



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:12 PM UTC

PDB ID : 1TNI / pdb_00001tni
Title : PREDICTION OF NOVEL SERINE PROTEASE INHIBITORS
Authors : Kurinov, I.; Harrison, R.W.
Deposited on : 1994-07-21
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

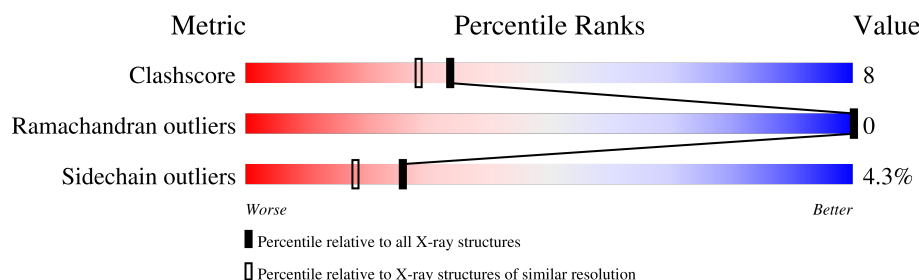
1 Overall quality at a glance

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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	

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	PBN	A	900	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2515 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.

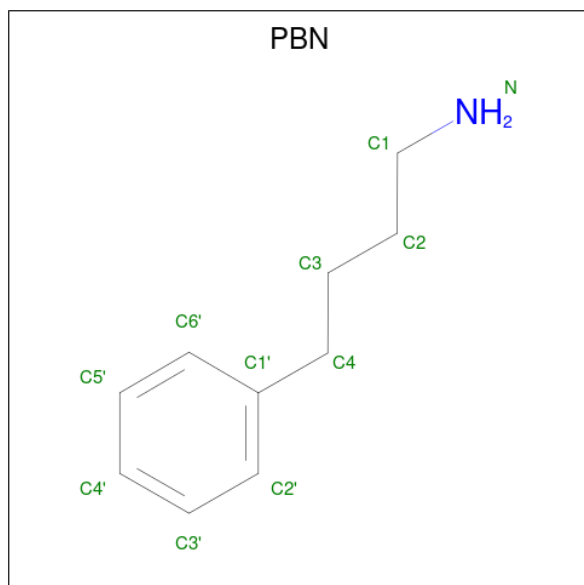
- Molecule 1 is a protein called TRYPSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	S	0	0	0
			2011	1012	382	279	324	14			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 4-PHENYLBUTYLAMINE (CCD ID: PBN) (formula: C₁₀H₁₅N).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			14	10	3	1		

- Molecule 4 is water.

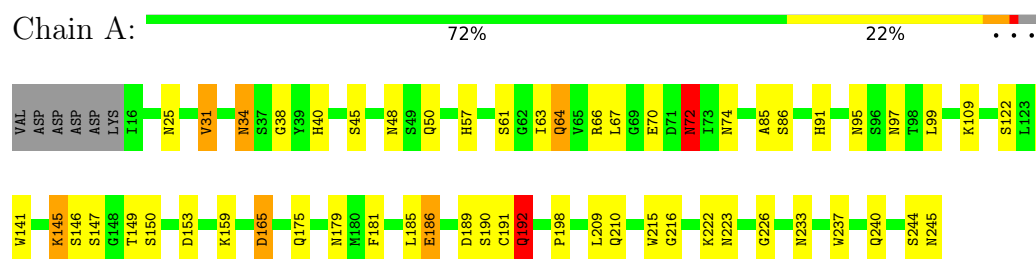
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	163	Total	H	O	0	0
			489	326	163		

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

Xtriage (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	54.85Å 58.55Å 67.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.02	5/1660 (0.3%)	1.84	42/2250 (1.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	57	HIS	CG-ND1	-6.01	1.31	1.38
1	A	57	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	40	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	63	ILE	CA-CB	5.26	1.60	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLN	OE1-CD-NE2	-11.86	110.75	122.60
1	A	72	ASN	OD1-CG-ND2	-9.98	112.62	122.60
1	A	165	ASP	CA-CB-CG	-9.33	103.27	112.60
1	A	210	GLN	CG-CD-NE2	8.53	129.19	116.40
1	A	64	GLN	OE1-CD-NE2	-8.09	114.51	122.60
1	A	50	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	A	223	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	A	175	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	A	165	ASP	N-CA-C	7.52	120.43	111.33
1	A	50	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	149	THR	N-CA-C	6.86	120.35	108.76
1	A	72	ASN	CB-CG-ND2	6.77	126.56	116.40
1	A	240	GLN	N-CA-CB	-6.68	100.30	110.12
1	A	189	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	190	SER	O-C-N	-6.58	114.55	122.65
1	A	244	SER	N-CA-C	6.43	121.91	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	95	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	245	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	240	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	A	240	GLN	CA-CB-CG	6.13	126.36	114.10
1	A	149	THR	CA-C-O	6.07	127.06	120.32
1	A	186	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	57	HIS	CA-CB-CG	5.92	119.72	113.80
1	A	175	GLN	CG-CD-NE2	5.83	125.15	116.40
1	A	70	GLU	N-CA-C	5.77	119.31	110.20
1	A	237	TRP	CG-CD2-CE3	5.76	139.66	133.90
1	A	192	GLN	CA-CB-CG	5.73	125.56	114.10
1	A	181	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	215	TRP	N-CA-C	5.52	115.83	108.38
1	A	122	SER	CB-CA-C	-5.50	100.24	109.65
1	A	141	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	A	97	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	48	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	34	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	141	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	85	ALA	O-C-N	-5.32	116.73	123.01
1	A	233	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	223	ASN	CB-CG-ND2	5.19	124.19	116.40
1	A	135	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	61	SER	O-C-N	-5.04	117.29	122.94
1	A	179	ASN	OD1-CG-ND2	-5.00	117.59	122.60

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	1629	382	1588	23	0
2	A	1	0	0	0	0
3	A	11	3	15	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	163	326	0	3	0
All	All	1804	711	1603	24	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 8.

All (24) 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:226:GLY:HA2	3:A:900:PBN:H11	1.62	0.81
1:A:216:GLY:HA3	3:A:900:PBN:H12	1.63	0.80
1:A:72:ASN:HD22	1:A:74:ASN:H	1.42	0.66
3:A:900:PBN:H3'	4:A:269:HOH:O	2.00	0.62
1:A:192:GLN:N	3:A:900:PBN:H6'	2.17	0.60
1:A:64:GLN:NE2	1:A:66:ARG:HE	1.99	0.59
1:A:45:SER:OG	1:A:198:PRO:HB3	2.03	0.58
1:A:34:ASN:ND2	1:A:38:GLY:H	2.02	0.57
1:A:186:GLU:CD	1:A:222:LYS:HZ2	2.17	0.53
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.62	0.47
1:A:86:SER:HB3	1:A:109:LYS:HG2	1.96	0.46
1:A:124:PRO:HD3	1:A:209:LEU:O	2.15	0.46
1:A:72:ASN:ND2	1:A:74:ASN:H	2.13	0.45
1:A:186:GLU:HB2	4:A:299:HOH:O	2.17	0.45
1:A:136:CYS:O	1:A:159:LYS:HA	2.17	0.45
1:A:145:LYS:NZ	1:A:147:SER:OG	2.50	0.44
1:A:145:LYS:HE3	4:A:302:HOH:O	2.18	0.43
1:A:186:GLU:HA	1:A:222:LYS:HG3	2.00	0.43
1:A:145:LYS:HD3	1:A:147:SER:O	2.20	0.42
1:A:226:GLY:CA	3:A:900:PBN:H11	2.42	0.42
1:A:145:LYS:HE2	1:A:146:SER:N	2.35	0.41
1:A:191:CYS:C	3:A:900:PBN:H6'	2.45	0.41
1:A:31:VAL:HG12	1:A:67:LEU:HD23	2.03	0.41
1:A:72:ASN:HA	1:A:153:ASP:O	2.22	0.40

There are no symmetry-related clashes.

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	221/229 (96%)	216 (98%)	5 (2%)	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	184/190 (97%)	176 (96%)	8 (4%)	26	18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	72	ASN
1	A	99	LEU
1	A	145	LYS
1	A	150	SER
1	A	165	ASP
1	A	185	LEU
1	A	192	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	72	ASN
1	A	192	GLN
1	A	221	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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PBN	A	900	-	11,11,11	0.40	0	12,12,12	1.11	1 (8%)

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	PBN	A	900	-	-	3/5/5/5	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	PBN	C4'-C3'-C2'	2.11	122.84	120.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	PBN	C1-C2-C3-C4
3	A	900	PBN	C6'-C1'-C4-C3
3	A	900	PBN	C2'-C1'-C4-C3

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	PBN	6	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

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.