

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

May 14, 2020 – 06:03 am BST

PDB ID : 4PEP

Title: THE MOLECULAR AND CRYSTAL STRUCTURES OF MONOCLINIC

PORCINE PEPSIN REFINED AT 1.8 ANGSTROMS RESOLUTION

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Deposited on : 1989-12-18

Resolution : 1.80 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:

 $Mol Probity \quad : \quad 4.02 \, b\text{--}467$ 

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)

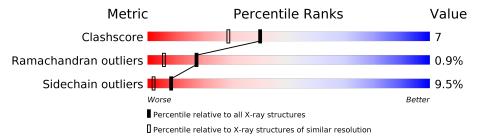
Validation Pipeline (wwPDB-VP) : 2.11

## 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 1.80 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ \ range(\AA)}) \end{array}$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 chair	ı	
		222			
1	A	326	64%	29%	5% •



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2620 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	Δ	326	Total	С	N	О	Р	S	0	0	0
1	Λ	320	2433	1530	365	527	1	10			0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP P00791
A	263	ASP	ASN	CONFLICT	UNP P00791

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	187	Total O 187 187	0	0

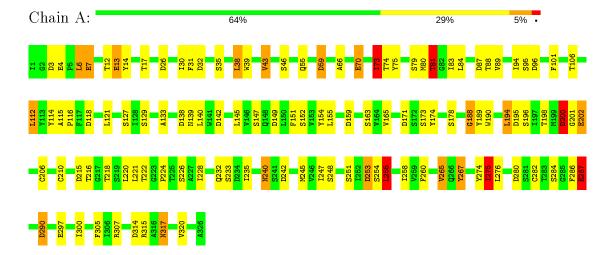


## 3 Residue-property plots (i)

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 1 21 1	Depositor
Cell constants	54.83Å 36.44Å 73.68Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.80^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	8.00 - 1.80	Depositor
% Data completeness	(Not available) (8.00-1.80)	Depositor
(in resolution range)	(1101 available) (0.00 1.00)	Беровног
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
$R, R_{free}$	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2620	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: SEP

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	Bond	lengths	Bo	ond angles
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	1.02	0/2477	2.07	90/3389~(2.7%)

There are no bond length outliers.

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
1	A	215	ASP	CB-CG-OD2	16.73	133.36	118.30
1	A	118	ASP	CB-CG-OD1	11.95	129.06	118.30
1	A	73	ILE	CA-CB-CG2	9.78	130.46	110.90
1	A	87	ASP	CB-CG-OD2	9.39	126.75	118.30
1	A	159	ASP	CB-CG-OD1	9.23	126.61	118.30

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	2433	0	2251	34	0
2	A	187	0	0	2	0
All	All	2620	0	2251	34	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.



The worst 5 of 34 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap} & ( ext{Å}) \end{aligned}$
1:A:251:SER:HB3	1:A:255:LEU:HD22	1.76	0.68
1:A:171:ASP:HB3	1:A:174:TYR:HD1	1.59	0.67
1:A:235:ILE:O	1:A:247:ILE:HD11	1.95	0.66
1:A:275:ILE:HG21	1:A:282:CYS:HB3	1.79	0.64
1:A:265:VAL:HG13	1:A:267:TYR:CE1	2.33	0.63

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	323/326 (99%)	307 (95%)	13 (4%)	3 (1%)	17 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASP
1	A	201	GLY
1	A	188	GLY

#### 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	Analysed Rotameric		Percentiles	
1	A	274/274 (100%)	248 (90%)	26 (10%)	8 2	

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	SER
1	A	202	GLU
1	A	280	ASP
1	A	178	SER
1	A	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN

#### 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 Cl		Chain Res		Chain	Chain	Chain	Chain	Chain	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
	Type	1 tes	LIIIK		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2					
1	SEP	A	68	1	8,9,10	0.96	0	8,12,14	4.16	3 (37%)					

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	SEP	A	68	1	-	3/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	68	SEP	P-OG-CB	8.56	141.86	118.30
1	A	68	SEP	OG-P-O1P	7.13	126.47	106.47
1	A	68	SEP	O3P-P-OG	-3.46	97.54	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$
1	A	68	SEP	CB-OG-P-O3P
1	A	68	SEP	N-CA-CB-OG
1	A	68	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

There are no carbohydrates 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.

