



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 1TGB / pdb_00001tgb
Title : CRYSTAL STRUCTURE OF BOVINE TRYPSINOGEN AT 1.8
ANGSTROMS RESOLUTION. II. CRYSTALLOGRAPHIC REFINEMENT,
REFINED CRYSTAL STRUCTURE AND COMPARISON WITH BOVINE TRYPSIN
Authors : Bode, W.; Fehllhammer, H.; Huber, R.
Deposited on : 1979-03-07
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
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

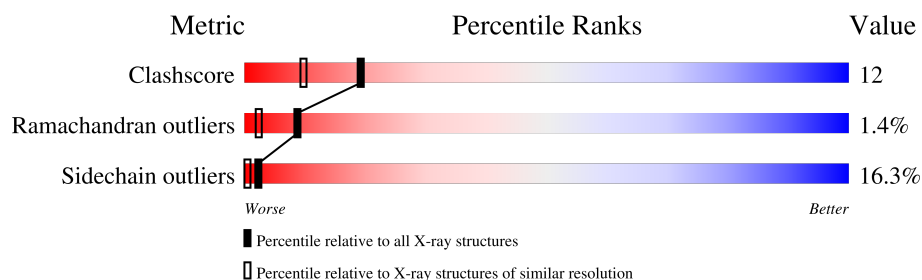
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	229	48% 36% 11% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1750 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 TRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	143	0	0
			1629	1012	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	25	0
			120	120		

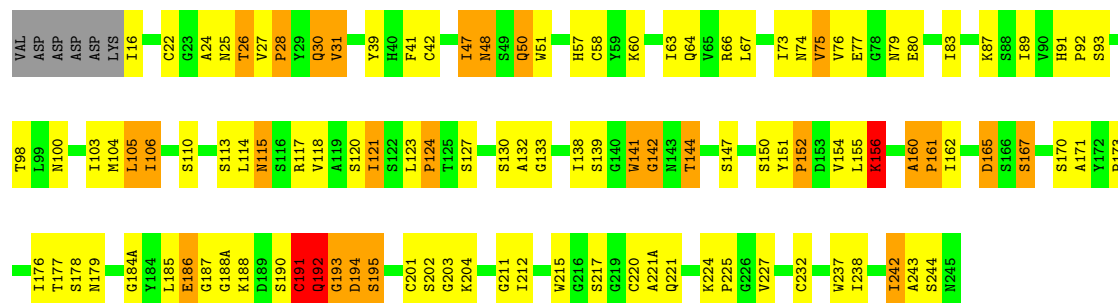
3 Residue-property plots

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: TRYPSINOGEN

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	55.10Å 55.10Å 109.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1750	wwPDB-VP
Average B, all atoms (Å ²)	1.0	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

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	1.79	16/1660 (1.0%)	2.07	92/2250 (4.1%)

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	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	CYS	N-CA	-41.68	0.92	1.46
1	A	188(A)	GLY	N-CA	14.63	1.66	1.45
1	A	186	GLU	CA-CB	-13.58	1.29	1.53
1	A	191	CYS	CA-CB	12.80	1.75	1.53
1	A	192	GLN	CA-C	-10.80	1.38	1.52
1	A	215	TRP	NE1-CE2	-8.81	1.27	1.37
1	A	51	TRP	NE1-CE2	-8.71	1.27	1.37
1	A	141	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	237	TRP	NE1-CE2	-8.51	1.28	1.37
1	A	221(A)	ALA	N-CA	7.69	1.56	1.46
1	A	151	TYR	CA-CB	7.65	1.65	1.53
1	A	165	ASP	CG-OD2	7.40	1.39	1.25
1	A	162	ILE	CA-CB	-6.08	1.46	1.54
1	A	42	CYS	N-CA	5.71	1.53	1.46
1	A	188	LYS	N-CA	-5.46	1.39	1.46
1	A	195	SER	N-CA	5.35	1.52	1.46

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	PRO	CB-CA-C	17.30	134.21	111.71
1	A	192	GLN	CA-C-O	-14.42	99.89	120.51
1	A	162	ILE	N-CA-C	-13.01	91.72	108.89
1	A	193	GLY	N-CA-C	-12.70	83.08	113.18
1	A	170	SER	N-CA-C	12.09	124.45	111.28
1	A	244	SER	N-CA-C	12.01	127.73	113.20
1	A	192	GLN	CB-CA-C	11.89	134.08	110.42
1	A	51	TRP	N-CA-C	10.18	126.24	109.24
1	A	124	PRO	CB-CA-C	10.10	124.47	111.64
1	A	124	PRO	N-CA-C	9.95	127.47	111.26
1	A	47	ILE	CB-CA-C	-9.72	100.28	110.88
1	A	28	PRO	CA-CB-CG	-9.59	86.27	104.50
1	A	211	GLY	N-CA-C	9.53	128.84	110.73
1	A	74	ASN	N-CA-C	9.49	125.12	113.17
1	A	28	PRO	CB-CA-C	9.34	126.97	111.56
1	A	191	CYS	N-CA-C	-9.26	91.08	110.80
1	A	144	THR	N-CA-C	9.10	124.11	112.92
1	A	237	TRP	N-CA-C	9.05	121.15	111.28
1	A	114	LEU	N-CA-C	-9.00	95.01	109.76
1	A	26	THR	N-CA-C	8.95	124.01	113.18
1	A	154	VAL	N-CA-C	8.95	122.95	109.17
1	A	39	TYR	N-CA-C	-8.88	95.02	108.52
1	A	156	LYS	N-CA-C	8.86	124.04	109.95
1	A	171	ALA	N-CA-C	8.70	121.91	111.82
1	A	220	CYS	N-CA-C	-8.51	95.03	109.24
1	A	47	ILE	N-CA-C	8.43	123.28	113.42
1	A	60	LYS	N-CA-C	-8.29	96.48	109.07
1	A	203	GLY	N-CA-C	8.14	126.19	115.36
1	A	243	ALA	N-CA-C	8.05	121.16	111.82
1	A	167	SER	N-CA-C	-7.96	103.36	113.23
1	A	41	PHE	N-CA-C	7.93	125.15	114.12
1	A	124	PRO	CA-N-CD	-7.66	101.28	112.00
1	A	195	SER	CB-CA-C	7.66	123.19	109.64
1	A	221(A)	ALA	N-CA-CB	-7.57	97.70	110.49
1	A	187	GLY	CA-C-N	7.32	135.76	121.41
1	A	187	GLY	C-N-CA	7.32	135.76	121.41
1	A	161	PRO	N-CA-C	7.20	123.70	111.68
1	A	58	CYS	CB-CA-C	-7.20	98.07	110.09
1	A	142	GLY	N-CA-C	7.14	130.10	113.18
1	A	133	GLY	N-CA-C	7.11	130.04	113.18
1	A	187	GLY	N-CA-C	-7.00	103.87	112.33
1	A	195	SER	N-CA-C	-6.87	101.32	110.24
1	A	191	CYS	CA-CB-SG	6.85	130.16	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	SER	N-CA-C	-6.74	98.78	109.23
1	A	188(A)	GLY	N-CA-C	6.71	129.08	113.18
1	A	242	ILE	N-CA-C	-6.68	102.93	112.35
1	A	16	ILE	CA-CB-CG2	-6.61	99.27	110.50
1	A	186	GLU	N-CA-CB	6.51	121.39	110.32
1	A	28	PRO	CA-N-CD	-6.47	102.94	112.00
1	A	225	PRO	CB-CA-C	6.46	119.41	110.95
1	A	28	PRO	N-CA-C	6.39	125.63	112.47
1	A	176	ILE	CA-CB-CG2	-6.33	99.75	110.50
1	A	132	ALA	N-CA-C	6.13	118.68	110.35
1	A	150	SER	N-CA-C	6.07	118.17	107.61
1	A	79	ASN	N-CA-C	5.97	120.26	112.92
1	A	58	CYS	N-CA-C	5.96	120.68	113.17
1	A	215	TRP	N-CA-C	5.88	115.86	108.45
1	A	93	SER	N-CA-C	5.86	119.74	112.59
1	A	130	SER	N-CA-C	5.85	119.12	110.46
1	A	185	LEU	N-CA-C	-5.71	104.52	112.45
1	A	232	CYS	N-CA-C	5.67	119.01	111.75
1	A	185	LEU	CA-C-N	5.62	129.60	120.60
1	A	185	LEU	C-N-CA	5.62	129.60	120.60
1	A	162	ILE	CA-CB-CG2	-5.62	100.94	110.50
1	A	147	SER	N-CA-C	-5.56	99.36	108.76
1	A	178	SER	N-CA-C	5.56	119.57	112.34
1	A	39	TYR	CB-CA-C	5.53	118.89	109.99
1	A	47	ILE	CA-CB-CG2	-5.44	101.25	110.50
1	A	98	THR	N-CA-C	5.43	119.91	113.28
1	A	162	ILE	CB-CA-C	5.43	118.22	111.15
1	A	154	VAL	CB-CA-C	-5.42	103.79	111.38
1	A	170	SER	CB-CA-C	-5.40	101.82	110.79
1	A	160	ALA	N-CA-C	5.35	116.90	108.23
1	A	30	GLN	N-CA-C	5.33	118.24	109.76
1	A	227	VAL	N-CA-C	5.33	116.25	108.53
1	A	244	SER	CB-CA-C	-5.31	100.02	110.11
1	A	220	CYS	CB-CA-C	5.30	119.84	109.35
1	A	212	ILE	CA-CB-CG2	-5.29	101.51	110.50
1	A	50	GLN	N-CA-C	5.26	120.56	113.72
1	A	138	ILE	CA-CB-CG2	-5.25	101.57	110.50
1	A	103	ILE	CA-CB-CG2	-5.25	101.58	110.50
1	A	121	ILE	CA-CB-CG2	-5.22	101.63	110.50
1	A	242	ILE	CA-CB-CG2	-5.22	101.63	110.50
1	A	83	ILE	CA-CB-CG2	-5.22	101.63	110.50
1	A	89	ILE	CA-CB-CG2	-5.21	101.64	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ILE	CA-CB-CG2	-5.18	101.69	110.50
1	A	190	SER	N-CA-C	-5.12	101.98	109.81
1	A	238	ILE	CA-CB-CG2	-5.08	101.86	110.50
1	A	106	ILE	CA-CB-CG2	-5.05	101.91	110.50
1	A	161	PRO	CB-CA-C	5.05	117.85	110.63
1	A	177	THR	CA-CB-OG1	-5.04	102.03	109.60
1	A	63	ILE	CA-CB-CG2	-5.03	101.95	110.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	GLN	Peptide
1	A	193	GLY	Peptide
1	A	47	ILE	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	1629	0	1590	34	0
2	A	1	0	0	0	0
3	A	120	0	0	0	0
All	All	1750	0	1590	34	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 12.

All (34) 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:57:HIS:NE2	1:A:195:SER:HB3	1.72	1.04
1:A:115:ASN:HD22	1:A:117:ARG:H	1.24	0.83
1:A:31:VAL:CG2	1:A:67:LEU:HD23	2.11	0.80
1:A:115:ASN:ND2	1:A:117:ARG:H	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.31	0.66
1:A:48:ASN:HD22	1:A:48:ASN:C	2.04	0.64
1:A:26:THR:O	1:A:26:THR:CG2	2.47	0.63
1:A:31:VAL:HG22	1:A:67:LEU:HD23	1.81	0.62
1:A:100:ASN:HD21	1:A:179:ASN:HD22	1.48	0.61
1:A:57:HIS:NE2	1:A:195:SER:CB	2.58	0.61
1:A:31:VAL:HG23	1:A:67:LEU:HD23	1.82	0.60
1:A:104:MET:HE3	1:A:106:ILE:HD11	1.84	0.59
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.49	0.58
1:A:26:THR:O	1:A:26:THR:HG22	2.03	0.57
1:A:48:ASN:HD22	1:A:50:GLN:H	1.52	0.57
1:A:64:GLN:NE2	1:A:66:ARG:HE	2.04	0.56
1:A:57:HIS:CE1	1:A:195:SER:HB3	2.40	0.55
1:A:24:ALA:O	1:A:25:ASN:HB2	2.06	0.55
1:A:31:VAL:CG2	1:A:67:LEU:CD2	2.87	0.53
1:A:27:VAL:HG12	1:A:30:GLN:HB2	1.91	0.52
1:A:30:GLN:NE2	1:A:139:SER:OG	2.44	0.51
1:A:48:ASN:C	1:A:48:ASN:ND2	2.69	0.51
1:A:121:ILE:O	1:A:121:ILE:HG23	2.12	0.48
1:A:67:LEU:O	1:A:80:GLU:HA	2.14	0.48
1:A:144:THR:HG23	1:A:152:PRO:HD3	1.95	0.47
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.63	0.47
1:A:115:ASN:HD22	1:A:115:ASN:C	2.23	0.47
1:A:141:TRP:O	1:A:152:PRO:HD2	2.15	0.46
1:A:160:ALA:HB1	1:A:184(A):GLY:HA2	1.99	0.44
1:A:48:ASN:ND2	1:A:50:GLN:H	2.15	0.43
1:A:75:VAL:HG22	1:A:77:GLU:CG	2.50	0.42
1:A:115:ASN:ND2	1:A:118:VAL:H	2.19	0.41
1:A:22:CYS:SG	1:A:156:LYS:C	3.04	0.40
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.86	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%)	202 (91%)	16 (7%)	3 (1%)	9 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLY
1	A	191	CYS
1	A	194	ASP

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%)	154 (84%)	30 (16%)	2 0

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	31	VAL
1	A	48	ASN
1	A	75	VAL
1	A	76	VAL
1	A	87	LYS
1	A	105	LEU
1	A	113	SER
1	A	115	ASN
1	A	120	SER
1	A	123	LEU
1	A	124	PRO
1	A	127	SER
1	A	152	PRO
1	A	155	LEU
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	161	PRO
1	A	165	ASP
1	A	167	SER
1	A	186	GLU
1	A	191	CYS
1	A	192	GLN
1	A	194	ASP
1	A	201	CYS
1	A	202	SER
1	A	204	LYS
1	A	217	SER
1	A	221	GLN
1	A	224	LYS
1	A	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	ASN
1	A	64	GLN
1	A	100	ASN
1	A	101	ASN
1	A	115	ASN
1	A	175	GLN
1	A	210	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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.