



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:38 PM BST

PDB ID : 1UON
Title : REOVIRUS POLYMERASE LAMBDA-3 LOCALIZED BY ELECTRON CRYOMICROSCOPY OF VIRIONS AT 7.6-Å RESOLUTION
Authors : Zhang, X.; Walker, S.B.; Chipman, P.R.; Nibert, M.L.; Baker, T.S.
Deposited on : 2003-09-21
Resolution : 7.60 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>

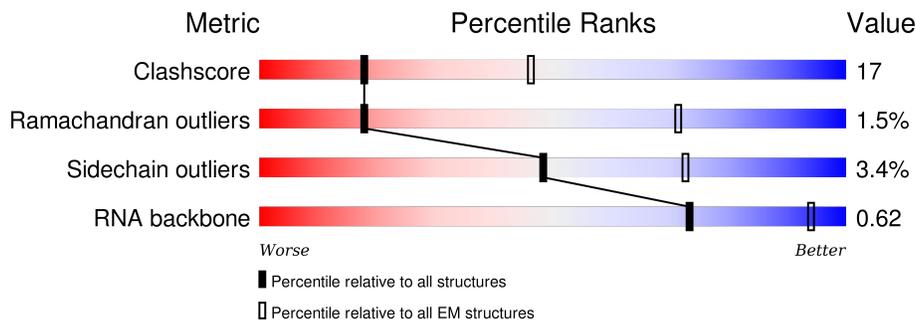
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 7.60 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 ≥ 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	1267	 68% 30% .
2	B	5	 20% 80%
3	C	8	 75% 25%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10703 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 MINOR CORE PROTEIN LAMBDA 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1264	Total	C	N	O	S	0	0
			9986	6369	1712	1841	64		

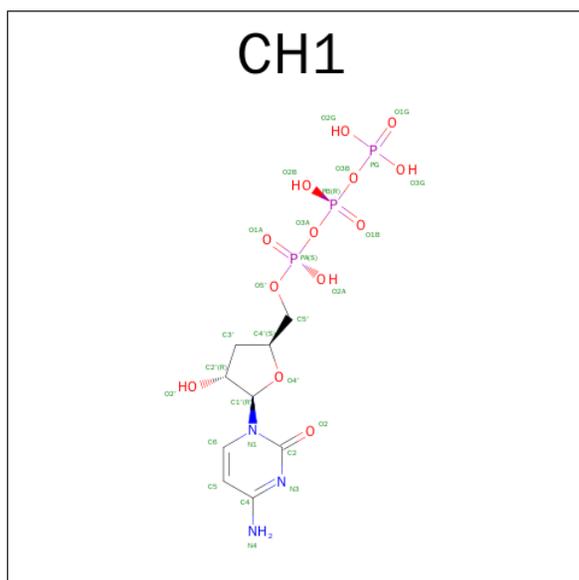
- Molecule 2 is a RNA chain called 5'-R(*GP*GP*GP*GP*GP*)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	5	Total	C	N	O	P	0	0
			116	50	25	36	5		

- Molecule 3 is a RNA chain called 5'-R(*UP*AP*GP*CP*CP*CP*CP*CP*)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	8	Total	C	N	O	P	0	0
			165	74	27	56	8		

- Molecule 4 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	
4	A	1	Total	C	N	O	P	0
			84	27	9	39	9	

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mn	0
			2	2	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	Z	350	Total	O	0
			350	350	

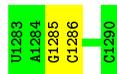
- Molecule 2: 5'-R(*GP*GP*GP*GP*GP*)-3'

Chain B:  20% 80%


G1272
G1273
G1274
G1275
G1276

- Molecule 3: 5'-R(*UP*AP*GP*CP*CP*CP*CP*CP*)-3'

Chain C:  75% 25%


U1283
A1284
G1285
C1286
G1290

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	INDIVIDUAL PARTICLES, PHASE AND AMPLITUDE	Depositor
Microscope	PHILIPS CM200, PHILIPS CM300 FEG	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000, Not provided	Depositor
Minimum defocus (nm)	1300, Not provided	Depositor
Maximum defocus (nm)	3200, Not provided	Depositor
Magnification	38000, 45000	Depositor
Image detector	KODAK SO-163 FILM, Not provided	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: CH1, MN

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	0.38	0/10239	0.61	1/13905 (0.0%)
2	B	0.81	1/130 (0.8%)	0.68	0/201
3	C	0.52	0/182	0.71	0/280
All	All	0.39	1/10551 (0.0%)	0.61	1/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1272	G	OP3-P	-7.08	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ILE	N-CA-C	-5.48	96.20	111.00

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	9986	0	9903	356	0
2	B	116	0	56	7	0
3	C	165	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	84	0	36	3	0
5	A	2	0	0	0	0
6	Z	350	0	0	8	0
All	All	10703	0	10083	357	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 17.

The worst 5 of 357 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:223:THR:HG22	1:A:225:ALA:H	1.14	1.12
1:A:1112:MET:HE1	1:A:1150:LEU:HD11	1.31	1.08
1:A:562:ALA:HB2	2:B:1274:G:H21	1.22	1.04
1:A:410:GLU:H	1:A:649:GLN:NE2	1.58	1.01
1:A:724:THR:HG22	1:A:726:GLN:H	1.31	0.96

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	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	13 57

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	A	559	SER
1	A	561	SER
1	A	814	TRP

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Mol	Chain	Res	Type
1	A	564	ILE

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	1081/1083 (100%)	1044 (97%)	37 (3%)	44 75

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	735	ASP
1	A	804	GLU
1	A	1151	GLN
1	A	778	THR
1	A	784	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	GLN
1	A	675	HIS
1	A	1005	ASN
1	A	664	ASN
1	A	671	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	4/5 (80%)	0	0
3	C	7/8 (87%)	0	0
All	All	11/13 (84%)	0	0

There are no RNA backbone outliers to report.

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	CH1	A	2267	5	22,29,29	1.12	1 (4%)	23,45,45	2.88	10 (43%)
4	CH1	A	2268	-	22,29,29	1.16	2 (9%)	23,45,45	2.87	9 (39%)
4	CH1	A	2269	-	22,29,29	1.16	1 (4%)	23,45,45	2.91	8 (34%)

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	CH1	A	2267	5	-	0/18/34/34	0/2/2/2
4	CH1	A	2268	-	-	0/18/34/34	0/2/2/2
4	CH1	A	2269	-	-	0/18/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2267	CH1	C6-N1	2.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2268	CH1	PG-O1G	2.10	1.57	1.50
4	A	2268	CH1	C6-N1	2.29	1.38	1.35
4	A	2269	CH1	C6-N1	2.49	1.39	1.35

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2269	CH1	O3G-PG-O1G	-9.17	80.70	110.63
4	A	2268	CH1	O3G-PG-O1G	-8.83	81.81	110.63
4	A	2267	CH1	O3G-PG-O1G	-8.78	81.97	110.63
4	A	2267	CH1	O3G-PG-O2G	-5.32	87.91	107.44
4	A	2269	CH1	O3G-PG-O2G	-5.29	88.04	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2267	CH1	2	0
4	A	2268	CH1	1	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.