



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 1AZ8 / pdb_00001az8
Title : BOVINE TRYPSIN COMPLEXED TO BIS-PHENYLAMIDINE INHIBITOR
Authors : Alexander, R.; Smallwood, A.
Deposited on : 1997-11-26
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 ⓘ 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

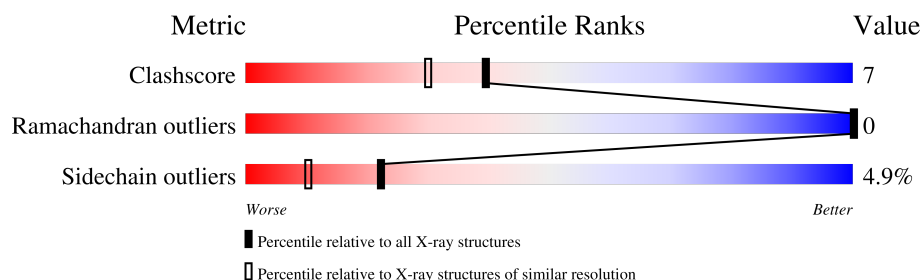
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 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	223	 79% 19% .

2 Entry composition [i](#)

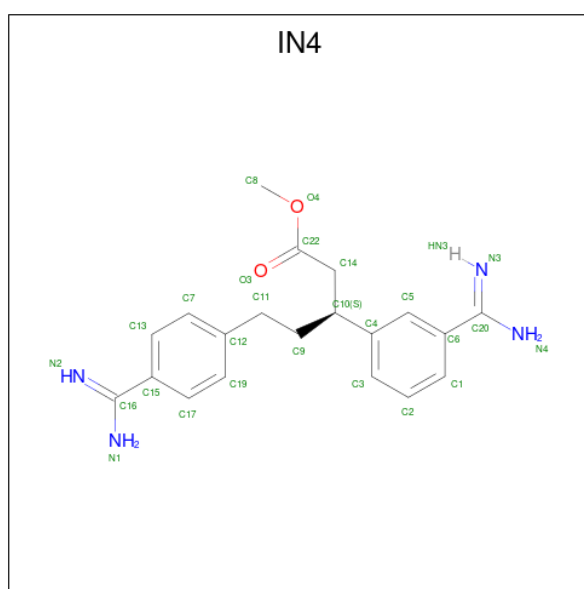
There are 3 unique types of molecules in this entry. The entry contains 1724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is +/-METHYL 4-(AMINOIMINOMETHYL)-BETA-[3- INH (AMINOIMINO) PHENYL]BENZENE PENTANOATE (CCD ID: IN4) (formula: C₂₀H₂₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total	0	0
			69		

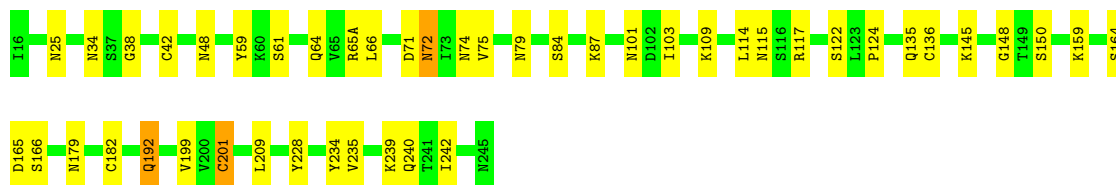
3 Residue-property plots

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

Chain A:  79% 19%



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	54.80Å 58.70Å 67.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	90.0 (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1724	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: IN4

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	1.00	8/1660 (0.5%)	0.90	7/2250 (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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	CYS	CA-C	-6.47	1.44	1.52
1	A	114	LEU	CA-C	-6.16	1.45	1.52
1	A	75	VAL	CA-CB	5.68	1.61	1.54
1	A	103	ILE	CA-CB	5.61	1.61	1.55
1	A	242	ILE	CA-CB	5.59	1.61	1.54
1	A	182	CYS	CA-C	-5.23	1.46	1.52
1	A	42	CYS	CA-C	-5.22	1.46	1.52
1	A	164	SER	CA-C	-5.15	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CA-CB-CG	-9.15	103.45	112.60
1	A	192	GLN	CB-CG-CD	-8.58	98.01	112.60
1	A	71	ASP	CA-CB-CG	-7.16	105.44	112.60
1	A	48	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	179	ASN	CA-CB-CG	-6.29	106.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASN	CA-CB-CG	-6.03	106.57	112.60
1	A	115	ASN	CA-CB-CG	-5.66	106.94	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	TYR	Sidechain

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	0	1588	18	0
2	A	26	0	22	0	0
3	A	69	0	0	0	0
All	All	1724	0	1610	18	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 7.

All (18) 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:72:ASN:HD22	1:A:74:ASN:H	1.30	0.77
1:A:64:GLN:HE21	1:A:65(A):ARG:HE	1.45	0.64
1:A:84:SER:HB2	1:A:109:LYS:HD2	1.80	0.64
1:A:72:ASN:ND2	1:A:74:ASN:H	1.98	0.61
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	2.01	0.59
1:A:145:LYS:HE2	1:A:150:SER:HB3	1.85	0.58
1:A:25:ASN:HD22	1:A:117:ARG:HH21	1.53	0.55
1:A:64:GLN:HE22	1:A:65(A):ARG:HH21	1.53	0.55
1:A:235:VAL:HG12	1:A:239:LYS:HD2	1.90	0.53
1:A:34:ASN:ND2	1:A:38:GLY:H	2.07	0.52
1:A:66:LEU:N	1:A:66:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:CYS:O	1:A:159:LYS:HA	2.17	0.45
1:A:199:VAL:HG21	1:A:228:TYR:CD1	2.53	0.43
1:A:25:ASN:HD22	1:A:117:ARG:NH2	2.15	0.43
1:A:101:ASN:HA	1:A:234:TYR:OH	2.19	0.43
1:A:72:ASN:HD22	1:A:72:ASN:C	2.28	0.42
1:A:145:LYS:HB2	1:A:148:GLY:O	2.21	0.41
1:A:124:PRO:HD3	1:A:209:LEU:O	2.21	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	221/223 (99%)	217 (98%)	4 (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	184/184 (100%)	175 (95%)	9 (5%)	22	10

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

Mol	Chain	Res	Type
1	A	61	SER
1	A	72	ASN
1	A	87	LYS
1	A	122	SER
1	A	135	GLN
1	A	166	SER
1	A	192	GLN
1	A	201	CYS
1	A	240	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	25	ASN
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	72	ASN
1	A	223	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	IN4	A	1	-	27,27,27	1.22	2 (7%)	29,36,36	1.41	4 (13%)

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
2	IN4	A	1	-	-	10/23/23/23	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	IN4	C4-C10	-2.97	1.46	1.52
2	A	1	IN4	C15-C16	2.96	1.52	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	IN4	O4-C22-C14	2.98	117.90	111.47
2	A	1	IN4	C8-O4-C22	2.94	125.49	116.07
2	A	1	IN4	C15-C16-N1	2.77	122.21	118.01
2	A	1	IN4	C5-C4-C10	-2.28	115.23	120.88

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	IN4	N4-C20-C6-C1
2	A	1	IN4	N4-C20-C6-C5
2	A	1	IN4	C13-C15-C16-N1
2	A	1	IN4	C17-C15-C16-N1
2	A	1	IN4	C14-C10-C4-C3
2	A	1	IN4	N3-C20-C6-C1
2	A	1	IN4	N3-C20-C6-C5
2	A	1	IN4	C13-C15-C16-N2
2	A	1	IN4	C17-C15-C16-N2

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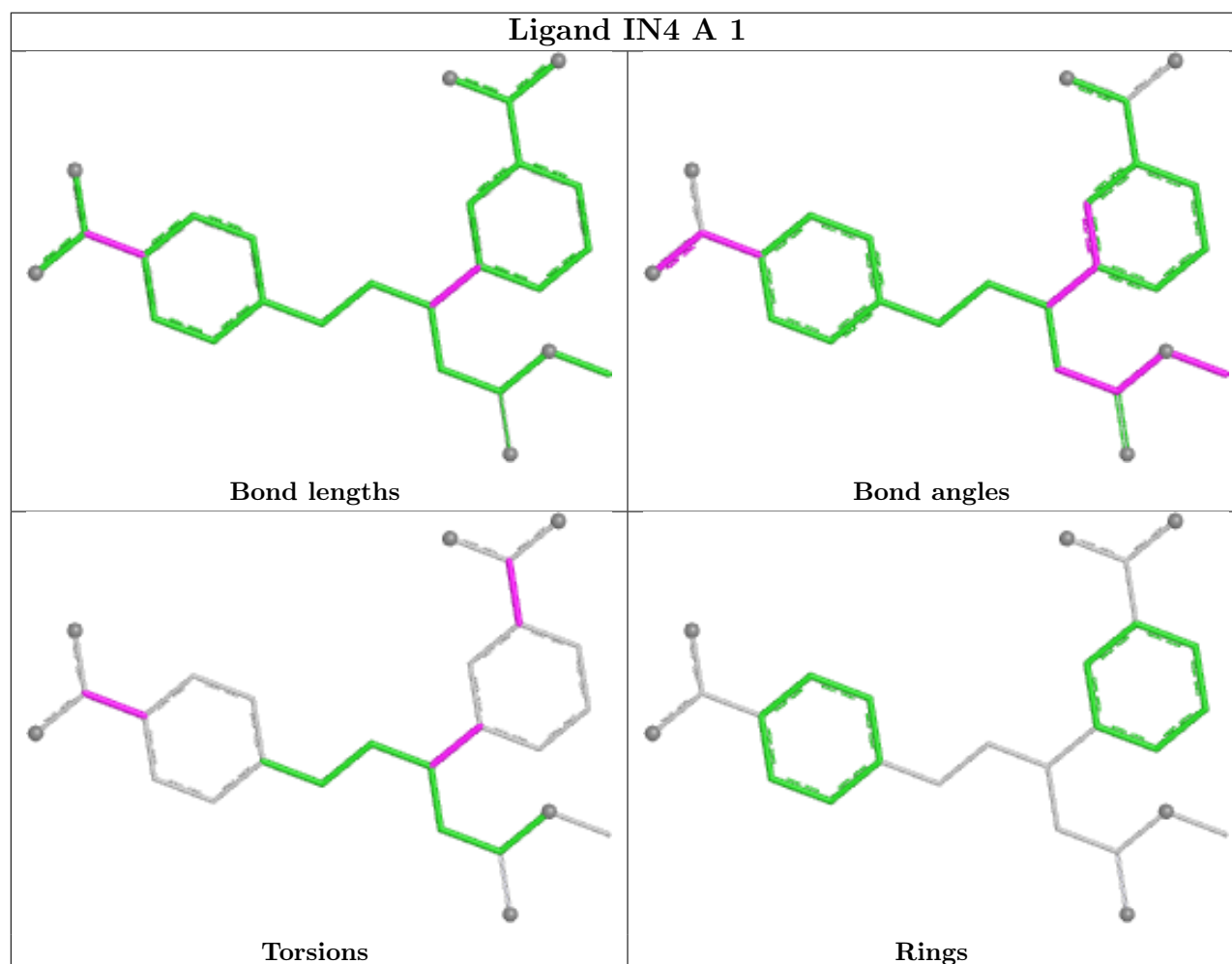
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Mol	Chain	Res	Type	Atoms
2	A	1	IN4	C14-C10-C4-C5

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.