Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1HAU
Title	:	X-RAY STRUCTURE OF A BLUE COPPER NITRITE REDUCTASE AT HIGH PH AND IN COPPER FREE FORM AT 1.9 A RESOLUTION
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Deposited on	:	2001-04-09
Resolution	:	1.90 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 (i) symbol.

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

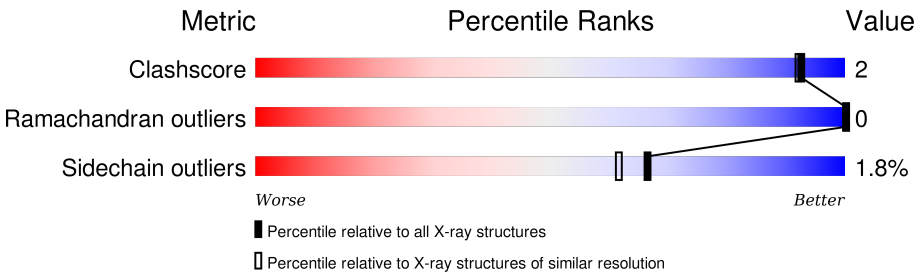
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 <=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	336	88% 11% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2757 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2578	1641	448	477	12	74	1	0

- 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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	177	177	177	0	0

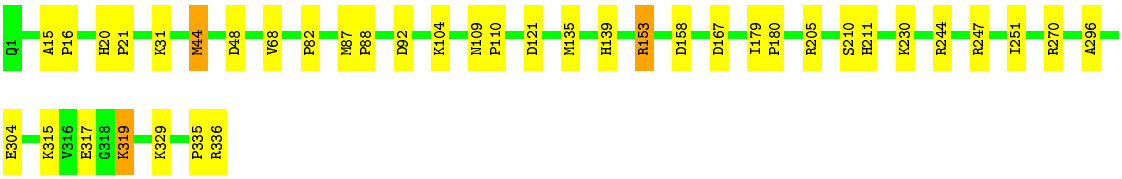
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	80.98Å 80.98Å 99.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	91.3 (20.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.154 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2757	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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	0.92	7/2654 (0.3%)	1.24	21/3613 (0.6%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLU	CG-CD	-31.75	1.04	1.51
1	A	329	LYS	CG-CD	-12.79	1.08	1.52
1	A	31	LYS	CG-CD	10.54	1.88	1.52
1	A	315	LYS	CG-CD	6.55	1.74	1.52
1	A	319	LYS	CG-CD	6.45	1.74	1.52
1	A	48	ASP	CB-CG	5.96	1.64	1.51
1	A	335	PRO	C-N	-5.27	1.22	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	LYS	CB-CG-CD	13.33	146.25	111.60
1	A	31	LYS	CB-CG-CD	-9.65	86.52	111.60
1	A	244	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	A	44	MET	CA-CB-CG	9.24	129.01	113.30
1	A	153	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	153	ARG	NE-CZ-NH2	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	319	LYS	CB-CG-CD	-6.33	95.13	111.60
1	A	336	ARG	CA-CB-CG	6.30	127.25	113.40
1	A	244	ARG	NH1-CZ-NH2	6.19	126.21	119.40
1	A	317	GLU	CB-CG-CD	6.06	130.56	114.20
1	A	121	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	153	ARG	CD-NE-CZ	5.86	131.81	123.60
1	A	158	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	335	PRO	O-C-N	5.61	131.68	122.70
1	A	270	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	315	LYS	CB-CG-CD	-5.38	97.61	111.60
1	A	205	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	230	LYS	CB-CG-CD	5.12	124.91	111.60
1	A	167	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	304	GLU	OE1-CD-OE2	-5.04	117.26	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	PRO	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	2578	0	2544	10	0
2	A	2	0	0	0	0
3	A	177	0	0	0	0
All	All	2757	0	2544	10	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 (10) 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:20:HIS:HE1	1:A:68:VAL:H	1.40	0.68
1:A:20:HIS:CE1	1:A:68:VAL:H	2.14	0.66
1:A:87:MET:HB3	1:A:88:PRO:HD2	1.88	0.56
1:A:179:ILE:HA	1:A:180:PRO:HD3	1.78	0.46
1:A:210:SER:OG	1:A:211:HIS:HD2	2.00	0.45
1:A:135[B]:MET:CE	1:A:139:HIS:HE2	2.29	0.44
1:A:15:ALA:HA	1:A:16:PRO:HD3	1.90	0.41
1:A:109:ASN:HB3	1:A:110:PRO:HD2	2.02	0.41
1:A:251:ILE:HD12	1:A:296:ALA:HB3	2.04	0.40
1:A:20:HIS:HA	1:A:21:PRO:HD3	1.98	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	335/336 (100%)	327 (98%)	8 (2%)	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	272/271 (100%)	267 (98%)	5 (2%)	66 61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	104	LYS
1	A	153	ARG
1	A	247	ARG
1	A	319	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	20	HIS
1	A	211	HIS

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 2 ligands modelled in this entry, 2 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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.