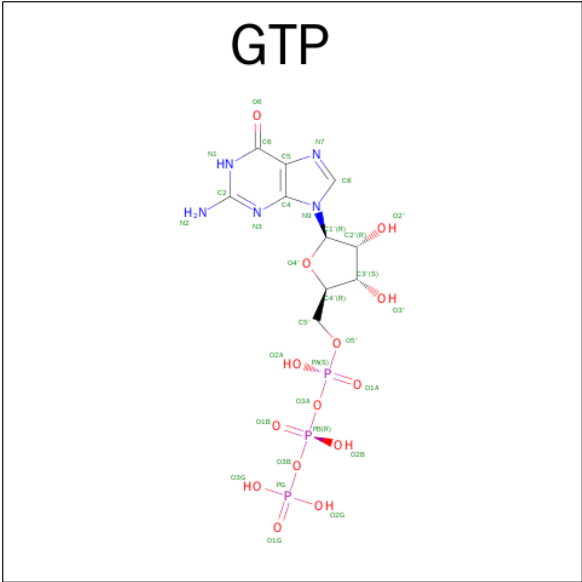
- Molecule 2 is a protein called Viral structural protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	498	Total	C	N	O	S	0	0
			3985	2553	666	749	17		

- Molecule 3 is a protein called VP1 CSP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	21	Total	C	N	O	S	0	0
			170	105	30	34	1		
3	D	16	Total	C	N	O		0	0
			129	81	22	26			

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

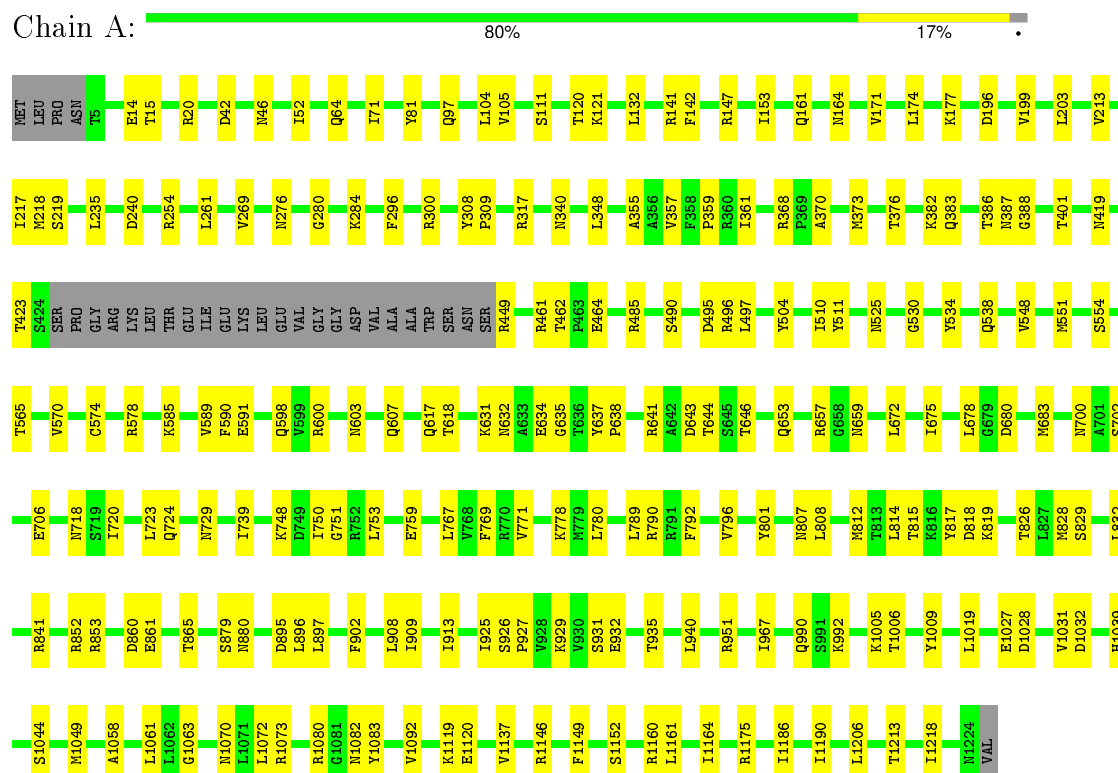


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

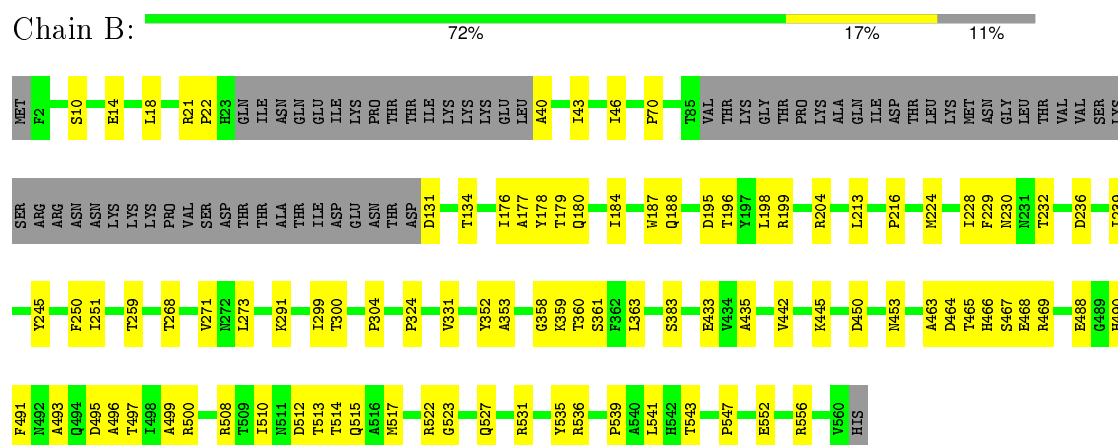
3 Residue-property plots

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: RNA-dependent RNA polymerase



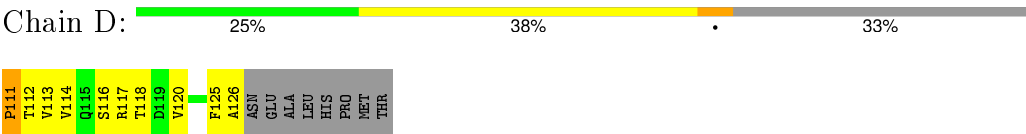
- Molecule 2: Viral structural protein 4



● Molecule 3: VP1 CSP



● Molecule 3: VP1 CSP



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	68526	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	49000	Depositor
Image detector	GATAN K2 (4k x 4k)	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

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	0/9760	0.49	0/13212
2	B	0.36	0/4071	0.47	0/5519
3	C	2.85	19/173 (11.0%)	2.08	10/234 (4.3%)
3	D	2.20	2/131 (1.5%)	0.77	1/177 (0.6%)
All	All	0.53	21/14135 (0.1%)	0.53	11/19142 (0.1%)

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	1
3	C	0	1
All	All	0	2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	111	PRO	N-CA	-20.90	1.11	1.47
3	D	111	PRO	N-CD	11.73	1.64	1.47
3	C	127	ASN	C-O	-8.09	1.07	1.23
3	C	129	ALA	C-O	-8.00	1.08	1.23
3	C	125	PHE	CG-CD1	-7.87	1.26	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	VAL	CG1-CB-CG2	-9.74	95.32	110.90
3	C	130	LEU	N-CA-C	8.44	133.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	130	LEU	CB-CG-CD2	-8.17	97.10	111.00
3	C	131	HIS	C-N-CD	7.10	143.31	128.40
3	D	111	PRO	N-CD-CG	-6.79	93.01	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	SER	Peptide
3	C	117	ARG	Sidechain

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	9556	0	9433	145	0
2	B	3985	0	3984	71	0
3	C	170	0	155	22	0
3	D	129	0	121	6	0
4	A	32	0	12	1	0
4	B	32	0	12	4	0
All	All	13904	0	13717	221	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 8.

The worst 5 of 221 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)
3:D:116:SER:O	3:D:120:VAL:HG23	1.75	0.86
2:B:442:VAL:CG1	3:C:128:GLU:HG3	2.09	0.83
1:A:386:THR:HG23	3:C:128:GLU:OE1	1.80	0.81
3:D:114:VAL:O	3:D:118:THR:HG23	1.81	0.81
2:B:271:VAL:HG12	2:B:273:LEU:H	1.45	0.80

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	1192/1225 (97%)	1160 (97%)	31 (3%)	1 (0%)	56	89
2	B	492/561 (88%)	483 (98%)	9 (2%)	0	100	100
3	C	19/24 (79%)	16 (84%)	2 (10%)	1 (5%)	2	17
3	D	14/24 (58%)	14 (100%)	0	0	100	100
All	All	1717/1834 (94%)	1673 (97%)	42 (2%)	2 (0%)	59	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
3	C	119	ASP

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	1038/1063 (98%)	1038 (100%)	0	100	100
2	B	434/493 (88%)	434 (100%)	0	100	100
3	C	19/22 (86%)	17 (90%)	2 (10%)	8	33
3	D	15/22 (68%)	14 (93%)	1 (7%)	20	58
All	All	1506/1600 (94%)	1503 (100%)	3 (0%)	95	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	123	GLU
3	C	130	LEU
3	D	112	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	413	HIS
1	A	718	ASN
1	A	364	HIS
1	A	696	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

2 ligands are 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	1301	-	26,34,34	0.92	1 (3%)	29,54,54	1.52	3 (10%)
4	GTP	B	601	-	26,34,34	0.92	1 (3%)	29,54,54	1.60	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	GTP	A	1301	-	-	0/18/38/38	0/3/3/3
4	GTP	B	601	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	GTP	C6-N1	2.88	1.38	1.33
4	A	1301	GTP	C6-N1	2.92	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GTP	N3-C2-N1	-5.49	120.09	127.56
4	A	1301	GTP	N3-C2-N1	-5.35	120.28	127.56
4	B	601	GTP	C5-C6-N1	-3.10	119.47	123.52
4	A	1301	GTP	C5-C6-N1	-2.98	119.63	123.52
4	B	601	GTP	C4'-O4'-C1'	2.37	112.15	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	GTP	1	0
4	B	601	GTP	4	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.