

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

Dec 3, 2023 - 03:57 pm GMT

PDB ID : 1EB8

Title : Structure Determinants of Substrate Specificity of Hydroxynitrile Lyase from

Manihot esculenta

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Deposited on : 2001-07-24

Resolution : 2.10 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 : 1.8.4, 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)

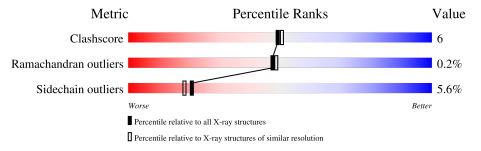
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	262	75%	21%	•••
1	В	262	79%	16%	



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4426 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.

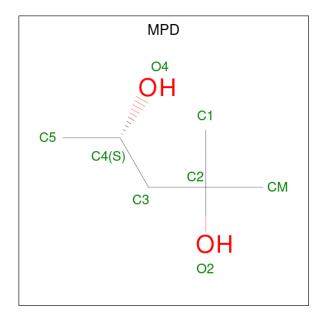
• Molecule 1 is a protein called (S)-ACETONE-CYANOHYDRIN LYASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	262	Total	С	N	О	S	0	0	0
1	A	202	2095	1351	348	388	8	0	U	U
1	D	258	Total	С	N	О	S	0	0	0
1	Б	200	2065	1331	343	383	8		U	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	TRP	engineered mutation	UNP P52705
В	128	ALA	TRP	engineered mutation	UNP P52705

• Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	C 6	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O 8 6 2	0	0

## $\bullet\,$ Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	В	134	Total O 134 134	0	0

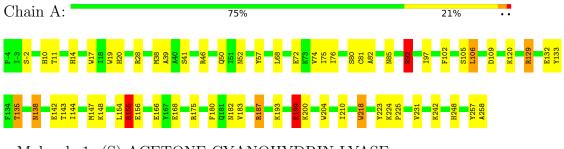


# 3 Residue-property plots (i)

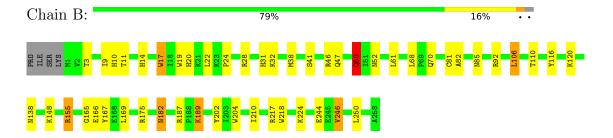
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: (S)-ACETONE-CYANOHYDRIN LYASE



• Molecule 1: (S)-ACETONE-CYANOHYDRIN LYASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 41 21 2	Depositor	
Cell constants	106.40Å 106.40Å 188.43Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	8.00 - 2.10	Depositor	
% Data completeness	86.6 (8.00-2.10)	Depositor	
(in resolution range)	00.0 (0.00 2.10)	Берозгог	
$R_{merge}$	0.04	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
$R, R_{free}$	0.192 , $0.234$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4426	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	26.0	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: MPD

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).

Mal	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.85	0/2145	1.47	25/2905~(0.9%)	
1	В	0.86	0/2114	1.49	33/2864 (1.2%)	
All	All	0.86	0/4259	1.48	58/5769 (1.0%)	

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	155	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	A	92	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	155	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	129	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	В	175	ARG	NE-CZ-NH1	9.70	125.15	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	2095	0	2096	33	0
1	В	2065	0	2060	18	0
2	A	8	0	14	0	0
2	В	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	116	0	0	2	0
3	В	134	0	0	2	0
All	All	4426	0	4184	49	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 6.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:10:HIS:HE1	1:A:38:MET:H	1.18	0.89
1:B:10:HIS:HE1	1:B:38:MET:H	1.21	0.85
1:B:52:ASN:HD22	1:B:138:ASN:HB2	1.52	0.75
1:A:52:ASN:HD22	1:A:138:ASN:HB2	1.53	0.74
1:A:10:HIS:HD2	1:A:11:THR:O	1.73	0.71

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	entiles
1	A	$260/262 \ (99\%)$	251 (96%)	9 (4%)	0	100	100
1	В	$256/262 \ (98\%)$	244 (95%)	11 (4%)	1 (0%)	34	32
All	All	516/524~(98%)	495 (96%)	20 (4%)	1 (0%)	47	49

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	17	TRP



#### 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	226/226 (100%)	213 (94%)	13 (6%)	20	17	
1	В	222/226 (98%)	210 (95%)	12 (5%)	22	20	
All	All	448/452 (99%)	423 (94%)	25 (6%)	21	18	

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

Mol	Chain	Res	Type
1	В	68	LEU
1	В	120	LYS
1	В	250	LEU
1	В	106	LEU
1	В	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	В	10	HIS
1	В	182	ASN
1	В	52	ASN
1	В	85	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)

2 ligands are 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	Tuno	Chain Res Link		Bond lengths			Bond angles			
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	MPD	В	1301	-	7,7,7	0.59	0	9,10,10	0.53	0
2	MPD	A	1301	-	7,7,7	0.55	0	9,10,10	0.54	0

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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	MPD	В	1301	-	-	0/5/5/5	-
2	MPD	A	1301	-	-	0/5/5/5	-

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 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.

