



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:05 PM GMT

PDB ID : 1WE0
Title : Crystal structure of peroxiredoxin (AhpC) from *Amphibacillus xylanus*
Authors : Kitano, K.; Kita, A.; Hakoshima, T.; Niimura, Y.; Miki, K.
Deposited on : 2004-05-21
Resolution : 2.90 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

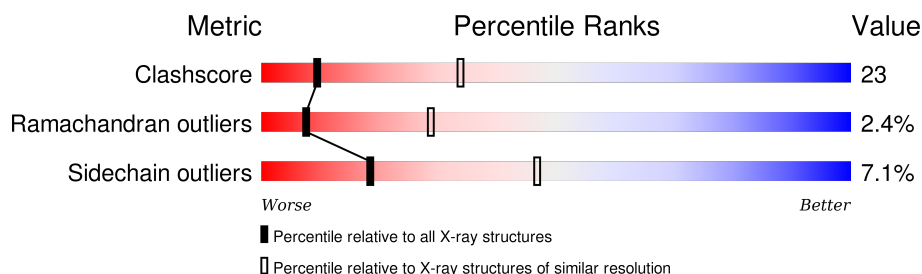
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	187	
1	B	187	
1	C	187	
1	D	187	
1	E	187	
1	F	187	
1	G	187	

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Mol	Chain	Length	Quality of chain
1	H	187	<div><div></div><div>47%36%5%11%</div></div>
1	I	187	<div><div></div><div>56%29%•11%</div></div>
1	J	187	<div><div></div><div>50%33%5%11%</div></div>

2 Entry composition

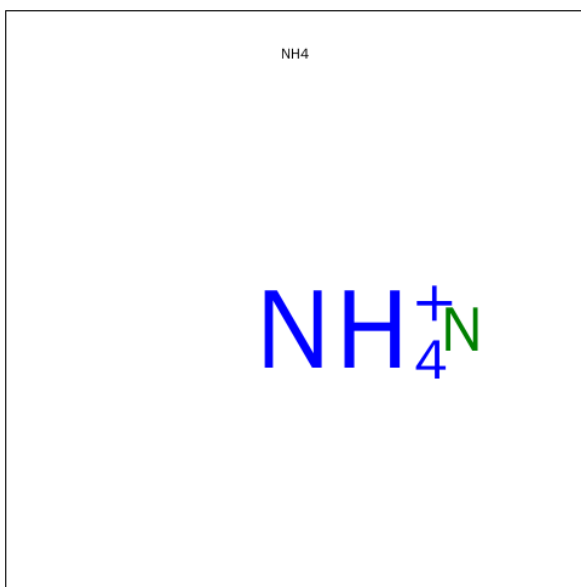
There are 2 unique types of molecules in this entry. The entry contains 12982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alkyl hydroperoxide reductase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	B	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	C	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	D	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	E	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	F	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	G	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	H	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	I	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	J	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total N 1 1	0	0
2	J	1	Total N 1 1	0	0

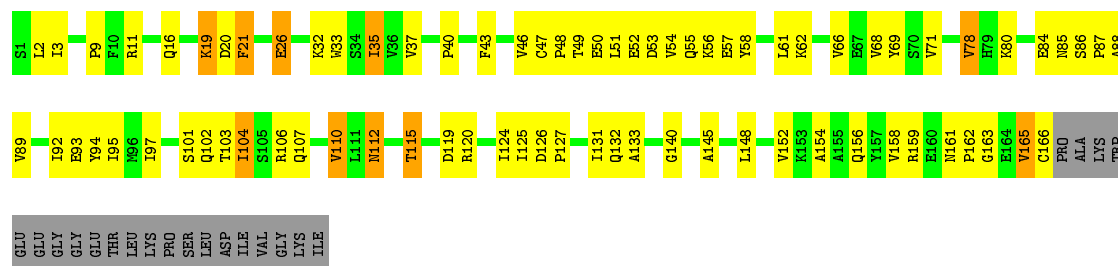
Note EDS was not executed.

- [illegible]

- Chain B:
-
- 49% 36% 11%
- | TRP | GLU | GLU | GLY | GLY | GLY | GLU | GLU | THR | LEU | LYS | PRO | SER | LEU | ASP | ILE | VAL | GLY | LYS | ILE |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V98 | I92 | E93 | Y94 | I95 | H96 | I97 | G98 | D99 | P100 | S101 | Q102 | T103 | I104 | S105 | R106 | Q107 | V110 | L111 | N112 |
| D119 | R120 | I125 | D126 | P127 | Q132 | I136 | G140 | A145 | S146 | T147 | L148 | I149 | N150 | K151 | V152 | A154 | A155 | Q156 | T157 |
| R158 | R159 | E160 | N161 | P162 | V165 | C166 | P167 | A168 | L169 | L170 | L171 | L172 | L173 | L174 | L175 | L176 | L177 | L178 | L179 |

- Chain C:**
-
- | Amino Acid | Category |
|------------|----------|
| S1 | Green |
| L2 | Green |
| I3 | Yellow |
| F10 | Yellow |
| Q16 | Green |
| K19 | Green |
| D20 | Green |
| F21 | Yellow |
| F22 | Yellow |
| E26 | Green |
| A27 | Green |
| D28 | Green |
| L29 | Yellow |
| M33 | Green |
| S34 | Green |
| I35 | Orange |
| V36 | Green |
| V37 | Green |
| F38 | Green |
| Y39 | Green |
| P40 | Yellow |
| C47 | Green |
| P48 | Yellow |
| T49 | Yellow |
| E50 | Yellow |
| L51 | Orange |
| E52 | Green |
| D53 | Green |
| W54 | Green |
| Q55 | Green |
| R56 | Yellow |
| G63 | Yellow |
| V66 | Yellow |
| V71 | Yellow |
| S72 | Orange |
| T73 | Green |
| D74 | Green |
| T75 | Yellow |
| V78 | Orange |
| N85 | Yellow |
| S86 | Yellow |
| P87 | Yellow |
| A88 | Yellow |
| V89 | Yellow |
| I92 | Grey |
| E93 | Grey |
| Y94 | Grey |
| I95 | Grey |
| N96 | Green |
| I97 | Grey |
| G98 | Green |
| D99 | Green |
| P100 | Yellow |
| S101 | Yellow |
| Q102 | Green |
| T103 | Orange |
| I104 | Orange |
| V110 | Yellow |
| L111 | Green |
| M112 | Orange |
| T115 | Yellow |
| R120 | Yellow |
| P127 | Yellow |
| G140 | Green |
| I141 | Yellow |
| D144 | Green |
| A145 | Yellow |
| S146 | Green |
| T147 | Green |
| L148 | Orange |
| I149 | Yellow |
| K153 | Yellow |
| Q156 | Yellow |
| Y157 | Green |
| V158 | Yellow |
| R159 | Yellow |
| E160 | Green |
| N161 | Yellow |
| P162 | Yellow |
| G163 | Yellow |
| E164 | Green |
| V165 | Yellow |
| C166 | Orange |
| P170 | Grey |
| A171 | Grey |
| L172 | Grey |
| T173 | Grey |
| T174 | Grey |
| G175 | Grey |
| G176 | Grey |
| G177 | Grey |
| G178 | Grey |
| G179 | Grey |
| L180 | Grey |
| L181 | Grey |
| L182 | Grey |
| L183 | Grey |
| P184 | Grey |
| S185 | Grey |
| L186 | Grey |
| ASP187 | Grey |
| I188 | Grey |
| VAL189 | Grey |
| G190 | Grey |

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.22Å 79.32Å 104.45Å 77.22° 82.33° 80.08°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.44	0/1326	0.62	0/1800
1	B	0.42	0/1326	0.59	0/1800
1	C	0.44	0/1326	0.60	0/1800
1	D	0.39	0/1326	0.59	0/1800
1	E	0.37	0/1326	0.58	0/1800
1	F	0.42	0/1326	0.63	0/1800
1	G	0.41	0/1326	0.62	0/1800
1	H	0.41	0/1326	0.59	0/1800
1	I	0.41	0/1326	0.60	0/1800
1	J	0.45	0/1326	0.61	0/1800
All	All	0.42	0/13260	0.60	0/18000

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

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	1298	0	1252	62	0
1	B	1298	0	1252	59	0
1	C	1298	0	1252	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1298	0	1252	69	0
1	E	1298	0	1252	55	0
1	F	1298	0	1252	66	0
1	G	1298	0	1252	61	0
1	H	1298	0	1252	73	0
1	I	1298	0	1252	57	0
1	J	1298	0	1252	68	0
2	F	1	0	0	0	0
2	J	1	0	0	0	0
All	All	12982	0	12520	576	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 23.

The worst 5 of 576 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:85:ASN:ND2	1:J:85:ASN:HD22	1.53	1.06
1:B:85:ASN:HD22	1:C:85:ASN:HD22	1.12	0.96
1:D:85:ASN:HD22	1:E:85:ASN:ND2	1.63	0.96
1:A:85:ASN:HD22	1:J:85:ASN:HD22	1.03	0.94
1:H:85:ASN:HD22	1:I:85:ASN:HD22	1.13	0.92

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	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	29
1	B	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	29
1	D	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	29
1	E	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	29
1	F	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	7	29
1	G	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	7	29
1	H	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	29
1	I	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	29
1	J	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	29
All	All	1640/1870 (88%)	1437 (88%)	163 (10%)	40 (2%)	7	29

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	E	21	PHE

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	141/158 (89%)	135 (96%)	6 (4%)	35	71
1	B	141/158 (89%)	132 (94%)	9 (6%)	22	53
1	C	141/158 (89%)	127 (90%)	14 (10%)	10	29
1	D	141/158 (89%)	130 (92%)	11 (8%)	16	41
1	E	141/158 (89%)	134 (95%)	7 (5%)	30	65
1	F	141/158 (89%)	132 (94%)	9 (6%)	22	53
1	G	141/158 (89%)	128 (91%)	13 (9%)	11	33
1	H	141/158 (89%)	129 (92%)	12 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	141/158 (89%)	134 (95%)	7 (5%)	30 65
1	J	141/158 (89%)	129 (92%)	12 (8%)	13 37
All	All	1410/1580 (89%)	1310 (93%)	100 (7%)	18 47

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	104	ILE
1	F	166	CYS
1	J	51	LEU
1	E	166	CYS
1	F	35	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	102	GLN
1	G	79	HIS
1	J	112	ASN
1	F	112	ASN
1	F	150	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are modelled with single atom - 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.