

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 12:39 PM EDT

PDB ID	:	1NPN
Title	:	Crystal structure of a copper reconstituted H145A mutant of nitrite reductase
		from Alcaligenes faecalis
Authors	:	Wijma, H.J.; Boulanger, M.J.; Molon, A.; Fittipaldi, M.; Huber, M.; Murphy,
		M.E.; Verbeet, M.P.; Canters, G.W.
Deposited on		
Resolution	:	1.80 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:

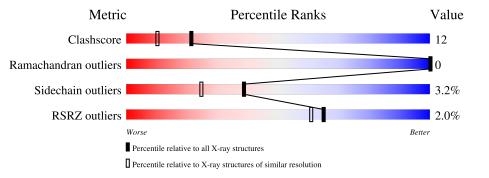
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	А	343	% • 84%	12%	•••		
1	В	343	83%	13%	•••		
1	С	343	76%	20%	•••		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9020 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	٨	A 990	Total	С	Ν	0	\mathbf{S}	0	0	0
	А	336	2555	1636	428	480	11	0		
1	В	336	Total	С	Ν	0	S	0	0	0
	D	550	2555	1636	428	480	11	0		
1	C	336	Total	С	Ν	0	S	0	0	0
	- 220	2555	1636	428	480	11	U	0	0	

• Molecule 1 is a protein called Copper-containing nitrite reductase.

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
А	145	ALA	HIS	engineered mutation	UNP P38501
В	145	ALA	HIS	engineered mutation	UNP P38501
С	145	ALA	HIS	engineered mutation	UNP P38501

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	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

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

Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0

Continued on next page...



Continued from previous page...

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

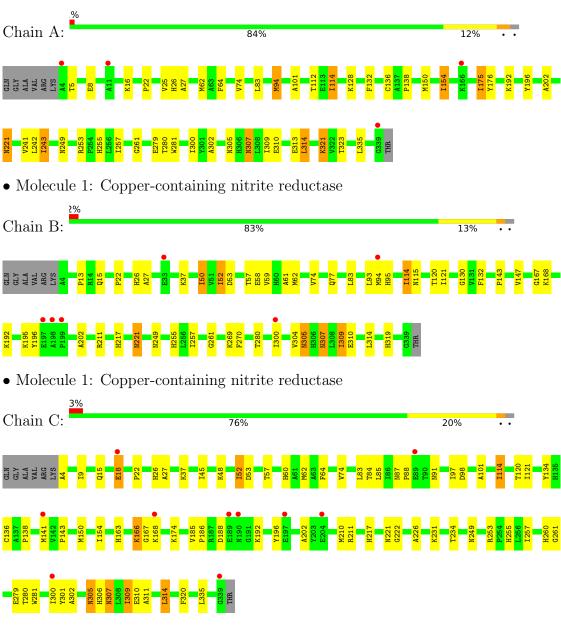
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	479	Total O 479 479	0	0
4	В	435	Total O 435 435	2	0
4	С	432	Total O 432 432	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	61.60Å 102.52Å 146.07Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.28 - 1.80	Depositor
Resolution (A)	33.27 - 1.79	EDS
% Data completeness	90.1 (33.28-1.80)	Depositor
(in resolution range)	88.1 (33.27-1.79)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.12 (at 1.79 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
D D.	0.156 , 0.195	Depositor
R, R_{free}	0.173 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	15.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 57.2	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9020	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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, 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	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.57	0/2625	0.81	4/3580~(0.1%)	
1	В	0.54	0/2625	0.80	3/3580~(0.1%)	
1	С	0.52	0/2625	0.80	5/3580~(0.1%)	
All	All	0.54	0/7875	0.80	12/10740~(0.1%)	

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	307	ASN	N-CA-C	-8.16	88.97	111.00
1	В	307	ASN	N-CA-C	-8.10	89.14	111.00
1	А	307	ASN	N-CA-C	-7.92	89.62	111.00
1	С	305	ASN	N-CA-C	-6.05	94.67	111.00
1	В	305	ASN	N-CA-C	-5.86	95.19	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	А	2555	0	2483	54	0
1	В	2555	0	2483	68	0
1	С	2555	0	2483	76	0

Continued on next page...



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	А	1	0	0	0	0
3	В	1	0	0	1	0
3	С	1	0	0	0	0
4	А	479	0	0	8	0
4	В	435	0	0	6	0
4	C	432	0	0	12	0
All	All	9020	0	7449	182	0

Continued from previous page...

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 12.

The worst 5 of 182 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:B:192:LYS:HD2	4:B:5028:HOH:O	1.61	0.98
1:A:25:VAL:HG21	1:A:175:ILE:HD12	1.49	0.95
1:B:62:MET:HE3	1:B:95:HIS:HE1	1.32	0.94
1:B:94:MET:CE	1:B:115:ASN:HD21	1.86	0.88
1:B:62:MET:CE	1:B:93:LEU:HD12	2.05	0.87

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	Perce	ntiles
1	А	334/343~(97%)	329~(98%)	5(2%)	0	100	100
1	В	334/343~(97%)	329~(98%)	5 (2%)	0	100	100

Continued on next page...



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	С	334/343~(97%)	328 (98%)	6~(2%)	0	100	100
All	All	1002/1029~(97%)	986 (98%)	16 (2%)	0	100	100

Continued from previous page...

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	263/268~(98%)	253~(96%)	10 (4%)	33 18
1	В	263/268~(98%)	255~(97%)	8 (3%)	41 27
1	С	263/268~(98%)	256~(97%)	7 (3%)	44 31
All	All	789/804~(98%)	764 (97%)	25 (3%)	39 25

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	168	LYS
1	В	309	ILE
1	С	314	LEU
1	В	305	ASN
1	С	18	GLU

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

Mol	Chain	Res	Type
1	С	115	ASN
1	С	255	HIS
1	С	221	ASN
1	В	221	ASN
1	С	77	GLN



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 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 (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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	336/343~(97%)	-0.11	4 (1%) 79 76	8, 13, 26, 39	0
1	В	336/343~(97%)	-0.07	6 (1%) 68 64	9, 14, 28, 40	0
1	С	336/343~(97%)	0.05	10 (2%) 50 44	10, 17, 32, 43	0
All	All	1008/1029~(97%)	-0.04	20 (1%) 65 61	8, 15, 29, 43	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	339	GLY	4.7
1	А	4	ALA	4.1
1	С	197	GLU	4.0
1	В	197	GLU	3.5
1	С	189	GLU	3.2

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
3	CL	В	499	1/1	0.95	0.13	$25,\!25,\!25,\!25$	0
3	CL	А	498	1/1	0.96	0.12	21,21,21,21	0
2	CU	С	501	1/1	0.96	0.05	22,22,22,22	0
3	CL	С	500	1/1	0.96	0.13	30,30,30,30	0
2	CU	А	501	1/1	0.98	0.07	17,17,17,17	0
2	CU	А	502	1/1	0.98	0.04	12,12,12,12	0
2	CU	В	502	1/1	0.99	0.05	$14,\!14,\!14,\!14$	0
2	CU	В	501	1/1	0.99	0.06	20,20,20,20	0
2	CU	С	502	1/1	0.99	0.04	$15,\!15,\!15,\!15$	0

6.5 Other polymers (i)

There are no such residues in this entry.

