

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

May 22, 2020 – 01:58 am BST

PDB ID : 1MPP

Title : X-RAY ANALYSES OF ASPARTIC PROTEINASES. V. STRUCTURE AND

REFINEMENT AT 2.0 ANGSTROMS RESOLUTION OF THE ASPARTIC

PROTEINASE FROM MUCOR PUSILLUS

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Deposited on : 1992-02-19

Resolution : 2.00 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 following versions of software and data (see references (1)) 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)

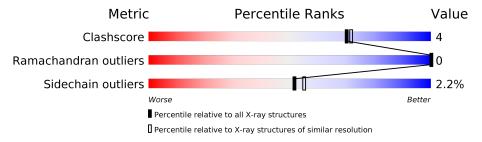
Validation Pipeline (wwPDB-VP) : 2.11

# 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 2.00 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	$(\# {\rm Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 >=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	361	66%	29%	• •		



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2864 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.

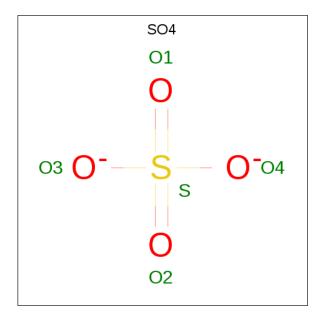
• Molecule 1 is a protein called PEPSIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	357	Total	С	N	О	S	0	0	0
1	A	397	2638	1686	414	530	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ILE	MET	CONFLICT	UNP P09177
A	170	VAL	ALA	CONFLICT	UNP P09177
A	202	SER	ALA	CONFLICT	UNP P09177

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	221	Total O 221 221	0	0

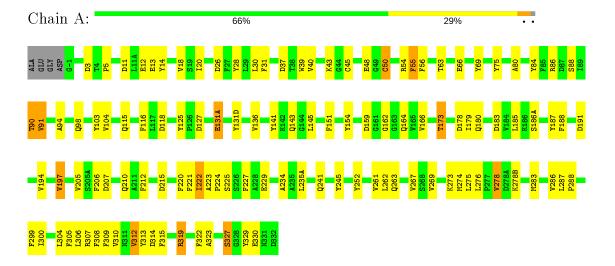


# 3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: PEPSIN





# 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 2	Depositor
Cell constants	70.00Å 104.00Å 46.30Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness	(Not available) ((Not available)-2.00)	Depositor
(in resolution range)	, , , ,	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
$R, R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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: SO4

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	Chain	Boı	nd lengths	Bond angles		
Mol   Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	1.42	8/2704 (0.3%)	2.35	$140/3693 \ (3.8\%)$	

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	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	A	88	SER	CA-CB	6.20	1.62	1.52
1	A	90	THR	CB-OG1	5.76	1.54	1.43
1	A	267	VAL	N-CA	5.34	1.57	1.46
1	A	305	PHE	CG-CD1	5.19	1.46	1.38
1	A	241	GLN	CD-OE1	5.17	1.35	1.24

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	54	ARG	NE-CZ-NH2	14.47	127.54	120.30
1	A	37	ASP	CB-CG-OD2	12.41	129.47	118.30
1	A	307	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	48	GLU	OE1-CD-OE2	-10.99	110.12	123.30
1	A	13	GLU	OE1-CD-OE2	-10.66	110.51	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



M	ol	Chain	Res	Type	Group
-	Ĺ	A	319	ARG	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	2638	0	2415	18	0
2	A	5	0	0	0	0
3	A	221	0	0	0	0
All	All	2864	0	2415	18	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 4.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$	
1:A:278:VAL:HG11	1:A:283:MET:HB2	1.57	0.86	
1:A:275:LEU:C	1:A:276:LEU:HD23	2.01	0.81	
1:A:276:LEU:HD23	1:A:276:LEU:N	2.07	0.68	
1:A:131(A):GLU:O	1:A:131(A):GLU:HG3	2.00	0.60	
1:A:278:VAL:CG1	1:A:283:MET:HB2	2.34	0.54	

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	355/361 (98%)	349 (98%)	6 (2%)	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	272/298 (91%)	266 (98%)	6 (2%)	52 55	

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	$\mathbf{Type}$	
1	A	221	PHE	
1	A	327	SER	
1	A	222	ILE	
1	A	131(A)	GLU	
1	A	263	GLN	

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	72	ASN
1	A	311	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 carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

1 ligand 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	ype Chain	in Res	Link	В	Bond lengths		Bond angles		
				Co	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	501	_	4,4,4	0.28	0	6,6,6	0.50	0

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.

