



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 10:57 PM EST

PDB ID : 1TGN
Title : STRUCTURE OF BOVINE TRYPSINOGEN AT 1.9 ANGSTROMS RESOLUTION
Authors : Kossiakoff, A.A.; Stroud, R.M.
Deposited on : unknown
Resolution : 1.65 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

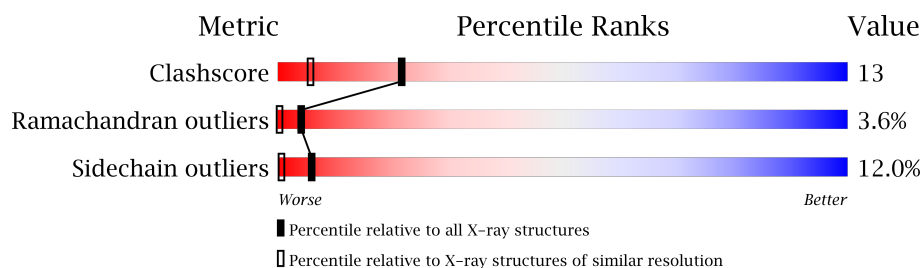
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	 64% 21% 7% 5% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1621 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.

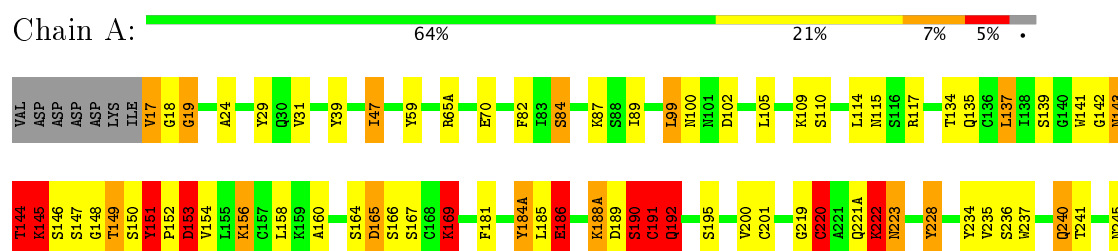
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1621	1006	278	323	14	0	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



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	55.15Å 55.15Å 109.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.65)	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	1621	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.34	4/1652 (0.2%)	2.39	86/2239 (3.8%)

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	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	CYS	CA-CB	14.35	1.85	1.53
1	A	151	TYR	CB-CG	10.70	1.67	1.51
1	A	151	TYR	CA-CB	6.10	1.67	1.53
1	A	84	SER	CB-OG	-6.06	1.34	1.42

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	TYR	CB-CG-CD2	29.23	138.54	121.00
1	A	117	ARG	NE-CZ-NH1	-23.98	108.31	120.30
1	A	151	TYR	CB-CG-CD1	-18.11	110.13	121.00
1	A	117	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	A	184(A)	TYR	CB-CG-CD1	-13.47	112.92	121.00
1	A	65(A)	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	A	151	TYR	CG-CD1-CE1	13.18	131.85	121.30
1	A	186	GLU	OE1-CD-OE2	-12.64	108.13	123.30
1	A	144	THR	CA-CB-CG2	11.86	129.00	112.40
1	A	150	SER	CB-CA-C	11.70	132.33	110.10
1	A	151	TYR	CB-CA-C	11.20	132.79	110.40
1	A	17	VAL	CA-CB-CG2	10.46	126.59	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	CYS	O-C-N	-10.05	106.62	122.70
1	A	220	CYS	CA-CB-SG	-9.21	97.41	114.00
1	A	190	SER	C-N-CA	8.30	142.46	121.70
1	A	59	TYR	CB-CG-CD1	-8.24	116.06	121.00
1	A	153	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	99	LEU	CB-CG-CD1	8.06	124.70	111.00
1	A	189	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	165	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	165	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	234	TYR	CB-CG-CD2	-7.64	116.41	121.00
1	A	188(A)	LYS	N-CA-CB	-7.56	96.98	110.60
1	A	47	ILE	CA-CB-CG2	7.44	125.78	110.90
1	A	17	VAL	CG1-CB-CG2	-7.44	99.00	110.90
1	A	188(A)	LYS	CD-CE-NZ	7.44	128.80	111.70
1	A	165	ASP	OD1-CG-OD2	-7.41	109.22	123.30
1	A	65(A)	ARG	NH1-CZ-NH2	7.40	127.54	119.40
1	A	190	SER	N-CA-CB	-7.39	99.41	110.50
1	A	222	LYS	O-C-N	-7.30	111.01	122.70
1	A	145	LYS	O-C-N	7.20	134.21	122.70
1	A	24	ALA	CB-CA-C	-7.09	99.46	110.10
1	A	235	VAL	CG1-CB-CG2	-7.09	99.56	110.90
1	A	137	LEU	CB-CG-CD2	6.91	122.75	111.00
1	A	59	TYR	CB-CG-CD2	6.90	125.14	121.00
1	A	144	THR	CA-C-N	-6.89	102.04	117.20
1	A	234	TYR	CD1-CG-CD2	6.82	125.41	117.90
1	A	184(A)	TYR	C-N-CA	-6.80	104.69	121.70
1	A	149	THR	N-CA-CB	6.67	122.97	110.30
1	A	145	LYS	CD-CE-NZ	-6.59	96.54	111.70
1	A	151	TYR	CD1-CG-CD2	-6.57	110.67	117.90
1	A	141	TRP	C-N-CA	-6.50	108.65	122.30
1	A	82	PHE	CB-CG-CD1	6.49	125.34	120.80
1	A	188(A)	LYS	O-C-N	-6.37	112.51	122.70
1	A	100	ASN	OD1-CG-ND2	-6.35	107.30	121.90
1	A	223	ASN	O-C-N	-6.33	112.56	122.70
1	A	190	SER	CB-CA-C	6.28	122.03	110.10
1	A	70	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	A	135	GLN	N-CA-CB	-6.13	99.56	110.60
1	A	144	THR	O-C-N	6.03	132.35	122.70
1	A	234	TYR	CG-CD1-CE1	-5.98	116.52	121.30
1	A	142	GLY	O-C-N	-5.93	113.21	122.70
1	A	149	THR	C-N-CA	-5.85	107.08	121.70
1	A	184(A)	TYR	CG-CD2-CE2	-5.79	116.67	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CB-CA-C	-5.75	98.89	110.40
1	A	184(A)	TYR	CA-CB-CG	-5.68	102.61	113.40
1	A	236	SER	CB-CA-C	5.63	120.79	110.10
1	A	240	GLN	CA-CB-CG	5.58	125.68	113.40
1	A	220	CYS	CA-C-N	5.55	129.41	117.20
1	A	222	LYS	CA-CB-CG	5.55	125.61	113.40
1	A	31	VAL	CA-CB-CG2	5.54	119.21	110.90
1	A	110	SER	CB-CA-C	-5.50	99.64	110.10
1	A	135	GLN	CA-CB-CG	-5.50	101.29	113.40
1	A	192	GLN	O-C-N	-5.49	113.87	123.20
1	A	192	GLN	CA-CB-CG	5.49	125.48	113.40
1	A	102	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	47	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	A	31	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	A	115	ASN	O-C-N	-5.42	114.03	122.70
1	A	135	GLN	CB-CG-CD	-5.39	97.58	111.60
1	A	222	LYS	N-CA-CB	-5.33	101.01	110.60
1	A	152	PRO	N-CA-C	-5.30	98.31	112.10
1	A	167	SER	CB-CA-C	-5.21	100.21	110.10
1	A	151	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	A	186	GLU	N-CA-C	5.18	124.98	111.00
1	A	236	SER	N-CA-CB	-5.16	102.76	110.50
1	A	102	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	141	TRP	CD1-CG-CD2	5.16	110.42	106.30
1	A	222	LYS	C-N-CA	5.14	134.56	121.70
1	A	222	LYS	CD-CE-NZ	-5.11	99.94	111.70
1	A	143	ASN	CB-CA-C	-5.09	100.23	110.40
1	A	134	THR	CA-C-N	-5.08	106.04	117.20
1	A	114	LEU	CB-CG-CD2	5.07	119.62	111.00
1	A	228	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	181	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	A	89	ILE	CG1-CB-CG2	-5.00	100.39	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	151	TYR	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	228	TYR	Sidechain
1	A	39	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	1621	0	1579	43	0
All	All	1621	0	1579	43	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 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:220:CYS:CB	1:A:220:CYS:CA	1.85	1.51
1:A:18:GLY:HA2	1:A:188(A):LYS:HG3	1.68	0.74
1:A:19:GLY:HA2	1:A:188(A):LYS:HE2	1.70	0.74
1:A:220:CYS:SG	1:A:220:CYS:CA	2.77	0.73
1:A:151:TYR:O	1:A:156:LYS:HE3	1.89	0.72
1:A:18:GLY:CA	1:A:188(A):LYS:HG3	2.26	0.65
1:A:105:LEU:CD1	1:A:241:THR:HG21	2.26	0.65
1:A:220:CYS:N	1:A:220:CYS:SG	2.72	0.63
1:A:105:LEU:CD1	1:A:241:THR:CG2	2.77	0.62
1:A:190:SER:O	1:A:220:CYS:HB3	2.01	0.60
1:A:19:GLY:HA2	1:A:188(A):LYS:CE	2.33	0.59
1:A:219:GLY:HA3	1:A:221(A):GLN:HG3	1.87	0.56
1:A:18:GLY:C	1:A:188(A):LYS:HE3	2.25	0.56
1:A:105:LEU:HD12	1:A:241:THR:HG21	1.88	0.55
1:A:237:TRP:O	1:A:241:THR:HG22	2.06	0.55
1:A:143:ASN:O	1:A:144:THR:HB	2.05	0.55
1:A:151:TYR:C	1:A:153:ASP:N	2.60	0.55
1:A:87:LYS:HE2	1:A:245:ASN:HD22	1.72	0.53
1:A:165:ASP:CG	1:A:169:LYS:HE2	2.30	0.52
1:A:144:THR:CG2	1:A:145:LYS:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:HB2	1:A:145:LYS:HG2	1.91	0.51
1:A:18:GLY:HA2	1:A:188(A):LYS:CG	2.38	0.51
1:A:18:GLY:O	1:A:188(A):LYS:HE3	2.11	0.51
1:A:185:LEU:HB3	1:A:186:GLU:OE1	2.12	0.49
1:A:18:GLY:CA	1:A:188(A):LYS:CG	2.90	0.49
1:A:29:TYR:CZ	1:A:200:VAL:HG21	2.47	0.49
1:A:165:ASP:OD1	1:A:169:LYS:HE2	2.13	0.48
1:A:158:LEU:CD2	1:A:160:ALA:HB2	2.43	0.48
1:A:84:SER:OG	1:A:109:LYS:CE	2.62	0.48
1:A:151:TYR:H	1:A:154:VAL:HG22	1.79	0.47
1:A:84:SER:OG	1:A:109:LYS:HE3	2.15	0.46
1:A:156:LYS:HD2	1:A:156:LYS:N	2.30	0.46
1:A:105:LEU:HD11	1:A:241:THR:CG2	2.45	0.45
1:A:165:ASP:OD2	1:A:169:LYS:HE2	2.16	0.45
1:A:143:ASN:O	1:A:191:CYS:HB3	2.17	0.44
1:A:186:GLU:OE1	1:A:223:ASN:HB3	2.18	0.44
1:A:105:LEU:CD1	1:A:241:THR:HG23	2.46	0.44
1:A:105:LEU:HD11	1:A:241:THR:HG21	1.99	0.44
1:A:151:TYR:C	1:A:153:ASP:H	2.21	0.43
1:A:184(A):TYR:CE1	1:A:188(A):LYS:HB3	2.56	0.41
1:A:18:GLY:C	1:A:188(A):LYS:HG3	2.41	0.41
1:A:18:GLY:HA2	1:A:188(A):LYS:HA	2.02	0.41
1:A:17:VAL:CB	1:A:145:LYS:NZ	2.84	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	Percentiles
1	A	220/229 (96%)	196 (89%)	16 (7%)	8 (4%)	4 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	THR
1	A	146	SER
1	A	191	CYS
1	A	192	GLN
1	A	145	LYS
1	A	19	GLY
1	A	222	LYS
1	A	148	GLY

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	183/190 (96%)	161 (88%)	22 (12%)	6 0

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	99	LEU
1	A	137	LEU
1	A	139	SER
1	A	144	THR
1	A	145	LYS
1	A	147	SER
1	A	149	THR
1	A	153	ASP
1	A	156	LYS
1	A	164	SER
1	A	166	SER
1	A	169	LYS
1	A	186	GLU
1	A	190	SER
1	A	191	CYS
1	A	192	GLN
1	A	195	SER
1	A	201	CYS

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Mol	Chain	Res	Type
1	A	220	CYS
1	A	222	LYS
1	A	240	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	100	ASN
1	A	101	ASN
1	A	233	ASN
1	A	245	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](#)

There are no ligands in this entry.

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.