



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2016 – 04:08 PM EDT

PDB ID : 5AOF
Title : Crystal structure of pneumolysin deletion mutant Delta146_147.
Authors : van Pee, K.; Yildiz, O.
Deposited on : 2015-09-10
Resolution : 2.45 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

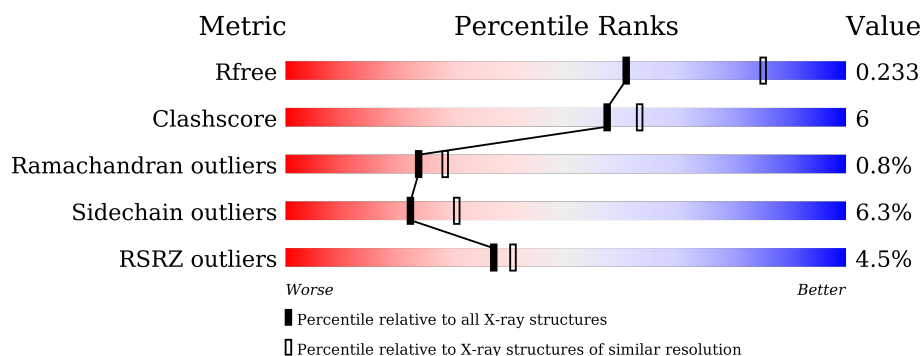
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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.

Mol	Chain	Length	Quality of chain
1	A	488	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4008 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 PNEUMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3856	2429	663	757	7			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	ALA	-	EXPRESSION TAG	UNP Q04IN8
A	-16	ALA	-	EXPRESSION TAG	UNP Q04IN8
A	-15	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-14	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-13	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-12	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-11	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-10	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	-9	SER	-	EXPRESSION TAG	UNP Q04IN8
A	-8	SER	-	EXPRESSION TAG	UNP Q04IN8
A	-7	GLY	-	EXPRESSION TAG	UNP Q04IN8
A	-6	LEU	-	EXPRESSION TAG	UNP Q04IN8
A	-5	VAL	-	EXPRESSION TAG	UNP Q04IN8
A	-4	PRO	-	EXPRESSION TAG	UNP Q04IN8
A	-3	ARG	-	EXPRESSION TAG	UNP Q04IN8
A	-2	GLY	-	EXPRESSION TAG	UNP Q04IN8
A	-1	SER	-	EXPRESSION TAG	UNP Q04IN8
A	0	HIS	-	EXPRESSION TAG	UNP Q04IN8
A	469	ALA	-	EXPRESSION TAG	UNP Q04IN8
A	470	ALA	-	EXPRESSION TAG	UNP Q04IN8
A	.	-	ALA	DELETION	UNP Q04IN8
A	.	-	ARG	DELETION	UNP Q04IN8

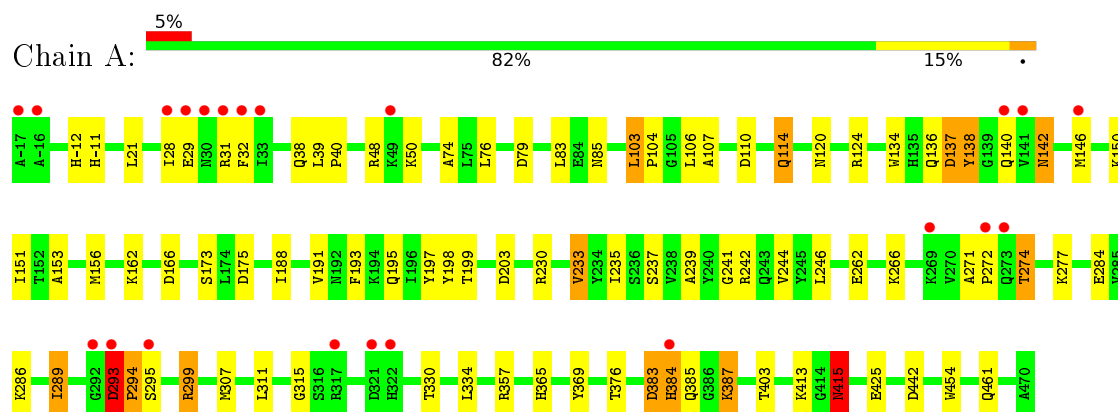
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total 152	O 152	0	0

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 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.

• Molecule 1: PNEUMOLYSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	24.73Å 163.50Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.45 48.26 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.26-2.45) 91.0 (48.26-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.234 0.207 , 0.233	Depositor DCC
R_{free} test set	1485 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4008	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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	0.21	0/3937	0.40	1/5352 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	293	ASP	C-N-CD	5.24	139.40	128.40

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	3856	0	3785	46	0
2	A	152	0	0	2	0
All	All	4008	0	3785	46	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 6.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:383:ASP:HB3	1:A:387:LYS:HG3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:HB3	1:A:294:PRO:HD3	1.76	0.67
1:A:150:LYS:NZ	1:A:262:GLU:OE1	2.28	0.66
1:A:173:SER:O	1:A:286:LYS:NZ	2.28	0.65
1:A:85:ASN:HB2	1:A:166:ASP:HB3	1.78	0.64
1:A:79:ASP:OD2	1:A:230:ARG:NH1	2.31	0.62
1:A:142:ASN:OD1	1:A:142:ASN:N	2.37	0.58
1:A:103:LEU:HD12	1:A:104:PRO:HD2	1.86	0.57
1:A:153:ALA:HB3	1:A:188:ILE:HB	1.87	0.55
1:A:21:LEU:HA	1:A:83:LEU:HD11	1.89	0.55
1:A:107:ALA:HB3	1:A:110:ASP:HB2	1.90	0.54
1:A:272:PRO:HA	1:A:277:LYS:HG2	1.88	0.54
1:A:151:ILE:HD13	1:A:162:LYS:HG2	1.91	0.53
1:A:74:ALA:HB3	1:A:235:ILE:HD12	1.93	0.51
1:A:289:ILE:HD11	1:A:311:LEU:HD22	1.94	0.50
1:A:120:ASN:O	1:A:124:ARG:HB2	2.12	0.49
1:A:237:SER:HG	1:A:330:THR:HG1	1.60	0.48
1:A:134:TRP:HH2	1:A:142:ASN:HD21	1.61	0.47
1:A:146:MET:SD	1:A:195:GLN:NE2	2.87	0.47
1:A:242:ARG:HD3	1:A:315:GLY:HA3	1.95	0.47
1:A:413:LYS:HB2	1:A:415:ASN:HB2	1.97	0.47
1:A:195:GLN:OE1	1:A:242:ARG:NH1	2.41	0.46
1:A:50:LYS:HB3	1:A:50:LYS:HE2	1.72	0.46
1:A:39:LEU:HB3	1:A:40:PRO:HD2	1.98	0.46
1:A:262:GLU:O	1:A:266:LYS:HG2	2.16	0.45
1:A:369:TYR:CG	1:A:425:GLU:HG3	2.51	0.45
1:A:114:GLN:NE2	2:A:2055:HOH:O	2.49	0.45
1:A:271:ALA:O	1:A:274:THR:OG1	2.31	0.45
1:A:76:LEU:HB2	1:A:233:VAL:HG12	1.97	0.45
1:A:193:PHE:HB2	1:A:244:VAL:HB	1.98	0.45
1:A:384:HIS:HD1	1:A:385:GLN:N	2.14	0.45
1:A:293:ASP:OD2	1:A:299:ARG:NH2	2.47	0.44
1:A:294:PRO:HB2	1:A:295:SER:H	1.47	0.44
1:A:137:ASP:HB3	1:A:138:TYR:CD1	2.51	0.44
1:A:32:PHE:HE2	1:A:50:LYS:HB2	1.82	0.44
1:A:197:TYR:CD2	1:A:241:GLY:HA2	2.53	0.43
1:A:38:GLN:NE2	1:A:39:LEU:O	2.52	0.43
1:A:146:MET:HE3	1:A:193:PHE:HB3	1.99	0.43
1:A:29:GLU:OE1	1:A:29:GLU:N	2.51	0.43
1:A:198:TYR:HA	2:A:2059:HOH:O	2.19	0.43
1:A:28:ILE:HG22	1:A:29:GLU:H	1.84	0.42
1:A:103:LEU:HB3	1:A:106:LEU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-12:HIS:O	1:A:-11:HIS:ND1	2.54	0.41
1:A:191:VAL:HB	1:A:246:LEU:HB3	2.02	0.41
1:A:454:TRP:CE2	1:A:461:GLN:HB2	2.56	0.41
1:A:199:THR:HG22	1:A:239:ALA:HA	2.02	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	486/488 (100%)	467 (96%)	15 (3%)	4 (1%)	24 28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASP
1	A	294	PRO
1	A	415	ASN
1	A	138	TYR

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	428/428 (100%)	401 (94%)	27 (6%)	22 30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	48	ARG
1	A	103	LEU
1	A	114	GLN
1	A	136	GLN
1	A	137	ASP
1	A	140	GLN
1	A	142	ASN
1	A	156	MET
1	A	175	ASP
1	A	203	ASP
1	A	233	VAL
1	A	274	THR
1	A	284	GLU
1	A	289	ILE
1	A	299	ARG
1	A	307	MET
1	A	334	LEU
1	A	357	ARG
1	A	365	HIS
1	A	376	THR
1	A	383	ASP
1	A	384	HIS
1	A	387	LYS
1	A	403	THR
1	A	415	ASN
1	A	442	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [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 [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	488/488 (100%)	-0.03	22 (4%)	37 40	24, 60, 123, 164	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-17	ALA	7.4
1	A	33	ILE	3.8
1	A	273	GLN	3.5
1	A	32	PHE	3.5
1	A	140	GLN	3.4
1	A	295	SER	3.4
1	A	31	ARG	3.2
1	A	317	ARG	2.9
1	A	141	VAL	2.9
1	A	272	PRO	2.8
1	A	29	GLU	2.8
1	A	292	GLY	2.6
1	A	384	HIS	2.6
1	A	293	ASP	2.5
1	A	269	LYS	2.5
1	A	322	HIS	2.4
1	A	321	ASP	2.4
1	A	-16	ALA	2.3
1	A	49	LYS	2.1
1	A	30	ASN	2.1
1	A	28	ILE	2.1
1	A	146	MET	2.1

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 carbohydrates 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.