



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:50 am GMT

PDB ID : 1GS6  
Title : Crystal structure of M144A mutant of *Alcaligenes xylosoxidans* Nitrite Reductase  
Authors : Ellis, M.J.; Prudencio, M.; Dodd, F.E.; Strange, R.W.; Sawers, G.; Eady, R.R.; Hasnain, S.S.  
Deposited on : 2002-01-02  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

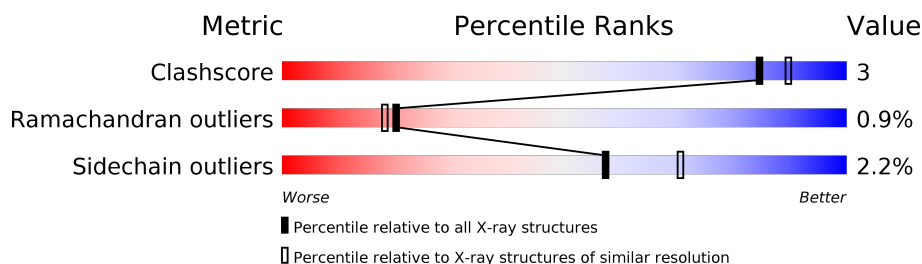
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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  $\geq 3$ , 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	X	336	 84%      13%      •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2728 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	336	Total	C	N	O	S	130	0	0
			2572	1637	448	477	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	144	ALA	MET	ENGINEERED MUTATION	UNP O68601

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

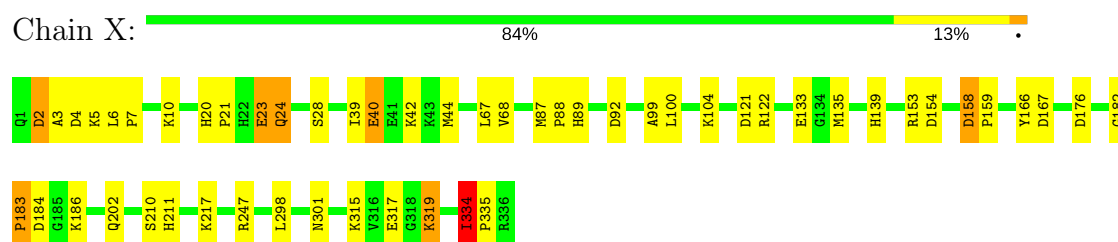
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	153	Total	O	0	0
			153	153		

### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

#### • Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.86Å 106.86Å 64.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.2 (60.00-2.20)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.148 , 0.181	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: MG, 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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	2.46	14/2643 (0.5%)	1.72	44/3600 (1.2%)

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
1	X	0	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	40	GLU	CG-CD	68.74	2.55	1.51
1	X	183	PRO	N-CD	53.27	2.22	1.47
1	X	183	PRO	CA-CB	48.76	2.51	1.53
1	X	154	ASP	CB-CG	33.85	2.22	1.51
1	X	334	ILE	C-N	-29.01	0.79	1.34
1	X	317	GLU	CG-CD	25.40	1.90	1.51
1	X	2	ASP	C-N	-21.35	0.84	1.34
1	X	183	PRO	C-O	-20.98	0.81	1.23
1	X	217	LYS	CG-CD	9.33	1.84	1.52
1	X	184	ASP	CA-CB	7.81	1.71	1.53
1	X	10	LYS	CB-CG	-6.88	1.33	1.52
1	X	319	LYS	CG-CD	-6.76	1.29	1.52
1	X	99	ALA	C-O	5.59	1.33	1.23
1	X	23	GLU	CG-CD	5.23	1.59	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	183	PRO	N-CA-CB	-32.88	63.84	103.30
1	X	183	PRO	CA-C-O	-28.48	51.86	120.20
1	X	334	ILE	O-C-N	-26.71	70.34	121.10
1	X	183	PRO	CA-N-CD	23.33	144.36	111.70
1	X	334	ILE	CA-C-N	17.64	166.50	117.10
1	X	40	GLU	CG-CD-OE1	-16.38	85.53	118.30
1	X	183	PRO	CB-CA-C	14.64	148.61	112.00
1	X	183	PRO	O-C-N	14.08	145.23	122.70
1	X	183	PRO	N-CD-CG	-14.05	82.12	103.20
1	X	182	GLY	C-N-CD	-13.39	91.15	120.60
1	X	334	ILE	C-N-CD	-13.06	91.86	120.60
1	X	40	GLU	CB-CG-CD	-13.01	79.07	114.20
1	X	2	ASP	O-C-N	-12.71	102.36	122.70
1	X	40	GLU	CG-CD-OE2	11.76	141.81	118.30
1	X	184	ASP	N-CA-CB	-9.83	92.90	110.60
1	X	167	ASP	CB-CG-OD2	9.32	126.69	118.30
1	X	40	GLU	OE1-CD-OE2	-8.97	112.53	123.30
1	X	217	LYS	CB-CG-CD	-8.51	89.46	111.60
1	X	4	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	X	5	LYS	N-CA-CB	8.20	125.36	110.60
1	X	154	ASP	CA-CB-CG	-8.14	95.50	113.40
1	X	42	LYS	CA-CB-CG	7.80	130.57	113.40
1	X	4	ASP	CA-CB-CG	-7.74	96.37	113.40
1	X	319	LYS	CB-CG-CD	7.70	131.62	111.60
1	X	23	GLU	CB-CG-CD	-7.69	93.45	114.20
1	X	154	ASP	CB-CG-OD2	7.65	125.19	118.30
1	X	334	ILE	C-N-CA	7.53	153.64	122.00
1	X	122	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	X	92	ASP	CB-CG-OD1	6.74	124.36	118.30
1	X	315	LYS	CB-CG-CD	-6.19	95.52	111.60
1	X	247	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	X	184	ASP	CA-CB-CG	5.76	126.07	113.40
1	X	2	ASP	CA-C-N	5.65	129.62	117.20
1	X	317	GLU	CG-CD-OE2	5.53	129.37	118.30
1	X	121	ASP	CB-CG-OD2	5.36	123.13	118.30
1	X	4	ASP	CB-CG-OD2	5.31	123.08	118.30
1	X	301	ASN	N-CA-C	-5.25	96.81	111.00
1	X	2	ASP	C-N-CA	5.25	134.83	121.70
1	X	186	LYS	CA-CB-CG	-5.23	101.90	113.40
1	X	158	ASP	CB-CG-OD1	5.21	122.99	118.30
1	X	3	ALA	CB-CA-C	5.18	117.87	110.10
1	X	176	ASP	CB-CG-OD1	5.15	122.94	118.30
1	X	317	GLU	OE1-CD-OE2	-5.06	117.22	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	133	GLU	CG-CD-OE1	-5.05	108.20	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	183	PRO	Mainchain
1	X	2	ASP	Mainchain
1	X	23	GLU	Sidechain
1	X	334	ILE	Mainchain
1	X	40	GLU	Sidechain

## 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	X	2572	0	2533	13	0
2	X	2	0	0	0	0
3	X	1	0	0	0	0
4	X	153	0	0	1	0
All	All	2728	0	2533	13	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 3.

All (13) 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:X:39:ILE:HD13	1:X:89:HIS:HB2	1.85	0.59
1:X:24:GLN:HE22	1:X:166:TYR:H	1.54	0.55
1:X:87:MET:HB3	1:X:88:PRO:HD2	1.89	0.54
1:X:39:ILE:CD1	1:X:89:HIS:HB2	2.39	0.53
1:X:210:SER:OG	1:X:211:HIS:HD2	1.92	0.52
1:X:20:HIS:HE1	1:X:68:VAL:H	1.57	0.51
1:X:6:LEU:HB3	1:X:7:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:135:MET:HE1	1:X:139:HIS:HE2	1.79	0.48
1:X:100:LEU:HD12	1:X:104:LYS:HD3	1.97	0.46
1:X:202:GLN:HG3	4:X:2098:HOH:O	2.20	0.41
1:X:20:HIS:HD2	1:X:21:PRO:O	2.03	0.41
1:X:158:ASP:HB2	1:X:159:PRO:CD	2.51	0.41
1:X:39:ILE:HG21	1:X:89:HIS:CD2	2.56	0.40

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	X	334/336 (99%)	323 (97%)	8 (2%)	3 (1%)	20	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	335	PRO
1	X	24	GLN
1	X	334	ILE

### 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	X	270/270 (100%)	264 (98%)	6 (2%)	57 70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	28	SER
1	X	44	MET
1	X	67	LEU
1	X	153	ARG
1	X	298	LEU
1	X	319	LYS

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

Mol	Chain	Res	Type
1	X	20	HIS
1	X	24	GLN
1	X	211	HIS

### 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 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.