



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:16 am BST

PDB ID : 1FMG  
Title : CRYSTAL STRUCTURE OF PORCINE BETA TRYPSIN WITH 0.04% POLYDOCANOL  
Authors : Deepthi, S.; Johnson, A.; Pattabhi, V.  
Deposited on : 2000-08-17  
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

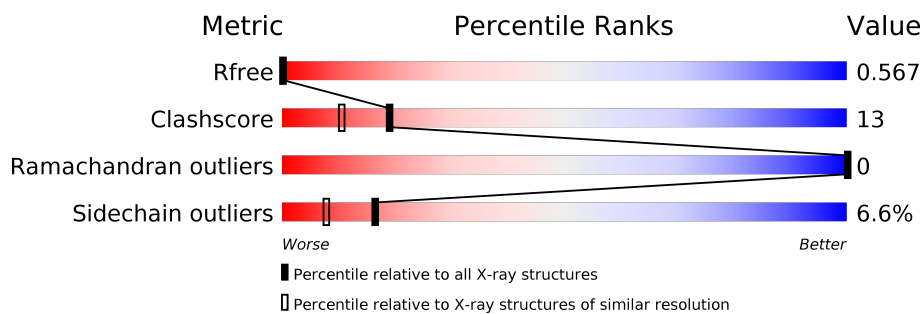
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 21%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>76% 21% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	434	-	-	X	-
4	EDO	A	438	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1842 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.

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

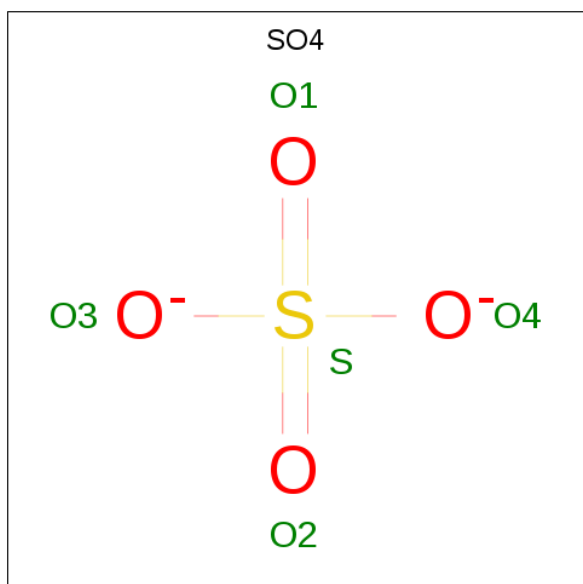
There are 2 discrepancies between the modelled and reference sequences:

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

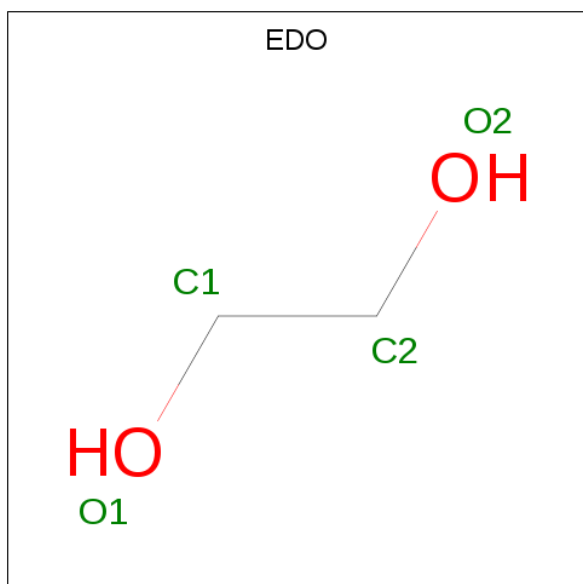
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

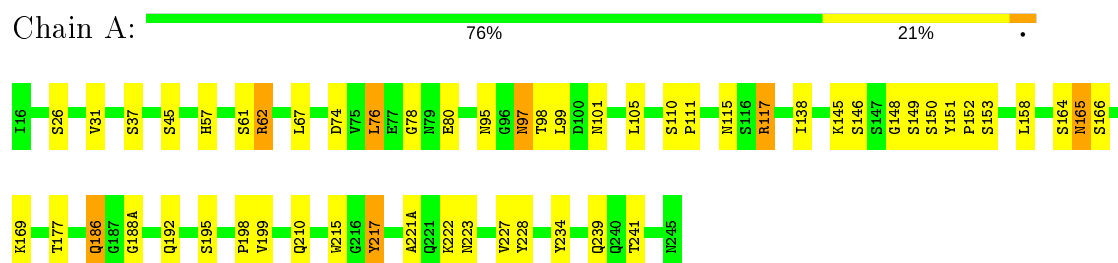
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		

### 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.

- Molecule 1: TRYPSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.95Å 54.16Å 47.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 44.47 – 1.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (8.00-1.90) 22.5 (44.47-1.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.36 (at 1.20Å)	Xtriage
Refinement program	X-PLOR, REFMAC	Depositor
R, $R_{free}$	0.158 , 0.234 0.573 , 0.567	Depositor DCC
$R_{free}$ test set	1240 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.6	Xtriage
Anisotropy	2.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 920.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.47	EDS
Total number of atoms	1842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, EDO

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	0.63	0/1674	1.20	6/2273 (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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	217	TYR	CB-CG-CD1	-11.03	114.38	121.00
1	A	217	TYR	CB-CG-CD2	10.07	127.05	121.00
1	A	164	SER	N-CA-CB	7.54	121.82	110.50
1	A	117	ARG	CA-CB-CG	6.42	127.53	113.40
1	A	164	SER	CB-CA-C	-6.08	98.55	110.10
1	A	117	ARG	CB-CG-CD	5.82	126.74	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLY	Peptide

## 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	1642	0	1599	41	2
2	A	1	0	0	0	0
3	A	5	0	0	3	0
4	A	20	0	30	7	0
5	A	174	0	0	12	2
All	All	1842	0	1629	43	4

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 13.

All (43) 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:195:SER:OG	5:A:573:HOH:O	1.81	0.97
1:A:215:TRP:CE2	1:A:227:VAL:HG21	2.02	0.94
1:A:98:THR:HG1	4:A:438:EDO:HO1	0.96	0.90
1:A:78:GLY:HA2	5:A:532:HOH:O	1.77	0.83
3:A:434:SO4:O3	5:A:588:HOH:O	2.02	0.78
1:A:115:ASN:HB2	4:A:437:EDO:H12	1.64	0.77
1:A:215:TRP:NE1	1:A:227:VAL:HG21	2.01	0.75
1:A:62:ARG:O	1:A:62:ARG:HG3	1.89	0.73
1:A:37:SER:HA	1:A:62:ARG:NH2	2.05	0.72
1:A:31:VAL:HG12	1:A:67:LEU:HD23	1.73	0.71
1:A:97:ASN:HD22	1:A:97:ASN:C	1.93	0.70
1:A:177:THR:HG21	4:A:438:EDO:H22	1.77	0.66
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.77	0.66
1:A:74:ASP:OD2	1:A:153:SER:HB3	1.98	0.62
1:A:62:ARG:HD2	5:A:574:HOH:O	2.01	0.60
1:A:215:TRP:CD1	1:A:227:VAL:CG2	2.85	0.60
1:A:95:ASN:ND2	4:A:438:EDO:O1	2.34	0.60
1:A:177:THR:CG2	4:A:438:EDO:H22	2.37	0.53
1:A:188(A):GLY:HA2	5:A:597:HOH:O	2.08	0.52
1:A:31:VAL:CG1	1:A:67:LEU:HD23	2.39	0.52
1:A:138:ILE:HG12	1:A:199:VAL:HG22	1.91	0.52
1:A:61:SER:H	4:A:435:EDO:H12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TRP:NE1	1:A:227:VAL:CG2	2.72	0.51
1:A:76:LEU:HD13	1:A:80:GLU:OE2	2.11	0.50
1:A:62:ARG:CD	5:A:574:HOH:O	2.59	0.50
1:A:221(A):ALA:HA	5:A:519:HOH:O	2.11	0.50
1:A:97:ASN:ND2	1:A:97:ASN:C	2.64	0.48
1:A:101:ASN:ND2	1:A:234:TYR:OH	2.46	0.47
1:A:105:LEU:HD12	1:A:241:THR:HG21	1.95	0.47
1:A:215:TRP:CD1	1:A:227:VAL:HG21	2.50	0.47
4:A:439:EDO:H22	5:A:468:HOH:O	2.15	0.46
1:A:45:SER:OG	1:A:198:PRO:HB3	2.16	0.46
1:A:98:THR:O	1:A:99:LEU:HB2	2.16	0.46
1:A:57:HIS:CE1	5:A:573:HOH:O	2.69	0.45
1:A:222:LYS:HG2	1:A:223:ASN:ND2	2.32	0.44
1:A:165:ASN:O	1:A:169:LYS:HG3	2.16	0.44
1:A:151:TYR:HA	1:A:152:PRO:HD3	1.83	0.43
1:A:195:SER:OG	3:A:434:SO4:O2	2.28	0.43
1:A:192:GLN:HG3	3:A:434:SO4:O3	2.19	0.42
1:A:210:GLN:NE2	5:A:482:HOH:O	2.49	0.42
1:A:26:SER:HB2	5:A:525:HOH:O	2.20	0.41
1:A:217:TYR:HB2	5:A:591:HOH:O	2.21	0.41
1:A:199:VAL:HG21	1:A:228:TYR:CD2	2.57	0.40

All (4) 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:217:TYR:CE1	1:A:239:GLN:NE2[3_645]	1.95	0.25
5:A:597:HOH:O	5:A:600:HOH:O[2_565]	1.98	0.22
1:A:153:SER:N	1:A:186:GLN:NE2[2_564]	2.05	0.15
5:A:473:HOH:O	5:A:569:HOH:O[2_564]	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	221/223 (99%)	213 (96%)	8 (4%)	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	183/183 (100%)	171 (93%)	12 (7%)	16	8

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	76	LEU
1	A	97	ASN
1	A	117	ARG
1	A	145	LYS
1	A	146	SER
1	A	149	SER
1	A	150	SER
1	A	158	LEU
1	A	165	ASN
1	A	166	SER
1	A	186	GLN

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

Mol	Chain	Res	Type
1	A	84	ASN
1	A	95	ASN
1	A	97	ASN
1	A	101	ASN
1	A	186	GLN

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Mol	Chain	Res	Type
1	A	192	GLN
1	A	210	GLN
1	A	223	ASN
1	A	236	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	434	-	4,4,4	0.66	0	6,6,6	0.13	0
4	EDO	A	436	-	3,3,3	0.49	0	2,2,2	0.15	0
4	EDO	A	438	1	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	A	439	-	3,3,3	0.54	0	2,2,2	0.28	0
4	EDO	A	437	-	3,3,3	0.54	0	2,2,2	0.29	0
4	EDO	A	435	1	3,3,3	0.49	0	2,2,2	0.29	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	438	1	-	1/1/1/1	-
4	EDO	A	436	-	-	1/1/1/1	-
4	EDO	A	439	-	-	1/1/1/1	-
4	EDO	A	437	-	-	1/1/1/1	-
4	EDO	A	435	1	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	438	EDO	O1-C1-C2-O2
4	A	439	EDO	O1-C1-C2-O2
4	A	436	EDO	O1-C1-C2-O2
4	A	437	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	434	SO4	3	0
4	A	438	EDO	4	0
4	A	439	EDO	1	0
4	A	437	EDO	1	0
4	A	435	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.