



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2016 – 05:32 AM EDT

PDB ID : 4YSC
Title : Completely oxidized structure of copper nitrite reductase from *Alcaligenes faecalis*
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Deposited on : 2015-03-17
Resolution : 2.03 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

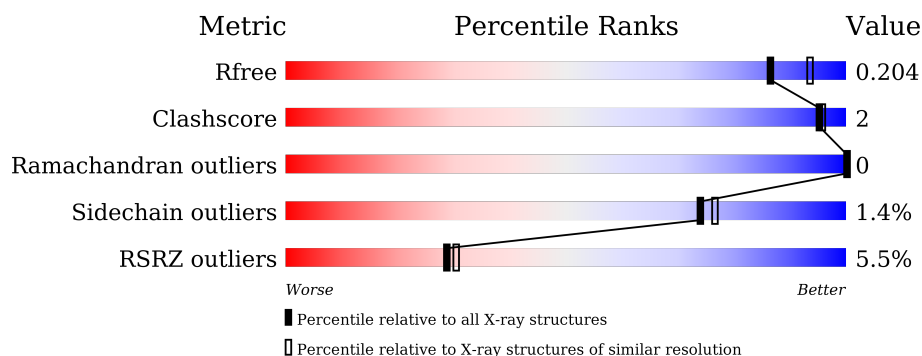
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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))
R_{free}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	342	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	342	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7931 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	336	Total	C	N	O	S	0	0	0
			2560	1639	430	480	11			
1	B	336	Total	C	N	O	S	0	0	0
			2560	1639	430	480	11			
1	C	335	Total	C	N	O	S	0	0	0
			2556	1637	429	479	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP P38501
A	341	LEU	-	expression tag	UNP P38501
A	342	VAL	-	expression tag	UNP P38501
A	343	PRO	-	expression tag	UNP P38501
A	344	ARG	-	expression tag	UNP P38501
B	3	MET	-	initiating methionine	UNP P38501
B	341	LEU	-	expression tag	UNP P38501
B	342	VAL	-	expression tag	UNP P38501
B	343	PRO	-	expression tag	UNP P38501
B	344	ARG	-	expression tag	UNP P38501
C	3	MET	-	initiating methionine	UNP P38501
C	341	LEU	-	expression tag	UNP P38501
C	342	VAL	-	expression tag	UNP P38501
C	343	PRO	-	expression tag	UNP P38501
C	344	ARG	-	expression tag	UNP P38501

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

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total 79	O 79	0	0
4	B	86	Total 86	O 86	0	0
4	C	81	Total 81	O 81	0	0

- Molecule 1: Copper-containing nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.10Å 103.80Å 147.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.90 – 2.03 44.51 – 2.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.90-2.03) 100.0 (44.51-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.164 , 0.203 0.165 , 0.204	Depositor DCC
R_{free} test set	2499 reflections (4.10%)	DCC
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7931	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, CL

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	0.96	0/2631	0.92	5/3588 (0.1%)
1	B	0.98	1/2631 (0.0%)	0.90	5/3588 (0.1%)
1	C	1.03	2/2627 (0.1%)	0.92	3/3583 (0.1%)
All	All	0.99	3/7889 (0.0%)	0.91	13/10759 (0.1%)

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	B	0	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	TYR	CG-CD2	5.68	1.46	1.39
1	C	281	TRP	CB-CG	5.58	1.60	1.50
1	C	310	GLU	CD-OE2	-5.26	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	54	ASP	CB-CG-OD1	7.55	125.09	118.30
1	C	211	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	B	159	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	164	ASP	CB-CG-OD1	6.80	124.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	C	211	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	B	14	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	251	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	98	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	159	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	98	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	211	ARG	NE-CZ-NH1	-5.17	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	HIS	Peptide
1	C	306	HIS	Peptide

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	A	2560	0	2485	12	0
1	B	2560	0	2485	10	0
1	C	2556	0	2482	3	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
4	A	79	0	0	1	0
4	B	86	0	0	0	0
4	C	81	0	0	0	0
All	All	7931	0	7452	24	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 2.

All (24) 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:A:141:MET:HG2	4:A:555:HOH:O	1.93	0.69
1:A:189:GLU:H	1:A:189:GLU:CD	1.95	0.68
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.87	0.56
1:A:188:ASP:HB2	1:A:189:GLU:OE1	2.06	0.55
1:B:143:PRO:HB2	1:B:210:MET:CE	2.39	0.52
1:A:29:SER:OG	1:A:31:VAL:O	2.28	0.51
1:C:257:ILE:HD12	1:C:302:ALA:HB3	1.95	0.49
1:B:143:PRO:HB2	1:B:210:MET:HE1	1.95	0.47
1:C:305:ASN:O	1:C:311:ALA:HB2	2.15	0.46
1:B:29:SER:OG	1:B:31:VAL:O	2.32	0.46
1:A:305:ASN:O	1:A:311:ALA:HB2	2.17	0.45
1:A:14:ARG:NH2	1:A:40:GLU:OE2	2.50	0.45
1:A:307:ASN:HA	1:B:249:ASN:O	2.18	0.44
1:A:33:GLU:O	1:A:37:LYS:NZ	2.52	0.43
1:A:253:ARG:HA	1:A:281:TRP:O	2.19	0.43
1:B:175:ILE:HD12	1:B:242:LEU:HD23	2.01	0.43
1:B:130:GLY:HA2	1:B:270:PHE:CD2	2.55	0.42
1:A:143:PRO:HB2	1:A:210:MET:HE1	2.01	0.42
1:A:83:LEU:HD22	1:A:99:PHE:HZ	1.84	0.41
1:B:141:MET:HE3	1:B:144:TRP:CE3	2.56	0.41
1:A:233:MET:O	1:A:320:PHE:HA	2.21	0.40
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.95	0.40
1:B:305:ASN:O	1:B:311:ALA:HB2	2.22	0.40
1:C:253:ARG:HA	1:C:281:TRP:O	2.21	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	A	334/342 (98%)	328 (98%)	6 (2%)	0	100	100
1	B	334/342 (98%)	328 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	333/342 (97%)	330 (99%)	3 (1%)	0	100	100
All	All	1001/1026 (98%)	986 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	264/270 (98%)	260 (98%)	4 (2%)	72	74
1	B	264/270 (98%)	261 (99%)	3 (1%)	80	82
1	C	264/270 (98%)	260 (98%)	4 (2%)	72	74
All	All	792/810 (98%)	781 (99%)	11 (1%)	74	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	166	LYS
1	A	189	GLU
1	A	208	LYS
1	B	16	LYS
1	B	141	MET
1	B	174	LYS
1	C	14	ARG
1	C	160	GLU
1	C	166	LYS
1	C	174	LYS

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 ⓘ

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, 95th 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>2	OWAB(Å ²)	Q<0.9
1	A	336/342 (98%)	0.28	17 (5%) 32 34	26, 36, 59, 86	0
1	B	336/342 (98%)	0.43	28 (8%) 14 15	24, 34, 62, 83	0
1	C	335/342 (97%)	0.13	10 (2%) 54 56	23, 31, 53, 73	0
All	All	1007/1026 (98%)	0.28	55 (5%) 29 30	23, 34, 59, 86	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	7.9
1	B	5	THR	5.4
1	B	4	ALA	5.3
1	B	6	ALA	4.5
1	A	4	ALA	4.4
1	B	282	PHE	4.0
1	B	283	ILE	3.7
1	B	11	ALA	3.6
1	B	12	LEU	3.5
1	C	282	PHE	3.5
1	B	8	GLU	3.5
1	A	189	GLU	3.3
1	B	10	ALA	3.3
1	B	33	GLU	3.3
1	A	5	THR	3.1
1	A	339	GLY	3.0
1	B	287	ALA	2.9
1	C	168	LYS	2.9
1	A	281	TRP	2.9
1	B	288	ALA	2.8
1	A	282	PHE	2.7
1	B	189	GLU	2.7
1	A	7	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	167	GLY	2.6
1	A	283	ILE	2.6
1	C	283	ILE	2.6
1	B	202	ALA	2.5
1	C	191	GLY	2.5
1	C	192	LYS	2.5
1	A	191	GLY	2.5
1	A	335	LEU	2.4
1	B	252	THR	2.4
1	B	286	GLY	2.4
1	B	244	VAL	2.4
1	B	281	TRP	2.4
1	B	284	PRO	2.3
1	A	202	ALA	2.3
1	B	9	ILE	2.3
1	C	166	LYS	2.3
1	A	338	SER	2.3
1	B	289	GLY	2.3
1	C	189	GLU	2.3
1	A	11	ALA	2.2
1	C	4	ALA	2.2
1	B	190	ASN	2.2
1	B	197	GLU	2.1
1	A	166	LYS	2.1
1	A	325	GLU	2.1
1	B	266	ALA	2.1
1	B	188	ASP	2.1
1	C	190	ASN	2.1
1	B	168	LYS	2.1
1	A	190	ASN	2.0
1	A	163	HIS	2.0
1	C	188	ASP	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	CL	B	403	1/1	0.96	0.14	-0.10	35,35,35,35	0
3	CL	A	403	1/1	0.98	0.13	-0.29	38,38,38,38	0
2	CU	B	402	1/1	0.99	0.10	-1.02	34,34,34,34	0
3	CL	A	404	1/1	0.99	0.10	-1.17	40,40,40,40	0
2	CU	A	402	1/1	1.00	0.11	-1.66	33,33,33,33	0
2	CU	B	401	1/1	0.99	0.07	-2.08	36,36,36,36	0
2	CU	C	402	1/1	1.00	0.09	-2.28	29,29,29,29	0
2	CU	C	401	1/1	1.00	0.07	-2.90	29,29,29,29	0
2	CU	A	401	1/1	1.00	0.06	-3.20	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.