



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:04 PM GMT

PDB ID : 1INC  
Title : CRYSTAL STRUCTURES OF THE COMPLEX OF PORCINE PANCREATIC ELASTASE WITH TWO VALINE-DERIVED BENZOXAZINONE INHIBITORS  
Authors : Meyer, E.  
Deposited on : 1993-03-19  
Resolution : 1.94 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

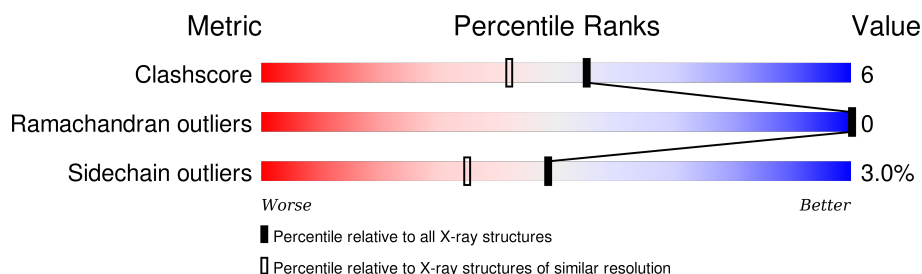
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1992 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
			Total	C	N	O	S			
1	A	240	1822	1135	330	347	10	0	0	0

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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).

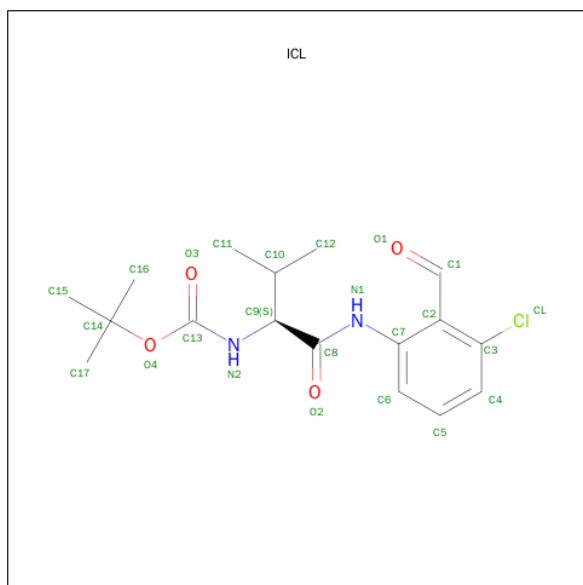


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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

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

- Molecule 4 is [1-(3-CHLORO-2-FORMYL-PHENYLCARBAMOYL)-2-METHYL-PROPYL]-CARBAMIC ACID TERT-BUTYL ESTER (three-letter code: ICL) (formula: C<sub>17</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 24 17 1 2 4	0	0

- Molecule 5 is water.

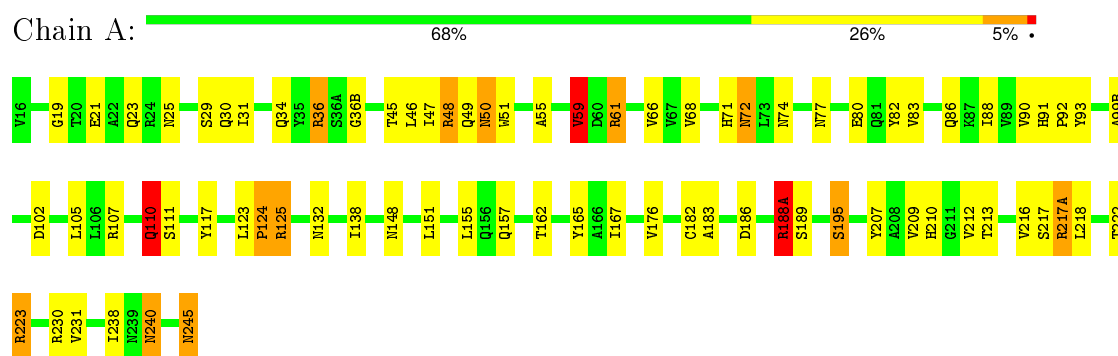
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	140	Total O 140 140	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.10 Å 58.00 Å 75.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.94	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.94)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	EREF	Depositor
R, $R_{free}$	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: CA, SO4, ICL

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	1.25	3/1862 (0.2%)	1.73	20/2543 (0.8%)

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	41

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	ARG	NE-CZ	6.42	1.41	1.33
1	A	223	ARG	NE-CZ	5.35	1.40	1.33
1	A	217(A)	ARG	CZ-NH1	5.33	1.40	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217(A)	ARG	NE-CZ-NH1	-13.61	113.50	120.30
1	A	125	ARG	NE-CZ-NH2	12.69	126.64	120.30
1	A	176	VAL	CA-CB-CG2	-10.84	94.64	110.90
1	A	188(A)	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	A	61	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	48	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	A	125	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	36	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	230	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	165	TYR	CB-CG-CD1	-6.25	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	124	PRO	N-CA-CB	6.18	110.71	103.30
1	A	186	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	66	VAL	CA-CB-CG1	5.59	119.29	110.90
1	A	117	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	A	195	SER	O-C-N	-5.40	114.02	123.20
1	A	80	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	82	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	91	HIS	CA-CB-CG	-5.14	104.86	113.60
1	A	59	VAL	CA-CB-CG2	5.13	118.60	110.90
1	A	90	VAL	CA-CB-CG1	5.00	118.41	110.90

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ASP	Mainchain
1	A	105	LEU	Mainchain
1	A	110	GLN	Sidechain
1	A	132	ASN	Sidechain
1	A	138	ILE	Mainchain
1	A	148	ASN	Sidechain
1	A	155	LEU	Mainchain
1	A	157	GLN	Mainchain
1	A	182	CYS	Mainchain
1	A	188(A)	ARG	Sidechain
1	A	189	SER	Mainchain
1	A	19	GLY	Mainchain
1	A	195	SER	Mainchain
1	A	207	TYR	Sidechain
1	A	21	GLU	Sidechain
1	A	210	HIS	Mainchain
1	A	212	VAL	Mainchain
1	A	213	THR	Mainchain
1	A	217	SER	Mainchain
1	A	218	LEU	Mainchain
1	A	238	ILE	Mainchain
1	A	240	ASN	Mainchain
1	A	245	ASN	Sidechain
1	A	25	ASN	Mainchain
1	A	29	SER	Mainchain
1	A	30	GLN	Sidechain
1	A	34	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	36	ARG	Mainchain
1	A	36(B)	GLY	Mainchain
1	A	46	LEU	Mainchain
1	A	49	GLN	Sidechain
1	A	50	ASN	Sidechain
1	A	55	ALA	Mainchain
1	A	59	VAL	Mainchain
1	A	61	ARG	Sidechain
1	A	71	HIS	Sidechain
1	A	72	ASN	Sidechain
1	A	74	ASN	Mainchain
1	A	86	GLN	Sidechain
1	A	93	TYR	Sidechain
1	A	99(B)	ALA	Mainchain

## 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	1822	0	1758	23	1
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	24	0	22	3	0
5	A	140	0	0	1	0
All	All	1992	0	1780	23	1

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.

All (23) 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:83:VAL:HG23	1:A:110:GLN:HG2	1.47	0.95
1:A:31:ILE:HG22	1:A:68:VAL:HG12	1.59	0.83
1:A:48:ARG:HB2	1:A:51:TRP:HB2	1.79	0.64
1:A:217(A):ARG:HD3	5:A:572:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG22	4:A:260:ICL:H4	1.84	0.59
1:A:151:LEU:HD21	4:A:260:ICL:C17	2.35	0.57
1:A:72:ASN:H	1:A:77:ASN:HD21	1.52	0.55
1:A:151:LEU:HD21	4:A:260:ICL:H171	1.88	0.55
1:A:31:ILE:CG2	1:A:68:VAL:HG12	2.34	0.50
1:A:83:VAL:HG23	1:A:110:GLN:CG	2.33	0.50
1:A:124:PRO:HD3	1:A:209:VAL:O	2.16	0.45
1:A:83:VAL:CG2	1:A:110:GLN:HG2	2.32	0.44
1:A:47:ILE:O	1:A:48:ARG:HD2	2.17	0.44
1:A:59:VAL:HG21	1:A:88:ILE:HG21	2.00	0.44
1:A:45:THR:HG21	1:A:209:VAL:HG21	2.00	0.42
1:A:59:VAL:HG21	1:A:88:ILE:CG2	2.49	0.42
1:A:162:THR:HA	1:A:183:ALA:HA	2.00	0.42
1:A:222:THR:HG22	1:A:223:ARG:HG3	2.02	0.42
1:A:125:ARG:HD3	1:A:125:ARG:HH11	1.60	0.41
1:A:240:ASN:HD22	1:A:240:ASN:HA	1.61	0.41
1:A:123:LEU:HD22	1:A:231:VAL:HG11	2.03	0.41
1:A:167:ILE:HD13	1:A:167:ILE:HG21	1.87	0.40
1:A:23:GLN:HE21	1:A:23:GLN:HB3	1.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:O	1:A:188(A):ARG:NH2[4_566]	2.11	0.09

## 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	238/240 (99%)	231 (97%)	7 (3%)	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	198/198 (100%)	192 (97%)	6 (3%)	48 35

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	92	PRO
1	A	110	GLN
1	A	111	SER
1	A	188(A)	ARG
1	A	245	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	75	GLN
1	A	91	HIS
1	A	153	GLN
1	A	240	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
2	SO4	A	250	-	4,4,4	0.38	0	6,6,6	0.11	0
4	ICL	A	260	1	24,24,24	1.37	3 (12%)	30,34,34	1.43	4 (13%)

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
2	SO4	A	250	-	-	0/0/0/0	0/0/0/0
4	ICL	A	260	1	-	0/23/23/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	260	ICL	C2-C1	-3.24	1.39	1.46
4	A	260	ICL	C3-CL	-3.07	1.66	1.73
4	A	260	ICL	C9-N2	2.36	1.51	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	260	ICL	C6-C7-N1	-3.49	113.83	121.90
4	A	260	ICL	O2-C8-C9	-2.88	114.75	120.68
4	A	260	ICL	C10-C9-C8	-2.43	104.94	111.31
4	A	260	ICL	C9-C8-N1	3.68	119.64	115.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	260	ICL	3	0

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.