

Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 - 10:39 am GMT

PDB ID	:	1OE2
Title	:	Atomic Resolution Structure of D92E Mutant of Alcaligenes xylosoxidans Ni-
		trite Reductase
Authors	:	Ellis, M.J.; Dodd, F.E.; Sawers, G.; Eady, R.R.; Hasnain, S.S.
Deposited on	:	2003-03-18
Resolution	:	1.12 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 (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:

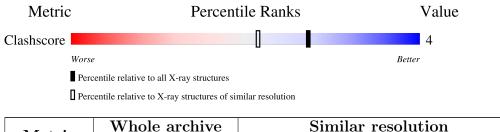
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.12 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
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1205 (1.14-1.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1		224		
	A	336	93%	7% •



 $\mathbf{2}$

Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5584 atoms, of which 2473 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	335	Total 5022	C 1624	Н 2473	N 434	0 480	S 11	0	5	0

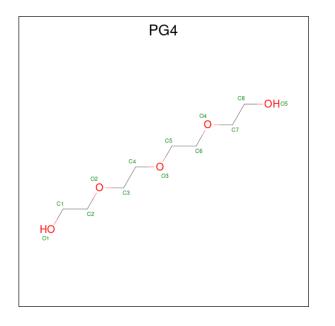
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	92	GLU	ASP	engineered mutation	UNP 068601

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Cu 2 2	0	0

• Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 13	C 8	O 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	547	Total O 547 547	0	0

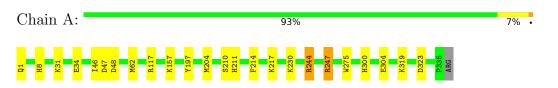


3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants	78.70Å 78.70Å 98.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 - 1.12	Depositor
% Data completeness	99.9 (60.00-1.12)	Depositor
(in resolution range)	33.3 (00.00-1.12)	Depositor
R_{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.119 , 0.179	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5584	wwPDB-VP
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP



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: PG4, PCA, CU

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		lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.71	0/2644	1.11	12/3609~(0.3%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

	Mol	Chain	#Chirality outliers	#Planarity outliers
ſ	1	А	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	244[A]	ARG	NE-CZ-NH2	-16.55	112.02	120.30
1	А	244[B]	ARG	NE-CZ-NH2	-16.55	112.02	120.30
1	А	197	TYR	CB-CG-CD2	-9.77	115.14	121.00
1	А	204	MET	CG-SD-CE	-6.81	89.31	100.20
1	А	244[A]	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	А	244[B]	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	А	247	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	А	157	LYS	CD-CE-NZ	-5.69	98.62	111.70
1	А	34	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	А	117	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	А	62	MET	CG-SD-CE	-5.08	92.06	100.20
1	А	214	PHE	CB-CG-CD1	5.02	124.32	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group	
1	А	300	HIS	Peptide	

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	А	2549	2473	2440	14	0
2	А	2	0	0	0	0
3	А	13	0	18	5	0
4	А	547	0	0	8	3
All	All	3111	2473	2458	19	3

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 4.

All (19) 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)
3:A:999:PG4:O1	3:A:999:PG4:C1	1.74	1.34
1:A:323[A]:ASP:OD1	4:A:2521:HOH:O	1.56	1.21
1:A:244[B]:ARG:NH2	1:A:304:GLU:OE2	1.84	1.11
3:A:999:PG4:O1	3:A:999:PG4:C2	1.99	1.10
1:A:244[B]:ARG:HH22	1:A:304:GLU:CD	1.65	0.99
3:A:999:PG4:O1	3:A:999:PG4:H22	1.68	0.91
3:A:999:PG4:O1	4:A:2546:HOH:O	1.94	0.85
1:A:323[A]:ASP:OD2	4:A:2520:HOH:O	1.97	0.82
1:A:31:LYS:CD	4:A:2098:HOH:O	2.33	0.76
1:A:319:LYS:CG	4:A:2511:HOH:O	2.37	0.71
1:A:8:HIS:NE2	4:A:2033:HOH:O	2.28	0.66
1:A:244[B]:ARG:NH2	1:A:304:GLU:CD	2.41	0.61
1:A:46:ILE:HA	1:A:217[B]:LYS:HG3	1.90	0.54
1:A:210:SER:OG	1:A:211:HIS:HD2	1.90	0.54
1:A:230:LYS:CG	4:A:2158:HOH:O	2.63	0.47
3:A:999:PG4:C1	3:A:999:PG4:HO1	2.17	0.45
1:A:47:ASP:OD2	1:A:211:HIS:HE1	2.00	0.45
1:A:48:ASP:CB	4:A:2167:HOH:O	2.69	0.40
1:A:247:ARG:HA	1:A:275:TRP:O	2.21	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2042:HOH:O	4:A:2165:HOH:O[5_565]	1.89	0.31
4:A:2132:HOH:O	4:A:2132:HOH:O[2_665]	2.02	0.18
4:A:2451:HOH:O	4:A:2451:HOH:O[2_665]	2.06	0.14

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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 Typ	Turne	Chain	Dec	Link	Bond lengths			Bond angles		
	туре		Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	PCA	А	1	1	7,8,9	0.84	0	$9,\!10,\!12$	1.42	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	А	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1	PCA	CB-CG-CD	-2.22	100.83	104.40
1	А	1	PCA	CG-CD-N	2.07	113.76	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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 7	Type	Chain	Res	Link	Bond lengths			Bond angles		
	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	PG4	А	999	-	12,12,12	1.96	1 (8%)	11,11,11	2.90	5 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	А	999	-	-	2/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	999	PG4	O1-C1	6.18	1.74	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	А	999	PG4	O1-C1-C2	-6.53	73.93	111.81
3	А	999	PG4	O5-C8-C7	4.19	136.13	111.81
3	А	999	PG4	O2-C3-C4	-3.02	96.79	110.39
3	А	999	PG4	O3-C5-C6	-2.88	97.41	110.39
3	А	999	PG4	O4-C7-C8	-2.62	98.55	110.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	999	PG4	O1-C1-C2-O2
3	А	999	PG4	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	999	PG4	5	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

