



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5CR6 / pdb_00005cr6
Title : Structure of pneumolysin at 1.98 Å resolution
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Deposited on : 2015-07-22
Resolution : 1.98 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 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

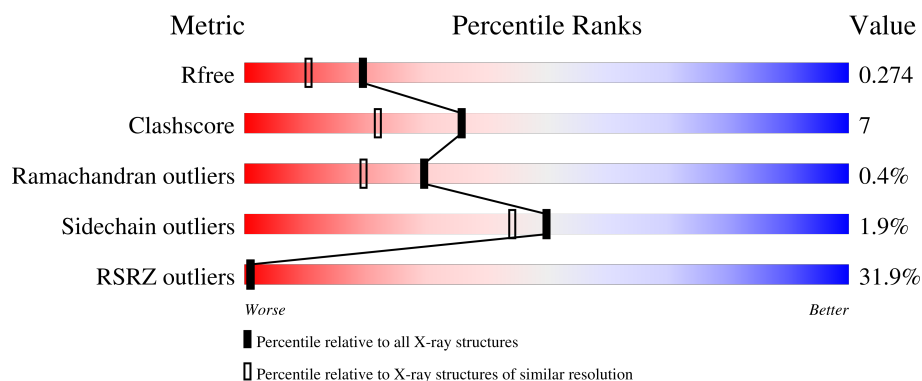
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	D	471	32% 85% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3907 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	D	467	Total	C	N	O	S	0	1	0
			3714	2343	633	733	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASN	ASP	engineered mutation	UNP Q04IN8
D	428	ALA	CYS	engineered mutation	UNP Q04IN8

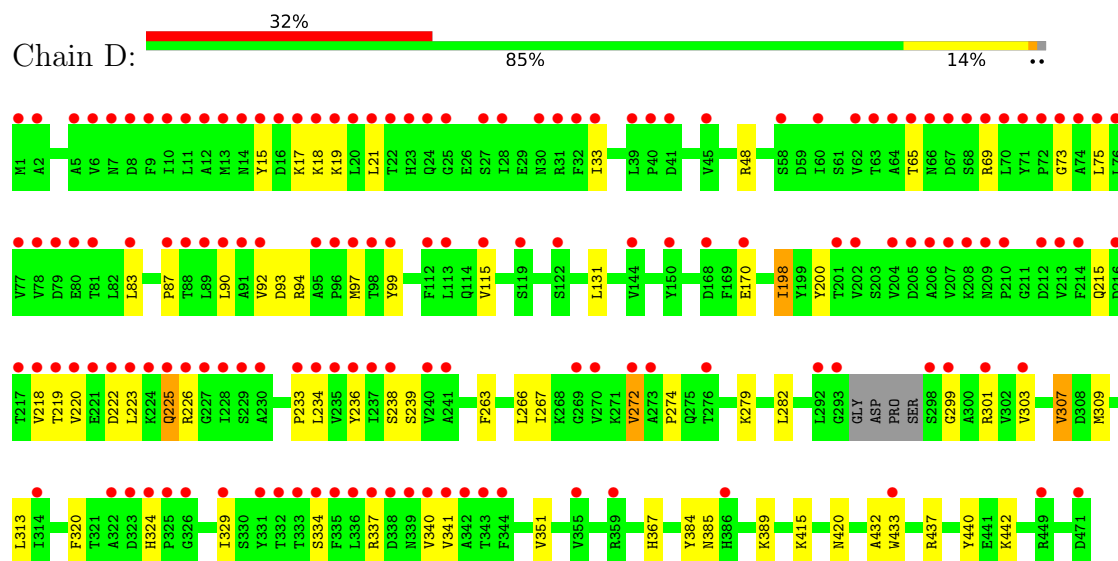
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	193	Total	O	0	0
			193	193		

3 Residue-property plots [i](#)

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

• 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	27.01Å 127.71Å 172.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.07 – 1.98 43.07 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.07-1.98) 99.3 (43.07-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.85 (at 1.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.248 , 0.266 0.254 , 0.274	Depositor DCC
R_{free} test set	2158 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.1	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	0.93	EDS
Total number of atoms	3907	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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	D	0.33	0/3785	0.72	0/5141

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	D	3714	0	3664	54	0
2	D	193	0	0	20	1
All	All	3907	0	3664	54	1

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 7.

All (54) 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:D:215:GLN:O	2:D:501:HOH:O	1.93	0.84
1:D:341:VAL:N	2:D:508:HOH:O	2.15	0.79
1:D:234:LEU:O	2:D:502:HOH:O	2.03	0.76
1:D:384:TYR:O	2:D:503:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:NH1	1:D:87:PRO:O	2.21	0.73
1:D:234:LEU:O	2:D:504:HOH:O	2.07	0.72
1:D:170:GLU:OE1	2:D:505:HOH:O	2.08	0.71
1:D:236:TYR:O	2:D:506:HOH:O	2.08	0.71
1:D:320:PHE:O	2:D:507:HOH:O	2.10	0.69
1:D:198:ILE:HD13	1:D:329:ILE:HD11	1.75	0.68
1:D:115:VAL:N	2:D:517:HOH:O	2.26	0.67
1:D:225:GLN:O	1:D:226:ARG:NH1	2.27	0.67
1:D:226:ARG:NH2	2:D:522:HOH:O	2.30	0.64
1:D:33:ILE:HG13	1:D:48:ARG:HB2	1.81	0.63
1:D:15:TYR:HE2	1:D:337:ARG:HD3	1.63	0.62
1:D:93:ASP:O	2:D:509:HOH:O	2.16	0.62
1:D:94:ARG:NH2	2:D:526:HOH:O	2.34	0.61
1:D:274:PRO:HA	1:D:279:LYS:HG2	1.83	0.60
1:D:238:SER:O	2:D:510:HOH:O	2.16	0.60
1:D:73:GLY:HA3	1:D:97:MET:HE1	1.85	0.58
1:D:17:LYS:HG3	1:D:18:LYS:HG3	1.88	0.56
1:D:218:VAL:HG22	1:D:219:THR:HG23	1.86	0.55
1:D:75:LEU:HD11	1:D:90:LEU:HB3	1.89	0.55
1:D:21:LEU:HA	1:D:83:LEU:HD21	1.88	0.55
1:D:223:LEU:C	1:D:225:GLN:H	2.17	0.51
1:D:437:ARG:NH2	2:D:518:HOH:O	2.26	0.51
1:D:97:MET:HE3	1:D:99:TYR:CZ	2.45	0.50
1:D:334:SER:N	2:D:506:HOH:O	2.42	0.50
1:D:385:ASN:HD21	1:D:389:LYS:HB3	1.77	0.49
1:D:21:LEU:N	2:D:528:HOH:O	2.34	0.49
1:D:233:PRO:HB2	2:D:504:HOH:O	2.13	0.49
1:D:420:ASN:OD1	2:D:512:HOH:O	2.20	0.48
1:D:15:TYR:CE2	1:D:337:ARG:HD3	2.48	0.48
1:D:239:SER:HB3	2:D:510:HOH:O	2.13	0.48
1:D:226:ARG:HD3	1:D:226:ARG:HA	1.72	0.47
1:D:222:ASP:O	1:D:225:GLN:NE2	2.36	0.46
1:D:75:LEU:HD23	1:D:94:ARG:HD3	1.98	0.46
1:D:223:LEU:O	2:D:513:HOH:O	2.21	0.46
1:D:219:THR:HA	1:D:222:ASP:HB3	1.98	0.46
1:D:432:ALA:HB1	1:D:433:TRP:CE3	2.51	0.46
1:D:266:LEU:HD13	1:D:307:VAL:HG13	1.98	0.46
1:D:65:THR:HG21	1:D:299:GLY:HA2	1.99	0.45
1:D:17:LYS:O	1:D:19:LYS:HG2	2.16	0.45
1:D:263:PHE:O	1:D:267:ILE:HG12	2.19	0.43
1:D:324:HIS:O	1:D:324:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:VAL:HG11	1:D:282:LEU:HD12	2.00	0.42
1:D:415:LYS:HE3	1:D:415:LYS:HB2	1.90	0.42
1:D:17:LYS:HE2	1:D:340:VAL:HG11	2.01	0.42
1:D:309:MET:HE2	1:D:313:LEU:HD11	2.02	0.42
1:D:131:LEU:HD11	1:D:200:TYR:CZ	2.56	0.41
1:D:440:TYR:OH	1:D:442:LYS:HD2	2.21	0.41
1:D:223:LEU:C	1:D:225:GLN:N	2.78	0.41
1:D:385:ASN:ND2	1:D:389:LYS:HB3	2.36	0.41
1:D:97:MET:HE3	1:D:99:TYR:OH	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:656:HOH:O	2:D:669:HOH:O[1_455]	2.19	0.01

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	D	464/471 (98%)	438 (94%)	24 (5%)	2 (0%)	30 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	225	GLN
1	D	92	VAL

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	D	412/415 (99%)	403 (98%)	9 (2%)	45 38

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	198	ILE
1	D	220	VAL
1	D	272	VAL
1	D	301[A]	ARG
1	D	301[B]	ARG
1	D	303	VAL
1	D	307	VAL
1	D	351	VAL
1	D	367	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	37	ASN
1	D	56	ASN
1	D	191	GLN

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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	D	467/471 (99%)	1.56	149 (31%) 1 1	22, 66, 125, 138	1 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	VAL	7.3
1	D	340	VAL	7.2
1	D	76	LEU	6.9
1	D	92	VAL	6.6
1	D	75	LEU	5.9
1	D	32	PHE	5.8
1	D	77	VAL	5.6
1	D	223	LEU	5.6
1	D	6	VAL	5.6
1	D	10	ILE	5.4
1	D	336	LEU	5.4
1	D	28	ILE	5.3
1	D	218	VAL	5.2
1	D	230	ALA	5.2
1	D	220	VAL	5.1
1	D	89	LEU	4.9
1	D	15	TYR	4.9
1	D	21	LEU	4.8
1	D	33	ILE	4.8
1	D	9	PHE	4.7
1	D	22	THR	4.6
1	D	213	VAL	4.6
1	D	70	LEU	4.6
1	D	433	TRP	4.5
1	D	214	PHE	4.5
1	D	20	LEU	4.4
1	D	342	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	219	THR	4.3
1	D	206	ALA	4.3
1	D	67	ASP	4.3
1	D	236	TYR	4.2
1	D	233	PRO	4.2
1	D	207	VAL	4.1
1	D	339	ASN	4.1
1	D	90	LEU	4.1
1	D	234	LEU	4.1
1	D	335	PHE	4.0
1	D	343	THR	3.9
1	D	224	LYS	3.9
1	D	210	PRO	3.9
1	D	217	THR	3.9
1	D	298	SER	3.8
1	D	95	ALA	3.7
1	D	331	TYR	3.7
1	D	16	ASP	3.6
1	D	78	VAL	3.6
1	D	292	LEU	3.6
1	D	204	VAL	3.6
1	D	12	ALA	3.5
1	D	62	VAL	3.5
1	D	74	ALA	3.5
1	D	2	ALA	3.5
1	D	325	PRO	3.4
1	D	13	MET	3.4
1	D	113	LEU	3.4
1	D	323	ASP	3.4
1	D	68	SER	3.3
1	D	8	ASP	3.3
1	D	30	ASN	3.3
1	D	303	VAL	3.3
1	D	322	ALA	3.3
1	D	221	GLU	3.3
1	D	11	LEU	3.3
1	D	64	ALA	3.2
1	D	273	ALA	3.2
1	D	88	THR	3.2
1	D	270	VAL	3.1
1	D	226	ARG	3.1
1	D	17	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	5	ALA	3.1
1	D	83	LEU	3.1
1	D	355	VAL	3.1
1	D	60	ILE	3.1
1	D	344	PHE	3.0
1	D	235	VAL	3.0
1	D	81	THR	3.0
1	D	227	GLY	3.0
1	D	23	HIS	3.0
1	D	98	THR	2.9
1	D	91	ALA	2.9
1	D	222	ASP	2.9
1	D	338	ASP	2.9
1	D	229	SER	2.9
1	D	65	THR	2.8
1	D	202	VAL	2.8
1	D	99	TYR	2.8
1	D	471	ASP	2.8
1	D	293	GLY	2.8
1	D	324	HIS	2.8
1	D	332	THR	2.8
1	D	205	ASP	2.8
1	D	228	ILE	2.7
1	D	333	THR	2.7
1	D	272	VAL	2.7
1	D	25	GLY	2.6
1	D	97	MET	2.6
1	D	276	THR	2.6
1	D	314	ILE	2.6
1	D	337	ARG	2.6
1	D	39	LEU	2.6
1	D	1	MET	2.6
1	D	79	ASP	2.6
1	D	241	ALA	2.6
1	D	72	PRO	2.6
1	D	359	ARG	2.6
1	D	216	ASP	2.6
1	D	329	ILE	2.6
1	D	269	GLY	2.6
1	D	112	PHE	2.5
1	D	122	SER	2.5
1	D	63	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	31	ARG	2.5
1	D	71	TYR	2.5
1	D	73	GLY	2.4
1	D	299	GLY	2.4
1	D	326	GLY	2.4
1	D	7	ASN	2.4
1	D	334	SER	2.4
1	D	237	ILE	2.4
1	D	45	VAL	2.4
1	D	301[A]	ARG	2.4
1	D	24	GLN	2.3
1	D	225	GLN	2.3
1	D	66	ASN	2.3
1	D	212	ASP	2.2
1	D	40	PRO	2.2
1	D	58	SER	2.2
1	D	386	HIS	2.2
1	D	19	LYS	2.2
1	D	170	GLU	2.2
1	D	14	ASN	2.2
1	D	41	ASP	2.1
1	D	168	ASP	2.1
1	D	115	VAL	2.1
1	D	87	PRO	2.1
1	D	27	SER	2.1
1	D	150	TYR	2.1
1	D	119	SER	2.1
1	D	18	LYS	2.1
1	D	80	GLU	2.1
1	D	96	PRO	2.1
1	D	449	ARG	2.1
1	D	209	ASN	2.0
1	D	144	VAL	2.0
1	D	240	VAL	2.0
1	D	69	ARG	2.0
1	D	208	LYS	2.0
1	D	238	SER	2.0
1	D	201	THR	2.0

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

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.