

# Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 05:30 am BST

PDB ID : 1TNH

Title : PREDICTION OF NOVEL SERINE PROTEASE INHIBITORS

Authors: Kurinov, I.; Harrison, R.W.

Deposited on : 1994-07-21

Resolution : 1.80 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 following versions of software and data (see references (1)) 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)

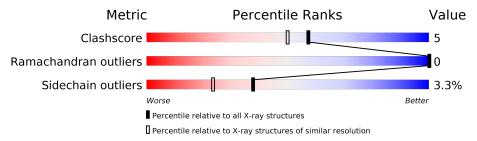
Validation Pipeline (wwPDB-VP) : 2.11

# 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 1.80 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	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$		
Clashscore	141614	6793 (1.80-1.80)		
Ramachandran outliers	138981	6697 (1.80-1.80)		
Sidechain outliers	138945	6696 (1.80-1.80)		

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	229	84%	11%	



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2513 atoms, of which 711 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.

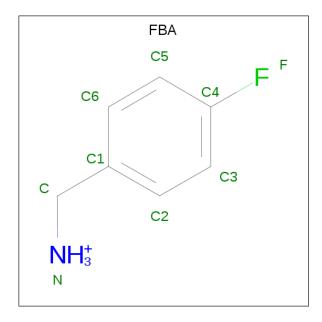
• Molecule 1 is a protein called TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Λ	223	Total	С	Н	N	О	S	0	0	0
1	A	223	2011	1012	382	279	324	14	U	U	

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

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

• Molecule 3 is 4-FLUOROBENZYLAMINE (three-letter code: FBA) (formula: C<sub>7</sub>H<sub>9</sub>FN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 12	C 7	F 1	H 3	N 1	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	163	Total 489	H 326	O 163	0	0

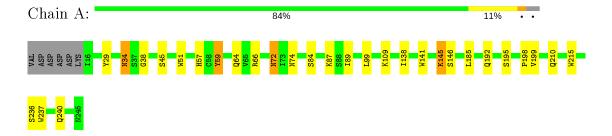


# 3 Residue-property plots (i)

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: 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	54.96Å 58.44Å 67.56Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	7.00 - 1.80	Depositor	
% Data completeness	(Not available) (7.00-1.80)	Depositor	
(in resolution range)	, , , , , , , , , , , , , , , , , , , ,		
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.168 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2513	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	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, FBA

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	Bond	lengths	Bond angles		
MIGI		RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.75	0/1660	1.42	$16/2250 \ (0.7\%)$	

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 maintain 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 (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	141	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	A	141	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	A	59	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	A	51	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	A	215	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	A	215	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	51	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	237	TRP	CD1-CG-CD2	6.41	111.43	106.30
1	A	237	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	A	141	TRP	CB-CG-CD1	-5.88	119.35	127.00
1	A	237	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	A	141	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	215	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	210	GLN	CG-CD-NE2	5.07	128.87	116.70
1	A	29	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	57	HIS	CA-CB-CG	5.04	122.17	113.60



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Chain Res		Group	
1	A	59	TYR	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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1629	382	1588	15	0
2	A	1	0	0	0	0
3	A	9	3	9	0	0
4	A	163	326	0	1	0
All	All	1802	711	1597	15	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 (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance} \ ( ext{\AA}) \end{array}$	Clash overlap (Å)
1:A:72:ASN:HD22	1:A:74:ASN:H	1.34	0.75
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.44	0.64
1:A:64:GLN:NE2	1:A:66:ARG:HE	1.97	0.62
1:A:145:LYS:HE2	1:A:146:SER:H	1.66	0.60
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.50	0.58
1:A:87:LYS:HD3	1:A:89:ILE:HD11	1.86	0.57
1:A:138:ILE:HG12	1:A:199:VAL:HG22	1.85	0.57
1:A:145:LYS:HE2	1:A:146:SER:N	2.21	0.56
1:A:34:ASN:ND2	1:A:38:GLY:H	2.06	0.53
1:A:72:ASN:ND2	1:A:74:ASN:H	2.05	0.53
1:A:195:SER:HB2	4:A:361:HOH:O	2.10	0.50
1:A:45:SER:OG	1:A:198:PRO:HB3	2.12	0.49
1:A:72:ASN:HD22	1:A:74:ASN:N	2.08	0.49
1:A:84:SER:HB3	1:A:109:LYS:HD2	1.95	0.48
1:A:236:SER:O	1:A:240:GLN:HG2	2.21	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	Perce	ntiles
1	A	221/229 (96%)	216 (98%)	5 (2%)	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	184/190 (97%)	178 (97%)	6 (3%)	38 23		

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

Mol	Chain	Res	Type
1	A	34	ASN
1	A	72	ASN
1	A	99	LEU
1	A	145	LYS
1	A	185	LEU
1	A	192	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	$\operatorname{Res}$	Type
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	72	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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Типо	Chain	Pos	Link	Bond lengths			Bond angles		
10101	туре	Chain	res		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FBA	A	900	-	9,9,9	0.67	0	11,11,11	0.75	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
3	FBA	A	900	_	_	0/2/2/2	0/1/1/1



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

