

**PDB**  
**(Protein Data Bank)**

Création : 1977  
Refonte: 25 Octobre 1996

**mmCIF**  
**(macro molecular Crytsallographic Information File)**

CIF: 1990  
mmCIF: 1997

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**HEADER**            **COMPLEX (SERINE PROTEASE/INHIBITOR)**            **15-JUL-98**            **3TGI**  
**TITLE**            **WILD-TYPE RAT ANIONIC TRYPSIN COMPLEXED WITH BOVINE**  
**TITLE**            **2 PANCREATIC TRYPSIN INHIBITOR (BPTI)**  
**COMPND**            **MOL\_ID: 1;**  
**COMPND**            **2 MOLECULE: TRYPSIN;**  
**COMPND**            **3 CHAIN: E;**  
**COMPND**            **4 EC: 3.4.21.4;**  
**COMPND**            **5 MOL\_ID: 2;**  
**COMPND**            **6 MOLECULE: BOVINE PANCREATIC TRYPSIN INHIBITOR;**  
**COMPND**            **7 CHAIN: I;**  
**COMPND**            **8 SYNONYM: BPTI**  
**SOURCE**            **MOL\_ID: 1;**  
**SOURCE**            **2 ORGANISM\_SCIENTIFIC: RATTUS NORVEGICUS;**

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SOURCE 6 ORGANISM\_COMMON: BOVINE  
KEYWDS COMPLEX (SERINE PROTEASE/INHIBITOR)  
EXPDTA X-RAY DIFFRACTION  
AUTHOR A.PASTERNAK,D.RINGE,L.HEDSTROM  
REVDAT 1 23-DEC-98 3TGI 0  
JRNL AUTH A.PASTERNAK,D.RINGE,L.HEDSTROM  
JRNL TITL COMPARISON OF ANIONIC AND CATIONIC TRYPSINOGENS:

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REMARK 2  
**REMARK 2 RESOLUTION. 1.8 ANGSTROMS.**  
REMARK 3  
REMARK 3 REFINEMENT.  
REMARK 3 PROGRAM : X-PLOR 3.851  
REMARK 3 AUTHORS : BRUNGER

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SEQRES	1	E	223	ILE	VAL	GLY	GLY	TYR	THR	CYS	GLN	GLU	ASN	SER	VAL	PRO
SEQRES	2	E	223	TYR	GLN	VAL	SER	LEU	ASN	SER	GLY	TYR	HIS	PHE	CYS	GLY
SEQRES	3	E	223	GLY	SER	LEU	ILE	ASN	ASP	GLN	TRP	VAL	VAL	SER	ALA	ALA
SEQRES	4	E	223	HIS	CYS	TYR	LYS	SER	ARG	ILE	GLN	VAL	ARG	LEU	GLY	GLU
SEQRES	5	E	223	HIS	ASN	ILE	ASN	VAL	LEU	GLU	GLY	ASN	GLU	GLN	PHE	VAL
SEQRES	6	E	223	ASN	ALA	ALA	LYS	ILE	ILE	LYS	HIS	PRO	ASN	PHE	ASP	ARG
SEQRES	7	E	223	LYS	THR	LEU	ASN	ASN	ASP	ILE	MET	LEU	ILE	LYS	LEU	SER
SEQRES	8	E	223	SER	PRO	VAL	LYS	LEU	ASN	ALA	ARG	VAL	ALA	THR	VAL	ALA
SEQRES	9	E	223	LEU	PRO	SER	SER	CYS	ALA	PRO	ALA	GLY	THR	GLN	CYS	LEU
SEQRES	10	E	223	ILE	SER	GLY	TRP	GLY	ASN	THR	LEU	SER	SER	GLY	VAL	ASN
SEQRES	11	E	223	GLU	PRO	ASP	LEU	LEU	GLN	CYS	LEU	ASP	ALA	PRO	LEU	LEU
SEQRES	12	E	223	PRO	GLN	ALA	ASP	CYS	GLU	ALA	SER	TYR	PRO	GLY	LYS	ILE

HELIX	1	1	ALA	E	56	CYS	E	58	5					
HELIX	2	2	GLN	E	165	SER	E	171	1					
HELIX	3	3	VAL	E	231	ASN	E	233	5					
HELIX	4	4	VAL	E	235	ALA	E	243	1					
HELIX	5	5	ASP	I	3	LEU	I	6	5					
HELIX	6	6	ALA	I	48	THR	I	54	1					
SHEET	1	A 7	GLN	E	81	ASN	E	84	0					
SHEET	2	A 7	GLN	E	64	LEU	E	68	-1	N	LEU	E	68	O GLN E 81
SHEET	3	A 7	GLN	E	30	ASN	E	34	-1	N	ASN	E	34	O GLN E 64
SHEET	4	A 7	HIS	E	40	ASN	E	48	-1	N	GLY	E	44	O VAL E 31

ATOM	9	N	VAL	E	17	-21.016	-84.840	-0.647	1.00	8.04
ATOM	10	CA	VAL	E	17	-22.339	-84.380	-0.246	1.00	8.43
ATOM	11	C	VAL	E	17	-22.231	-83.815	1.163	1.00	8.46
ATOM	12	O	VAL	E	17	-21.589	-84.408	2.030	1.00	6.70
ATOM	13	CB	VAL	E	17	-23.371	-85.539	-0.231	1.00	8.84
ATOM	14	CG1	VAL	E	17	-24.738	-85.013	0.170	1.00	9.11
ATOM	15	CG2	VAL	E	17	-23.443	-86.204	-1.592	1.00	11.01
ATOM	16	N	GLY	E	18	-22.845	-82.655	1.379	1.00	10.20
ATOM	17	CA	GLY	E	18	-22.832	-82.039	2.693	1.00	10.45
ATOM	18	C	GLY	E	18	-21.513	-81.431	3.120	1.00	11.25
ATOM	19	O	GLY	E	18	-21.303	-81.197	4.307	1.00	12.24
ATOM	20	N	GLY	E	19	-20.628	-81.172	2.160	1.00	10.69
ATOM	21	CA	GLY	E	19	-19.342	-80.582	2.478	1.00	10.12
ATOM	22	C	GLY	E	19	-19.323	-79.077	2.269	1.00	12.16
ATOM	23	O	GLY	E	19	-20.362	-78.412	2.294	1.00	13.16
ATOM	24	N	TYR	E	20	-18.132	-78.536	2.056	1.00	12.08

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