

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 - 02:29 pm GMT

PDB ID : 1WA6

Title : The structure of ACC oxidase

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Deposited on : 2004-10-25

Resolution : 2.55 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

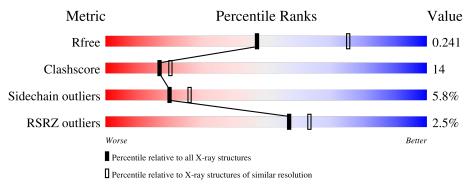
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.55 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	Similar resolution		
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
R_{free}	130704	1284 (2.56-2.52)		
Clashscore	141614	1332 (2.56-2.52)		
Sidechain outliers	138945	1315 (2.56-2.52)		
RSRZ outliers	127900	1272 (2.56-2.52)		

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 <=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					
			2%					
1	X	319	61%	25%	7% 7%			

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

\mathbf{Mol}	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	X	1308	-	X	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2460 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.

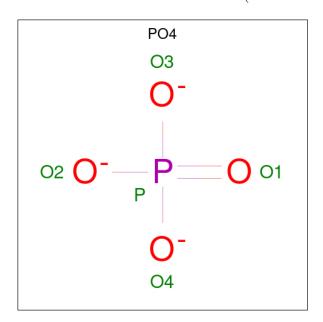
• Molecule 1 is a protein called 1-AMINOCYCLOPROPANE-1-CARBOXYLATE OXIDASE 1.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	X	298	Total 2372	C 1523	N 394	O 438	S 4	Se 13	0	0	0

• Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	X	1	Total Fe 1 1	0	0

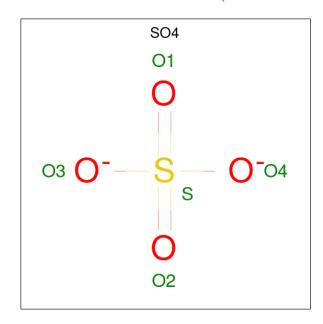
• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Y	1	Total O P	0	0	
9	3 A	1	5 4 1			
2	v	1	Total O P	0	0	
3	Λ	1	5 4 1	0	U	



 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total 5	O 4	S 1	0	0

• Molecule 5 is water.

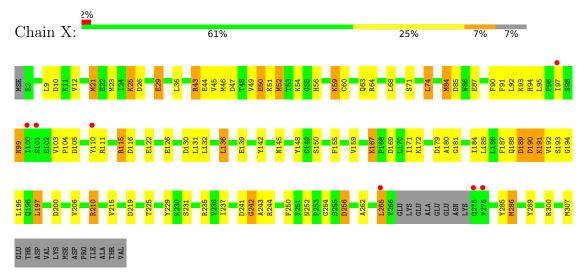
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	72	Total O 72 72	0	0



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: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE OXIDASE 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	70.34Å 107.06Å 108.38Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 2.55	Depositor
resolution (A)	39.84 - 2.55	EDS
% Data completeness	93.4 (40.00-2.55)	Depositor
(in resolution range)	93.4 (39.84-2.55)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.82 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
D D	0.186 , 0.236	Depositor
R, R_{free}	0.191 , 0.241	DCC
R_{free} test set	654 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 42.5	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2460	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: SO4, FE2, PO4

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	Bo	nd lengths	Bo	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	X	1.47	19/2411 (0.8%)	1.30	23/3228 (0.7%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	X	87	GLU	CD-OE1	-8.80	1.16	1.25
1	X	43	ARG	CG-CD	8.63	1.73	1.51
1	X	286	MSE	SE-CE	-7.85	1.49	1.95
1	X	167	LYS	CD-CE	7.39	1.69	1.51
1	X	139	GLU	CD-OE1	6.56	1.32	1.25

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	X	189	ASP	CB-CG-OD2	9.77	127.09	118.30
1	X	26	ASP	CB-CG-OD2	9.71	127.03	118.30
1	X	10	ASP	CB-CG-OD2	8.91	126.32	118.30
1	X	116	ASP	CB-CG-OD2	8.89	126.30	118.30
1	X	47	ASP	CB-CG-OD2	8.58	126.03	118.30

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	X	2372	0	2372	67	0
2	X	1	0	0	0	0
3	X	10	0	0	2	0
4	X	5	0	0	0	0
5	X	72	0	0	3	2
All	All	2460	0	2372	67	2

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 14.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:X:307:MSE:SE	1:X:307:MSE:CE	2.14	1.46
1:X:190:ASP:CG	1:X:191:LYS:H	1.60	1.03
1:X:52:MSE:CE	1:X:110:TYR:HA	1.93	0.99
1:X:52:MSE:HE1	1:X:110:TYR:HA	1.53	0.89
1:X:68:LEU:HD22	1:X:84:MSE:HE3	1.59	0.82

All (2) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:X:2025:HOH:O	5:X:2064:HOH:O[2_665]	0.52	1.68
5:X:2023:HOH:O	5:X:2050:HOH:O[2_665]	1.08	1.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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	Analysed Rotameric		Percentiles		
1	X	257/261 (98%)	242 (94%)	15 (6%)	20 26		

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	97	ILE
1	X	210	ARG
1	X	99	ASN
1	X	265	LEU
1	X	167	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	56	HIS
1	X	63	GLN
1	X	78	GLN
1	X	99	ASN
1	X	196	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

_	Mol Type	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
10	101	Type	Chain	nes		LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ
	3	PO4	X	1309	-	4,4,4	0.94	0	6,6,6	1.13	0
	3	PO4	X	1308	2	4,4,4	0.49	0	6,6,6	2.47	4 (66%)
	4	SO4	X	1310	-	4,4,4	0.51	0	6,6,6	1.62	1 (16%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	X	1308	PO4	O4-P-O2	3.87	120.38	107.97
4	X	1310	SO4	O4-S-O3	-3.47	94.26	109.06
3	X	1308	PO4	O2-P-O1	-2.91	100.23	110.89
3	X	1308	PO4	O3-P-O1	-2.22	102.77	110.89
3	X	1308	PO4	O3-P-O2	2.17	114.92	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1309	PO4	1	0
3	X	1308	PO4	1	0

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, 95^{th} 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	X	285/319 (89%)	-0.06	7 (2%)	57	63	32, 50, 73, 83	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	265	LEU	2.9
1	X	276	VAL	2.8
1	X	101	SER	2.7
1	X	100	ILE	2.7
1	X	110	TYR	2.4

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	${f B-factors(\AA^2)}$	Q<0.9
3	PO4	X	1308	5/5	0.86	0.22	86,86,93,96	0
4	SO4	X	1310	5/5	0.88	0.14	78,81,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
3	PO4	X	1309	5/5	0.91	0.32	101,103,105,106	0
2	FE2	X	1307	1/1	0.99	0.14	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.

