



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:02 PM EST

PDB ID : 1APA
Title : X-RAY STRUCTURE OF A POKEWEED ANTIVIRAL PROTEIN, CODED BY A NEW GENOMIC CLONE, AT 0.23 NM RESOLUTION. A MODEL STRUCTURE PROVIDES A SUITABLE ELECTROSTATIC FIELD FOR SUBSTRATE BINDING.
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Deposited on : unknown
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

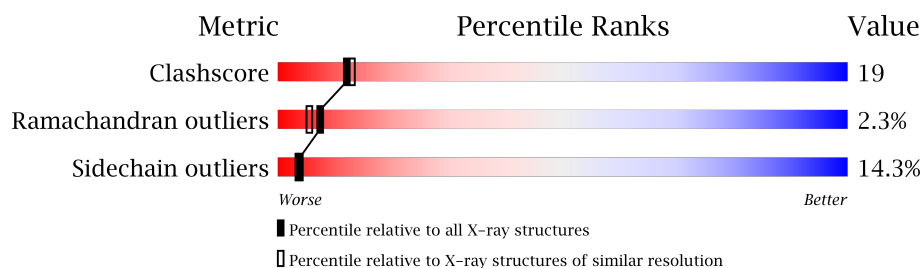
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2149 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 POKEWEED ANTIVIRAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2054	1303	351	390	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	LEU	TRP	CONFLICT	UNP Q03464
A	5	GLU	ALA	CONFLICT	UNP Q03464

- Molecule 2 is water.

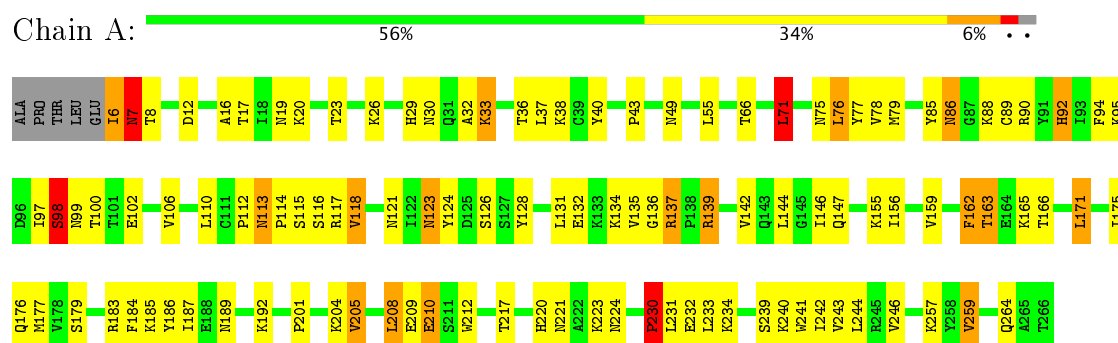
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: POKEWEED ANTIVIRAL PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	47.10Å 116.30Å 49.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2149	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

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	0.81	0/2092	0.97	4/2834 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	7	ASN	N-CA-C	-8.28	88.64	111.00
1	A	71	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	98	SER	N-CA-C	5.98	127.14	111.00
1	A	231	LEU	CA-CB-CG	5.92	128.92	115.30

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	2054	0	2079	79	0
2	A	95	0	0	9	0
All	All	2149	0	2079	79	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 19.

All (79) 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:128:TYR:O	1:A:132:GLU:HG3	1.65	0.96
1:A:163:THR:HG22	1:A:165:LYS:H	1.27	0.96
1:A:102:GLU:O	1:A:106:VAL:HG23	1.77	0.85
1:A:217:THR:HG22	1:A:221:ASN:HD21	1.46	0.81
1:A:185:LYS:HG3	2:A:347:HOH:O	1.85	0.76
1:A:139:ARG:HA	1:A:142:VAL:HG12	1.69	0.75
1:A:204:LYS:HE3	1:A:241:TRP:CZ3	2.24	0.73
1:A:38:LYS:HD3	1:A:43:PRO:HA	1.71	0.71
1:A:205:VAL:O	1:A:209:GLU:HG3	1.91	0.71
1:A:71:LEU:HD22	1:A:78:VAL:HG22	1.73	0.70
1:A:204:LYS:HG2	1:A:208:LEU:HD22	1.73	0.69
1:A:217:THR:HG22	1:A:221:ASN:ND2	2.08	0.68
1:A:240:LYS:HD3	1:A:242:ILE:HD11	1.74	0.67
1:A:7:ASN:N	1:A:7:ASN:OD1	2.28	0.66
1:A:6:ILE:HD11	1:A:112:PRO:CD	2.25	0.66
1:A:16:ALA:HA	1:A:20:LYS:HD2	1.76	0.66
1:A:89:CYS:O	1:A:117:ARG:HA	1.96	0.66
1:A:99:ASN:HB3	1:A:102:GLU:HG3	1.77	0.65
1:A:171:LEU:O	1:A:175:ILE:HG13	1.98	0.63
1:A:94:PHE:CG	1:A:126:SER:HB3	2.32	0.63
1:A:23:THR:HA	2:A:272:HOH:O	1.98	0.62
1:A:12:ASP:HB3	1:A:20:LYS:HE2	1.79	0.62
1:A:29:HIS:HB2	2:A:274:HOH:O	2.01	0.60
1:A:75:ASN:CG	1:A:77:TYR:HD2	2.05	0.60
1:A:85:TYR:O	1:A:88:LYS:HG2	2.02	0.60
1:A:163:THR:HG22	1:A:165:LYS:N	2.10	0.59
1:A:88:LYS:HG3	1:A:118:VAL:HG22	1.85	0.58
1:A:184:PHE:HB2	1:A:187:ILE:HD12	1.85	0.58
1:A:183:ARG:HD2	1:A:212:TRP:CE2	2.39	0.57
1:A:17:THR:OG1	1:A:20:LYS:HB2	2.05	0.56
1:A:179:SER:O	1:A:183:ARG:HG3	2.06	0.56
1:A:94:PHE:CD2	1:A:126:SER:HB3	2.43	0.53
1:A:123:ASN:HB2	2:A:304:HOH:O	2.07	0.53
1:A:204:LYS:HE3	1:A:241:TRP:HZ3	1.72	0.53
1:A:121:ASN:HB3	2:A:297:HOH:O	2.09	0.52
1:A:189:ASN:HD22	1:A:192:LYS:HE2	1.75	0.52
1:A:32:ALA:HB2	1:A:55:LEU:HD11	1.92	0.52
1:A:139:ARG:HA	1:A:142:VAL:CG1	2.37	0.51
1:A:114:PRO:O	1:A:115:SER:C	2.48	0.51
1:A:6:ILE:N	1:A:7:ASN:OD1	2.44	0.51
1:A:146:ILE:HD12	1:A:177:MET:CE	2.42	0.50
1:A:29:HIS:CE1	1:A:43:PRO:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD21	1:A:176:GLN:NE2	2.26	0.50
1:A:75:ASN:O	1:A:183:ARG:NH1	2.45	0.50
1:A:136:GLY:O	1:A:137:ARG:HG3	2.12	0.50
1:A:33:LYS:HE3	2:A:275:HOH:O	2.11	0.49
1:A:201:PRO:HB2	1:A:205:VAL:HG22	1.95	0.49
1:A:156:ILE:O	1:A:159:VAL:HG22	2.13	0.48
1:A:159:VAL:HG23	1:A:162:PHE:HD2	1.78	0.48
1:A:85:TYR:O	1:A:86:ASN:HB2	2.13	0.48
1:A:204:LYS:HG2	1:A:208:LEU:CD2	2.43	0.47
1:A:234:LYS:HE2	2:A:328:HOH:O	2.13	0.47
1:A:162:PHE:O	1:A:163:THR:CB	2.63	0.47
1:A:95:LYS:HE3	1:A:123:ASN:O	2.14	0.47
1:A:92:HIS:N	1:A:92:HIS:CD2	2.82	0.47
1:A:159:VAL:O	1:A:159:VAL:HG23	2.14	0.47
1:A:139:ARG:HH22	1:A:210:GLU:CD	2.18	0.46
1:A:90:ARG:HA	1:A:118:VAL:O	2.15	0.46
1:A:30:ASN:ND2	2:A:275:HOH:O	2.45	0.45
1:A:40:TYR:CD2	1:A:246:VAL:HG21	2.51	0.45
1:A:146:ILE:HD12	1:A:177:MET:HE2	1.98	0.45
1:A:212:TRP:CZ3	1:A:257:LYS:HG3	2.52	0.45
1:A:98:SER:O	1:A:99:ASN:C	2.56	0.44
1:A:124:TYR:CE1	1:A:131:LEU:HD23	2.53	0.43
1:A:132:GLU:O	1:A:136:GLY:N	2.49	0.43
1:A:139:ARG:NH1	1:A:209:GLU:OE1	2.51	0.43
1:A:204:LYS:O	1:A:208:LEU:HD22	2.19	0.43
1:A:94:PHE:HB2	1:A:97:ILE:HG12	2.01	0.43
1:A:113:ASN:C	1:A:113:ASN:ND2	2.71	0.42
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.90	0.42
1:A:186:TYR:CZ	1:A:204:LYS:HD3	2.55	0.42
1:A:75:ASN:O	1:A:76:LEU:HB2	2.19	0.42
1:A:113:ASN:C	1:A:113:ASN:HD22	2.21	0.41
1:A:223:LYS:O	1:A:224:ASN:C	2.58	0.41
1:A:147:GLN:HB3	2:A:314:HOH:O	2.20	0.41
1:A:155:LYS:HB3	1:A:166:THR:HG21	2.02	0.41
1:A:230:PRO:HG3	1:A:244:LEU:HD23	2.02	0.41
1:A:220:HIS:CE1	1:A:259:VAL:HG22	2.56	0.40
1:A:183:ARG:HD2	1:A:212:TRP:CZ2	2.57	0.40

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 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	259/266 (97%)	239 (92%)	14 (5%)	6 (2%)	7 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	163	THR
1	A	137	ARG
1	A	86	ASN
1	A	123	ASN
1	A	230	PRO

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 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	230/234 (98%)	197 (86%)	33 (14%)	4 3

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	7	ASN
1	A	8	THR
1	A	19	ASN
1	A	26	LYS

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Mol	Chain	Res	Type
1	A	33	LYS
1	A	36	THR
1	A	37	LEU
1	A	49	ASN
1	A	66	THR
1	A	71	LEU
1	A	76	LEU
1	A	79	MET
1	A	92	HIS
1	A	98	SER
1	A	100	THR
1	A	113	ASN
1	A	118	VAL
1	A	134	LYS
1	A	135	VAL
1	A	139	ARG
1	A	162	PHE
1	A	171	LEU
1	A	205	VAL
1	A	208	LEU
1	A	210	GLU
1	A	230	PRO
1	A	232	GLU
1	A	233	LEU
1	A	239	SER
1	A	243	VAL
1	A	259	VAL
1	A	264	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	60	GLN
1	A	113	ASN
1	A	150	ASN
1	A	176	GLN
1	A	189	ASN
1	A	207	ASN
1	A	221	ASN
1	A	260	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](#)

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](#)

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.