



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5AMR / pdb_00005amr
Title : Structure of the La Crosse Bunyavirus polymerase in complex with the 3' viral RNA
Authors : Reguera, J.; Gerlach, P.; Cusack, S.
Deposited on : 2015-03-12
Resolution : 2.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

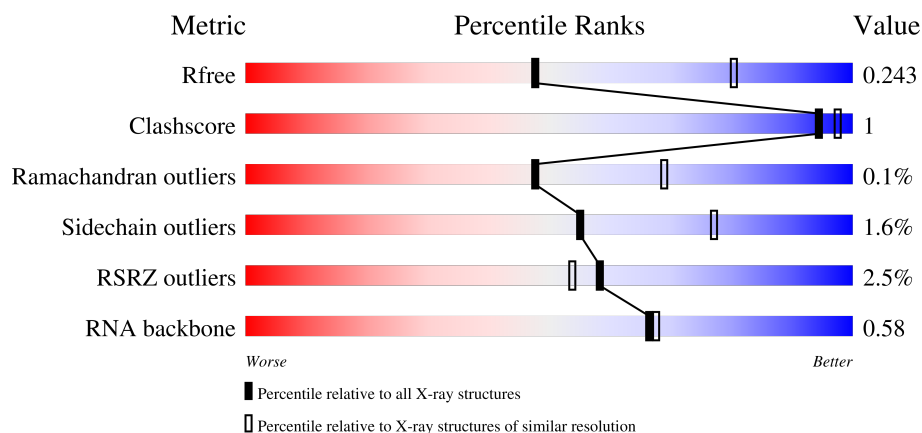
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)
RNA backbone	3983	1011 (2.82-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2264	 2% 70% 27%
2	B	16	 75% 25%
3	C	8	 75% 12% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14163 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 POLYMERASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1657	Total	C	N	O	S	0	0	0
			13571	8701	2256	2525	89			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A5HC98

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	P	0	0	0
			334	151	56	112	15			

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			166	76	31	52	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	1	Total	O	0	0
			1	1		
4	C	4	Total	O	0	0
			4	4		

- Molecule 1: RNA POLYMERASE L



SER	LEU	PRO	GLY	THR	ASP	ILE	PRO	PRO	TRP	ASN	VAL	MET	THR	GLU	ASN	PHE	LYS	LYS	LYS	CYS	ILE	ALA	LEU	LEU	ASN	SER	LYS	PHE	GLU	THR	THR	GLN	ARG	ASP	PHE	SER	GLU	GLU	PHE	THR	LYS	MET	LEU	LYS	GLY	ARG	SER	ASN	ILE	LEU	GLU	PHE	ASP
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Chain B: 75% 25%



Chain C: 75% 12% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.00Å 140.70Å 162.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 2.57 48.66 – 2.57	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.66-2.57) 94.7 (48.66-2.57)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.204 , 0.252 (Not available) , 0.243	Depositor DCC
R_{free} test set	3533 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14163	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/13841	0.60	0/18649
2	B	0.10	0/372	0.27	0/577
3	C	0.09	0/185	0.22	0/286
All	All	0.28	0/14398	0.58	0/19512

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	13571	0	13652	32	0
2	B	334	0	172	1	0
3	C	166	0	89	2	0
4	A	87	0	0	12	0
4	B	1	0	0	0	0
4	C	4	0	0	2	0
All	All	14163	0	13913	35	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 1.

The worst 5 of 35 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:334:ILE:O	4:A:3025:HOH:O	1.81	0.96
1:A:501:GLU:OE1	4:A:3037:HOH:O	1.82	0.95
1:A:741:TYR:OH	4:A:3046:HOH:O	2.05	0.73
4:A:3080:HOH:O	2:B:12:C:OP1	2.07	0.73
1:A:917:GLU:OE2	4:A:3054:HOH:O	2.10	0.68

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1629/2264 (72%)	1567 (96%)	60 (4%)	2 (0%)	48 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	ARG
1	A	1234	CYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1535/2087 (74%)	1511 (98%)	24 (2%)	55 77

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1138	LEU
1	A	1313	GLN
1	A	1305	LEU
1	A	1359	LYS
1	A	556	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1112	ASN
1	A	1145	GLN
1	A	1704	HIS
1	A	1571	GLN
1	A	578	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	15/16 (93%)	3 (20%)	0
3	C	7/8 (87%)	1 (14%)	0
All	All	22/24 (91%)	4 (18%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	A
2	B	10	C
2	B	14	A
3	C	16	A

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1657/2264 (73%)	0.17	42 (2%) 58 54	36, 62, 111, 145	0
2	B	16/16 (100%)	-0.76	0 100 100	49, 57, 62, 66	0
3	C	8/8 (100%)	-0.70	0 100 100	55, 62, 72, 73	0
All	All	1681/2288 (73%)	0.15	42 (2%) 58 54	36, 62, 111, 145	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	ALA	5.6
1	A	873	LEU	5.1
1	A	1432	PHE	4.9
1	A	721	ILE	4.6
1	A	1642	PRO	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.