



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:02 am BST

PDB ID : 1LLN
Title : 1.6Å CRYSTAL STRUCTURE OF POKEWEED ANTIVIRAL PROTEIN-III
(PAP-III) WITH METHYLATED LYSINES
Authors : Kurinov, I.V.; Uckun, F.M.
Deposited on : 2002-04-29
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

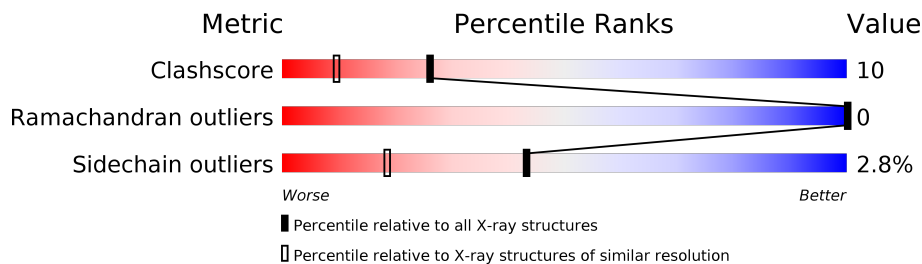
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	 81% 18%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2357 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 Antiviral Protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2097	1332	347	407	11	0	6	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	28	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	46	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	53	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	87	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	115	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	134	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	143	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	177	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	182	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	184	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	198	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	211	MLY	LYS	MODIFIED RESIDUE	UNP Q40772
A	231	MLY	LYS	MODIFIED RESIDUE	UNP Q40772

- Molecule 2 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	260	Total	O	0	0
			260	260		

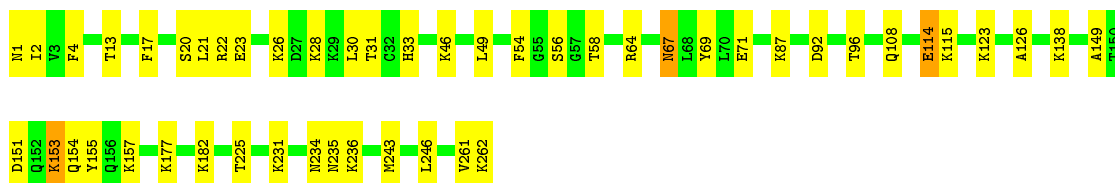
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: Antiviral Protein 3

Chain A:  81% 18%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.47Å 80.47Å 76.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 1.60	Depositor
% Data completeness (in resolution range)	97.1 (7.00-1.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.201 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2357	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

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: MLY

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	0.35	0/2001	0.65	0/2711

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	2097	0	2128	44	0
2	A	260	0	0	9	0
All	All	2357	0	2128	44	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 10.

All (44) 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:153:LYS:HD2	1:A:153:LYS:H	1.22	1.04
1:A:87:MLY:HE3	1:A:114:GLU:HG3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HE22	1:A:149:ALA:H	1.28	0.79
1:A:123:LYS:O	1:A:157:LYS:HD3	1.83	0.77
1:A:243:MET:SD	2:A:582:HOH:O	2.48	0.71
1:A:153:LYS:CD	1:A:153:LYS:H	1.99	0.71
1:A:234:ASN:HB2	1:A:236:LYS:HD3	1.75	0.69
1:A:46:MLY:HH13	1:A:92:ASP:OD2	1.95	0.67
1:A:46:MLY:HH23	1:A:64:ARG:NH2	2.11	0.65
1:A:153:LYS:HD2	1:A:153:LYS:N	2.06	0.63
1:A:1:ASN:HD22	1:A:49:LEU:H	1.44	0.62
1:A:234:ASN:HD22	1:A:236:LYS:NZ	1.98	0.61
1:A:1:ASN:ND2	1:A:49:LEU:H	2.00	0.60
1:A:225[B]:THR:HG23	2:A:509:HOH:O	2.02	0.59
1:A:151:ASP:O	1:A:155:TYR:HB3	2.07	0.54
1:A:243:MET:HA	1:A:243:MET:HE3	1.90	0.54
1:A:126:ALA:HB2	2:A:708:HOH:O	2.07	0.54
1:A:33:HIS:HD2	2:A:691:HOH:O	1.92	0.53
1:A:225[A]:THR:HG23	2:A:509:HOH:O	2.08	0.53
1:A:54:PHE:CZ	1:A:56:SER:HB2	2.43	0.53
1:A:243:MET:HE3	1:A:246:LEU:HB2	1.89	0.53
1:A:231:MLY:HD2	1:A:235:ASN:ND2	2.24	0.52
1:A:23:GLU:O	1:A:28:MLY:HH21	2.10	0.51
1:A:64:ARG:HB3	1:A:67:ASN:HD21	1.77	0.50
1:A:2[B]:ILE:HD12	1:A:20[B]:SER:HB2	1.94	0.50
1:A:157:LYS:HB2	1:A:157:LYS:HE2	1.65	0.48
1:A:22:ARG:NH1	1:A:177:MLY:HH13	2.29	0.48
1:A:26:MLY:CH2	1:A:28:MLY:HA	2.43	0.48
1:A:4:PHE:HB2	1:A:17:PHE:CD1	2.50	0.47
1:A:2[A]:ILE:CD1	1:A:21:LEU:HB2	2.46	0.46
1:A:13[B]:THR:HG21	2:A:501:HOH:O	2.16	0.45
1:A:26:MLY:HH21	1:A:28:MLY:HA	1.97	0.45
1:A:151:ASP:OD1	1:A:154:GLN:HB3	2.16	0.45
1:A:114:GLU:HG2	2:A:739:HOH:O	2.17	0.44
1:A:31:THR:OG1	1:A:262:LYS:HG2	2.17	0.44
1:A:67:ASN:HD22	1:A:67:ASN:C	2.21	0.43
1:A:58:THR:HG21	2:A:568:HOH:O	2.19	0.43
1:A:67:ASN:ND2	1:A:69:TYR:H	2.16	0.43
1:A:22:ARG:HH12	1:A:177:MLY:HH13	1.85	0.42
1:A:46:MLY:HH13	1:A:92:ASP:CG	2.41	0.41
1:A:49:LEU:HD21	1:A:96:THR:HG22	2.01	0.41
1:A:71:GLU:OE2	1:A:115:MLY:HH12	2.20	0.41
1:A:2[B]:ILE:HD12	1:A:20[B]:SER:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MLY:HH13	2:A:623:HOH:O	2.20	0.41

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	252/262 (96%)	246 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	219/213 (103%)	213 (97%)	6 (3%)	44 20

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	67	ASN
1	A	114	GLU
1	A	138	LYS
1	A	153	LYS

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Mol	Chain	Res	Type
1	A	261	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	33	HIS
1	A	67	ASN
1	A	78	ASN
1	A	94	GLN
1	A	108	GLN
1	A	154	GLN
1	A	194	GLN
1	A	234	ASN
1	A	235	ASN
1	A	244	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues 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
1	MLY	A	26	1	9,10,11	0.85	0	6,11,13	2.18	2 (33%)
1	MLY	A	115	1	9,10,11	0.61	0	6,11,13	2.14	3 (50%)
1	MLY	A	53	1	9,10,11	0.76	0	6,11,13	2.17	3 (50%)
1	MLY	A	143	1	9,10,11	0.80	0	6,11,13	2.30	3 (50%)
1	MLY	A	177	1	9,10,11	0.79	0	6,11,13	2.13	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	211	1	9,10,11	0.77	0	6,11,13	2.17	2 (33%)
1	MLY	A	184	1	9,10,11	0.75	0	6,11,13	2.12	3 (50%)
1	MLY	A	87	1	9,10,11	0.75	0	6,11,13	2.23	2 (33%)
1	MLY	A	198	1	9,10,11	0.63	0	6,11,13	2.18	2 (33%)
1	MLY	A	28	1	9,10,11	0.89	0	6,11,13	2.10	3 (50%)
1	MLY	A	182	1	9,10,11	0.69	0	6,11,13	2.19	3 (50%)
1	MLY	A	231	1	9,10,11	0.74	0	6,11,13	2.10	3 (50%)
1	MLY	A	46	1	9,10,11	0.69	0	6,11,13	2.20	3 (50%)
1	MLY	A	134	1	9,10,11	0.82	0	6,11,13	2.16	3 (50%)

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
1	MLY	A	26	1	-	1/8/9/11	-
1	MLY	A	115	1	-	2/8/9/11	-
1	MLY	A	53	1	-	1/8/9/11	-
1	MLY	A	143	1	-	1/8/9/11	-
1	MLY	A	177	1	-	1/8/9/11	-
1	MLY	A	211	1	-	2/8/9/11	-
1	MLY	A	184	1	-	2/8/9/11	-
1	MLY	A	87	1	-	1/8/9/11	-
1	MLY	A	198	1	-	1/8/9/11	-
1	MLY	A	28	1	-	4/8/9/11	-
1	MLY	A	182	1	-	1/8/9/11	-
1	MLY	A	231	1	-	1/8/9/11	-
1	MLY	A	46	1	-	1/8/9/11	-
1	MLY	A	134	1	-	1/8/9/11	-

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	MLY	CH2-NZ-CH1	4.15	120.47	109.73
1	A	87	MLY	CH2-NZ-CH1	4.13	120.42	109.73
1	A	211	MLY	CH2-NZ-CH1	4.07	120.26	109.73
1	A	182	MLY	CH2-NZ-CH1	4.07	120.26	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	MLY	CH2-NZ-CH1	4.06	120.24	109.73
1	A	134	MLY	CH2-NZ-CH1	4.06	120.24	109.73
1	A	198	MLY	CH2-NZ-CH1	4.05	120.19	109.73
1	A	177	MLY	CH2-NZ-CH1	3.98	120.03	109.73
1	A	26	MLY	CH2-NZ-CH1	3.98	120.01	109.73
1	A	184	MLY	CH2-NZ-CH1	3.90	119.81	109.73
1	A	231	MLY	CH2-NZ-CH1	3.81	119.58	109.73
1	A	28	MLY	CH2-NZ-CH1	3.80	119.56	109.73
1	A	115	MLY	CH2-NZ-CH1	3.80	119.55	109.73
1	A	46	MLY	CH2-NZ-CH1	3.40	118.52	109.73
1	A	198	MLY	CH1-NZ-CE	2.84	121.99	110.74
1	A	46	MLY	CH1-NZ-CE	2.80	121.85	110.74
1	A	28	MLY	CH2-NZ-CE	2.75	121.64	110.74
1	A	26	MLY	CH1-NZ-CE	2.72	121.50	110.74
1	A	87	MLY	CH1-NZ-CE	2.70	121.44	110.74
1	A	231	MLY	CH2-NZ-CE	2.64	121.21	110.74
1	A	211	MLY	CH1-NZ-CE	2.61	121.08	110.74
1	A	53	MLY	CH2-NZ-CE	2.58	120.96	110.74
1	A	115	MLY	CH1-NZ-CE	2.51	120.68	110.74
1	A	134	MLY	CH2-NZ-CE	2.51	120.66	110.74
1	A	143	MLY	CH2-NZ-CE	2.51	120.66	110.74
1	A	177	MLY	CH2-NZ-CE	2.49	120.62	110.74
1	A	182	MLY	CH1-NZ-CE	2.46	120.47	110.74
1	A	184	MLY	CH1-NZ-CE	2.39	120.23	110.74
1	A	184	MLY	CH2-NZ-CE	2.33	119.95	110.74
1	A	115	MLY	CH2-NZ-CE	2.27	119.75	110.74
1	A	46	MLY	CH2-NZ-CE	2.24	119.61	110.74
1	A	177	MLY	CH1-NZ-CE	2.17	119.32	110.74
1	A	182	MLY	CH2-NZ-CE	2.15	119.27	110.74
1	A	231	MLY	CH1-NZ-CE	2.14	119.21	110.74
1	A	134	MLY	CH1-NZ-CE	2.11	119.08	110.74
1	A	143	MLY	CH1-NZ-CE	2.05	118.86	110.74
1	A	28	MLY	CH1-NZ-CE	2.04	118.81	110.74
1	A	53	MLY	CH1-NZ-CE	2.03	118.77	110.74

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	MLY	O-C-CA-CB
1	A	115	MLY	CD-CE-NZ-CH2
1	A	184	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	198	MLY	CD-CE-NZ-CH1
1	A	28	MLY	CD-CE-NZ-CH1
1	A	182	MLY	CD-CE-NZ-CH2
1	A	46	MLY	CD-CE-NZ-CH1
1	A	115	MLY	CG-CD-CE-NZ
1	A	26	MLY	CD-CE-NZ-CH2
1	A	53	MLY	CD-CE-NZ-CH2
1	A	177	MLY	CD-CE-NZ-CH2
1	A	211	MLY	CD-CE-NZ-CH1
1	A	87	MLY	CD-CE-NZ-CH1
1	A	134	MLY	CD-CE-NZ-CH2
1	A	143	MLY	CD-CE-NZ-CH2
1	A	184	MLY	CD-CE-NZ-CH1
1	A	28	MLY	C-CA-CB-CG
1	A	231	MLY	CD-CE-NZ-CH2
1	A	28	MLY	CA-CB-CG-CD
1	A	28	MLY	CD-CE-NZ-CH2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	26	MLY	2	0
1	A	115	MLY	1	0
1	A	177	MLY	2	0
1	A	87	MLY	1	0
1	A	28	MLY	3	0
1	A	182	MLY	1	0
1	A	231	MLY	1	0
1	A	46	MLY	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.