

wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 04:29 AM EDT

PDB ID : 1L9P

Title : CRYSTAL STRUCTURE OF NITRITE SOAKED I257G VARIANT OF THE

COPPER-CONTAINING NITRITE REDUCTASE FROM ALCALIGENES

FAECALIES S-6

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Deposited on : 2002-03-26

Resolution : 1.75 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

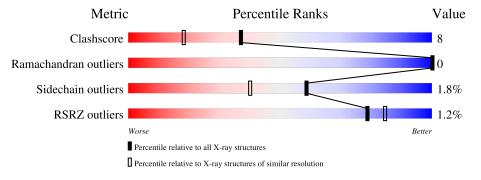
Validation Pipeline (wwPDB-VP) : 2.23.2

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 1.75 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
Menic	(# Entries)	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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		
1	A	341	87%	11%	
1	В	341	87%	11%	
1	С	341	83%	14%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9043 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	۸	336	Total	otal C N	О	S	0	0	0		
1	A	330	2556	1635	430	480	11	0	U	0	
1	В	336	Total	С	N	О	S	0	0	0	
1	Б	330	2556	1635	430	480	11	0	0		
1	С	336	Total	С	N	О	S	0	0	0	
1		330	2556	1635	430	480	11	U			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	GLY	ILE	engineered mutation	UNP P38501
A	341	ILE	-	cloning artifact	UNP P38501
A	342	GLU	-	cloning artifact	UNP P38501
A	343	GLY	-	cloning artifact	UNP P38501
A	344	ARG	-	cloning artifact	UNP P38501
В	257	GLY	ILE	engineered mutation	UNP P38501
В	341	ILE	-	cloning artifact	UNP P38501
В	342	GLU	-	cloning artifact	UNP P38501
В	343	GLY	-	cloning artifact	UNP P38501
В	344	ARG	-	cloning artifact	UNP P38501
С	257	GLY	ILE	engineered mutation	UNP P38501
С	341	ILE	-	cloning artifact	UNP P38501
С	342	GLU	-	cloning artifact	UNP P38501
С	343	GLY	-	cloning artifact	UNP P38501
С	344	ARG	-	cloning artifact	UNP P38501

• 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

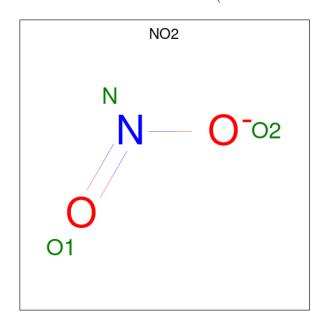
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Cu 2 2	0	0
2	С	2	Total Cu 2 2	0	0

 \bullet Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 6 2 4	0	1
3	В	1	Total N O 6 2 4	0	1
3	С	1	Total N O 6 2 4	0	1

• Molecule 4 is water.

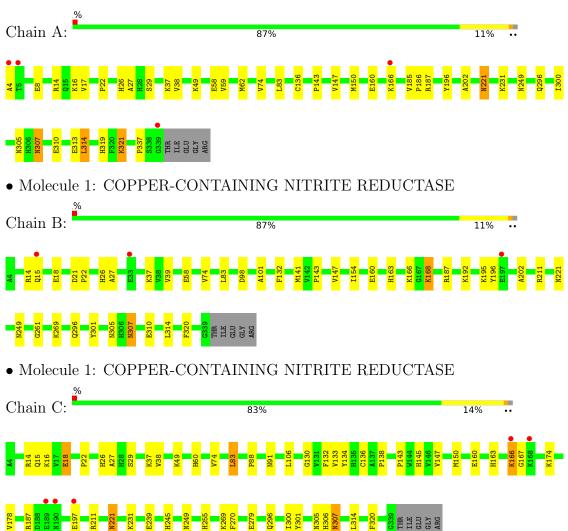
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	481	Total O 481 481	0	0
4	В	450	Total O 450 450	0	0
4	С	420	Total O 420 420	0	0



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: COPPER-CONTAINING NITRITE REDUCTASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	62.05Å 102.45Å 146.21Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.61 - 1.75	Depositor
rtesolution (A)	49.89 - 1.75	EDS
% Data completeness	97.9 (25.61-1.75)	Depositor
(in resolution range)	93.6 (49.89-1.75)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.91 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
P. P.	0.159 , 0.194	Depositor
R, R_{free}	0.156 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 51.1	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9043	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.08% 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: CU, NO2

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	Clasia	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/2627	0.79	3/3582~(0.1%)	
1	В	0.48	0/2627	0.78	3/3582~(0.1%)	
1	С	0.46	0/2627	0.77	$3/3582 \ (0.1\%)$	
All	All	0.48	0/7881	0.78	9/10746 (0.1%)	

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	307	ASN	N-CA-C	-8.21	88.83	111.00
1	В	307	ASN	N-CA-C	-7.75	90.07	111.00
1	С	307	ASN	N-CA-C	-7.64	90.38	111.00
1	В	305	ASN	N-CA-C	-6.09	94.56	111.00
1	A	305	ASN	N-CA-C	-6.00	94.80	111.00

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	A	2556	0	2477	37	1
1	В	2556	0	2477	39	0
1	С	2556	0	2477	46	0

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	J	1	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	A	6	0	0	0	0
3	В	6	0	0	0	0
3	С	6	0	0	0	0
4	A	481	0	0	15	0
4	В	450	0	0	15	1
4	С	420	0	0	16	0
All	All	9043	0	7431	118	1

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 8.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:29:SER:HB2	4:C:5372:HOH:O	1.42	1.19
1:A:296:GLN:HG2	4:A:5449:HOH:O	1.56	1.04
1:B:192:LYS:HD2	4:B:5292:HOH:O	1.67	0.93
1:A:29:SER:HB3	4:A:5447:HOH:O	1.70	0.91
1:A:26:HIS:HE1	1:A:74:VAL:H	1.22	0.88

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:4:ALA:O	4:B:5125:HOH:O[4_456]	2.19	0.01

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	Perce	ntiles
1	A	334/341 (98%)	331 (99%)	3 (1%)	0	100	100
1	В	334/341 (98%)	329 (98%)	5 (2%)	0	100	100
1	С	334/341 (98%)	329 (98%)	5 (2%)	0	100	100
All	All	1002/1023 (98%)	989 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	263/267 (98%)	258 (98%)	5 (2%)	57 37
1	В	263/267 (98%)	260 (99%)	3 (1%)	73 60
1	С	263/267 (98%)	257 (98%)	6 (2%)	50 28
All	All	789/801 (98%)	775 (98%)	14 (2%)	59 40

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	168	LYS
1	С	18	GLU
1	С	314	LEU
1	С	197	GLU
1	С	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	115	ASN
1	С	221	ASN
1	В	221	ASN
1	С	296	GLN
1	С	115	ASN



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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	Tuno	Chain	Res	Link	В	ond len	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NO2	A	1504[B]	2	1,2,2	4.32	1 (100%)	0,1,1	-	-
3	NO2	С	3504[B]	2	1,2,2	4.35	1 (100%)	0,1,1	-	-
3	NO2	В	2504[A]	2	1,2,2	4.31	1 (100%)	0,1,1	-	-
3	NO2	A	1504[A]	2	1,2,2	4.07	1 (100%)	0,1,1	-	-
3	NO2	В	2504[B]	2	1,2,2	4.19	1 (100%)	0,1,1	-	-
3	NO2	С	3504[A]	2	1,2,2	3.96	1 (100%)	0,1,1	-	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	С	3504[B]	NO2	O1-N	4.35	1.44	1.22
3	A	1504[B]	NO2	O1-N	4.32	1.44	1.22
3	В	2504[A]	NO2	O1-N	4.31	1.44	1.22
3	В	2504[B]	NO2	O1-N	4.19	1.43	1.22
3	A	1504[A]	NO2	O1-N	4.07	1.42	1.22



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)

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>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	336/341 (98%)	-0.29	4 (1%) 79 84	12, 17, 31, 49	0
1	В	336/341 (98%)	-0.18	3 (0%) 84 89	13, 18, 33, 44	0
1	С	336/341 (98%)	-0.02	5 (1%) 73 80	14, 22, 35, 47	0
All	All	1008/1023 (98%)	-0.16	12 (1%) 79 84	12, 19, 33, 49	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	5.4
1	A	339	GLY	3.9
1	С	168	LYS	3.8
1	В	33	GLU	3.6
1	С	197	GLU	3.4

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	NO2	A	1504[A]	3/3	0.90	0.16	27,27,29,29	3
3	NO2	A	1504[B]	3/3	0.90	0.16	11,11,12,13	3
3	NO2	В	2504[A]	3/3	0.93	0.17	21,21,21,22	3
3	NO2	В	2504[B]	3/3	0.93	0.17	23,23,25,26	3
3	NO2	С	3504[A]	3/3	0.96	0.10	28,28,28,29	3
3	NO2	С	3504[B]	3/3	0.96	0.10	10,10,11,11	3
2	CU	С	501	1/1	0.99	0.04	23,23,23,23	0
2	CU	В	501	1/1	1.00	0.03	20,20,20,20	0
2	CU	В	502	1/1	1.00	0.02	20,20,20,20	0
2	CU	A	501	1/1	1.00	0.03	16,16,16,16	0
2	CU	С	502	1/1	1.00	0.02	22,22,22,22	0
2	CU	A	502	1/1	1.00	0.04	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

