

wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2024 – 06:30 AM JST

PDB ID : 9IXF

Title : Crystal structure of Manganese-free N(omega)-hydroxy-L-arginine hydrolase

with oxidized Cys86.

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Deposited on : 2024-07-27

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 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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

Xtriage (Phenix) : 1.13 EDS : 3.0

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.003 (Gargrove)

Density-Fitness : 1.0.11

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

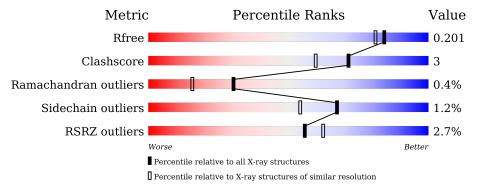
Validation Pipeline (wwPDB-VP) : 2.39

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (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	282	85%	12%	-
1	В	282	92%	5%	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4532 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 N(omega)-hydroxy-L-arginine amidinohydrolase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1 A	272	Total	С	N	О	S	0	0	0	
	A	212	2027	1269	355	396	7		0	
1	D	274	Total	С	N	О	S	0	1	0
1	B 274	214	2049	1283	358	400	8		1	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	LEU	-	expression tag	UNP D2Z025
A	275	GLU	-	expression tag	UNP D2Z025
A	276	HIS	-	expression tag	UNP D2Z025
A	277	HIS	-	expression tag	UNP D2Z025
A	278	HIS	-	expression tag	UNP D2Z025
A	279	HIS	-	expression tag	UNP D2Z025
A	280	HIS	-	expression tag	UNP D2Z025
A	281	HIS	-	expression tag	UNP D2Z025
В	274	LEU	-	expression tag	UNP D2Z025
В	275	GLU	-	expression tag	UNP D2Z025
В	276	HIS	-	expression tag	UNP D2Z025
В	277	HIS	-	expression tag	UNP D2Z025
В	278	HIS	-	expression tag	UNP D2Z025
В	279	HIS	-	expression tag	UNP D2Z025
В	280	HIS	-	expression tag	UNP D2Z025
В	281	HIS	-	expression tag	UNP D2Z025

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0



• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	В	3	Total Mg 3 3	0	0

• Molecule 4 is water.

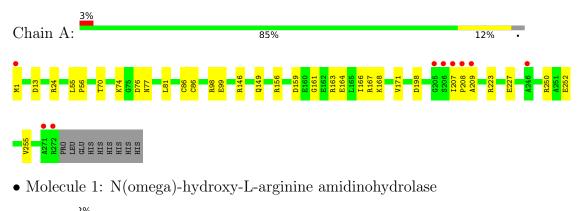
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	223	Total O 223 223	0	0
4	В	228	Total O 228 228	0	0

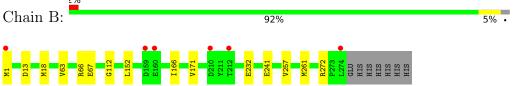


3 Residue-property plots (i)

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: N(omega)-hydroxy-L-arginine amidinohydrolase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	45.88Å 46.68Å 58.22Å	Donositon
a, b, c, α , β , γ	85.39° 86.78° 70.54°	Depositor
Resolution (Å)	43.92 - 1.75	Depositor
rtesolution (A)	43.92 - 1.75	EDS
% Data completeness	96.8 (43.92-1.75)	Depositor
(in resolution range)	96.8 (43.92-1.75)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.78 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
P.P.	0.158 , 0.201	Depositor
R, R_{free}	0.157 , 0.201	DCC
R_{free} test set	2254 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37 , 41.2	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4532	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.16% 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: CSO, MG, MN

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
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.38	0/2067	0.57	0/2827
1	В	0.38	0/2082	0.58	0/2847
All	All	0.38	0/4149	0.57	0/5674

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	2027	0	1992	18	0
1	В	2049	0	2013	10	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	В	3	0	0	0	0
4	A	223	0	0	1	0
4	В	228	0	0	3	0
All	All	4532	0	4005	26	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 3.



The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:250:ARG:HH22	1:B:1:MET:HG2	1.60	0.66
1:B:272:ARG:NH1	4:B:501:HOH:O	2.28	0.65
1:A:98:ARG:NH2	4:A:501:HOH:O	2.24	0.63
1:B:63:VAL:O	1:B:67:GLU:HG3	2.00	0.61
1:A:164:GLU:OE1	1:A:168:LYS:HE3	2.02	0.60

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	Percentile	es
1	A	$270/282\ (96\%)$	262 (97%)	7 (3%)	1 (0%)	30 16	
1	В	$271/282\ (96\%)$	265 (98%)	5 (2%)	1 (0%)	30 16	
All	All	541/564 (96%)	527 (97%)	12 (2%)	2 (0%)	30 16	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
1	В	241	GLU

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 Outlie		Percentiles
1	A	$206/215 \; (96\%)$	202 (98%)	4 (2%)	52 34
1	В	208/215 (97%)	207 (100%)	1 (0%)	86 82
All	All	414/430 (96%)	409 (99%)	5 (1%)	67 54

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

Mol	Chain	Res	Type
1	A	13	ASP
1	A	76	ASP
1	A	81	LEU
1	A	156	ARG
1	В	13	ASP

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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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 Type Chain Res		Res	Link	Bond lengths			Bond angles			
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	В	86[B]	1,3	3,6,7	0.76	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	В	86[B]	1,3	-	0/1/5/7	-

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.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$273/282 \ (96\%)$	-0.05	9 (3%) 49 56	9, 20, 38, 75	0
1	В	273/282 (96%)	-0.19	6 (2%) 62 68	11, 19, 35, 47	0
All	All	546/564 (96%)	-0.12	15 (2%) 56 62	9, 19, 36, 75	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	5.1
1	A	208	PRO	4.5
1	A	205	GLY	3.6
1	A	272	ARG	3.1
1	A	206	SER	2.8

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CSO	В	86[B]	7/8	-	-	13,14,17,17	7

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



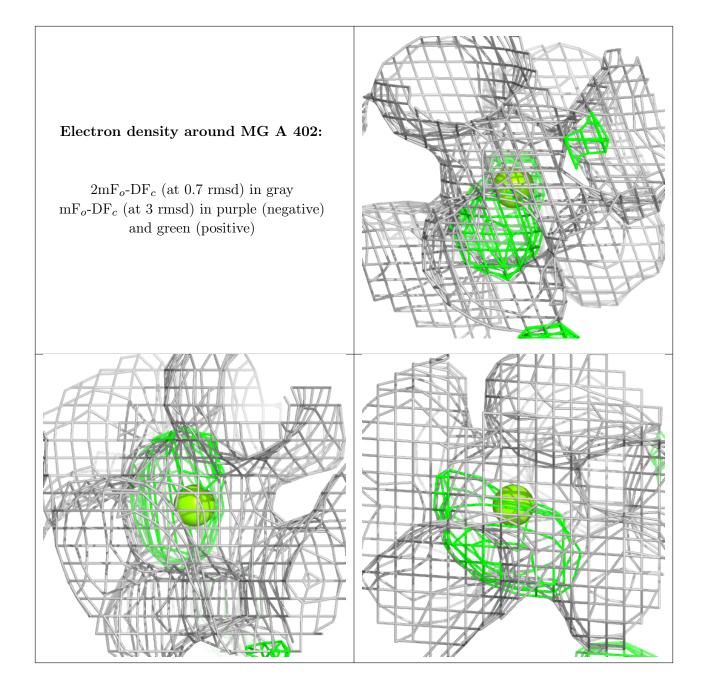
6.4 Ligands (i)

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	MG	A	402	1/1	0.98	0.07	5,5,5,5	0
3	MG	В	402	1/1	0.99	0.04	12,12,12,12	1
3	MG	В	403	1/1	0.99	0.02	21,21,21,21	1
2	MN	A	401	1/1	1.00	0.03	8,8,8,8	1
3	MG	В	401	1/1	1.00	0.02	7,7,7,7	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





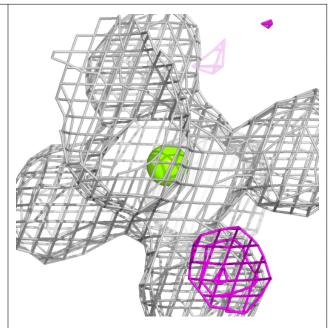


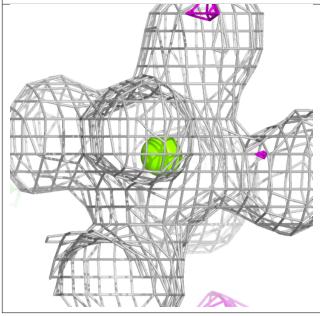
Electron density around MG B 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

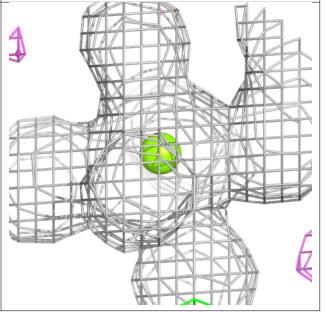


Electron density around MG B 403:

 $2 {
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m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



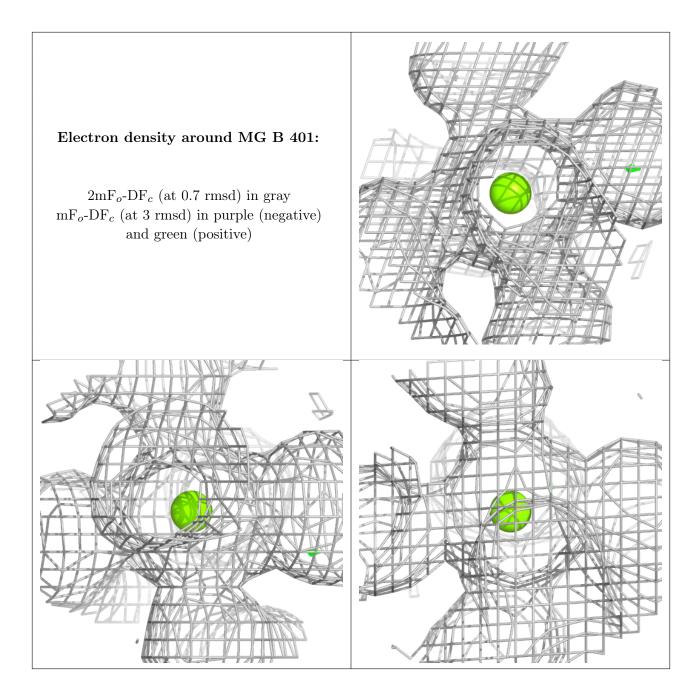






Electron density around MN A 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

