

# wwPDB X-ray Structure Validation Summary Report (i)

#### Jan 28, 2024 – 12:11 PM EST

PDB ID : 1ELS

Title : CATALYTIC METAL ION BINDING IN ENOLASE: THE CRYSTAL

STRUCTURE OF ENOLASE-MN2+-PHOSPHONOACETOHYDROXA

MATE COMPLEX AT 2.4 ANGSTROMS RESOLUTION

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Deposited on : 1994-04-05

Resolution : 2.40 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

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

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

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

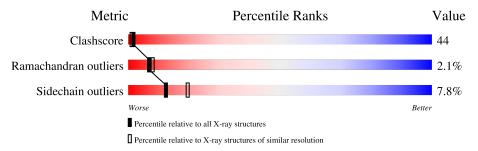
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.40 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$		
Clashscore	141614	4398 (2.40-2.40)		
Ramachandran outliers	138981	4318 (2.40-2.40)		
Sidechain outliers	138945	4319 (2.40-2.40)		

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%

Note EDS was not executed.

Mol	Chain	Length		Quality of chain					
1	A	436	37%	42%	19%	•			

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PAH	A	439	-	X	X	-



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3643 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 ENOLASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	436	Total	С	N	О	S	0	0	0
1	11	100	3289	2076	569	638	6			

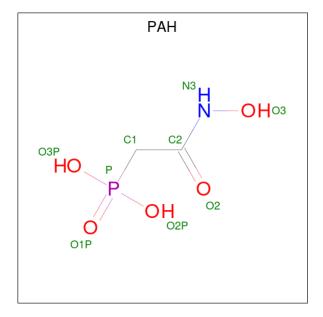
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	conflict	UNP P00924

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

• Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (three-letter code: PAH) (formula: C<sub>2</sub>H<sub>6</sub>NO<sub>5</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	Λ	1	Total	С	N	О	Р	0	0
)	A	1	9	2	1	5	1	0	0

## • Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	343	Total O 343 343	0	0

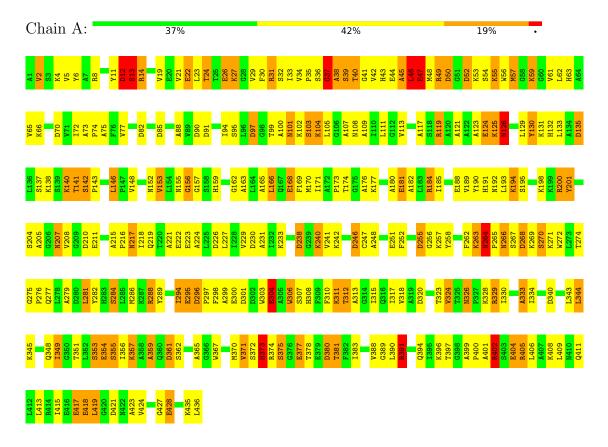


# 3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: ENOLASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	124.10Å 124.10Å 66.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness	(Not available) ((Not available)-2.40)	Depositor
(in resolution range)	, , , , , , , , , , , , , , , , , , , ,	Берозгог
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
$R, R_{free}$	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: MN, PAH

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	Bo	nd lengths	В	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	1.04	2/3349 (0.1%)	2.49	189/4531 (4.2%)

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	A	404	GLU	CD-OE1	-5.73	1.19	1.25
1	A	377	GLU	CD-OE2	-5.01	1.20	1.25

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	391	ARG	NE-CZ-NH1	-23.27	108.67	120.30
1	A	8	ARG	NE-CZ-NH1	21.99	131.29	120.30
1	A	49	ARG	NE-CZ-NH1	20.78	130.69	120.30
1	A	49	ARG	NE-CZ-NH2	-16.67	111.96	120.30
1	A	200	ARG	NE-CZ-NH2	-15.29	112.65	120.30

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	3289	0	3291	288	5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	9	0	3	9	0
4	A	343	0	0	111	6
All	All	3643	0	3294	290	6

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 44.

The worst 5 of 290 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:142:SER:HA	4:A:586:HOH:O	1.33	1.23
1:A:255:ASP:HB3	4:A:708:HOH:O	1.39	1.18
1:A:435:LYS:HE3	4:A:694:HOH:O	1.43	1.17
1:A:227:LEU:HB2	4:A:597:HOH:O	1.52	1.08
1:A:345:LYS:NZ	3:A:439:PAH:H12	1.66	1.08

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:207:ASN:C	4:A:630:HOH:O[8_666]	0.80	1.40
1:A:207:ASN:CA	4:A:630:HOH:O[8_666]	1.06	1.14
1:A:208:VAL:N	4:A:630:HOH:O[8_666]	1.40	0.80
1:A:288:ARG:NH2	4:A:672:HOH:O[4_565]	1.72	0.48
1:A:207:ASN:O	4:A:630:HOH:O[8_666]	2.00	0.20

## 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	434/436 (100%)	394 (91%)	31 (7%)	9 (2%)	7 8	

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	264	ASN
1	A	270	SER
1	A	37	GLY
1	A	263	LYS

#### 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	344/344 (100%)	317 (92%)	27 (8%)	12 19	

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ASP
1	A	284	SER
1	A	372	SER
1	A	268	ASP
1	A	304	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	326	ASN
1	A	373	HIS
1	A	348	GLN
1	A	155	ASN



#### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	Link	Bond lengths		Bond angles			
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	$\mid \# Z  > 2 \mid$
3	PAH	A	439	2	8,8,8	6.32	5 (62%)	10,11,11	6.00	7 (70%)

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
3	PAH	A	439	2	-	4/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(\AA)$	$\operatorname{Ideal}( ext{\AA})$
3	A	439	PAH	C2-N3	16.78	1.50	1.32
3	A	439	PAH	P-C1	4.09	1.86	1.79
3	A	439	PAH	P-O1P	-3.41	1.43	1.50

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(\AA)$	$\operatorname{Ideal}( ext{\AA})$
3	A	439	PAH	O2-C2	2.32	1.28	1.23
3	A	439	PAH	C1-C2	-2.19	1.47	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	439	PAH	O3-N3-C2	13.23	139.34	119.79
3	A	439	PAH	C1-C2-N3	10.08	125.91	115.08
3	A	439	PAH	O2-C2-N3	-5.69	116.29	123.27
3	A	439	PAH	O2-C2-C1	-4.14	111.61	121.16
3	A	439	PAH	O2P-P-C1	-3.48	99.53	106.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	439	PAH	C1-C2-N3-O3
3	A	439	PAH	O2-C2-N3-O3
3	A	439	PAH	C2-C1-P-O2P
3	A	439	PAH	C2-C1-P-O3P

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	PAH	9	0

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

