



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:48 AM UTC

PDB ID : 1PPE / pdb_00001ppe

Title : THE REFINED 2.0 ANGSTROMS X-RAY CRYSTAL STRUCTURE OF THE COMPLEX FORMED BETWEEN BOVINE BETA-TRYPSIN AND CMTI-I, A TRYPSIN INHIBITOR FROM SQUASH SEEDS (CUCURBITA MAXIMA): TOPOLOGICAL SIMILARITY OF THE SQUASH SEED INHIBITORS WITH THE CARBOXYPEPTIDASE A INHIBITOR FROM POTATOES

Authors : Bode, W.; Huber, R.

Deposited on : 1991-10-24

Resolution : 2.00 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

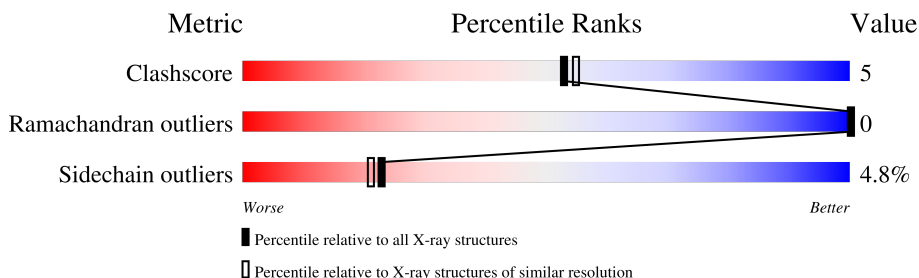
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	E	223	
2	I	29	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1991 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	E	223	Total	C	N	O	S	13	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called TRYPSIN INHIBITOR CMTI-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	29	Total	C	N	O	S	4	0	0
			222	134	39	42	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	126	Total	O	0	0
			126	126		
3	I	14	Total	O	0	0
			14	14		

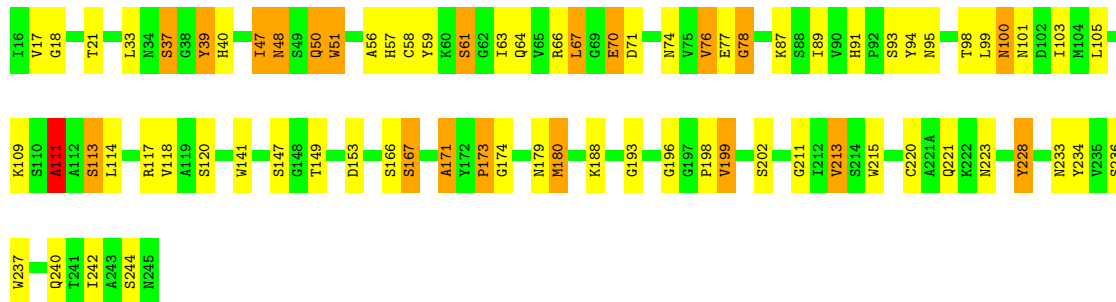
3 Residue-property plots

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 E: 



• Molecule 2: TRYPSIN INHIBITOR CMTI-I

Chain I: 



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	59.28Å 55.47Å 74.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1991	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	E	1.62	17/1660 (1.0%)	2.01	55/2250 (2.4%)
2	I	1.71	5/224 (2.2%)	2.08	4/297 (1.3%)
All	All	1.63	22/1884 (1.2%)	2.02	59/2547 (2.3%)

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	E	0	18
2	I	0	2
All	All	0	20

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	40	HIS	CE1-NE2	11.41	1.44	1.32
2	I	25	HIS	CE1-NE2	10.93	1.43	1.32
1	E	215	TRP	NE1-CE2	-9.64	1.26	1.37
2	I	25	HIS	ND1-CE1	9.36	1.42	1.32
1	E	40	HIS	ND1-CE1	9.20	1.41	1.32
1	E	237	TRP	NE1-CE2	-8.47	1.28	1.37
1	E	91	HIS	ND1-CE1	7.93	1.40	1.32
1	E	57	HIS	ND1-CE1	7.71	1.40	1.32
1	E	141	TRP	NE1-CE2	-7.48	1.29	1.37
2	I	25	HIS	N-CA	7.31	1.54	1.46
2	I	6	ILE	N-CA	7.04	1.54	1.46
1	E	51	TRP	NE1-CE2	-6.34	1.30	1.37
1	E	91	HIS	CE1-NE2	6.28	1.38	1.32
1	E	211	GLY	N-CA	5.81	1.51	1.45
1	E	113	SER	N-CA	5.63	1.53	1.46
1	E	94	TYR	N-CA	5.59	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	213	VAL	N-CA	5.42	1.53	1.46
1	E	114	LEU	C-N	-5.32	1.28	1.33
2	I	25	HIS	CG-ND1	5.27	1.44	1.38
1	E	57	HIS	CE1-NE2	5.25	1.37	1.32
1	E	18	GLY	C-N	-5.22	1.28	1.33
1	E	63	ILE	N-CA	5.04	1.52	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173	PRO	CA-C-N	-9.21	109.01	122.46
1	E	173	PRO	C-N-CA	-9.21	109.01	122.46
2	I	1	ARG	NE-CZ-NH2	-9.16	110.95	119.20
1	E	50	GLN	OE1-CD-NE2	8.90	131.50	122.60
1	E	71	ASP	CA-CB-CG	-8.68	103.92	112.60
1	E	171	ALA	N-CA-C	-7.91	102.73	111.36
1	E	78	GLY	CA-C-N	-7.60	109.99	122.54
1	E	78	GLY	C-N-CA	-7.60	109.99	122.54
1	E	180	MET	CA-C-O	-7.39	112.81	121.46
1	E	153	ASP	CA-CB-CG	-7.38	105.22	112.60
2	I	25	HIS	CA-CB-CG	-7.35	106.45	113.80
1	E	236	SER	O-C-N	7.33	130.01	122.09
1	E	18	GLY	CA-C-N	-7.13	115.28	122.69
1	E	18	GLY	C-N-CA	-7.13	115.28	122.69
1	E	174	GLY	CA-C-N	-7.02	111.10	122.26
1	E	174	GLY	C-N-CA	-7.02	111.10	122.26
1	E	39	TYR	N-CA-CB	-6.75	100.90	111.56
1	E	91	HIS	CA-CB-CG	-6.74	107.06	113.80
1	E	167	SER	CA-CB-OG	-6.56	97.98	111.10
1	E	223	ASN	CA-CB-CG	-6.47	106.13	112.60
1	E	74	ASN	CA-CB-CG	-6.46	106.14	112.60
1	E	77	GLU	O-C-N	6.29	129.85	122.24
2	I	1	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	E	244	SER	N-CA-C	6.27	120.64	112.92
1	E	213	VAL	CA-C-N	-6.23	114.05	121.90
1	E	213	VAL	C-N-CA	-6.23	114.05	121.90
1	E	233	ASN	N-CA-C	-6.14	105.75	113.18
1	E	71	ASP	CA-C-O	6.05	126.06	119.40
1	E	61	SER	N-CA-CB	-5.97	101.37	110.45
1	E	193	GLY	N-CA-C	-5.96	106.86	115.27
1	E	141	TRP	CA-C-N	-5.92	114.84	121.83
1	E	141	TRP	C-N-CA	-5.92	114.84	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	SER	CB-CA-C	-5.88	100.40	110.22
1	E	50	GLN	CA-CB-CG	-5.85	102.40	114.10
1	E	166	SER	CB-CA-C	-5.81	101.76	110.88
1	E	244	SER	CA-CB-OG	-5.79	99.53	111.10
1	E	95	ASN	CB-CA-C	-5.75	101.47	110.74
1	E	196	GLY	N-CA-C	-5.74	107.75	115.21
1	E	56	ALA	CA-C-O	-5.71	114.49	120.55
1	E	93	SER	O-C-N	5.53	129.06	122.26
1	E	117	ARG	CA-CB-CG	-5.52	103.06	114.10
1	E	103	ILE	CA-CB-CG2	5.50	119.86	110.50
2	I	18	ALA	CB-CA-C	-5.42	110.34	116.63
1	E	147	SER	CA-C-N	-5.41	112.08	121.39
1	E	147	SER	C-N-CA	-5.41	112.08	121.39
1	E	111	ALA	N-CA-C	-5.33	102.99	110.50
1	E	89	ILE	N-CA-CB	-5.31	105.73	112.15
1	E	91	HIS	CA-C-N	5.22	125.53	119.47
1	E	91	HIS	C-N-CA	5.22	125.53	119.47
1	E	87	LYS	N-CA-CB	-5.21	101.70	111.13
1	E	199	VAL	CA-C-N	-5.17	116.78	123.19
1	E	199	VAL	C-N-CA	-5.17	116.78	123.19
1	E	50	GLN	CG-CD-NE2	-5.13	108.70	116.40
1	E	37	SER	O-C-N	-5.13	115.61	122.28
1	E	113	SER	N-CA-CB	5.07	118.69	110.17
1	E	67	LEU	CD1-CG-CD2	-5.04	99.72	110.80
1	E	202	SER	CB-CA-C	-5.04	104.58	111.73
1	E	100	ASN	CA-C-O	-5.03	115.52	121.16
1	E	70	GLU	CB-CG-CD	-5.00	104.10	112.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	109	LYS	Mainchain
1	E	111	ALA	Mainchain
1	E	120	SER	Mainchain
1	E	167	SER	Mainchain
1	E	180	MET	Mainchain
1	E	198	PRO	Mainchain
1	E	21	THR	Mainchain
1	E	228	TYR	Sidechain
1	E	33	LEU	Mainchain
1	E	37	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	E	39	TYR	Sidechain
1	E	47	ILE	Mainchain
1	E	58	CYS	Mainchain
1	E	59	TYR	Sidechain
1	E	70	GLU	Mainchain,Peptide
1	E	76	VAL	Mainchain
1	E	78	GLY	Mainchain
2	I	17	LEU	Mainchain
2	I	19	GLU	Mainchain

5.2 Too-close contacts [i](#)

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	E	1629	0	1588	17	0
2	I	222	0	214	1	0
3	E	126	0	0	0	1
3	I	14	0	0	0	0
All	All	1991	0	1802	18	1

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 (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:E:48:ASN:C	1:E:48:ASN:HD22	2.09	0.61
1:E:47:ILE:HD11	1:E:242:ILE:HD11	1.84	0.60
1:E:48:ASN:HD22	1:E:50:GLN:H	1.52	0.57
1:E:64:GLN:NE2	1:E:66:ARG:HE	2.03	0.56
1:E:64:GLN:HE22	1:E:66:ARG:HH21	1.56	0.53
1:E:100:ASN:HD21	1:E:179:ASN:HD22	1.57	0.53
1:E:98:THR:O	1:E:99:LEU:HB2	2.13	0.49
1:E:17:VAL:O	1:E:188:LYS:HA	2.14	0.48
1:E:199:VAL:HG21	1:E:228:TYR:CD1	2.49	0.47
2:I:3:CYS:HA	2:I:4:PRO:HD2	1.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLN:HG3	1:E:111:ALA:HA	1.98	0.46
1:E:48:ASN:HD21	1:E:51:TRP:HD1	1.64	0.45
1:E:67:LEU:HD23	1:E:118:VAL:CG1	2.47	0.44
1:E:101:ASN:ND2	1:E:234:TYR:OH	2.50	0.43
1:E:171:ALA:C	1:E:173:PRO:HD3	2.43	0.43
1:E:220:CYS:H	1:E:221:GLN:NE2	2.18	0.42
1:E:48:ASN:ND2	1:E:50:GLN:H	2.16	0.42
1:E:213:VAL:HG22	1:E:228:TYR:HE1	1.86	0.40

All (1) 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)
3:E:968:HOH:O	3:E:970:HOH:O[3_555]	0.15	2.05

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	E	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	I	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
All	All	248/252 (98%)	239 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	184/184 (100%)	177 (96%)	7 (4%)	29	29
2	I	26/26 (100%)	23 (88%)	3 (12%)	5	3
All	All	210/210 (100%)	200 (95%)	10 (5%)	23	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	48	ASN
1	E	61	SER
1	E	76	VAL
1	E	105	LEU
1	E	113	SER
1	E	149	THR
1	E	240	GLN
2	I	1	ARG
2	I	12	LYS
2	I	19	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	GLN
1	E	48	ASN
1	E	50	GLN
1	E	64	GLN
1	E	97	ASN
1	E	100	ASN
1	E	101	ASN
1	E	175	GLN
1	E	210	GLN
1	E	221	GLN
1	E	240	GLN

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 oligosaccharides 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.