

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 6, 2023 – 08:11 am GMT

PDB ID : 2JFC

Title : M144L mutant of Nitrite Reductase from Alcaligenes xylosoxidans in space

group P212121

Authors: Paraskevopoulos, K.; Hough, M.A.; Sawers, R.G.; Eady, R.R.; Hasnain, S.S.

Deposited on : 2007-01-31

Resolution : 2.40 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

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)

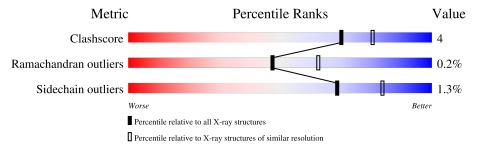
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	A	335	93%	7%
1	В	335	94%	6%
1	С	335	91%	8% •
1	D	335	92%	7% •
1	Е	335	93%	7%
1	F	335	90%	10%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16613 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 RE-DUCTASE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	335	Total	С	N	О	S	0	0	0
1	Λ	333	2556	1632	440	474	10	U	0	
1	В	335	Total	С	N	О	S	0	0	0
1	Ъ	333	2556	1632	440	474	10	U	0	
1	С	335	Total	С	N	О	S	0	0	0
1		333	2553	1630	439	474	10			
1	D	335	Total	С	N	O	S	0	0	0
1	ט	333	2549	1627	438	474	10	U	0	
1	E	335	Total	С	N	О	S	0	0	0
1	12	333	2549	1627	438	474	10	U	0	
1	F	335	Total	С	N	О	S	0	0	0
1	I'	333	2552	1629	439	474	10	0		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	LEU	MET	engineered mutation	UNP O68601
В	144	LEU	MET	engineered mutation	UNP O68601
С	144	LEU	MET	engineered mutation	UNP O68601
D	144	LEU	MET	engineered mutation	UNP O68601
Е	144	LEU	MET	engineered mutation	UNP O68601
F	144	LEU	MET	engineered mutation	UNP O68601

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	В	2	Total Cu 2 2	0	0
2	С	2	Total Cu 2 2	0	0

Continued on next page...



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	208	Total O 208 208	0	0
4	В	211	Total O 211 211	0	0
4	С	214	Total O 214 214	0	0
4	D	211	Total O 211 211	0	0
4	E	217	Total O 217 217	0	0
4	F	221	Total O 221 221	0	0

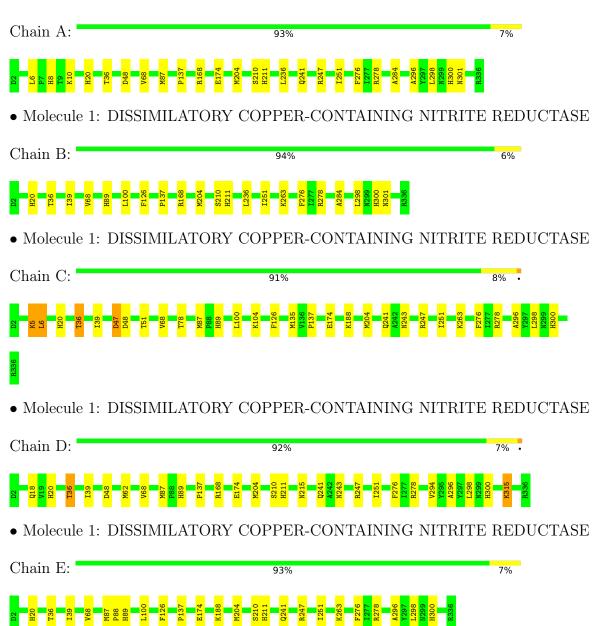


# 3 Residue-property plots (i)

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.

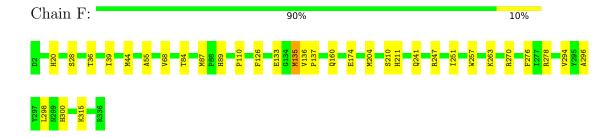
Note EDS was not executed.

• Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE



• 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 21 21 21	Depositor	
Cell constants	171.96Å 175.91Å 181.06Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	49.70 - 2.40	Depositor	
% Data completeness	97.6 (49.70-2.40)	Depositor	
(in resolution range)	31.0 (43.10 2.40)	Берозног	
$R_{merge}$	0.08	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	REFMAC 5.2.0005	Depositor	
$R, R_{free}$	0.171 , 0.193	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	16613	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	47.0	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: CL, 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.47	0/2627	0.60	0/3581	
1	В	0.46	0/2627	0.60	0/3581	
1	С	0.46	0/2624	0.61	1/3578 (0.0%)	
1	D	0.46	0/2620	0.61	1/3574~(0.0%)	
1	Е	0.47	0/2620	0.59	0/3574	
1	F	0.46	0/2623	0.61	0/3577	
All	All	0.46	0/15741	0.60	$2/21465 \ (0.0\%)$	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
1	С	0	1
1	D	0	1
1	Е	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	47	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	48	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.



5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Peptide
1	В	300	HIS	Peptide
1	С	300	HIS	Peptide
1	D	300	HIS	Peptide
1	Е	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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2556	0	2504	16	0
1	В	2556	0	2504	14	0
1	С	2553	0	2495	28	0
1	D	2549	0	2484	19	0
1	Е	2549	0	2484	19	0
1	F	2552	0	2493	26	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Ε	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	F	1	0	0	0	0
4	A	208	0	0	3	0
4	В	211	0	0	0	0
4	С	214	0	0	3	0
4	D	211	0	0	2	0
4	Е	217	0	0	1	0
4	F	221	0	0	4	0
All	All	16613	0	14964	109	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 4.

The worst 5 of 109 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:C:87:MET:SD	4:C:2141:HOH:O	2.10	1.09
1:F:160:GLN:OE1	4:F:2130:HOH:O	1.72	1.07
1:A:168:ARG:HD3	4:A:2111:HOH:O	1.54	1.05
1:E:87:MET:HE2	4:F:2080:HOH:O	1.61	1.00
1:F:44:MET:HE3	1:F:55:ALA:CB	1.96	0.95

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	Percentil	les
1	A	333/335~(99%)	325 (98%)	8 (2%)	0	100 10	00
1	В	333/335 (99%)	325 (98%)	8 (2%)	0	100 10	00
1	С	333/335 (99%)	324 (97%)	7 (2%)	2 (1%)	25 36	3
1	D	333/335 (99%)	326 (98%)	7 (2%)	0	100 10	)0
1	Е	333/335 (99%)	325 (98%)	8 (2%)	0	100 10	00
1	F	333/335 (99%)	323 (97%)	9 (3%)	1 (0%)	41 55	5
All	All	1998/2010 (99%)	1948 (98%)	47 (2%)	3 (0%)	47 62	2

#### All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	28	SER
1	С	5	LYS
1	С	6	LEU



#### 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	A	$266/270 \ (98\%)$	262 (98%)	4 (2%)	65 80
1	В	266/270 (98%)	264 (99%)	2 (1%)	81 91
1	C	265/270~(98%)	260 (98%)	5 (2%)	57 75
1	D	264/270 (98%)	261 (99%)	3 (1%)	73 87
1	${ m E}$	264/270 (98%)	262 (99%)	2 (1%)	81 91
1	F	265/270 (98%)	261 (98%)	4 (2%)	65 80
All	All	1590/1620 (98%)	1570 (99%)	20 (1%)	69 84

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ε	36	THR
1	F	133	GLU
1	F	247	ARG
1	F	135	MET
1	С	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	HIS
1	Е	18	GLN
1	F	20	HIS
1	Е	8	HIS
1	Е	20	HIS

#### 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 16 ligands modelled in this entry, 16 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)

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.

