

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

#### Dec 17, 2023 – 07:46 PM EST

PDB ID : 1GGV

Title : CRYSTAL STRUCTURE OF THE C123S MUTANT OF DIENELACTONE

HYDROLASE (DLH) BOUND WITH THE PMS MOIETY OF THE PROTEASE INHIBITOR, PHENYLMETHYLSULFONYL FLUORIDE (PMSF)

Authors: Robinson, A.; Edwards, K.J.; Carr, P.D.; Barton, J.D.; Ewart, G.D.; Ollis,

D.L.

Deposited on : 2000-09-27

Resolution : 2.50 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
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)

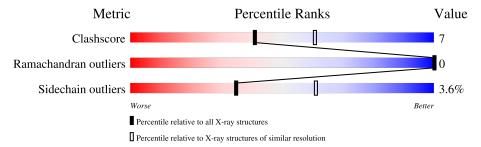
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.50 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	$(\# \mathrm{Entries})$	$(\# \text{Entries, resolution range}(\mathring{A}))$	
Clashscore	141614	5346 (2.50-2.50)	
Ramachandran outliers	138981	5231 (2.50-2.50)	
Sidechain outliers	138945	5233 (2.50-2.50)	

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 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	232	82%	16%			



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1806 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 DIENELACTONE HYDROLASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	232	Total 1742	C 1118	N 293	O 326	S 5	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	ARG	conflict	UNP P0A114
A	123	SEB	CYS	SEE REMARK 999	UNP P0A114
A	154	ASN	LYS	conflict	UNP P0A114
A	224	THR	ARG	conflict	UNP P0A114

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0

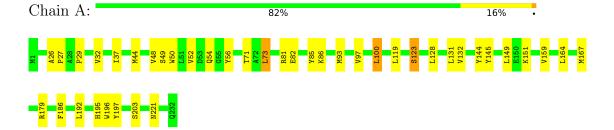


# 3 Residue-property plots (i)

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: DIENELACTONE HYDROLASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	51.08Å 51.86Å 82.61Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	7.00 - 2.50	Depositor	
% Data completeness	(Not available) (7.00-2.50)	Depositor	
(in resolution range)	(1100 available) (1.00 2.00)	Depositor	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR 3.1	Depositor	
$R, R_{free}$	0.151 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1806	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	14.0	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: SEB

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).

ſ	Mol	Chain	Bond	lengths	Bond angles		
			RMSZ	# Z  > 5	RMSZ	# Z  > 5	
ſ	1	A	0.50	0/1770	0.68	0/2411	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TYR	Sidechain

## 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	1742	0	1665	24	0
2	A	64	0	0	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1806	0	1665	24	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 7.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:85:TYR:OH	1:A:123:SEB:HI1	1.74	0.87
1:A:85:TYR:CZ	1:A:123:SEB:HI1	2.21	0.76
1:A:81:ARG:NH2	1:A:123:SEB:HJ	2.00	0.75
1:A:32:VAL:O	1:A:119:LEU:HD12	1.89	0.72
1:A:179:ARG:HG2	1:A:196:TRP:CH2	2.25	0.71
1:A:49:SER:HA	1:A:52:VAL:HG22	1.79	0.65
1:A:145:TYR:CZ	1:A:203:SER:HA	2.33	0.63
1:A:50:TRP:O	1:A:54:GLN:HG2	1.99	0.63
1:A:37:ILE:HG23	1:A:123:SEB:OD1	1.99	0.62
1:A:82:GLU:O	1:A:86:LYS:HG2	2.06	0.54
1:A:26:ALA:HB1	1:A:27:PRO:HA	1.92	0.51
1:A:44:MET:O	1:A:48:VAL:HG23	2.10	0.51
1:A:179:ARG:HG2	1:A:196:TRP:CZ3	2.48	0.48
1:A:167:MET:O	1:A:196:TRP:HA	2.16	0.45
1:A:29:PRO:HG2	1:A:56:TYR:CD1	2.51	0.45
1:A:144:TYR:OH	1:A:221:ASN:ND2	2.48	0.45
1:A:93:MET:O	1:A:97:VAL:HG23	2.18	0.43
1:A:151:LYS:HA	1:A:151:LYS:HE2	2.00	0.43
1:A:71:THR:HG22	1:A:73:LEU:HD22	2.01	0.42
1:A:100:LEU:HD23	1:A:132:VAL:HG21	2.01	0.42
1:A:186:PHE:CD1	1:A:192:LEU:HD22	2.55	0.42
1:A:81:ARG:CZ	1:A:123:SEB:HJ	2.51	0.41
1:A:123:SEB:HA	1:A:145:TYR:O	2.21	0.41
1:A:164:LEU:HD11	1:A:195:HIS:CD2	2.56	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	229/232 (99%)	222 (97%)	7 (3%)	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	165/173~(95%)	159 (96%)	6 (4%)	35 61	

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	100	LEU
1	A	128	LEU
1	A	131	LEU
1	A	149	LEU
1	A	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	67	GLN

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	161	HIS
1	A	221	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)

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	Pog	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	eles
MIOI	туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEB	A	123	1	15,16,17	1.26	1 (6%)	15,21,23	1.89	5 (33%)

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	SEB	A	123	1	-	5/9/13/15	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
1	A	123	SEB	CE-SD	4.35	1.82	1.78

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	123	SEB	OG-SD-CE	3.73	114.47	104.18
1	A	123	SEB	OD1-SD-OD2	-3.45	103.53	116.40

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	123	SEB	CB-OG-SD	-3.32	112.10	119.23
1	A	123	SEB	OD2-SD-CE	2.93	115.80	108.82
1	A	123	SEB	OG-SD-OD1	-2.34	99.01	107.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	123	SEB	SD-CE-CZ-CH2
1	A	123	SEB	SD-CE-CZ-CH1
1	A	123	SEB	CZ-CE-SD-OD2
1	A	123	SEB	CB-OG-SD-CE
1	A	123	SEB	CB-OG-SD-OD1

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	123	SEB	6	0

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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.

