



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:22 AM UTC

PDB ID : 4CAA / pdb_00004caa
Title : CLEAVED ANTICHYMOTRYPSIN T345R
Authors : Lukacs, C.M.; Christianson, D.W.
Deposited on : 1997-08-14
Resolution : 2.90 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

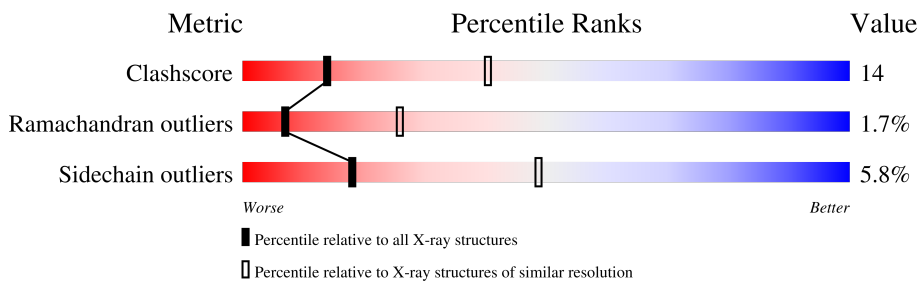
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	341	
2	B	37	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2927 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 ANTICHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	26	0	0
			2657	1703	436	507	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	ARG	THR	engineered mutation	UNP P01011

- Molecule 2 is a protein called ANTICHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	33	Total	C	N	O	S	0	0	0
			270	177	46	45	2			

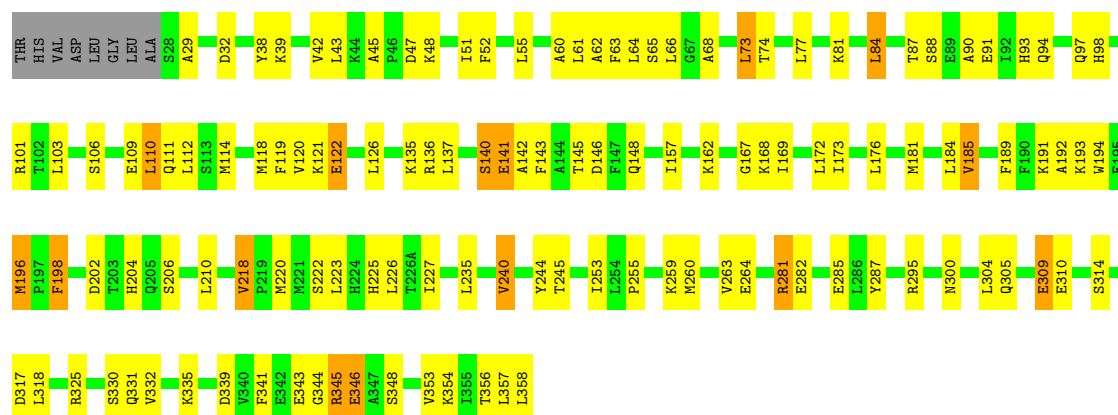
3 Residue-property plots

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.

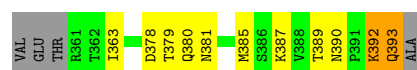
• Molecule 1: ANTICHYMOTRYPSIN

Chain A: 



• Molecule 2: ANTICHYMOTRYPSIN

Chain B: 



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	72.83Å 83.51Å 82.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	89.4 (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2927	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.73	4/2707 (0.1%)	1.06	14/3656 (0.4%)
2	B	0.70	0/276	1.20	2/373 (0.5%)
All	All	0.73	4/2983 (0.1%)	1.07	16/4029 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	SER	C-N	-10.86	1.19	1.33
1	A	141	GLU	N-CA	-10.72	1.31	1.45
1	A	140	SER	CA-C	-6.14	1.44	1.53
1	A	141	GLU	CA-C	-5.65	1.45	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	CA-C-N	9.39	131.58	119.84
1	A	45	ALA	C-N-CA	9.39	131.58	119.84
2	B	392	LYS	N-CA-C	-7.46	96.58	108.73
2	B	381	ASN	N-CA-C	-7.31	98.55	108.86
1	A	346	GLU	N-CA-C	7.07	118.93	108.60
1	A	137	LEU	N-CA-C	6.22	120.07	112.23
1	A	196	MET	N-CA-C	-6.00	98.91	108.82
1	A	198	PHE	N-CA-C	-5.81	101.09	110.32
1	A	172	LEU	N-CA-C	-5.59	104.58	111.40
1	A	309	GLU	N-CA-C	5.55	120.31	112.93
1	A	47	ASP	N-CA-C	5.49	118.97	112.72
1	A	244	TYR	N-CA-C	-5.44	102.00	110.42
1	A	202	ASP	N-CA-C	5.33	119.77	113.16
1	A	204	HIS	N-CA-C	5.28	117.27	108.99
1	A	141	GLU	CB-CA-C	5.14	122.12	110.67
1	A	84	LEU	N-CA-C	5.12	119.01	112.87

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	2657	0	2672	82	0
2	B	270	0	280	9	0
All	All	2927	0	2952	84	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 14.

All (84) 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:285:GLU:HG2	2:B:363:ILE:HD12	1.53	0.91
1:A:140:SER:C	1:A:141:GLU:HG3	2.06	0.79
1:A:341:PHE:HD2	1:A:345:ARG:HG3	1.49	0.77
1:A:295:ARG:HH22	2:B:393:GLN:HG3	1.52	0.73
1:A:305:GLN:HE21	1:A:305:GLN:HA	1.54	0.72
1:A:339:ASP:HB3	1:A:341:PHE:CE2	2.24	0.71
1:A:181:MET:SD	1:A:357:LEU:HD13	2.29	0.71
1:A:39:LYS:HE2	1:A:264:GLU:O	1.92	0.68
1:A:253:ILE:O	1:A:255:PRO:HD3	1.92	0.68
1:A:341:PHE:CD2	1:A:345:ARG:HG3	2.29	0.68
1:A:110:LEU:HB2	1:A:192:ALA:HB2	1.76	0.65
1:A:330:SER:HB2	1:A:356:THR:HG23	1.79	0.64
1:A:119:PHE:HB3	1:A:145:THR:OG1	1.97	0.64
1:A:140:SER:C	1:A:141:GLU:CG	2.71	0.63
1:A:88:SER:OG	1:A:91:GLU:HG3	1.98	0.63
1:A:285:GLU:HG3	1:A:287:TYR:HE1	1.64	0.61
1:A:118:MET:HB3	1:A:184:LEU:HD23	1.85	0.59
1:A:198:PHE:HD1	1:A:222:SER:O	1.85	0.59
1:A:55:LEU:HG	1:A:114:MET:HE1	1.85	0.58
1:A:77:LEU:HD13	1:A:84:LEU:HD21	1.86	0.58
1:A:38:TYR:O	1:A:42:VAL:HG23	2.04	0.57
1:A:259:LYS:O	1:A:263:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CE1	2:B:385:MET:HG2	2.40	0.56
1:A:285:GLU:HG3	1:A:287:TYR:CE1	2.41	0.55
1:A:111:GLN:HB2	1:A:191:LYS:HB3	1.88	0.55
1:A:305:GLN:HA	1:A:305:GLN:NE2	2.18	0.55
1:A:339:ASP:HB3	1:A:341:PHE:HE2	1.70	0.55
1:A:343:GLU:HG2	1:A:345:ARG:HG2	1.89	0.55
1:A:61:LEU:O	1:A:64:LEU:HB3	2.06	0.54
1:A:173:ILE:HG21	1:A:176:LEU:HD13	1.88	0.54
1:A:29:ALA:O	1:A:32:ASP:HB3	2.08	0.54
1:A:281:ARG:HH11	1:A:281:ARG:HB2	1.72	0.54
1:A:66:LEU:HD23	1:A:93:HIS:NE2	2.21	0.53
1:A:90:ALA:O	1:A:94:GLN:HG2	2.09	0.53
1:A:227:ILE:HD12	1:A:240:VAL:HG13	1.90	0.52
1:A:39:LYS:O	1:A:43:LEU:HD13	2.11	0.50
1:A:206:SER:OG	1:A:220:MET:HB2	2.12	0.49
1:A:295:ARG:NH2	2:B:393:GLN:HG3	2.24	0.48
1:A:81:LYS:N	1:A:81:LYS:HD2	2.28	0.48
1:A:52:PHE:HE1	2:B:385:MET:HG2	1.79	0.48
1:A:281:ARG:HG2	1:A:282:GLU:N	2.29	0.48
1:A:162:LYS:HG3	1:A:167:GLY:HA2	1.97	0.47
1:A:194:TRP:O	1:A:245:THR:HG23	2.14	0.47
1:A:226:LEU:HG	1:A:227:ILE:HG23	1.95	0.47
1:A:77:LEU:CD1	1:A:84:LEU:HD21	2.44	0.47
1:A:253:ILE:HD12	1:A:253:ILE:N	2.29	0.47
1:A:168:LYS:HD2	1:A:346:GLU:OE1	2.15	0.46
2:B:387:LYS:HD2	2:B:389:THR:HG23	1.96	0.46
1:A:98:HIS:O	1:A:101:ARG:HB2	2.15	0.46
1:A:112:LEU:HA	1:A:189:PHE:O	2.17	0.45
1:A:119:PHE:CD1	1:A:157:ILE:HG12	2.51	0.45
1:A:119:PHE:HE1	1:A:185:VAL:HG11	1.81	0.45
1:A:73:LEU:HD23	1:A:74:THR:N	2.31	0.45
1:A:169:ILE:HG23	1:A:335:LYS:HD3	1.99	0.45
1:A:304:LEU:HD23	1:A:309:GLU:HA	1.98	0.45
1:A:135:LYS:HA	1:A:140:SER:H	1.83	0.45
1:A:260:MET:O	1:A:264:GLU:HG3	2.18	0.44
1:A:118:MET:HE2	1:A:142:ALA:HB2	1.99	0.44
1:A:330:SER:HB3	1:A:354:LYS:O	2.17	0.44
1:A:62:ALA:O	1:A:65:SER:HB2	2.18	0.43
1:A:198:PHE:CE1	1:A:223:LEU:HG	2.53	0.43
1:A:122:GLU:OE2	1:A:146:ASP:HB2	2.18	0.43
1:A:87:THR:HA	1:A:91:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	1:A:331:GLN:HA	2.19	0.43
1:A:332:VAL:HG22	1:A:353:VAL:HG22	2.00	0.43
1:A:110:LEU:HB2	1:A:192:ALA:CB	2.45	0.43
1:A:196:MET:SD	1:A:226:LEU:CD1	3.07	0.42
1:A:210:LEU:HD21	2:B:390:ASN:ND2	2.34	0.42
1:A:344:GLY:O	1:A:345:ARG:HB2	2.19	0.42
1:A:118:MET:CB	1:A:184:LEU:HD23	2.48	0.42
1:A:168:LYS:HD3	1:A:348:SER:OG	2.19	0.42
1:A:118:MET:HG2	1:A:141:GLU:O	2.20	0.42
2:B:387:LYS:CD	2:B:389:THR:HG23	2.50	0.41
1:A:68:ALA:HA	1:A:318:LEU:HD23	2.02	0.41
1:A:94:GLN:O	1:A:97:GLN:HB3	2.21	0.41
1:A:255:PRO:HG2	1:A:260:MET:SD	2.60	0.41
1:A:218:VAL:HG12	2:B:392:LYS:HE3	2.03	0.41
1:A:88:SER:H	1:A:91:GLU:CD	2.29	0.41
1:A:255:PRO:HB3	1:A:263:VAL:HG21	2.03	0.41
1:A:317:ASP:HA	1:A:325:ARG:HG3	2.03	0.41
1:A:314:SER:HA	1:A:358:LEU:HD13	2.03	0.40
1:A:60:ALA:O	1:A:63:PHE:HB3	2.22	0.40
1:A:121:LYS:HA	1:A:145:THR:O	2.22	0.40
1:A:141:GLU:OE1	1:A:143:PHE:CZ	2.74	0.40

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	331/341 (97%)	299 (90%)	28 (8%)	4 (1%)	10	34
2	B	31/37 (84%)	27 (87%)	2 (6%)	2 (6%)	1	3
All	All	362/378 (96%)	326 (90%)	30 (8%)	6 (2%)	7	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	379	THR
1	A	106	SER
1	A	109	GLU
1	A	345	ARG
1	A	122	GLU
2	B	378	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	294/300 (98%)	277 (94%)	17 (6%)	18	49
2	B	32/36 (89%)	30 (94%)	2 (6%)	16	45
All	All	326/336 (97%)	307 (94%)	19 (6%)	18	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	51	ILE
1	A	73	LEU
1	A	103	LEU
1	A	110	LEU
1	A	120	VAL
1	A	126	LEU
1	A	136	ARG
1	A	148	GLN
1	A	185	VAL
1	A	193	LYS
1	A	218	VAL
1	A	225	HIS
1	A	235	LEU
1	A	240	VAL
1	A	281	ARG
1	A	310	GLU

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Mol	Chain	Res	Type
2	B	380	GLN
2	B	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	331	GLN
2	B	393	GLN

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	140:SER	C	141:GLU	N	1.19

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.