

Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 02:05 AM EDT

PDB ID : 1FNI

Title : CRYSTAL STRUCTURE OF PORCINE BETA TRYPSIN WITH 0.01%

POLYDOCANOL

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Deposited on : 2000-08-22

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 (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)

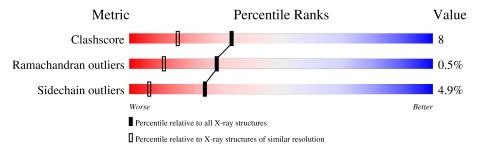
Validation Pipeline (wwPDB-VP) : 2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\AA))$
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 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.

Mo	Chain	Length	Quality of chain		
1	A	223	84%	13%	. .



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1822 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.

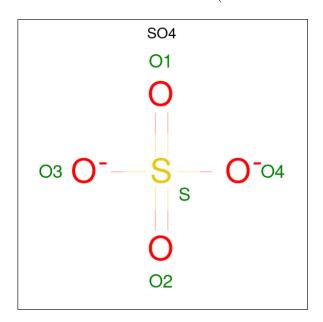
• Molecule 1 is a protein called TRYPSIN.

Mo	ol (Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1		A	223	Total 1642	C 1020	N 289	O 319	S 14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ASN	ASP	SEE REMARK 999	UNP P00761
A	186	GLN	GLU	SEE REMARK 999	UNP P00761

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



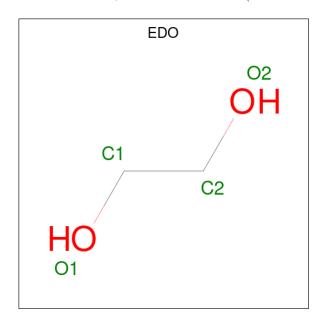
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

• 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

 \bullet Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	158	Total O 158 158	0	0

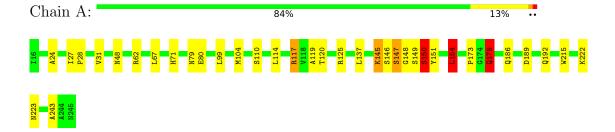


3 Residue-property plots (i)

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: TRYPSIN





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	77.80Å 53.95Å 47.20Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 1.60	Depositor	
% Data completeness	82.6 (8.00-1.60)	Depositor	
(in resolution range)	02.0 (0.00 1.00)	Depositor	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR, REFMAC	Depositor	
R, R_{free}	0.183 , 0.233	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1822	wwPDB-VP	
Average B, all atoms (Å ²)	25.0	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, EDO, 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).

Mal	Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.58	0/1674	1.25	$13/2273 \ (0.6\%)$	

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	125	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	125	ARG	CD-NE-CZ	9.63	137.08	123.60
1	A	125	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	80	GLU	OE1-CD-OE2	-7.39	114.43	123.30
1	A	117	ARG	CD-NE-CZ	6.46	132.64	123.60
1	A	117	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	175	GLN	CA-CB-CG	-5.73	100.80	113.40
1	A	62	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	151	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	154	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	104	MET	CG-SD-CE	5.20	108.53	100.20
1	A	80	GLU	CG-CD-OE1	5.12	128.55	118.30
1	A	189	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1642	0	1605	22	0
2	A	5	0	0	1	0
3	A	1	0	0	0	0
4	A	16	0	24	4	0
5	A	158	0	0	3	0
All	All	1822	0	1629	23	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 8.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)	
1:A:145:LYS:HE2	1:A:147:SER:H	1.46	0.80	
4:A:426:EDO:H22	5:A:482:HOH:O	1.95	0.66	
1:A:99:LEU:HD22	1:A:215:TRP:HB3	1.82	0.61	
1:A:149:SER:O	1:A:150:SER:HB3	2.00	0.60	
1:A:28:PRO:HG3	4:A:425:EDO:H11	1.87	0.56	
1:A:148:GLY:O	1:A:149:SER:HB3	2.07	0.55	
1:A:31:VAL:HG12	1:A:67:LEU:HD23	1.90	0.54	
1:A:24:ALA:HB2	1:A:71:HIS:CD2	2.41	0.54	
1:A:175:GLN:CD	5:A:546:HOH:O	2.45	0.54	
1:A:154:LEU:HD12	5:A:516:HOH:O	2.07	0.53	
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.74	0.52	
1:A:149:SER:O	1:A:150:SER:CB	2.61	0.49	
1:A:145:LYS:NZ	1:A:147:SER:HB2	2.29	0.47	
1:A:48:ASN:HA	1:A:120:THR:HG21	1.98	0.46	
1:A:145:LYS:CE	1:A:147:SER:H	2.23	0.44	
1:A:192:GLN:HG3	2:A:422:SO4:O3	2.19	0.43	
1:A:222:LYS:HG2	1:A:223:ASN:ND2	2.34	0.42	
1:A:222:LYS:HG2	1:A:223:ASN:HD22	1.83	0.42	
1:A:119:ALA:HB1	4:A:425:EDO:H22	2.02	0.42	
1:A:173:PRO:O	1:A:175:GLN:NE2	2.52	0.41	
1:A:243:ALA:HA	4:A:427:EDO:H12	2.01	0.41	
1:A:27:ILE:CD1	1:A:137:LEU:HD21	2.51	0.41	
1:A:79:ASN:ND2	1:A:117:ARG:HD2	2.36	0.41	

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	221/223 (99%)	213 (96%)	7 (3%)	1 (0%)	29 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	\mathbf{Type}	
1	A	150	SER	

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	183/183 (100%)	174 (95%)	9 (5%)	25 6		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	SER
1	A	114	LEU
1	A	145	LYS
1	A	146	SER
1	A	147	SER
1	A	150	SER
1	A	154	LEU
1	A	175	GLN
1	A	186	GLN



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	79	ASN
1	A	84	ASN
1	A	93	ASN
1	A	101	ASN
1	A	210	GLN
1	A	221	GLN
1	A	223	ASN
1	A	236	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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	Tuno	Chain	Res	Link	В	ond leng	gths	В	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	422	-	4,4,4	0.73	0	6,6,6	0.35	0
4	EDO	A	424	-	3,3,3	0.75	0	2,2,2	0.54	0
4	EDO	A	425	-	3,3,3	0.55	0	2,2,2	0.38	0



Mol	T	Chain	Dag	Timle	В	ond leng	${ m gths}$	В	ond ang	gles
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	426	-	3,3,3	0.45	0	2,2,2	0.20	0
4	EDO	A	427	-	3,3,3	0.57	0	2,2,2	0.38	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	EDO	A	425	-	-	0/1/1/1	-
4	EDO	A	427	-	-	1/1/1/1	-
4	EDO	A	426	-	-	1/1/1/1	-
4	EDO	A	424	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	424	EDO	O1-C1-C2-O2
4	A	426	EDO	O1-C1-C2-O2
4	A	427	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	422	SO4	1	0
4	A	425	EDO	2	0
4	A	426	EDO	1	0
4	A	427	EDO	1	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 (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.

