Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 10:56 AM EDT

PDB ID	:	8EST
Title	:	REACTION OF PORCINE PANCREATIC ELASTASE WITH 7-SUBSTITUTED 3-ALKOXY-4-CHLOROISOCOUMARINS: DESIGN OF POTENT INHIBITORS USING THE CRYSTAL STRUCTURE OF THE COMPLEX FORMED WITH 4-CHLORO-3-ETHOXY-7-GUANIDINO-ISOCOUMARIN
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Deposited on	:	1990-02-21
Resolution	:	1.78 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:

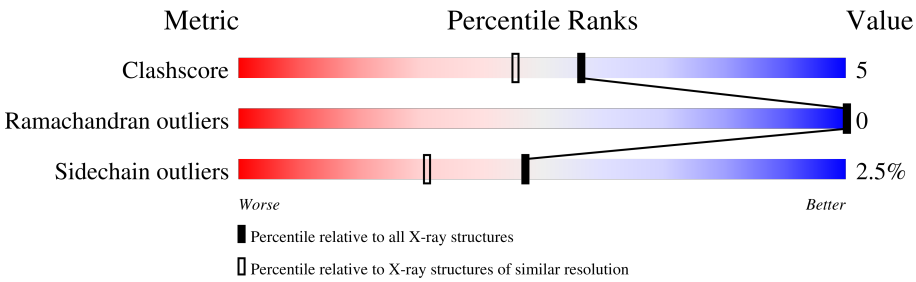
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.78 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	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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	E	240	83% 15% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2016 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.

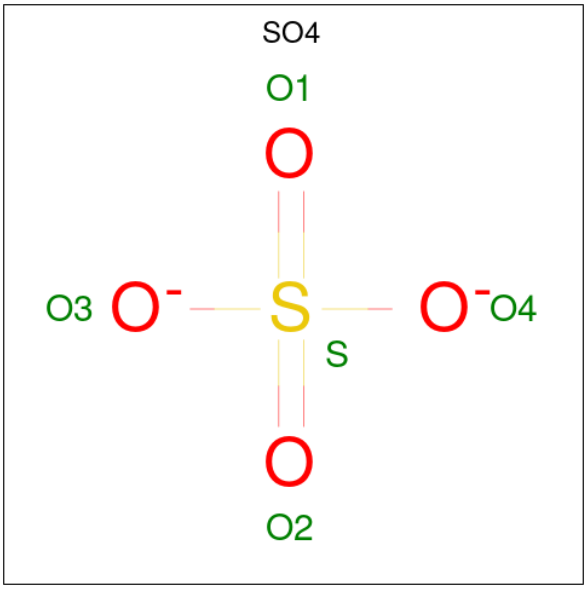
- Molecule 1 is a protein called PORCINE PANCREATIC ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	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
E	77	ASN	ASP	conflict	UNP P00772

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

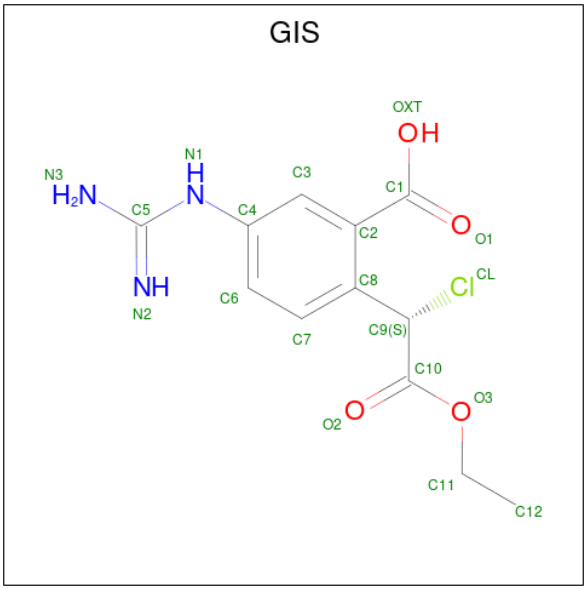


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	E	1	5	4	1	0	0

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

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

- Molecule 4 is ETHYL-(2-CARBOXY-4-GUANIDINIUM-PHENYL)-CHLOROACETATE (three-letter code: GIS) (formula: $C_{12}H_{14}ClN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	E	1	19	12	1	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	169	169	169	0	0

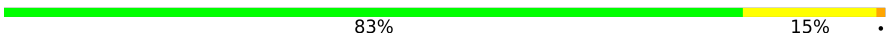
3 Residue-property plots (i)

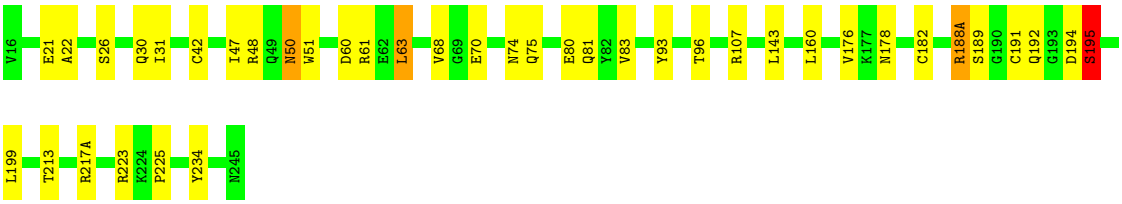
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

Chain E:





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 a, b, c, α, β, γ	50.62Å 58.26Å 75.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.78	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-1.78)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2016	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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, GIS, CA

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	E	1.05	1/1862 (0.1%)	1.35	7/2543 (0.3%)

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	E	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	107	ARG	NE-CZ	6.01	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	188(A)	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	E	107	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	225	PRO	N-CA-CB	5.38	109.76	103.30
1	E	93	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	E	80	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	E	223	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	E	195	SER	N-CA-CB	5.04	118.06	110.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	178	ASN	Sidechain
1	E	189	SER	Mainchain
1	E	192	GLN	Sidechain
1	E	194	ASP	Sidechain
1	E	195	SER	Mainchain
1	E	21	GLU	Sidechain
1	E	234	TYR	Sidechain
1	E	42	CYS	Mainchain
1	E	70	GLU	Sidechain
1	E	74	ASN	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	E	1822	0	1758	18	0
2	E	5	0	0	0	0
3	E	1	0	0	0	0
4	E	19	0	12	0	0
5	E	169	0	0	6	0
All	All	2016	0	1770	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 5.

All (18) 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:E:31:ILE:HG22	1:E:68:VAL:HG12	1.78	0.65
1:E:26:SER:HB2	5:E:698:HOH:O	1.98	0.64
1:E:22:ALA:HB1	5:E:698:HOH:O	1.97	0.63
1:E:50:ASN:HD22	1:E:50:ASN:H	1.47	0.62
1:E:47:ILE:O	1:E:48:ARG:HD2	2.02	0.60
1:E:48:ARG:HB2	1:E:51:TRP:HB2	1.85	0.59
1:E:61:ARG:HB2	1:E:63:LEU:HD22	1.89	0.55
1:E:217(A):ARG:NH1	5:E:702:HOH:O	2.40	0.53
1:E:68:VAL:CG2	1:E:81:GLN:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LEU:HD23	5:E:666:HOH:O	2.09	0.51
1:E:50:ASN:HD22	1:E:50:ASN:N	2.09	0.51
1:E:68:VAL:HG22	1:E:81:GLN:HB2	1.98	0.46
1:E:143:LEU:HB2	1:E:191:CYS:SG	2.57	0.45
1:E:176:VAL:HG21	1:E:182:CYS:SG	2.57	0.45
1:E:75:GLN:NE2	5:E:686:HOH:O	2.50	0.44
1:E:30:GLN:HB2	5:E:703:HOH:O	2.17	0.44
1:E:195:SER:HA	1:E:213:THR:HB	2.00	0.43
1:E:60:ASP:OD2	1:E:96:THR:HG23	2.19	0.42

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	E	238/240 (99%)	228 (96%)	10 (4%)	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	E	198/198 (100%)	193 (98%)	5 (2%)	47 31

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	50	ASN
1	E	63	LEU
1	E	83	VAL
1	E	160	LEU
1	E	188(A)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	49	GLN
1	E	50	ASN
1	E	75	GLN
1	E	110	GLN
1	E	153	GLN
1	E	204	ASN
1	E	239	ASN
1	E	240	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 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	$\#\|Z\| > 2$
4	GIS	E	269	1	17,19,20	2.06	2 (11%)	18,25,27	1.16	2 (11%)
2	SO4	E	247	-	4,4,4	0.45	0	6,6,6	0.42	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
4	GIS	E	269	1	-	5/17/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	269	GIS	C9-CL	-6.69	1.73	1.80
4	E	269	GIS	C2-C1	-3.32	1.39	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	269	GIS	C4-N1-C5	-2.87	120.91	127.85
4	E	269	GIS	C7-C8-C9	-2.51	116.29	120.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	269	GIS	N3-C5-N1-C4
4	E	269	GIS	O1-C1-C2-C3
4	E	269	GIS	O2-C10-C9-C8
4	E	269	GIS	O1-C1-C2-C8
4	E	269	GIS	O3-C10-C9-C8

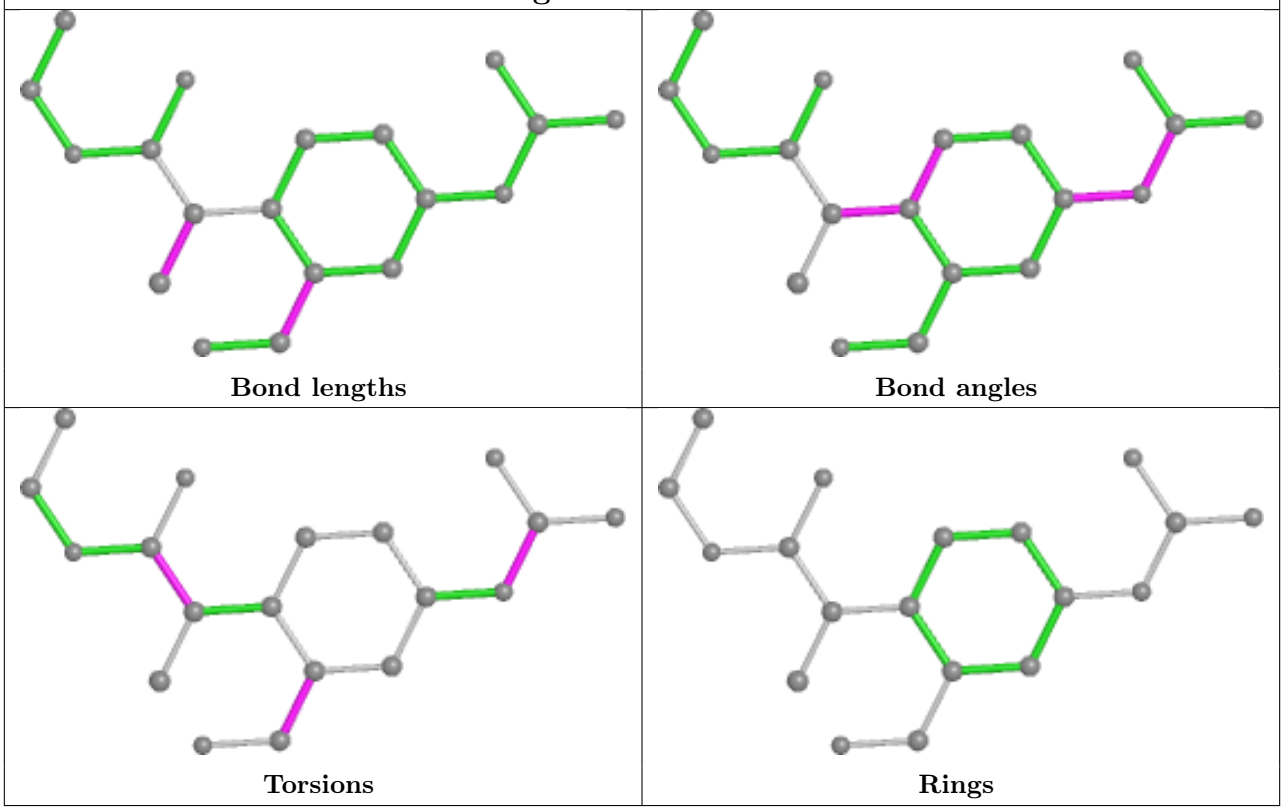
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GIS E 269



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.