

表四 Serine ligand test sets

PBD ID	Classification	HEM group	Structure	Source	Resolution	R-factor	R-free
1a3b	serine protease/inhibitor	T29	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	1.80Å	0.17	0.23
1a3e	serine protease/inhibitor	T16	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	1.85Å	0.17	0.22
1a46	serine protease/inhibitor	ASP-PHE-GLU-GLU-ILE-PRO-GLU-GLU-TYS-LEU RNG-BCY-LYS-OHO	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.12Å	0.155	
1a4w	serine protease/inhibitor	ASP-PHE-GLU-GLU-ILE-PRO-GLU-GLU-TYS ANS-ARG-2EP-KTH	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	1.80Å	0.155	
1a5g	serine protease/inhibitor	BIC-ARG-EOA	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.06Å	0.158	
1abj	serine protease/inhibitor	PHE-PRO-ARG-CH2	<i>Alpha-thrombin</i>	<i>Human plasma</i>	2.40Å	0.144	
1ae8	serine protease/inhibitor	AZL	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.00Å	0.169	
1aht	serine protease/inhibitor	APA	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	1.60Å	0.187	
1aq7	Serine protease	AEB	<i>Trypsin.</i>	<i>Bos taurus. Bovine</i>	2.20Å	0.164	0.237
1auj	Hydrolase	PPB	<i>Trypsin.</i>	<i>Bos taurus. Bovine</i>	2.10Å	0.169	
1awf	protease/inhibitor	GR4	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.20Å	0.196	
1awh	protease/inhibitor	GR3	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	3.00Å	0.202	
1ay6	serine protease/inhibitor	HMF-PRO-ARG-HHO	<i>Thrombin</i>	<i>Homo sapiens. Human</i>	1.80Å	0.166	
1az8	Serine protease	IN4	<i>Trypsin.</i>	<i>Bos taurus. Bovine</i>	1.80Å	0.188	
1b5g	serine protease/inhibitor	BCC-ARG-THZ	<i>Alpha-thrombin.</i>	<i>Homo sapiens. Human</i>	2.07Å	0.164	
1ba8	serine protease/inhibitor	PHE-GLU-GLY-ILE-PRO-GLY-GLU-TYS PMS-RON-GLY-ARG	<i>Thrombin</i>	<i>Homo sapiens. Human</i>	1.80Å	0.152	
1bb0	serine protease/inhibitor	PMS-RON-GLY-3GA	<i>Thrombin. Chain</i>	<i>Homo sapiens. Human</i>	2.10Å	0.157	
1bcr	serine protease/inhibitor	AIP	<i>Serine carboxypeptidase ii</i>	<i>Triticum vulgare</i>	2.50Å	0.162	
1bcs	serine protease/inhibitor	CST	<i>Serine carboxypeptidase ii</i>	<i>Triticum vulgare</i>	2.10Å	0.174	
1bcu	serine protease/inhibitor	PRL	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.00Å	0.189	0.212
1bhx	Serine protease	ASP-PHE-GLU-GLU-ILE	<i>Alpha thrombin</i>	<i>Homo sapiens. Human</i>	2.30Å.	0.187	0.232.
1bjv	Serine protease	GB6	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.80Å	0.171	
1bjv	Serine protease	GB8	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.80Å	0.196	
1bmm	serine protease/inhibitor	ASP-PHE-GLU-GLU-ILE-PRO-GLU-GLU-TYR BM2	<i>Alpha-thrombin</i>	<i>Homo sapiens. Human</i>	2.60Å	0.177.	
1btw	Hydrolase (serine proteinase)	BOC-ALA-VAL-BLY-HPG	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.80Å	0.164	
1btx	Hydrolase (serine proteinase)	BOC-ALA-VAL-BLY-ETY	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.80Å	0.14	
1c1n	Hydrolase/Hydrolase Inhibitor	BAM	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	1.40Å	0.186	0.214
1c1p	Hydrolase/hydrolase inhibitor	BAI	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	1.37Å	0.178	0.192
1c1s	Hydrolase/hydrolase inhibitor	BAB	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	1.63Å	0.185	0.206
1c1w	Blood clotting	BAH	<i>Alpha thrombin</i>	<i>Homo sapiens. Human</i>	1.90Å	0.203	0.242
		TYS					
1c2d	Hydrolase/hydrolase inhibitor	BAK	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	1.65Å	0.193	0.211
1c2k	Hydrolase/hydrolase inhibitor	ABI	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	1.65Å	0.202	0.243
1eb1	Serine proteinase	ALC-PRO-MMO	<i>Thrombin heavy chain</i>	<i>Homo sapiens. Human</i>	1.80Å	0.191	0.22
1eb2	Hydrolase	BPO	<i>Trypsin</i>	<i>Bos taurus. Bovine</i>	2.00Å	0.178	0.244
1gbt	Hydrolase(serine proteinase)	GBS	<i>Beta-trypsin</i>	<i>Bovine</i>	2.00Å	0.162	
1gi0	Hydrolase	BMZ	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.42Å	0.179	0.219
1gi2	Hydrolase	122	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.38Å	0.184	0.205
1gi5	Hydrolase	123	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.60Å	0.2	0.216
1gi6	Hydrolase	124	<i>Beta-trypsin</i>	<i>Bos taurus. Bovine</i>	1.49Å	0.186	0.209
1gi7	Blood clotting, hydrolase	120	<i>Urokinase-type plasminogen activator</i>	<i>Homo sapiens. Human</i>	1.79Å	0.185	0.22
1gi4	Blood clotting, hydrolase	132	<i>Thrombin</i>	<i>Homo sapiens. Human</i>	1.81Å	0.202	0.236
1h8d	Serine protease	PHW	<i>Thrombin</i>	<i>Homo sapiens. Human</i>	1.40Å	0.17	0.220.
1hpg	Hydrolase (serine protease)	BOC-ALA-ALA-PRO-GLU	<i>Glutamic acid-specific protease</i>	<i>Glutamic acid-specific protease</i>	1.50Å	0.181	
1o2g	Blood clotting, hydrolase	696	<i>Thrombin</i>	<i>Homo sapiens. Human</i>	1.58Å	0.219	0.25
1tng	Hydrolase(serine proteinase)	AMC	<i>Trypsin</i>	<i>Bovine</i>	1.80Å	0.172	
1dy8	Serine protease	CBZ-ILE-LEU-FKI	<i>Protease/helicase ns.3</i>	<i>Hepatitis c virus (isolate 1)</i>	2.40Å	0.216	0.318
1dy9	Serine protease	BOC-GLU-LEU-FKI	<i>Protease/helicase ns.3</i>	<i>Hepatitis c virus (isolate 1)</i>	2.10Å	0.207	0.275
MbBBI	Virus/viral protein/inhibitor		<i>ns3 protease domain</i>	<i>Dengue virus. Virus</i>	2.10Å	0.199	0.243
1rt1	Nucleotidyltransferase	MKC	<i>HIV-1 reverse transcriptase</i>	<i>Human immunodeficiency virus</i>	2.55Å	0.197	