

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 10:05 AM EDT

PDB ID : 1EST

Title: THE ATOMIC STRUCTURE OF CRYSTALLINE PORCINE PANCRE-

ATIC ELASTASE AT 2.5 ANGSTROMS RESOLUTION. COMPARISONS

WITH THE STRUCTURE OF ALPHA-CHYMOTRYPSIN

Authors: Sawyer, L.; Shotton, D.M.; Watson, H.C.

Deposited on : 1976-05-17

Resolution : 2.50 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 : 1.8.5 (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)

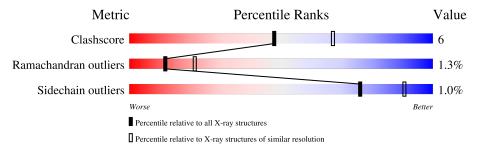
Validation Pipeline (wwPDB-VP) : 2.36.2

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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
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	240	55%	37%	8%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1858 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.

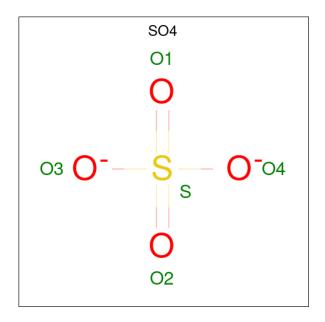
• Molecule 1 is a protein called PORCINE PANCREATIC ELASTASE.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	240	Total	С	N	О	S	0	0	0
1	Λ	240	1822	1135	330	347	10	0	0	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ASN	ASP	conflict	UNP P00772

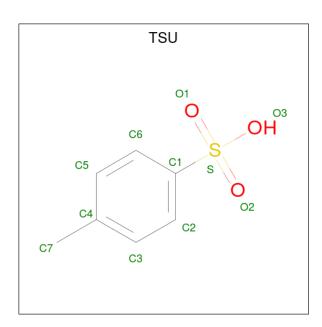
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

• Molecule 3 is PARA-TOLUENE SULFONATE (three-letter code: TSU) (formula: C₇H₈O₃S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 7	O 2	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0

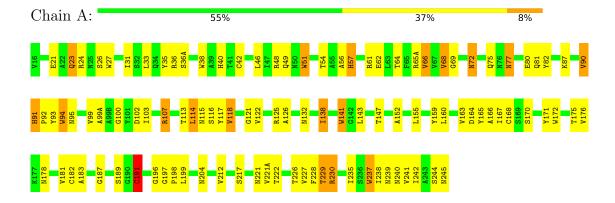


3 Residue-property plots (i)

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: PORCINE PANCREATIC ELASTASE





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	51.50Å 58.00Å 75.50Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	(Not available) – 2.50	Depositor	
% Data completeness	(Not available) ((Not available)-2.50)	Depositor	
(in resolution range)	, , ,	•	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	unknown	Depositor	
R, R_{free}	(Not available) , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1858	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	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, TSU

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.72	7/1862 (0.4%)	0.93	0/2543	

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	87

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\mathring{A}})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	A	172	TRP	NE1-CE2	-7.47	1.27	1.37
1	A	51	TRP	NE1-CE2	-7.42	1.27	1.37
1	A	38	TRP	NE1-CE2	-7.41	1.27	1.37
1	A	237	TRP	NE1-CE2	-7.38	1.27	1.37
1	A	94	TRP	NE1-CE2	-7.37	1.27	1.37

There are no bond angle outliers.

There are no chirality outliers.

5 of 87 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLU	Mainchain
1	A	23	GLN	Mainchain
1	A	33	LEU	Mainchain
1	A	35	TYR	Sidechain
1	A	36	ARG	Mainchain



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	1822	0	1758	22	0
2	A	1	0	0	1	0
3	A	10	0	7	0	0
4	A	25	0	0	6	0
All	All	1858	0	1765	22	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 22 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:75:GLN:O	4:A:272:HOH:O	1.92	0.87	
1:A:77:ASN:OD1	4:A:272:HOH:O	2.07	0.72	
1:A:230:ARG:NH1	2:A:246:SO4:S	2.63	0.71	
1:A:72:ASN:O	4:A:272:HOH:O	2.10	0.70	
1:A:31:ILE:HG22	1:A:68:VAL:HG12	1.74	0.69	

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 Allower		Outliers	Percentiles		
1	A	238/240 (99%)	207 (87%)	28 (12%)	3 (1%)	12	21	

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	62	GLU
1	A	230	ARG
1	A	24	ARG

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	198/198 (100%)	196 (99%)	2 (1%)	76 90	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	191	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	240	ASN
1	A	153	GLN
1	A	178	ASN
1	A	204	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)

Of 2 ligands modelled in this entry, 1 is modelled with single atom - 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 Ty	Trino	Chain	Chain	Chain	Chain	Chain Bog	Pog Link	Bond lengths			Bond angles		
	туре		nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
3	TSU	A	247	-	9,10,11	1.10	1 (11%)	11,13,16	0.89	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
3	TSU	A	247	-	-	0/2/4/6	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	A	247	TSU	C1-S	-2.20	1.75	1.80

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.

