



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:07 am GMT

PDB ID : 2CGA  
Title : BOVINE CHYMOTRYPSINOGEN A. X-RAY CRYSTAL STRUCTURE ANALYSIS AND REFINEMENT OF A NEW CRYSTAL FORM AT 1.8 ANGSTROMS RESOLUTION  
Authors : Wang, D.; Bode, W.; Huber, R.  
Deposited on : 1987-01-16  
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](mailto: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.

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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)	:	recalc28949

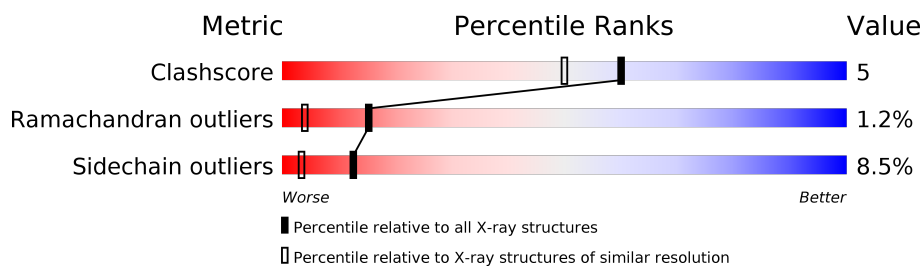
# 1 Overall quality at a glance

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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (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  $\geq 3$ , 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	245	 73% 22% 5%
1	B	245	 71% 22% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3927 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 CHYMOTRYPSINOGEN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1799	1127	307	353	12			
1	B	245	Total	C	N	O	S	0	0	0
			1799	1127	307	353	12			

- Molecule 2 is water.

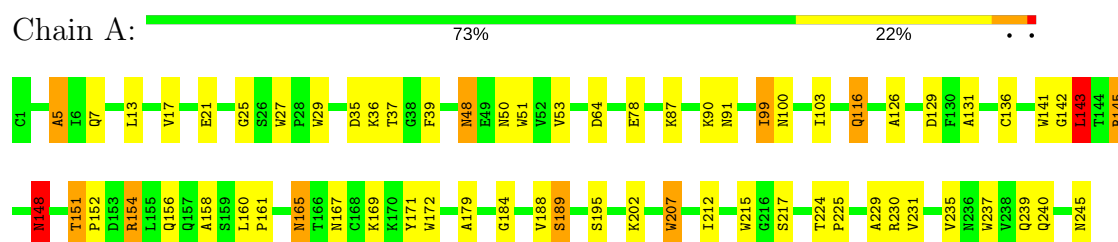
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	179	Total	O	0	0
			179	179		

### 3 Residue-property plots

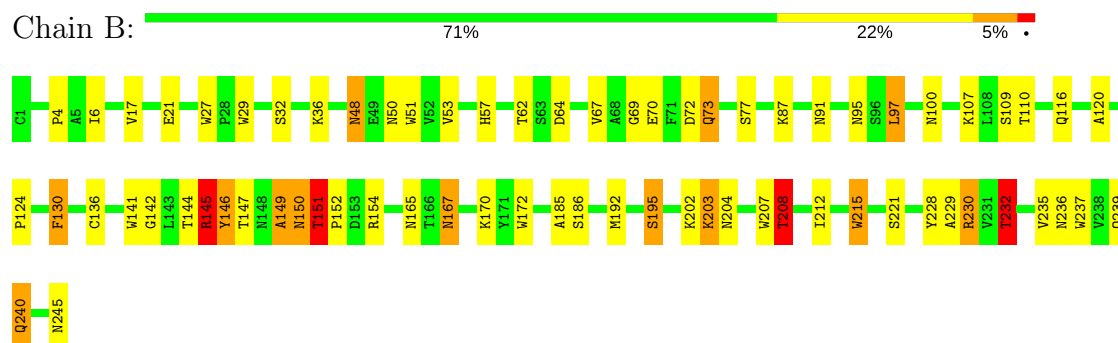
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $RSRZ > 2$ ). 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: CHYMOTRYPSINOGEN A



#### • Molecule 1: CHYMOTRYPSINOGEN A



## 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, $\alpha$ , $\beta$ , $\gamma$	59.30Å 77.10Å 110.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	EREF	Depositor
R, $R_{free}$	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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	1.23	9/1835 (0.5%)	1.40	10/2502 (0.4%)
1	B	1.22	8/1835 (0.4%)	1.49	18/2502 (0.7%)
All	All	1.22	17/3670 (0.5%)	1.45	28/5004 (0.6%)

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	21
1	B	0	29
All	All	0	50

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	TRP	NE1-CE2	-8.98	1.25	1.37
1	B	207	TRP	NE1-CE2	-8.48	1.26	1.37
1	B	215	TRP	NE1-CE2	-8.45	1.26	1.37
1	A	215	TRP	NE1-CE2	-8.23	1.26	1.37
1	A	172	TRP	NE1-CE2	-7.54	1.27	1.37
1	B	237	TRP	NE1-CE2	-7.54	1.27	1.37
1	B	172	TRP	NE1-CE2	-7.19	1.28	1.37
1	A	141	TRP	NE1-CE2	-6.85	1.28	1.37
1	B	51	TRP	NE1-CE2	-6.79	1.28	1.37
1	A	237	TRP	NE1-CE2	-6.76	1.28	1.37
1	B	29	TRP	NE1-CE2	-6.73	1.28	1.37
1	A	51	TRP	NE1-CE2	-6.70	1.28	1.37
1	B	27	TRP	NE1-CE2	-6.61	1.28	1.37
1	B	141	TRP	NE1-CE2	-6.49	1.29	1.37
1	A	207	TRP	NE1-CE2	-6.25	1.29	1.37
1	A	231	VAL	C-N	6.24	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TRP	NE1-CE2	-6.16	1.29	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	B	230	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	186	SER	N-CA-CB	-9.15	96.77	110.50
1	B	154	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	B	230	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	144	THR	C-N-CA	8.53	143.01	121.70
1	A	230	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	154	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	171	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	87	LYS	CB-CA-C	-6.11	98.17	110.40
1	B	6	ILE	CA-CB-CG1	6.06	122.51	111.00
1	A	53	VAL	CB-CA-C	-5.78	100.43	111.40
1	A	145	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	215	TRP	CG-CD2-CE3	-5.64	128.82	133.90
1	B	232	THR	CA-CB-CG2	5.55	120.17	112.40
1	A	225	PRO	N-CA-CB	5.51	109.91	103.30
1	A	5	ALA	CB-CA-C	-5.49	101.86	110.10
1	B	215	TRP	NE1-CE2-CZ2	-5.44	124.42	130.40
1	A	143	LEU	CB-CG-CD1	5.31	120.03	111.00
1	B	208	THR	CA-CB-OG1	5.25	120.01	109.00
1	B	215	TRP	CH2-CZ2-CE2	-5.23	112.17	117.40
1	A	154	ARG	CA-CB-CG	-5.17	102.03	113.40
1	B	215	TRP	CD1-NE1-CE2	-5.14	104.37	109.00
1	B	144	THR	O-C-N	5.12	130.89	122.70
1	B	215	TRP	CD2-CE3-CZ3	-5.08	112.19	118.80
1	B	72	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	145	ARG	N-CA-CB	5.04	119.67	110.60
1	A	158	ALA	CB-CA-C	-5.03	102.55	110.10

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ALA	Mainchain
1	A	129	ASP	Sidechain
1	A	131	ALA	Mainchain
1	A	136	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	148	ASN	Sidechain,Mainchain
1	A	156	GLN	Sidechain,Mainchain
1	A	160	LEU	Mainchain
1	A	167	ASN	Sidechain
1	A	188	VAL	Mainchain
1	A	189	SER	Mainchain
1	A	21	GLU	Sidechain
1	A	240	GLN	Sidechain
1	A	245	ASN	Sidechain
1	A	25	GLY	Mainchain
1	A	35	ASP	Sidechain
1	A	64	ASP	Sidechain
1	A	78	GLU	Sidechain
1	A	91	ASN	Sidechain,Mainchain
1	B	100	ASN	Sidechain
1	B	120	ALA	Mainchain
1	B	124	PRO	Mainchain
1	B	130	PHE	Mainchain
1	B	136	CYS	Mainchain
1	B	142	GLY	Mainchain
1	B	150	ASN	Sidechain
1	B	151	THR	Mainchain
1	B	165	ASN	Mainchain
1	B	185	ALA	Mainchain
1	B	195	SER	Mainchain
1	B	202	LYS	Mainchain
1	B	203	LYS	Mainchain
1	B	204	ASN	Sidechain
1	B	21	GLU	Sidechain
1	B	228	TYR	Mainchain
1	B	236	ASN	Sidechain
1	B	240	GLN	Sidechain
1	B	245	ASN	Sidechain
1	B	36	LYS	Mainchain
1	B	4	PRO	Mainchain
1	B	62	THR	Mainchain
1	B	64	ASP	Sidechain
1	B	69	GLY	Mainchain
1	B	70	GLU	Mainchain
1	B	73	GLN	Sidechain
1	B	77	SER	Mainchain
1	B	91	ASN	Sidechain

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Mol	Chain	Res	Type	Group
1	B	95	ASN	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	1799	0	1777	20	2
1	B	1799	0	1777	18	2
2	A	150	0	0	1	1
2	B	179	0	0	0	1
All	All	3927	0	3554	38	3

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 (38) 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:B:151:THR:HG23	1:B:152:PRO:CD	1.87	1.04
1:B:151:THR:CG2	1:B:152:PRO:HD2	1.85	1.04
1:B:151:THR:HG23	1:B:152:PRO:HD2	0.96	0.94
1:A:165:ASN:O	1:A:169:LYS:HG3	1.98	0.63
1:A:100:ASN:HD21	1:A:179:ALA:HB3	1.69	0.57
1:A:48:ASN:HD22	1:A:50:ASN:H	1.53	0.56
1:B:151:THR:CG2	1:B:152:PRO:CD	2.64	0.55
1:A:100:ASN:ND2	1:A:179:ALA:HB3	2.22	0.54
1:B:230:ARG:HG2	1:B:232:THR:HG22	1.91	0.53
1:B:57:HIS:NE2	1:B:195:SER:HB2	2.25	0.52
1:B:130:PHE:CZ	1:B:203:LYS:HE3	2.46	0.50
1:A:143:LEU:C	1:A:151:THR:HG21	2.32	0.48
1:B:48:ASN:HD22	1:B:50:ASN:H	1.61	0.48
1:A:151:THR:HG23	1:A:152:PRO:O	2.14	0.47
1:B:212:ILE:HB	1:B:229:ALA:HB3	1.97	0.47
1:B:146:TYR:HB3	1:B:147:THR:H	1.56	0.47
1:A:5:ALA:HB1	1:A:116:GLN:HG2	1.97	0.46
1:B:203:LYS:HB3	1:B:208:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HB3	1:B:208:THR:HG21	1.98	0.45
1:A:161:PRO:HD2	1:A:184:GLY:HA2	1.98	0.45
1:A:212:ILE:HB	1:A:229:ALA:HB3	2.00	0.44
1:A:148:ASN:HD22	1:A:148:ASN:H	1.64	0.44
1:A:36:LYS:HG3	1:A:37:THR:HG23	2.00	0.43
1:A:143:LEU:HB2	2:A:713:HOH:O	2.18	0.43
1:B:97:LEU:HD12	1:B:97:LEU:HA	1.83	0.42
1:A:103:ILE:HG13	1:A:212:ILE:CD1	2.50	0.42
1:A:202:LYS:HD3	1:A:207:TRP:CE2	2.55	0.42
1:A:142:GLY:O	1:A:145:ARG:HG2	2.20	0.42
1:B:149:ALA:HB1	1:B:150:ASN:H	1.45	0.42
1:B:167:ASN:HA	1:B:170:LYS:HE3	2.01	0.41
1:A:90:LYS:HB3	1:A:90:LYS:HE2	1.89	0.41
1:B:151:THR:CG2	1:B:152:PRO:N	2.84	0.41
1:A:154:ARG:HH21	1:A:154:ARG:HD2	1.73	0.40
1:A:48:ASN:ND2	1:A:50:ASN:H	2.18	0.40
1:B:130:PHE:CE2	1:B:203:LYS:HE3	2.55	0.40
1:B:32:SER:HB3	1:B:67:VAL:HB	2.04	0.40
1:A:5:ALA:CB	1:A:116:GLN:HG2	2.50	0.40
1:A:99:ILE:HD13	1:A:99:ILE:HG21	1.78	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	2:B:745:HOH:O[4_566]	2.05	0.15
1:B:147:THR:CG2	2:A:851:HOH:O[3_545]	2.07	0.13
1:A:39:PHE:CE2	1:B:146:TYR:CZ[3_555]	2.17	0.03

## 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	243/245 (99%)	231 (95%)	10 (4%)	2 (1%)	22	8
1	B	243/245 (99%)	228 (94%)	11 (4%)	4 (2%)	11	2
All	All	486/490 (99%)	459 (94%)	21 (4%)	6 (1%)	15	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	ARG
1	B	146	TYR
1	B	149	ALA
1	B	17	VAL
1	A	17	VAL
1	A	99	ILE

### 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	200/200 (100%)	186 (93%)	14 (7%)	18	5
1	B	200/200 (100%)	180 (90%)	20 (10%)	9	2
All	All	400/400 (100%)	366 (92%)	34 (8%)	12	3

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	LEU
1	A	48	ASN
1	A	116	GLN
1	A	143	LEU
1	A	148	ASN
1	A	151	THR
1	A	165	ASN
1	A	189	SER
1	A	195	SER

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Mol	Chain	Res	Type
1	A	217	SER
1	A	224	THR
1	A	235	VAL
1	A	239	GLN
1	B	48	ASN
1	B	53	VAL
1	B	73	GLN
1	B	87	LYS
1	B	97	LEU
1	B	107	LYS
1	B	109	SER
1	B	110	THR
1	B	116	GLN
1	B	145	ARG
1	B	151	THR
1	B	167	ASN
1	B	192	MET
1	B	208	THR
1	B	215	TRP
1	B	221	SER
1	B	232	THR
1	B	235	VAL
1	B	239	GLN
1	B	240	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	73	GLN
1	A	100	ASN
1	A	148	ASN
1	A	165	ASN
1	B	48	ASN
1	B	100	ASN
1	B	165	ASN
1	B	167	ASN

### 5.3.3 RNA ⓘ

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.