Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 12:34 AM EDT

PDB ID	:	1NDR
Title	:	CRYSTALLOGRAPHIC STRUCTURE OF A BLUE COPPER NITRITE REDUCTASE FROM ALCALIGENES XYLOSOXIDANS
Authors	:	Dodd, F.E.; Hasnain, S.S.; Abraham, Z.H.L.; Eady, R.R.; Smith, B.E.
Deposited on	:	1997-01-23
Resolution	:	3.00 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:

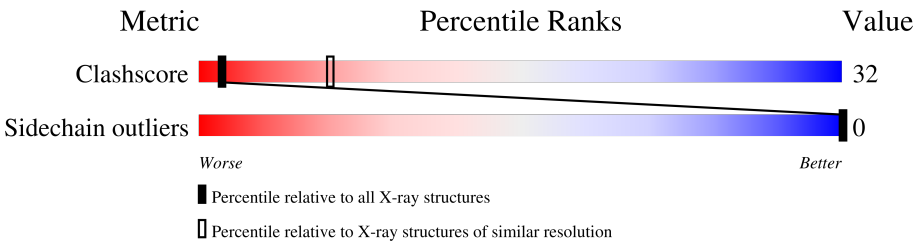
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 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	141614	2416 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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%

Mol	Chain	Length	Quality of chain
1	A	330	94% 6%
1	B	330	94% 6%
1	C	330	94% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1170 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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	387	361	17	7	2	0	0	323
1	B	330	387	361	17	7	2	0	0	323
1	C	330	387	361	17	7	2	0	0	323

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	PRO	GLN	conflict	UNP P81445
A	16	ALA	LYS	conflict	UNP P81445
A	29	SER	GLU	conflict	UNP P81445
A	32	ALA	VAL	conflict	UNP P81445
A	33	ALA	SER	conflict	UNP P81445
A	35	ALA	PRO	conflict	UNP P81445
A	52	ALA	ILE	conflict	UNP P81445
A	55	ASP	GLN	conflict	UNP P81445
A	59	ALA	LEU	conflict	UNP P81445
A	68	VAL	MET	conflict	UNP P81445
A	120	ALA	VAL	conflict	UNP P81445
A	139	ALA	GLN	conflict	UNP P81445
A	165	ALA	PRO	conflict	UNP P81445
A	166	ALA	GLN	conflict	UNP P81445
A	168	ALA	LYS	conflict	UNP P81445
A	169	ALA	LEU	conflict	UNP P81445
A	171	ALA	HIS	conflict	UNP P81445
A	185	VAL	ILE	conflict	UNP P81445
A	188	ALA	ASP	conflict	UNP P81445
A	189	ALA	LYS	conflict	UNP P81445
A	192	ASN	HIS	conflict	UNP P81445
A	194	SER	LYS	conflict	UNP P81445
A	198	ALA	ASP	conflict	UNP P81445

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Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	SER	conflict	UNP P81445
A	204	ALA	GLN	conflict	UNP P81445
A	207	VAL	ARG	conflict	UNP P81445
A	218	ALA	VAL	conflict	UNP P81445
A	223	ALA	ARG	conflict	UNP P81445
A	235	ALA	SER	conflict	UNP P81445
A	236	ALA	LYS	conflict	UNP P81445
A	243	ILE	PHE	conflict	UNP P81445
A	276	LEU	ARG	conflict	UNP P81445
A	289	ALA	VAL	conflict	UNP P81445
A	302	ALA	VAL	conflict	UNP P81445
A	317	ALA	LEU	conflict	UNP P81445
A	320	ALA	ILE	conflict	UNP P81445
A	321	SER	LYS	conflict	UNP P81445
A	333	SER	GLN	conflict	UNP P81445
A	335	ALA	LYS	conflict	UNP P81445
B	13	PRO	GLN	conflict	UNP P81445
B	16	ALA	LYS	conflict	UNP P81445
B	29	SER	GLU	conflict	UNP P81445
B	32	ALA	VAL	conflict	UNP P81445
B	33	ALA	SER	conflict	UNP P81445
B	35	ALA	PRO	conflict	UNP P81445
B	52	ALA	ILE	conflict	UNP P81445
B	55	ASP	GLN	conflict	UNP P81445
B	59	ALA	LEU	conflict	UNP P81445
B	68	VAL	MET	conflict	UNP P81445
B	120	ALA	VAL	conflict	UNP P81445
B	139	ALA	GLN	conflict	UNP P81445
B	165	ALA	PRO	conflict	UNP P81445
B	166	ALA	GLN	conflict	UNP P81445
B	168	ALA	LYS	conflict	UNP P81445
B	169	ALA	LEU	conflict	UNP P81445
B	171	ALA	HIS	conflict	UNP P81445
B	185	VAL	ILE	conflict	UNP P81445
B	188	ALA	ASP	conflict	UNP P81445
B	189	ALA	LYS	conflict	UNP P81445
B	192	ASN	HIS	conflict	UNP P81445
B	194	SER	LYS	conflict	UNP P81445
B	198	ALA	ASP	conflict	UNP P81445
B	202	ALA	SER	conflict	UNP P81445
B	204	ALA	GLN	conflict	UNP P81445
B	207	VAL	ARG	conflict	UNP P81445

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Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ALA	VAL	conflict	UNP P81445
B	223	ALA	ARG	conflict	UNP P81445
B	235	ALA	SER	conflict	UNP P81445
B	236	ALA	LYS	conflict	UNP P81445
B	243	ILE	PHE	conflict	UNP P81445
B	276	LEU	ARG	conflict	UNP P81445
B	289	ALA	VAL	conflict	UNP P81445
B	302	ALA	VAL	conflict	UNP P81445
B	317	ALA	LEU	conflict	UNP P81445
B	320	ALA	ILE	conflict	UNP P81445
B	321	SER	LYS	conflict	UNP P81445
B	333	SER	GLN	conflict	UNP P81445
B	335	ALA	LYS	conflict	UNP P81445
C	13	PRO	GLN	conflict	UNP P81445
C	16	ALA	LYS	conflict	UNP P81445
C	29	SER	GLU	conflict	UNP P81445
C	32	ALA	VAL	conflict	UNP P81445
C	33	ALA	SER	conflict	UNP P81445
C	35	ALA	PRO	conflict	UNP P81445
C	52	ALA	ILE	conflict	UNP P81445
C	55	ASP	GLN	conflict	UNP P81445
C	59	ALA	LEU	conflict	UNP P81445
C	68	VAL	MET	conflict	UNP P81445
C	120	ALA	VAL	conflict	UNP P81445
C	139	ALA	GLN	conflict	UNP P81445
C	165	ALA	PRO	conflict	UNP P81445
C	166	ALA	GLN	conflict	UNP P81445
C	168	ALA	LYS	conflict	UNP P81445
C	169	ALA	LEU	conflict	UNP P81445
C	171	ALA	HIS	conflict	UNP P81445
C	185	VAL	ILE	conflict	UNP P81445
C	188	ALA	ASP	conflict	UNP P81445
C	189	ALA	LYS	conflict	UNP P81445
C	192	ASN	HIS	conflict	UNP P81445
C	194	SER	LYS	conflict	UNP P81445
C	198	ALA	ASP	conflict	UNP P81445
C	202	ALA	SER	conflict	UNP P81445
C	204	ALA	GLN	conflict	UNP P81445
C	207	VAL	ARG	conflict	UNP P81445
C	218	ALA	VAL	conflict	UNP P81445
C	223	ALA	ARG	conflict	UNP P81445
C	235	ALA	SER	conflict	UNP P81445

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Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ALA	LYS	conflict	UNP P81445
C	243	ILE	PHE	conflict	UNP P81445
C	276	LEU	ARG	conflict	UNP P81445
C	289	ALA	VAL	conflict	UNP P81445
C	302	ALA	VAL	conflict	UNP P81445
C	317	ALA	LEU	conflict	UNP P81445
C	320	ALA	ILE	conflict	UNP P81445
C	321	SER	LYS	conflict	UNP P81445
C	333	SER	GLN	conflict	UNP P81445
C	335	ALA	LYS	conflict	UNP P81445

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

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

- Molecule 3 is water.

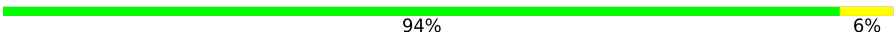
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
			Total	O		
3	B	1	1	1	0	0

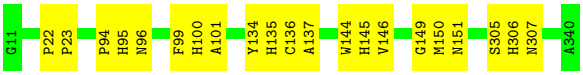
3 Residue-property plots (i)

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.

- Molecule 1: NITRITE REDUCTASE

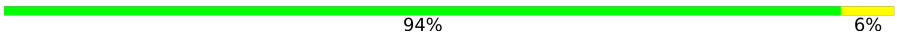
Chain A:

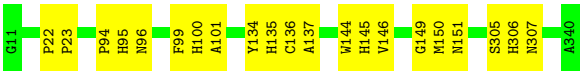




- Molecule 1: NITRITE REDUCTASE

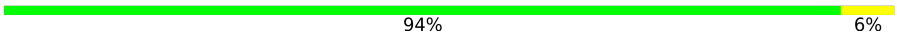
Chain B:

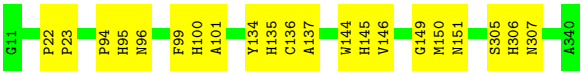




- Molecule 1: NITRITE REDUCTASE

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.15Å 101.72Å 150.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 60.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.8 (8.00-3.00) 78.4 (60.46-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.78 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.270 0.433 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.24 , 660.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.35	EDS
Total number of atoms	1170	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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

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	0.48	0/63	0.85	0/75
1	B	0.37	0/63	0.79	0/75
1	C	0.51	0/63	0.79	0/75
All	All	0.46	0/189	0.81	0/225

There are no bond length outliers.

There are no bond angle outliers.

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	387	0	42	14	0
1	B	387	0	42	13	0
1	C	387	0	42	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	1170	0	126	41	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 32.

All (41) 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:150:MET:C	1:C:151:ASN:CA	2.40	0.90
1:C:136:CYS:C	1:C:137:ALA:CA	2.41	0.90
1:B:150:MET:C	1:B:151:ASN:CA	2.41	0.89
1:A:136:CYS:C	1:A:137:ALA:CA	2.42	0.89
1:A:100:HIS:C	1:A:101:ALA:CA	2.41	0.88
1:B:95:HIS:C	1:B:96:ASN:CA	2.43	0.87
1:B:100:HIS:C	1:B:101:ALA:CA	2.43	0.87
1:B:136:CYS:C	1:B:137:ALA:CA	2.43	0.87
1:B:306:HIS:C	1:B:307:ASN:CA	2.43	0.87
1:A:150:MET:C	1:A:151:ASN:CA	2.43	0.86
1:B:145:HIS:C	1:B:146:VAL:CA	2.43	0.86
1:A:306:HIS:C	1:A:307:ASN:CA	2.43	0.86
1:A:145:HIS:C	1:A:146:VAL:CA	2.43	0.86
1:C:100:HIS:C	1:C:101:ALA:CA	2.43	0.86
1:C:306:HIS:C	1:C:307:ASN:CA	2.45	0.85
1:C:145:HIS:C	1:C:146:VAL:CA	2.45	0.85
1:A:95:HIS:C	1:A:96:ASN:CA	2.45	0.84
1:B:144:TRP:CA	1:B:145:HIS:N	2.41	0.84
1:C:95:HIS:C	1:C:96:ASN:CA	2.47	0.83
1:B:94:PRO:CA	1:B:95:HIS:N	2.41	0.83
1:A:99:PHE:CA	1:A:100:HIS:N	2.41	0.83
1:C:134:TYR:CA	1:C:135:HIS:N	2.43	0.82
1:B:99:PHE:CA	1:B:100:HIS:N	2.42	0.82
1:C:144:TRP:CA	1:C:145:HIS:N	2.42	0.82
1:B:149:GLY:CA	1:B:150:MET:N	2.43	0.82
1:A:134:TYR:CA	1:A:135:HIS:N	2.43	0.82
1:A:144:TRP:CA	1:A:145:HIS:N	2.42	0.81
1:B:134:TYR:CA	1:B:135:HIS:N	2.44	0.81
1:C:99:PHE:CA	1:C:100:HIS:N	2.44	0.81
1:C:149:GLY:CA	1:C:150:MET:N	2.43	0.81
1:A:149:GLY:CA	1:A:150:MET:N	2.45	0.80
1:A:94:PRO:CA	1:A:95:HIS:N	2.45	0.80
1:A:305:SER:CA	1:A:306:HIS:N	2.46	0.79
1:C:305:SER:CA	1:C:306:HIS:N	2.46	0.78
1:C:94:PRO:CA	1:C:95:HIS:N	2.46	0.78
1:B:305:SER:CA	1:B:306:HIS:N	2.49	0.75
1:C:22:PRO:CA	1:C:23:PRO:CA	2.94	0.46
1:A:22:PRO:CA	1:A:23:PRO:CA	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PRO:CA	1:B:23:PRO:CA	2.96	0.44
1:C:136:CYS:HB2	1:C:150:MET:HB3	2.02	0.42
1:A:136:CYS:HB2	1:A:150:MET:HB3	2.02	0.41

There are no symmetry-related clashes.

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)

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	7/245 (3%)	7 (100%)	0	100	100
1	B	7/245 (3%)	7 (100%)	0	100	100
1	C	7/245 (3%)	7 (100%)	0	100	100
All	All	21/735 (3%)	21 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.