



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:27 pm BST

PDB ID : 1BTU
Title : PORCINE PANCREATIC ELASTASE COMPLEXED WITH (3S, 4R)-1-T
OLUENESULPHONYL-3-ETHYL-AZETIDIN-2-ONE-4-CARBOXYLIC
ACID
Authors : Wilmouth, R.C.; Clifton, I.J.; Schofield, C.J.
Deposited on : 1998-09-01
Resolution : 1.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.11

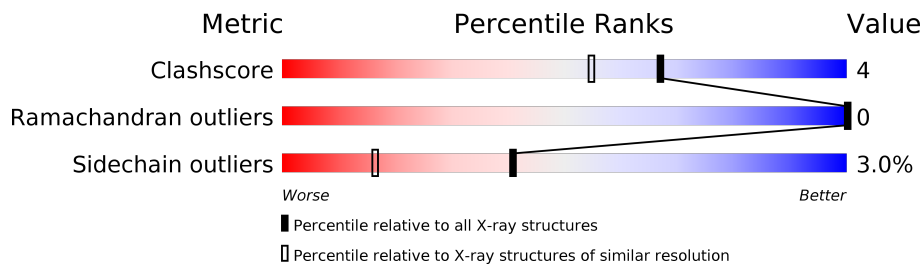
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 $\leq 5\%$.

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 2054 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 ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1822	1135	330	347	10	0	0	0

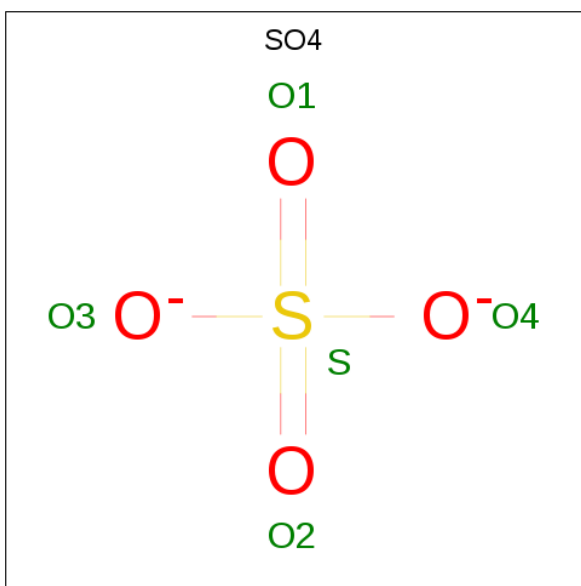
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

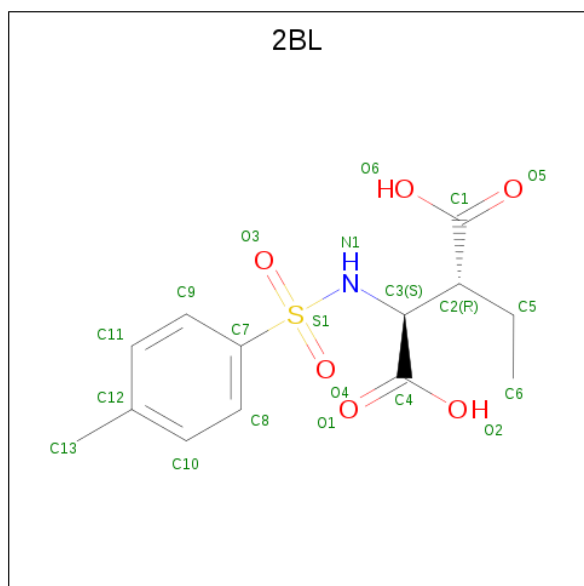
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is (3R)-3-ethyl-N-[(4-methylphenyl)sulfonyl]-L-aspartic acid (three-letter code: 2BL) (formula: C₁₃H₁₇NO₆S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	S	0	0
			20	13	1	5	1		

- Molecule 5 is water.

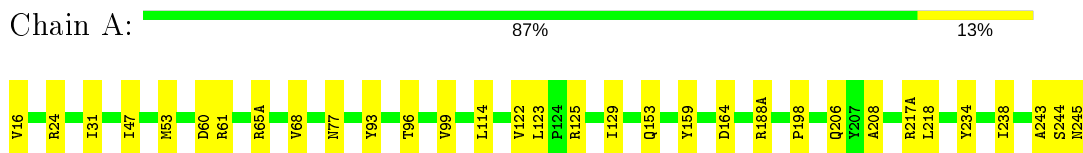
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		

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: ELASTASE



4 Data and refinement statistics

Xtrriage (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	50.57Å 57.93Å 74.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.80 – 1.60	Depositor
% Data completeness (in resolution range)	98.7 (23.80-1.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97, X-PLOR	Depositor
R, R_{free}	0.192 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2054	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: CA, 2BL, 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	1/1862 (0.1%)	1.25	14/2543 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ASN	C-OXT	18.40	1.58	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TYR	CB-CG-CD2	8.88	126.33	121.00
1	A	234	TYR	CG-CD2-CE2	8.58	128.16	121.30
1	A	164	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	188(A)	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	206	GLN	CA-CB-CG	6.45	127.58	113.40
1	A	159	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	A	217(A)	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	65(A)	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	A	217(A)	ARG	CD-NE-CZ	5.53	131.34	123.60
1	A	188(A)	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	A	188(A)	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	234	TYR	CZ-CE2-CD2	-5.27	115.06	119.80
1	A	65(A)	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	61	ARG	CD-NE-CZ	5.09	130.72	123.60

There are no chirality outliers.

There are no planarity outliers.

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	14	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	20	0	15	0	0
5	A	206	0	0	6	0
All	All	2054	0	1773	14	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 4.

All (14) 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:47:ILE:HG21	1:A:53:MET:HE3	1.75	0.69
1:A:198:PRO:HG3	5:A:465:HOH:O	2.07	0.55
1:A:218:LEU:HD21	5:A:497:HOH:O	2.07	0.55
1:A:244:SER:HB3	5:A:456:HOH:O	2.14	0.48
1:A:24:ARG:HH12	1:A:77:ASN:HD22	1.64	0.46
1:A:243:ALA:HB3	5:A:456:HOH:O	2.17	0.45
1:A:47:ILE:HD13	1:A:53:MET:CE	2.48	0.44
1:A:153:GLN:NE2	5:A:458:HOH:O	2.51	0.43
1:A:122:VAL:CG2	1:A:208:ALA:HA	2.49	0.43
1:A:99:VAL:HB	5:A:476:HOH:O	2.19	0.42
1:A:53:MET:HE1	1:A:238:ILE:HD13	2.03	0.41
1:A:31:ILE:HG22	1:A:68:VAL:HG12	2.03	0.41
1:A:24:ARG:HH12	1:A:77:ASN:ND2	2.18	0.41
1:A:60:ASP:CG	1:A:96:THR:HG1	2.25	0.40

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	238/240 (99%)	231 (97%)	7 (3%)	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	A	198/198 (100%)	192 (97%)	6 (3%)	41	16

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

Mol	Chain	Res	Type
1	A	16	VAL
1	A	93	TYR
1	A	114	LEU
1	A	123	LEU
1	A	125	ARG
1	A	129	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	153	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
3	SO4	A	270	-	4,4,4	0.57	0	6,6,6	0.44	0
4	2BL	A	7	1	17,20,21	2.16	7 (41%)	21,28,30	3.07	10 (47%)

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	2BL	A	7	1	-	5/19/23/25	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7	2BL	O6-C1	-5.06	1.21	1.42
4	A	7	2BL	C7-S1	-3.13	1.71	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7	2BL	C11-C9	2.93	1.44	1.38
4	A	7	2BL	C10-C8	2.91	1.44	1.38
4	A	7	2BL	O4-S1	2.69	1.46	1.43
4	A	7	2BL	S1-N1	2.53	1.66	1.61
4	A	7	2BL	C9-C7	-2.43	1.35	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7	2BL	O6-C1-C2	6.21	125.60	111.36
4	A	7	2BL	C8-C10-C12	-5.47	114.05	121.38
4	A	7	2BL	C8-C7-S1	-4.65	114.71	119.77
4	A	7	2BL	C9-C7-C8	4.20	126.30	120.44
4	A	7	2BL	C11-C12-C10	4.19	127.29	118.11
4	A	7	2BL	O4-S1-O3	-4.17	114.42	119.55
4	A	7	2BL	C9-C11-C12	-3.55	116.62	121.38
4	A	7	2BL	O4-S1-C7	3.25	111.97	107.97
4	A	7	2BL	O3-S1-C7	3.21	111.92	107.97
4	A	7	2BL	C11-C9-C7	-2.44	116.92	119.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

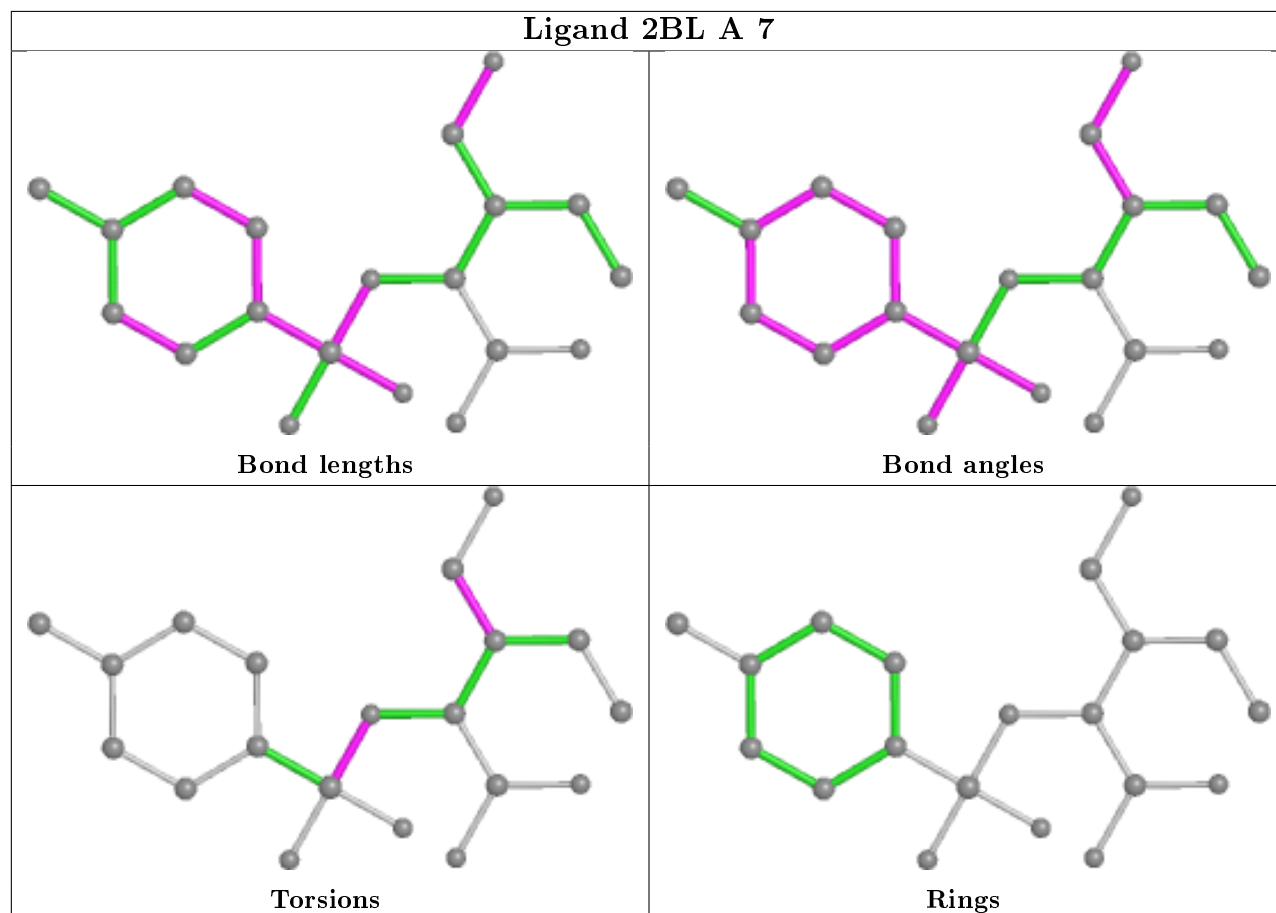
Mol	Chain	Res	Type	Atoms
4	A	7	2BL	O6-C1-C2-C3
4	A	7	2BL	O6-C1-C2-C5
4	A	7	2BL	C3-N1-S1-O3
4	A	7	2BL	C3-N1-S1-O4
4	A	7	2BL	C3-N1-S1-C7

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 than 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.



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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.