



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:13 PM UTC

PDB ID : 2IPP / pdb\_00002ipp  
Title : Crystal Structure of the tetragonal form of human liver cathepsin B  
Authors : Huber, C.P.; Campbell, R.L.; Hasnain, S.; Hiramama, T.; To, R.  
Deposited on : 2006-10-12  
Resolution : 2.15 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

<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)  
Xtrriage (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

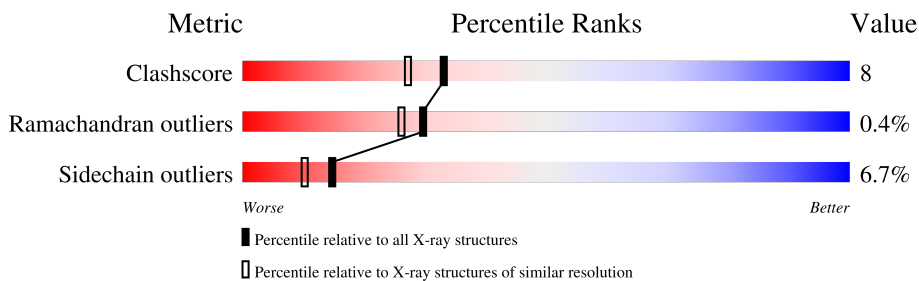
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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  $\geq 3$ , 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	47	
2	B	205	

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	PYS	A	255	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2097 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.

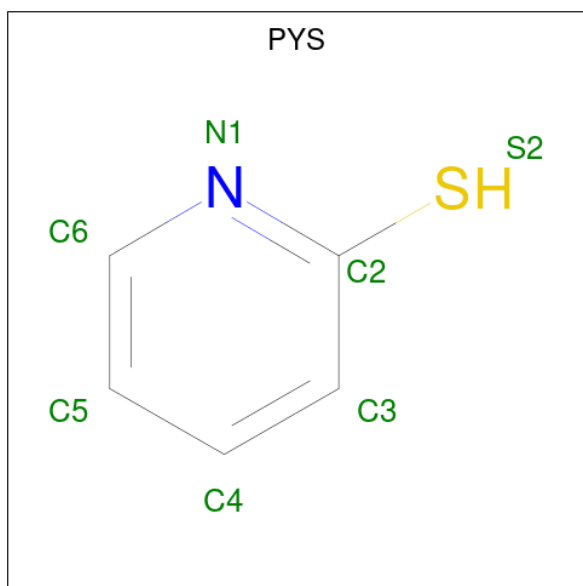
- Molecule 1 is a protein called Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	47	364	225	65	70	4	0	0	0

- Molecule 2 is a protein called Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	205	1574	988	265	307	14	0	0	0

- Molecule 3 is 2-PYRIDINETHIOL (CCD ID: PYS) (formula: C<sub>5</sub>H<sub>5</sub>NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
3	A	1	7	5	1	1	0	0

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	24	Total 24	O 24	0	0
4	B	128	Total 128	O 128	0	0

### 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.

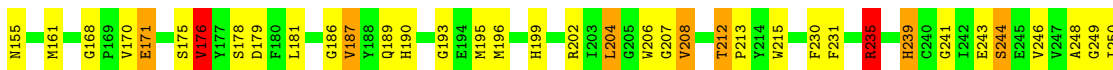
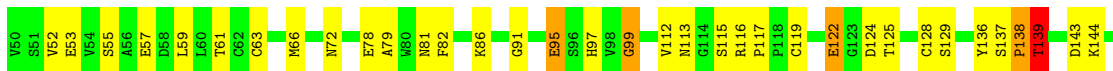
- Molecule 1: Cathepsin B

Chain A:  77% 21%



- Molecule 2: Cathepsin B

Chain B:  64% 29% 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.58Å 85.58Å 34.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.15)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	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: PYS

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	1.07	0/373	1.81	5/505 (1.0%)
2	B	1.07	1/1622 (0.1%)	2.02	48/2203 (2.2%)
All	All	1.07	1/1995 (0.1%)	1.98	53/2708 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	235	ARG	CD-NE	-5.11	1.39	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	ARG	CD-NE-CZ	17.28	148.59	124.40
2	B	116	ARG	CD-NE-CZ	14.10	144.14	124.40
2	B	231	PHE	CA-CB-CG	9.74	123.54	113.80
2	B	97	HIS	CA-CB-CG	-9.24	104.56	113.80
2	B	202	ARG	NE-CZ-NH2	8.55	126.90	119.20
2	B	72	ASN	CA-CB-CG	8.17	120.77	112.60
2	B	119	CYS	CA-C-N	8.16	131.22	120.28
2	B	119	CYS	C-N-CA	8.16	131.22	120.28
2	B	116	ARG	NE-CZ-NH1	8.13	129.63	121.50
2	B	122	GLU	CA-CB-CG	7.39	128.88	114.10
2	B	116	ARG	NE-CZ-NH2	-7.20	112.72	119.20
2	B	139	THR	CA-CB-CG2	6.93	122.28	110.50
2	B	250	ILE	O-C-N	6.73	127.47	121.41
2	B	199	HIS	CA-CB-CG	6.72	120.52	113.80
2	B	249	GLY	CA-C-N	-6.59	116.18	123.43
2	B	249	GLY	C-N-CA	-6.59	116.18	123.43
1	A	5	PHE	CA-CB-CG	6.35	120.15	113.80
2	B	125	THR	O-C-N	6.29	126.66	121.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	GLN	OE1-CD-NE2	6.29	128.89	122.60
2	B	99	GLY	CA-C-N	6.24	128.88	120.65
2	B	99	GLY	C-N-CA	6.24	128.88	120.65
2	B	95	GLU	CA-CB-CG	6.22	126.54	114.10
2	B	122	GLU	N-CA-CB	6.22	122.69	111.37
1	A	42	ILE	N-CA-C	-6.09	104.57	110.42
1	A	42	ILE	O-C-N	6.07	127.86	121.91
2	B	129	SER	O-C-N	6.07	130.37	123.27
2	B	63	CYS	N-CA-C	-5.94	100.32	109.76
2	B	117	PRO	N-CA-C	-5.91	103.49	110.70
2	B	57	GLU	CB-CA-C	-5.88	101.39	110.81
2	B	230	PHE	CA-CB-CG	5.81	119.61	113.80
2	B	176	VAL	CB-CA-C	5.81	118.11	110.91
2	B	124	ASP	O-C-N	5.74	129.82	123.16
2	B	187	VAL	CB-CA-C	5.73	118.83	110.98
2	B	113	ASN	OD1-CG-ND2	5.72	128.32	122.60
2	B	204	LEU	N-CA-CB	-5.60	102.19	111.49
2	B	212	THR	O-C-N	5.58	126.44	121.19
2	B	208	VAL	O-C-N	5.51	129.03	123.07
1	A	34	ALA	N-CA-C	5.49	116.95	110.97
2	B	129	SER	CA-C-O	-5.45	114.47	120.24
2	B	112	VAL	O-C-N	5.42	128.97	122.95
2	B	53	GLU	N-CA-CB	5.37	118.35	110.35
2	B	72	ASN	CB-CA-C	5.36	119.37	111.06
2	B	112	VAL	CA-C-O	-5.33	116.42	121.64
2	B	139	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	4	SER	CA-C-O	-5.23	114.99	121.11
2	B	186	GLY	O-C-N	5.18	127.18	122.88
2	B	82	PHE	O-C-N	5.14	127.57	122.12
2	B	143	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	239	HIS	N-CA-C	5.13	117.13	109.59
2	B	168	GLY	O-C-N	5.07	126.84	121.77
2	B	179	ASP	CA-C-N	5.07	127.07	120.28
2	B	179	ASP	C-N-CA	5.07	127.07	120.28
2	B	171	GLU	CG-CD-OE2	-5.04	106.82	118.40

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	364	0	339	6	0
2	B	1574	0	1444	25	1
3	A	7	0	4	0	0
4	A	24	0	0	3	0
4	B	128	0	0	2	1
All	All	2097	0	1787	29	2

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 (29) 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)
2:B:59:LEU:HD21	2:B:79:ALA:HB1	1.71	0.72
2:B:190:HIS:H	2:B:239:HIS:HE1	1.41	0.69
2:B:181:LEU:HD11	2:B:196:MET:HE2	1.76	0.67
1:A:42:ILE:HG21	2:B:52:VAL:HG12	1.82	0.61
2:B:190:HIS:H	2:B:239:HIS:CE1	2.21	0.56
2:B:176:VAL:HG22	2:B:196:MET:HG3	1.88	0.56
2:B:178:SER:HB3	2:B:193:GLY:HA3	1.88	0.56
2:B:253:THR:N	4:B:368:HOH:O	2.41	0.53
2:B:139:THR:HG23	4:B:545:HOH:O	2.11	0.50
1:A:47:ASN:ND2	4:A:573:HOH:O	2.44	0.50
2:B:66:MET:HE3	2:B:78:GLU:OE1	2.13	0.49
2:B:170:VAL:HG12	2:B:248:ALA:HB2	1.95	0.48
2:B:66:MET:HE1	2:B:81:ASN:OD1	2.17	0.45
1:A:9:GLU:O	1:A:12:PRO:HD3	2.16	0.45
2:B:207:GLY:O	2:B:235:ARG:NH2	2.50	0.45
2:B:241:GLY:O	2:B:244:SER:HB2	2.18	0.44
2:B:208:VAL:HA	2:B:213:PRO:HA	2.00	0.43
2:B:99:GLY:HA2	2:B:136:TYR:CE1	2.54	0.43
2:B:55:SER:HB2	2:B:91:GLY:HA3	2.00	0.43
1:A:23:GLN:HA	1:A:32:PHE:CZ	2.55	0.42
2:B:171:GLU:O	2:B:246:VAL:HA	2.19	0.42
2:B:161:MET:HE3	2:B:206:TRP:CE2	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:VAL:HG11	2:B:212:THR:HG22	2.01	0.41
4:A:427:HOH:O	2:B:161:MET:HE1	2.19	0.41
1:A:1:LEU:HD13	2:B:161:MET:HB3	2.02	0.41
1:A:18:LYS:HE3	4:A:571:HOH:O	2.21	0.40
2:B:155:ASN:HA	2:B:243:GLU:O	2.21	0.40
2:B:61:THR:O	2:B:128:CYS:HB2	2.21	0.40
2:B:215:TRP:CD1	2:B:235:ARG:HB2	2.55	0.40

All (2) 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)
2:B:78:GLU:OE1	2:B:95:GLU:OE2[1_556]	2.09	0.11
4:B:423:HOH:O	4:B:470:HOH:O[1_556]	2.18	0.02

## 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	45/47 (96%)	45 (100%)	0	0	100	100
2	B	203/205 (99%)	185 (91%)	17 (8%)	1 (0%)	24	20
All	All	248/252 (98%)	230 (93%)	17 (7%)	1 (0%)	30	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	138	PRO

### 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	39/39 (100%)	39 (100%)	0	100	100
2	B	169/169 (100%)	155 (92%)	14 (8%)	10	6
All	All	208/208 (100%)	194 (93%)	14 (7%)	15	10

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	LYS
2	B	115	SER
2	B	122	GLU
2	B	137	SER
2	B	138	PRO
2	B	139	THR
2	B	144	LYS
2	B	175	SER
2	B	176	VAL
2	B	195	MET
2	B	204	LEU
2	B	235	ARG
2	B	244	SER
2	B	252	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
2	B	167	ASN
2	B	237	GLN
2	B	239	HIS

### 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
3	PYS	A	255	1	6,7,7	2.45	2 (33%)	6,8,8	2.86	5 (83%)

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	PYS	A	255	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	255	PYS	C2-N1	4.38	1.39	1.33
3	A	255	PYS	C5-C4	2.81	1.44	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	255	PYS	C6-N1-C2	4.48	124.60	117.10
3	A	255	PYS	C5-C4-C3	2.98	123.92	120.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	255	PYS	C3-C2-N1	-2.63	118.38	122.98
3	A	255	PYS	C5-C6-N1	-2.24	119.88	123.42
3	A	255	PYS	C4-C5-C6	-2.14	114.69	118.62

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 [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.