



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:49 AM GMT

PDB ID : 1ESB
Title : DIRECT STRUCTURE OBSERVATION OF AN ACYL-ENZYME INTERMEDIATE IN THE HYDROLYSIS OF AN ESTER SUBSTRATE BY ELASTASE
Authors : Ding, X.; Rasmussen, B.; Petsko, G.A.; Ringe, D.
Deposited on : 1994-02-04
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

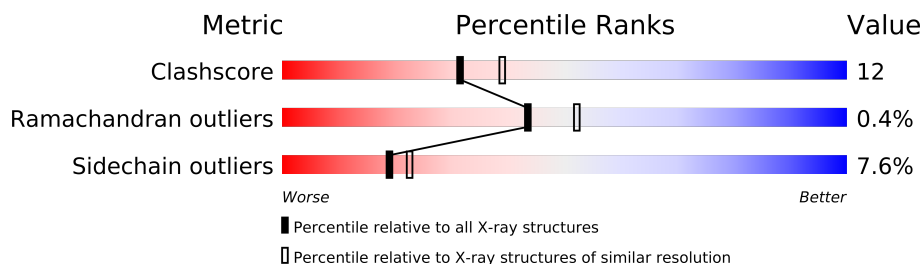
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1968 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

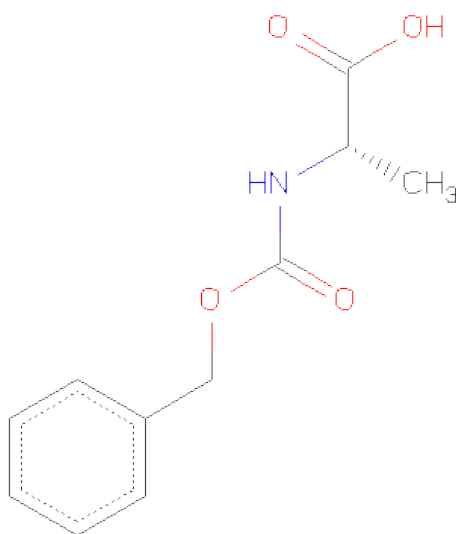
- Molecule 1 is a protein called PORCINE PANCREATIC ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1821	1135	330	346	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ASN	ASP	CONFLICT	UNP P00772

- Molecule 2 is N-[(BENZYLOXY)CARBONYL]-L-ALANINE (three-letter code: BBL) (formula: $C_{11}H_{13}NO_4$).

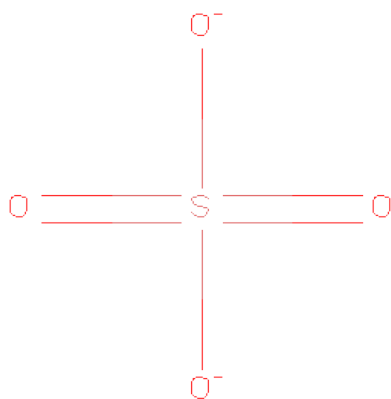


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	1	3	0	0

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

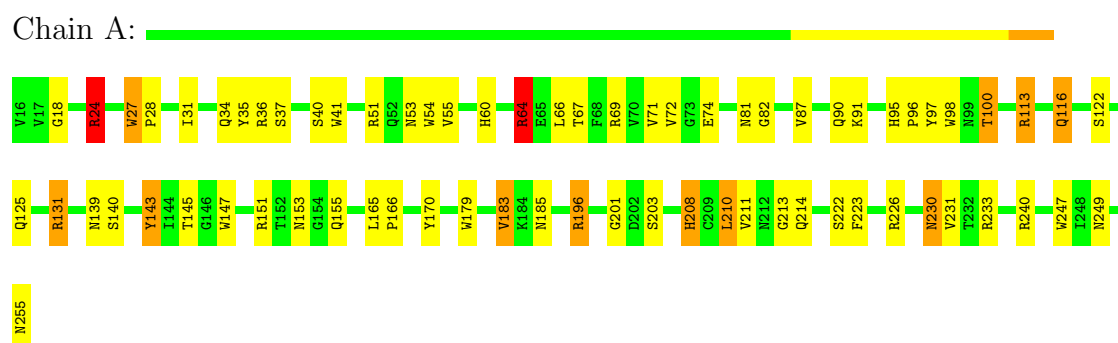
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total	O	0	0
			126	126		

3 Residue-property plots

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, α , β , γ	52.02Å 57.22Å 74.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1968	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, BBL, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	0/1861	1.75	49/2543 (1.9%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	NE-CZ-NH2	-11.43	114.58	120.30
1	A	24	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	41	TRP	CD1-CG-CD2	9.86	114.19	106.30
1	A	240	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	179	TRP	CD1-CG-CD2	9.49	113.89	106.30
1	A	51	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	151	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	247	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	A	51	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	179	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	247	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	A	41	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	A	64	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	98	TRP	CD1-CG-CD2	6.83	111.76	106.30
1	A	41	TRP	CG-CD1-NE1	-6.82	103.28	110.10
1	A	131	ARG	CA-CB-CG	6.62	127.95	113.40
1	A	98	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	147	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	A	226	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	196	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	147	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	A	100	THR	CA-CB-CG2	-6.22	103.69	112.40
1	A	196	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	36	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	A	27	TRP	CE2-CD2-CG	-6.01	102.49	107.30
1	A	41	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	A	55	VAL	CG1-CB-CG2	-5.98	101.34	110.90
1	A	113	ARG	CA-CB-CG	5.94	126.48	113.40
1	A	27	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	A	27	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	A	179	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	A	247	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	54	TRP	CG-CD2-CE3	5.65	138.99	133.90
1	A	247	TRP	CG-CD2-CE3	5.64	138.98	133.90
1	A	183	VAL	CA-CB-CG2	-5.59	102.51	110.90
1	A	54	TRP	CE2-CD2-CG	-5.53	102.87	107.30
1	A	98	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	A	247	TRP	CB-CG-CD1	-5.31	120.10	127.00
1	A	240	ARG	CB-CG-CD	-5.30	97.83	111.60
1	A	41	TRP	CB-CG-CD1	-5.28	120.13	127.00
1	A	95	HIS	CA-CB-CG	-5.26	104.65	113.60
1	A	143	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	27	TRP	CD1-CG-CD2	5.18	110.44	106.30
1	A	179	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	A	36	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	170	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	97	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	A	131	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	1758	40	5
2	A	15	0	12	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	5	0	0	0	1
5	A	126	0	0	7	3
All	All	1968	0	1770	41	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:SER:CB	2:A:256:BBL:CB2	2.38	1.01
1:A:213:GLY:N	5:A:349:HOH:O	1.96	0.97
1:A:81:ASN:HB3	5:A:310:HOH:O	1.66	0.94
2:A:256:BBL:HD1	5:A:505:HOH:O	1.72	0.90
1:A:222:SER:O	2:A:256:BBL:HE1	1.85	0.77
1:A:34:GLN:HE22	1:A:69:ARG:HH21	1.31	0.77
1:A:230:ASN:H	1:A:230:ASN:HD22	1.36	0.71
1:A:122:SER:O	5:A:393:HOH:O	2.07	0.71
1:A:203:SER:HB2	2:A:256:BBL:CB2	2.20	0.71
1:A:34:GLN:NE2	1:A:69:ARG:HH21	1.91	0.68
1:A:91:LYS:HB3	1:A:113:ARG:HG2	1.78	0.66
1:A:28:PRO:HB2	1:A:125:GLN:HB2	1.82	0.62
1:A:60:HIS:CD2	2:A:256:BBL:CE2	2.82	0.62
1:A:223:PHE:HB3	2:A:256:BBL:HE1	1.83	0.60
1:A:222:SER:O	2:A:256:BBL:CE1	2.51	0.58
1:A:31:ILE:HG22	1:A:72:VAL:HG12	1.85	0.58
1:A:24:ARG:HH22	1:A:81:ASN:HD22	1.50	0.57
1:A:60:HIS:CG	2:A:256:BBL:HE2	2.40	0.56
1:A:87:VAL:HG23	1:A:116:GLN:HE21	1.70	0.56
1:A:60:HIS:CE1	2:A:256:BBL:CZ	2.89	0.55
1:A:28:PRO:HD2	5:A:334:HOH:O	2.08	0.54
1:A:60:HIS:CG	2:A:256:BBL:CE2	2.92	0.52
1:A:230:ASN:H	1:A:230:ASN:ND2	2.06	0.51
1:A:34:GLN:HE21	1:A:69:ARG:HE	1.60	0.49
1:A:24:ARG:NH2	1:A:81:ASN:HD22	2.11	0.48
1:A:64:ARG:HB3	1:A:66:LEU:HG	1.96	0.48
1:A:201:GLY:N	2:A:256:BBL:OG1	2.46	0.47
1:A:210:LEU:HD12	5:A:536:HOH:O	2.15	0.47
1:A:211:VAL:O	1:A:214:GLN:HG2	2.16	0.46
1:A:18:GLY:O	1:A:196:ARG:HG2	2.15	0.46
1:A:31:ILE:CG2	1:A:72:VAL:HG12	2.46	0.46
1:A:35:TYR:HA	1:A:67:THR:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:TRP:CD1	1:A:145:THR:HG21	2.53	0.44
1:A:140:SER:O	1:A:166:PRO:HA	2.19	0.43
1:A:64:ARG:HE	1:A:66:LEU:HD21	1.84	0.43
1:A:74:GLU:HB3	5:A:322:HOH:O	2.19	0.42
1:A:143:TYR:O	1:A:208:HIS:HD2	2.02	0.42
1:A:71:VAL:HG12	1:A:74:GLU:HB2	2.02	0.42
1:A:233:ARG:HH11	1:A:233:ARG:HD3	1.73	0.41
1:A:201:GLY:H	2:A:256:BBL:HBZ3	1.86	0.40
1:A:53:ASN:HD22	1:A:113:ARG:NH2	2.19	0.40

All (7) 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	Distance(Å)	Clash(Å)
1:A:82:GLY:O	5:A:502:HOH:O[4.566]	1.44	0.76
4:A:290:SO4:O1	5:A:513:HOH:O[2.665]	1.56	0.64
1:A:81:ASN:O	1:A:196:ARG:NH1[4.566]	1.70	0.50
5:A:520:HOH:O	5:A:558:HOH:O[4.566]	1.99	0.21
1:A:131:ARG:NH2	1:A:153:ASN:ND2[2.665]	2.15	0.05
1:A:155:GLN:OE1	1:A:185:ASN:OD1[2.664]	2.16	0.04
1:A:131:ARG:NE	1:A:153:ASN:ND2[2.665]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	228 (96%)	9 (4%)	1 (0%)	43 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO

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%)	183 (92%)	15 (8%)	19	22

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	37	SER
1	A	40	SER
1	A	64	ARG
1	A	90	GLN
1	A	100	THR
1	A	116	GLN
1	A	139	ASN
1	A	165	LEU
1	A	183	VAL
1	A	208	HIS
1	A	210	LEU
1	A	230	ASN
1	A	249	ASN
1	A	255	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	78	ASN
1	A	95	HIS
1	A	116	GLN
1	A	125	GLN
1	A	155	GLN
1	A	158	GLN
1	A	230	ASN
1	A	249	ASN
1	A	250	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	BBL	A	256	1	15,15,16	4.03	4 (26%)	16,18,20	2.27	3 (18%)
4	SO4	A	290	-	4,4,4	1.33	0	6,6,6	0.35	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
2	BBL	A	256	1	-	0/9/11/13	0/1/1/1
4	SO4	A	290	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	256	BBL	OG1-CB2	13.09	1.20	1.11
2	A	256	BBL	OEZ-C	7.21	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	256	BBL	CA-CB2	2.61	1.53	1.48
2	A	256	BBL	CA-N	-2.29	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	256	BBL	CBZ-CA-CB2	-7.05	105.32	108.46
2	A	256	BBL	CBZ-CA-N	-4.93	102.74	110.24
2	A	256	BBL	CA-N-C	2.12	127.13	121.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.