



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:17 pm GMT

PDB ID : 1MZZ  
Title : Crystal Structure of Mutant (M182T)of Nitrite Reductase  
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Deposited on : 2002-10-10  
Resolution : 2.00 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](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

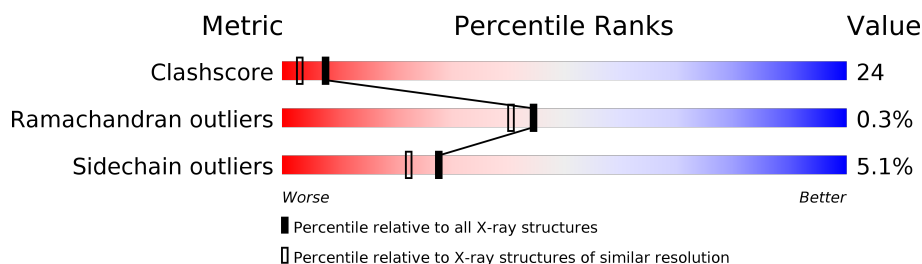
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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	A	334	
1	B	334	
1	C	334	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8561 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	B	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	C	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	MET	ENGINEERED	UNP Q53239
A	230	ASP	THR	CONFLICT	UNP Q53239
A	281	ASN	LYS	CONFLICT	UNP Q53239
A	351	HIS	SER	CONFLICT	UNP Q53239
A	367	VAL	TRP	CONFLICT	UNP Q53239
A	368	ALA	PRO	CONFLICT	UNP Q53239
A	372	LEU	-	CLONING ARTIFACT	UNP Q53239
B	1182	THR	MET	ENGINEERED	UNP Q53239
B	1230	ASP	THR	CONFLICT	UNP Q53239
B	1281	ASN	LYS	CONFLICT	UNP Q53239
B	1351	HIS	SER	CONFLICT	UNP Q53239
B	1367	VAL	TRP	CONFLICT	UNP Q53239
B	1368	ALA	PRO	CONFLICT	UNP Q53239
B	1372	LEU	-	CLONING ARTIFACT	UNP Q53239
C	2182	THR	MET	ENGINEERED	UNP Q53239
C	2230	ASP	THR	CONFLICT	UNP Q53239
C	2281	ASN	LYS	CONFLICT	UNP Q53239
C	2351	HIS	SER	CONFLICT	UNP Q53239
C	2367	VAL	TRP	CONFLICT	UNP Q53239
C	2368	ALA	PRO	CONFLICT	UNP Q53239
C	2372	LEU	-	CLONING ARTIFACT	UNP Q53239

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Cu 2	0	0
2	A	2	Total 2	Cu 2	0	0
2	C	2	Total 2	Cu 2	0	0

- Molecule 3 is water.

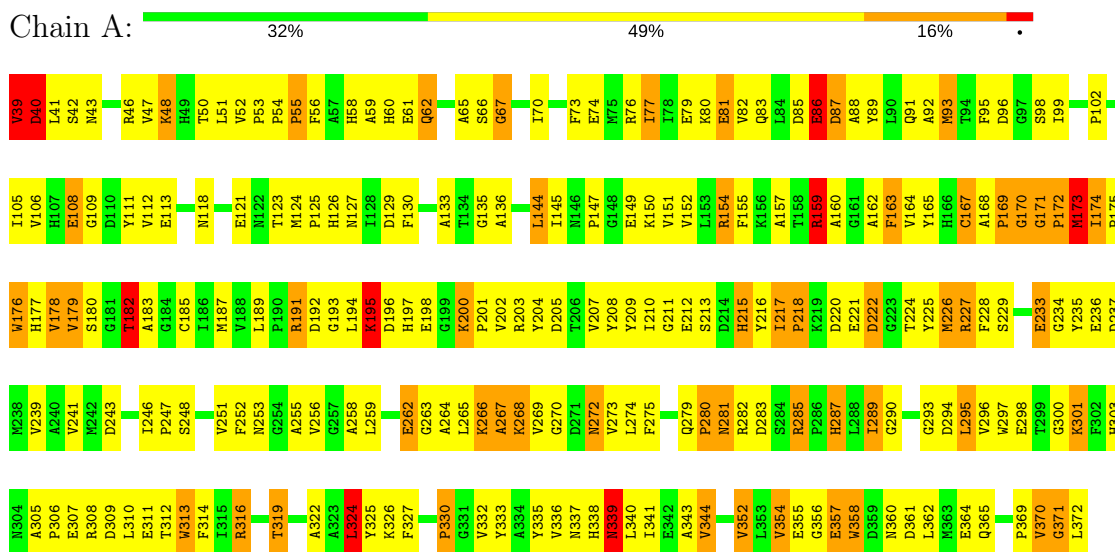
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	289	Total 289	O 289	0	0
3	B	276	Total 276	O 276	0	0
3	C	289	Total 289	O 289	0	0

### 3 Residue-property plots

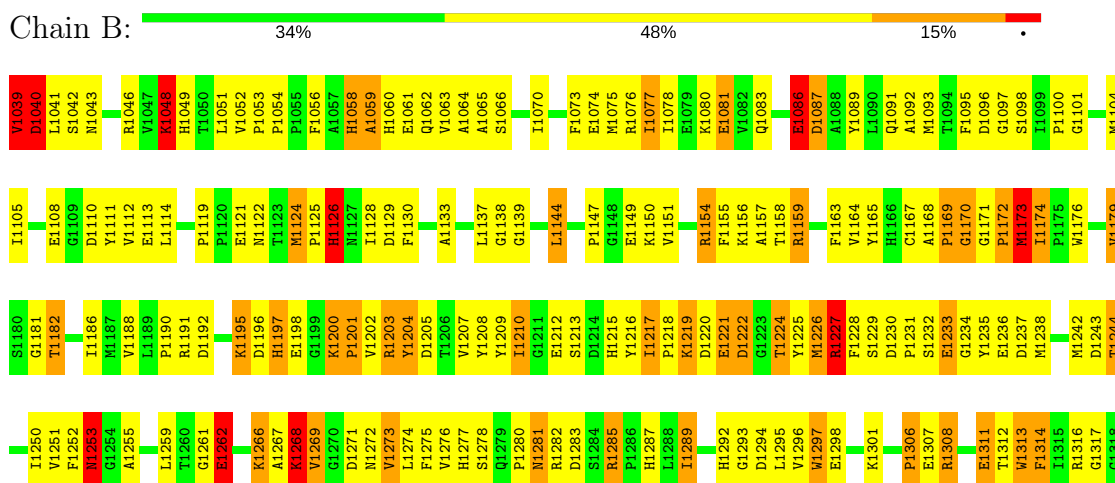
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Copper-containing nitrite reductase



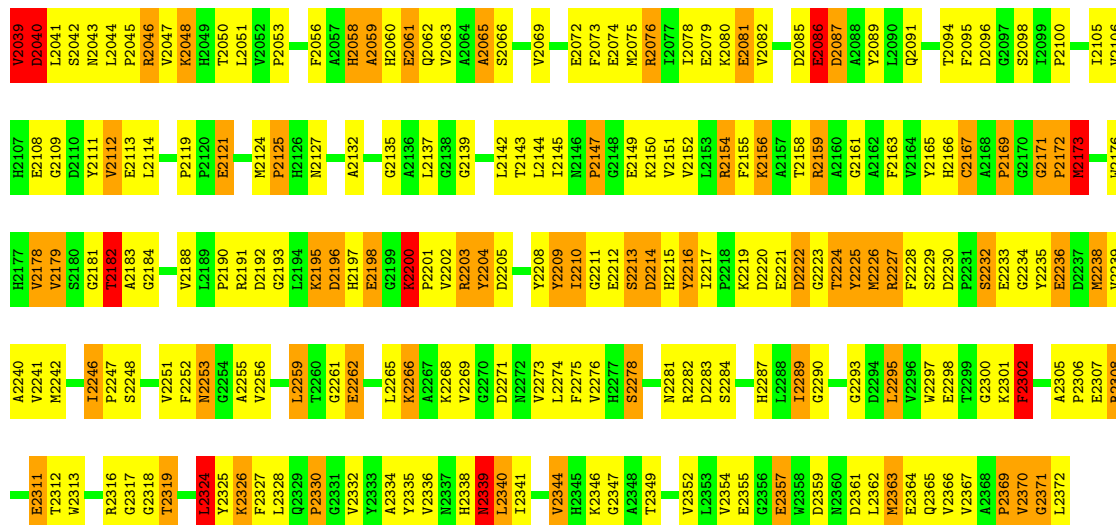
#### • Molecule 1: Copper-containing nitrite reductase





• Molecule 1: Copper-containing nitrite reductase

Chain C: 35% 44% 18%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.50Å 123.73Å 130.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.4 (30.00-2.00)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.170 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: 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	A	3.64	298/2640 (11.3%)	2.69	149/3599 (4.1%)
1	B	3.59	304/2640 (11.5%)	2.51	157/3599 (4.4%)
1	C	3.67	267/2640 (10.1%)	2.53	155/3599 (4.3%)
All	All	3.63	869/7920 (11.0%)	2.58	461/10797 (4.3%)

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
1	A	0	5
1	B	0	8
1	C	0	7
All	All	0	20

The worst 5 of 869 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ARG	CZ-NH1	44.61	1.91	1.33
1	C	2121	GLU	CD-OE2	30.47	1.59	1.25
1	C	2262	GLU	CD-OE2	28.84	1.57	1.25
1	A	86	GLU	CD-OE1	27.63	1.56	1.25
1	C	2262	GLU	CG-CD	27.51	1.93	1.51

The worst 5 of 461 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	-42.44	99.08	120.30
1	C	2227	ARG	NE-CZ-NH2	-34.08	103.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	NE-CZ-NH2	-33.63	103.48	120.30
1	A	227	ARG	NE-CZ-NH1	30.69	135.64	120.30
1	A	124	MET	CG-SD-CE	-29.68	52.72	100.20

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Mainchain
1	A	159	ARG	Sidechain
1	A	173	MET	Mainchain
1	A	272	ASN	Mainchain
1	A	352	VAL	Mainchain

## 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	A	2567	0	2477	139	0
1	B	2567	0	2476	116	0
1	C	2567	0	2477	137	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	289	0	0	11	0
3	B	276	0	0	7	0
3	C	289	0	0	9	0
All	All	8561	0	7430	367	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 24.

The worst 5 of 367 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:C:2178:VAL:CG1	1:C:2178:VAL:CB	1.74	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:CA	1:A:173:MET:CB	1.74	1.64
1:B:1086:GLU:CG	1:B:1086:GLU:CB	1.75	1.63
1:C:2295:LEU:CG	1:C:2295:LEU:CD1	1.75	1.62
1:A:289:ILE:CG2	1:A:289:ILE:CB	1.75	1.62

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	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	44	40
1	B	332/334 (99%)	319 (96%)	12 (4%)	1 (0%)	44	40
1	C	332/334 (99%)	316 (95%)	15 (4%)	1 (0%)	44	40
All	All	996/1002 (99%)	956 (96%)	37 (4%)	3 (0%)	44	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	B	1040	ASP
1	C	2040	ASP

### 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	270/270 (100%)	258 (96%)	12 (4%)	33	28
1	B	270/270 (100%)	254 (94%)	16 (6%)	23	17
1	C	270/270 (100%)	257 (95%)	13 (5%)	30	25
All	All	810/810 (100%)	769 (95%)	41 (5%)	28	22

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1173	MET
1	B	1253	ASN
1	C	2324	LEU
1	B	1182	THR
1	B	1227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1215	HIS
1	B	1253	ASN
1	C	2215	HIS
1	B	1058	HIS
1	B	1060	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 6 ligands modelled in this entry, 6 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

### 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.