



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:36 am GMT

PDB ID : 1PWW
Title : Crystal structure of Anthrax Lethal Factor active site mutant protein complexed with an optimised peptide substrate in the presence of zinc.
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 2.80 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

<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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

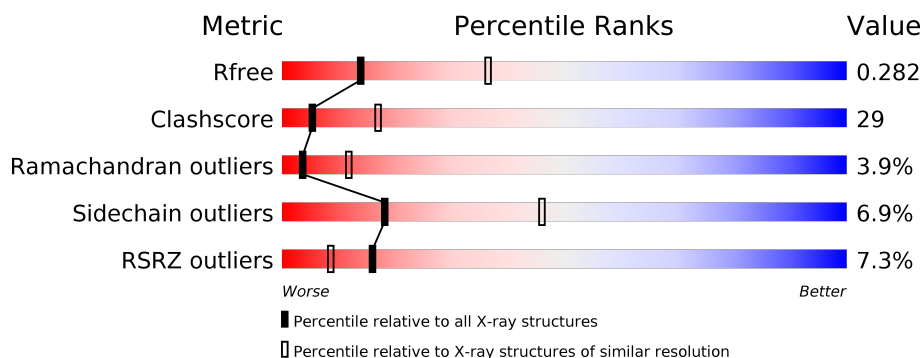
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	776	<div> <div>6%</div> <div> <div>43%</div> <div>44%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	776	<div> <div>6%</div> <div> <div>48%</div> <div>42%</div> <div>•</div> <div>5%</div> </div> </div>
2	C	20	<div> <div>35%</div> <div> <div>15%</div> <div>15%</div> <div>20%</div> <div>5%</div> <div>45%</div> </div> </div>
2	D	20	<div> <div>40%</div> <div> <div>5%</div> <div>30%</div> <div>10%</div> <div>10%</div> <div>45%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12185 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 Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5965	3796	1002	1159	8			
1	B	734	Total	C	N	O	S	0	0	0
			6030	3833	1017	1172	8			

There are 2 discrepancies between the modelled and reference sequences:

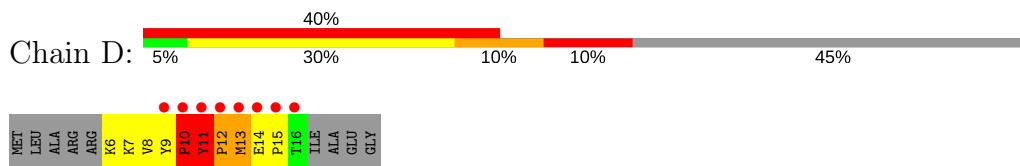
Chain	Residue	Modelled	Actual	Comment	Reference
A	687	CYS	GLU	engineered	UNP P15917
B	687	CYS	GLU	engineered	UNP P15917

- Molecule 2 is a protein called LF20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			
2	D	11	Total	C	N	O	S	0	0	0
			94	64	13	16	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	22.69 – 2.80 46.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.7 (22.69-2.80) 81.6 (46.05-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.288 0.237 , 0.282	Depositor DCC
R_{free} test set	2583 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.40	0/6072	0.65	0/8178
1	B	0.42	0/6138	0.66	1/8267 (0.0%)
2	C	0.69	0/98	1.01	0/133
2	D	0.44	0/98	1.08	1/133 (0.8%)
All	All	0.41	0/12406	0.66	2/16711 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	PRO	CA-N-CD	-10.49	96.81	111.50
2	D	10	PRO	CA-N-CD	-7.20	101.42	111.50

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	5965	0	5957	368	0
1	B	6030	0	6021	332	0
2	C	94	0	95	23	0
2	D	94	0	95	23	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
All	All	12185	0	12168	706	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 29.

The worst 5 of 706 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:B:653:VAL:HG11	2:D:10:PRO:HG3	1.34	1.06
1:B:551:PRO:HD2	1:B:554:LYS:HE2	1.36	1.05
1:B:319:LEU:HD23	1:B:345:ILE:HD12	1.39	1.05
1:B:366:ASN:HB3	1:B:367:PRO:HD3	1.38	1.01
1:A:563:GLN:NE2	1:A:585:PHE:H	1.57	1.00

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	722/776 (93%)	617 (86%)	74 (10%)	31 (4%)	3	10
1	B	730/776 (94%)	635 (87%)	76 (10%)	19 (3%)	6	21
2	C	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
2	D	9/20 (45%)	4 (44%)	1 (11%)	4 (44%)	0	0
All	All	1470/1592 (92%)	1260 (86%)	152 (10%)	58 (4%)	3	12

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLN

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Mol	Chain	Res	Type
1	A	181	SER
1	A	370	GLU
1	A	473	LYS
1	A	675	VAL

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	665/710 (94%)	616 (93%)	49 (7%)	16	42
1	B	673/710 (95%)	636 (94%)	37 (6%)	25	57
2	C	11/17 (65%)	8 (73%)	3 (27%)	0	1
2	D	11/17 (65%)	6 (54%)	5 (46%)	0	0
All	All	1360/1454 (94%)	1266 (93%)	94 (7%)	18	46

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	HIS
1	B	80	LYS
2	C	11	TYR
1	A	701	ASP
1	A	767	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	GLN
1	B	248	ASN
1	B	645	HIS
1	B	186	GLN
1	B	209	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	726/776 (93%)	0.16	50 (6%) 18 10	14, 40, 88, 94	0
1	B	734/776 (94%)	0.07	43 (5%) 23 15	13, 39, 85, 123	0
2	C	11/20 (55%)	3.00	7 (63%) 0 0	89, 98, 108, 108	0
2	D	11/20 (55%)	3.28	8 (72%) 0 0	88, 98, 108, 108	0
All	All	1482/1592 (93%)	0.16	108 (7%) 16 8	13, 40, 88, 123	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ASN	8.8
2	D	16	THR	7.6
2	C	11	TYR	5.9
2	D	11	TYR	5.5
1	A	321	ARG	5.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	9001	1/1	0.99	0.21	-0.57	45,45,45,45	0
3	ZN	B	9002	1/1	0.98	0.19	-0.59	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.