



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:07 am BST

PDB ID : 3FW0  
Title : Structure of Peptidyl-alpha-hydroxyglycine alpha-Amidating Lyase (PAL)  
bound to alpha-hydroxyhippuric acid (non-peptidic substrate)  
Authors : Chufan, E.E.; De, M.; Eipper, B.A.; Mains, R.E.; Amzel, L.M.  
Deposited on : 2009-01-16  
Resolution : 2.52 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](mailto: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 ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

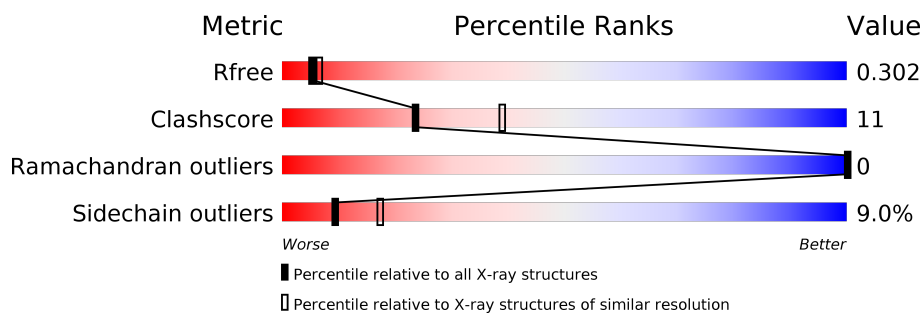
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 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))
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	329	 78% 18% •

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2754 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 Peptidyl-glycine alpha-amidating monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2619	1667	453	491	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	EXPRESSION TAG	UNP P14925
A	493	HIS	-	EXPRESSION TAG	UNP P14925
A	494	HIS	-	EXPRESSION TAG	UNP P14925
A	495	HIS	-	EXPRESSION TAG	UNP P14925
A	496	HIS	-	EXPRESSION TAG	UNP P14925
A	497	HIS	-	EXPRESSION TAG	UNP P14925

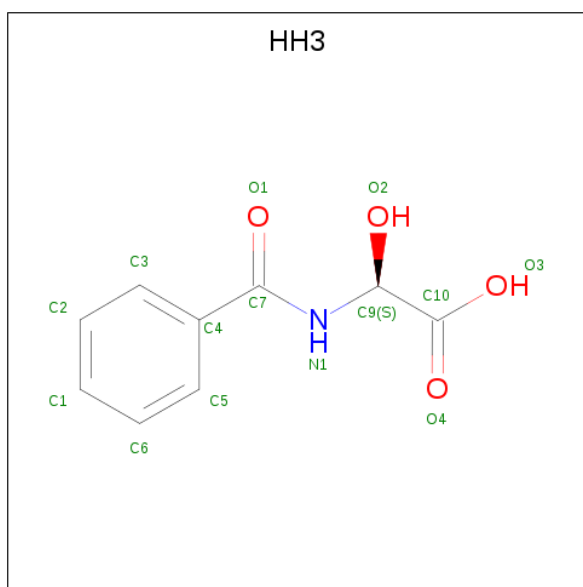
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (2S)-hydroxy[(phenylcarbonyl)amino]ethanoic acid (three-letter code: HH3) (formula: C<sub>9</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	9	1	4		

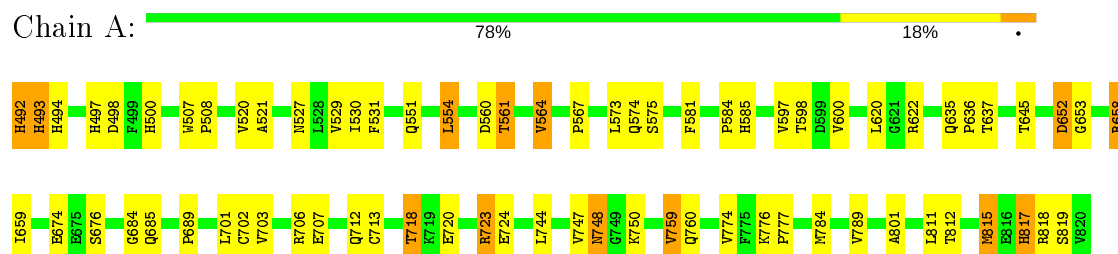
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		

### 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 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.

- Molecule 1: Peptidyl-glycine alpha-amidating monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.93Å 75.08Å 97.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.34 – 2.52 48.51 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (59.34-2.52) 99.1 (48.51-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.207 , 0.260 0.258 , 0.302	Depositor DCC
$R_{free}$ test set	655 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HH3, CA, HG

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	0.40	0/2700	0.60	0/3671

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	493	HIS	Peptide
1	A	652	ASP	Peptide

### 5.2 Too-close contacts

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	2619	0	2468	57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	14	0	7	0	0
5	A	118	0	0	2	0
All	All	2754	0	2475	57	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 11.

All (57) 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:500[B]:HIS:NE2	1:A:817:HIS:HB3	1.46	1.29
1:A:500[B]:HIS:NE2	1:A:817:HIS:CB	2.26	0.99
1:A:520:VAL:HG23	1:A:789:VAL:HG23	1.44	0.97
1:A:500[B]:HIS:CE1	1:A:817:HIS:HA	2.04	0.92
1:A:500[B]:HIS:CE1	1:A:817:HIS:HB3	2.10	0.84
1:A:684:GLY:H	1:A:712:GLN:HE22	1.26	0.83
1:A:748:ASN:HD21	1:A:760:GLN:H	1.34	0.76
1:A:500[B]:HIS:CE1	1:A:817:HIS:CA	2.70	0.74
1:A:500[B]:HIS:CD2	1:A:817:HIS:HB3	2.22	0.73
1:A:500[B]:HIS:CE1	1:A:817:HIS:CB	2.69	0.72
1:A:659:ILE:HD11	1:A:703:VAL:HG21	1.70	0.72
1:A:676:SER:HA	1:A:685:GLN:HB3	1.71	0.71
1:A:748:ASN:ND2	1:A:760:GLN:H	1.93	0.67
1:A:784:MET:HE2	1:A:801:ALA:HB3	1.76	0.66
1:A:561:THR:HG21	1:A:581:PHE:CD1	2.31	0.65
1:A:492:HIS:HA	5:A:73:HOH:O	1.98	0.64
1:A:500[B]:HIS:NE2	1:A:817:HIS:CG	2.68	0.61
1:A:561:THR:HG21	1:A:581:PHE:HD1	1.66	0.60
1:A:500[B]:HIS:NE2	1:A:817:HIS:CD2	2.70	0.60
1:A:527:ASN:HD22	1:A:567:PRO:HD3	1.66	0.58
1:A:520:VAL:HG23	1:A:789:VAL:CG2	2.27	0.56
1:A:531:PHE:HE1	1:A:561:THR:HG23	1.71	0.54
1:A:784:MET:CE	1:A:801:ALA:HB3	2.36	0.54
1:A:748:ASN:HD21	1:A:760:GLN:N	2.05	0.54
1:A:674:GLU:HG3	1:A:685:GLN:HG2	1.88	0.54
1:A:521:ALA:HA	1:A:789:VAL:HG21	1.90	0.54
1:A:531:PHE:CE1	1:A:561:THR:HG23	2.43	0.53
1:A:520:VAL:HG12	1:A:530:ILE:HG22	1.92	0.52
1:A:723:ARG:HG2	1:A:724:GLU:N	2.25	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:PHE:CZ	1:A:584:PRO:HB3	2.46	0.51
1:A:702:CYS:HG	1:A:713:CYS:HG	1.53	0.50
1:A:520:VAL:CG2	1:A:789:VAL:HG23	2.30	0.50
1:A:652:ASP:HB3	1:A:658:ARG:HG2	1.93	0.49
1:A:750:LYS:HA	1:A:759:VAL:HG22	1.93	0.49
1:A:585:HIS:HB3	1:A:598:THR:HG22	1.95	0.48
1:A:748:ASN:HD22	1:A:748:ASN:H	1.62	0.47
1:A:564:VAL:HG13	1:A:574:GLN:HB2	1.95	0.47
1:A:815:MET:HB2	5:A:12:HOH:O	2.16	0.46
1:A:507:TRP:HA	1:A:508:PRO:HD3	1.72	0.46
1:A:748:ASN:HD21	1:A:759:VAL:HA	1.81	0.45
1:A:551:GLN:HG3	1:A:554:LEU:HG	1.98	0.45
1:A:585:HIS:ND1	1:A:637:THR:O	2.49	0.44
1:A:529:VAL:HG22	1:A:564:VAL:HB	2.00	0.44
1:A:659:ILE:CD1	1:A:703:VAL:HG21	2.45	0.44
1:A:776:LYS:HB2	1:A:777:PRO:HD2	1.99	0.44
1:A:531:PHE:HE1	1:A:561:THR:CG2	2.31	0.43
1:A:702:CYS:SG	1:A:713:CYS:SG	3.11	0.43
1:A:817:HIS:O	1:A:818:ARG:C	2.56	0.43
1:A:492:HIS:C	1:A:492:HIS:CD2	2.92	0.43
1:A:498:ASP:HA	1:A:817:HIS:HD2	1.84	0.43
1:A:653:GLY:HA2	1:A:689:PRO:HD2	2.01	0.43
1:A:718:THR:HB	1:A:720:GLU:HG3	2.00	0.42
1:A:560:ASP:HB3	1:A:575:SER:HB2	2.02	0.42
1:A:600:VAL:HG13	1:A:635:GLN:HG2	2.01	0.42
1:A:598:THR:CG2	1:A:636:PRO:O	2.68	0.42
1:A:564:VAL:HG22	1:A:573:LEU:HB2	2.01	0.41
1:A:531:PHE:CE2	1:A:597:VAL:HG22	2.55	0.41

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	328/329 (100%)	312 (95%)	16 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	290/289 (100%)	264 (91%)	26 (9%)	9	17

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	HIS
1	A	493	HIS
1	A	494	HIS
1	A	497	HIS
1	A	554	LEU
1	A	561	THR
1	A	564	VAL
1	A	620	LEU
1	A	622	ARG
1	A	645	THR
1	A	658	ARG
1	A	701	LEU
1	A	706	ARG
1	A	707	GLU
1	A	718	THR
1	A	723	ARG
1	A	744	LEU
1	A	747	VAL
1	A	748	ASN
1	A	759	VAL
1	A	774	VAL
1	A	811	LEU
1	A	812	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	815	MET
1	A	817	HIS
1	A	819	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	ASN
1	A	579	ASN
1	A	708	ASN
1	A	712	GLN
1	A	748	ASN
1	A	817	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 4 ligands modelled in this entry, 3 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HH3	A	1	-	10,14,14	0.51	0	11,18,18	0.66	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	Res	Link	Chirals	Torsions	Rings
4	HH3	A	1	-	-	5/8/12/12	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	HH3	C10-C9-N1-C7
4	A	1	HH3	C5-C4-C7-N1
4	A	1	HH3	C5-C4-C7-O1
4	A	1	HH3	C3-C4-C7-O1
4	A	1	HH3	C3-C4-C7-N1

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.