Supplementary Materials: Crystal Structure of Bovine Alpha-Chymotrypsin in Space Group $P6_5$

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Table S1. Summary of space groups and unit cell parameters for representative bovine α-chymotrypsin crystal structures currently deposited at the PDB.

PDB ID	Space Group	*a*, *b*, *c* (Å)	α, β, γ (°)	Ligand Present?
3RU4	P 1	49.477, 54.571, 69.286	67.28, 71.04, 73.55	Yes
2CHA	P 1 21 1	49.1, 67.4, 65.9	90, 101.7, 90	Yes
4CHA	P 1 21 1	49.23, 67.39, 65.99	90, 101.8, 90	No
5CHA	P 1 21 1	49.29, 67.48, 65.94	90, 102.2, 90	No
6CHA	P 1 21 1	49.27, 67.16, 65.91	90, 101.68, 90	Yes
1CHO	P 1 21 1	44.92, 54.52, 57.18	90, 103.9, 90	Yes
1ACB	P 1 21 1	55.3, 59.4, 42.5	90, 99.1, 90	Yes
1N8O	P 1 21 1	95.5, 63.8, 79.6	90, 91.7, 90	Yes
1YPH	P 1 21 1	43.83, 77.51, 62.77	90, 106.3, 90	No
2Y6T	P 1 21 1	97.31, 48.278, 174.636	90, 103.96, 90	Yes
4Q2K	P 1 21 1	45.61, 109.34, 89.07	90, 93.47, 90	Yes
1CA0	P 21 21 2	70.522, 181.488, 46.328	90, 90, 90	Yes
5J4Q	P 21 21 2	76.163, 79.28, 51.529	90, 90, 90	Yes
5J4S	P 21 21 2	74.745, 78.793, 48.003	90, 90, 90	Yes
1CHG	P 21 21 21	52, 63.9, 77.1	90, 90, 90	No
2CGA	P 21 21 21	59.3, 77.1, 110.1	90, 90, 90	No
3BG4	P 21 21 21	44.274, 43.992, 122.57	90, 90, 90	Yes
2GCH	P 42 21 2	69.6, 69.6, 97.4	90, 90, 90	No
3GCH	P 42 21 2	69.7, 69.7, 97.5	90, 90, 90	Yes
4GCH	P 42 21 2	69.7, 69.7, 97.5	90, 90, 90	Yes
5GCH	P 42 21 2	69.7, 69.7, 97.5	90, 90, 90	Yes
6GCH	P 42 21 2	69.3, 69.3, 97.2	90, 90, 90	Yes
7GCH	P 42 21 2	69.3, 69.3, 97.6	90, 90, 90	Yes
1GCT	P 42 21 2	69.8, 69.8, 98.1	90, 90, 90	Yes
2GCT	P 42 21 2	69.8, 69.8, 98.1	90, 90, 90	Yes
3GCT	P 42 21 2	70, 70, 97.7	90, 90, 90	Yes
8GCH	P 42 21 2	69, 69, 95.3	90, 90, 90	Yes
1CGI	P 42 21 2	84.4, 84.4, 86.7	90, 90, 90	Yes
1CGJ	P 42 21 2	84.4, 84.4, 86.7	90, 90, 90	Yes
1GMC	P 42 21 2	69.54, 69.52, 98.01	90, 90, 90	Yes
1GMD	P 42 21 2	69.34, 69.32, 97.51	90, 90, 90	Yes
1GCD	P 42 21 2	69, 69, 95.3	90, 90, 90	Yes
1GHA	P 42 21 2	69.6, 69.6, 97.51	90, 90, 90	Yes
1GHB	P 42 21 2	69.6, 69.6, 97.51	90, 90, 90	Yes
1GMH	P 42 21 2	69.9, 69.9, 96.7	90, 90, 90	Yes
2GMT	P 42 21 2	69.5, 69.5, 97.6	90, 90, 90	Yes
1AB9	P 42 21 2	69.52, 69.52, 97.81	90, 90, 90	Yes
1AFQ	P 42 21 2	69.84, 69.84, 97.36	90, 90, 90	Yes
1VGC	P 42 21 2	69.86, 69.86, 97.15	90, 90, 90	Yes
2VGC	P 42 21 2	69.689, 69.689, 96.787	90, 90, 90	Yes
3VGC	P 42 21 2	69.895, 69.895, 97.142	90, 90, 90	Yes
4VGC	P 42 21 2	69.89, 69.89, 96.14	90, 90, 90	Yes
1DLK	P 42 21 2	121.17, 121.17,116.08	90, 90, 90	Yes
1EX3	P 42 21 2	114.9, 114.9, 52.8	90, 90, 90	No
1GG6	P 42 21 2	69.19, 69.19, 95.44	90, 90, 90	Yes
1GGD	P 42 21 2	69.6, 69.6, 97.55	90, 90, 90	Yes
1K2I	P 42 21 2	69.852, 69.852, 97.38	90, 90, 90	Yes
2P8O	P 42 21 2	68.989, 68.989, 95.892	90, 90, 90	Yes

1MTN	P 61	102.45, 102.45, 207,57	90, 90, 120	Yes
1CBW	P 61	101.6, 101.6, 205.9	90, 90, 120	Yes
1HJA	P 61	103.47, 103.47, 47.12	90, 90, 120	Yes
1P2M	P 61	100.34, 100.34, 204.68	90, 90, 120	Yes
1P2N	P 61	100.01, 100.01, 205.1	90, 90, 120	Yes
1P2O	P 61	100.17, 100.17, 206.14	90, 90, 120	Yes
1P2Q	P 61	99.57, 99.57, 205.22	90, 90, 120	Yes
1T7C	P 61	99.98, 99.98, 205.37	90, 90, 120	Yes
1T8L	P 61	99.52, 99.52, 205.38	90, 90, 120	Yes
1T8M	P 61	99.91, 99.91, 205	90, 90, 120	Yes
1T8N	P 61	99.96, 99.96, 205.36	90, 90, 120	Yes
1T8O	P 61	100.23, 100.23, 204.65	90, 90, 120	Yes
1GL1	P 65	92.958, 92.958, 165.841	90, 90, 120	Yes
*6DI8	*P 65	*126.81, 126.81, 122.03	*90, 90, 120	*No
1GL0	P 65 2 2	85.853, 85.853, 187.983	90, 90, 120	Yes
1OXG	I 2 2 2	56.187, 76.382, 105.098	90, 90, 90	Yes
3T62	H 3	199.706, 199.706, 54.572	90, 90, 120	Yes

† "Ligand" includes small molecule, peptide and small protein protease inhibitors. *Current study.

Table S2: Crystallographic interfaces with areas greater than 100 Å^2 for unliganded bovine α-chymotrypsin in space group $P2_1$ (PDB: 4CHA).

Interface #	Symmetry Operation	Interface Area (Å^2)	Subunits†
1	X, Y, Z	1035	B, A
2	-X, Y-1/2, -Z+1	522	A, B
3	X, Y, Z-1	448	B, A
4	-X+1, Y-1/2,-Z+1	336	A, B
5	-X+1, Y-1/2,-Z+1	163	B, A
6	X-1, Y, Z	148	A, A
7	X-1, Y, Z	136	B, B

† Subunits A and B constitute the asymmetric unit. Each subunit is composed of three separate polypeptide chains, crosslinked by disulphide bonds.