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Supporting information for article:

The thrombospondin module 1 domain (TSP1) of the matricellular protein CCN3 shows an atypical disulfide pattern and incomplete CWR layers

Emma-Ruoqi Xu, Aleix Lafita, Alex Bateman and Marko Hyvönen

Table S1 Currently available TSP1 domain structures in the Protein Data Bank

The last column describes the connectivity of the top disulfide bond, with those that lacking it marked as n/a.

UniProt entry	UniProt residues	PDB ID	PDB residues	Connectivity
ATS13_HUMAN	388 - 438	3VN4 , 3GHN, 3GHM	388 - 438	3-4
CO6_HUMAN	28 - 78	3T5O , 4A5W, 4E0S	7-57	1-4
	566 - 612	3T5O , 4A5W, 4E0S	545 - 591	3-4
	85 - 133	3T5O , 4A5W, 4E0S	64 - 112	1-4
CO8A_HUMAN	540 - 582	3OJY	510 - 552	3-4
CO8B_HUMAN	546 - 590	3OJY	492 - 536	n/a
	68 - 116	3OJY	14 - 62	1-4
M1V0B0_PLAFA	329 - 377	6B0S	326 - 374	n/a
O00816_TOXGO	274 - 331	4OKR , 4OKU	274 - 331	1-4 (+)
Q7K740_PLAF7	326 - 374	3VDJ, 3VDK, 3VDL	326 - 374	n/a
Q9TVF0_PLAVI	241 - 283	4HQL, 4HQN , 4HQO	241 - 283	1-4
SPON1_RAT	446 - 494	1SZL	446 - 494	1-4
	618 - 665	1VEX	618 - 665	1-4
TRAP_PLAFA	245 - 288	2BBX	6-49	1-4
TSP1_HUMAN	383 - 428	5FOE	1006 - 1051	3-4
	439 - 489	1LSL , 3R6B	421 - 471	3-4
	496 - 546	1LSL , 3R6B	478 - 528	3-4
UNC5D_RAT	254 - 303	5FTT	254 - 303	3-4
UNC5A_HUMAN	240-288	4V2A	240-288	3-4
PROP_HUMAN	77-134	6S08, 6S0A , 6S0B,	77-134	3-4
	136-186	6RUR, 6RUS, 6SEJ,	136-186	3-4
	191-254	6SV6	191-254	3-4
	255-313		255-313	3-4
	314-376		314-376	3-4
	377-461		377-461	3-4

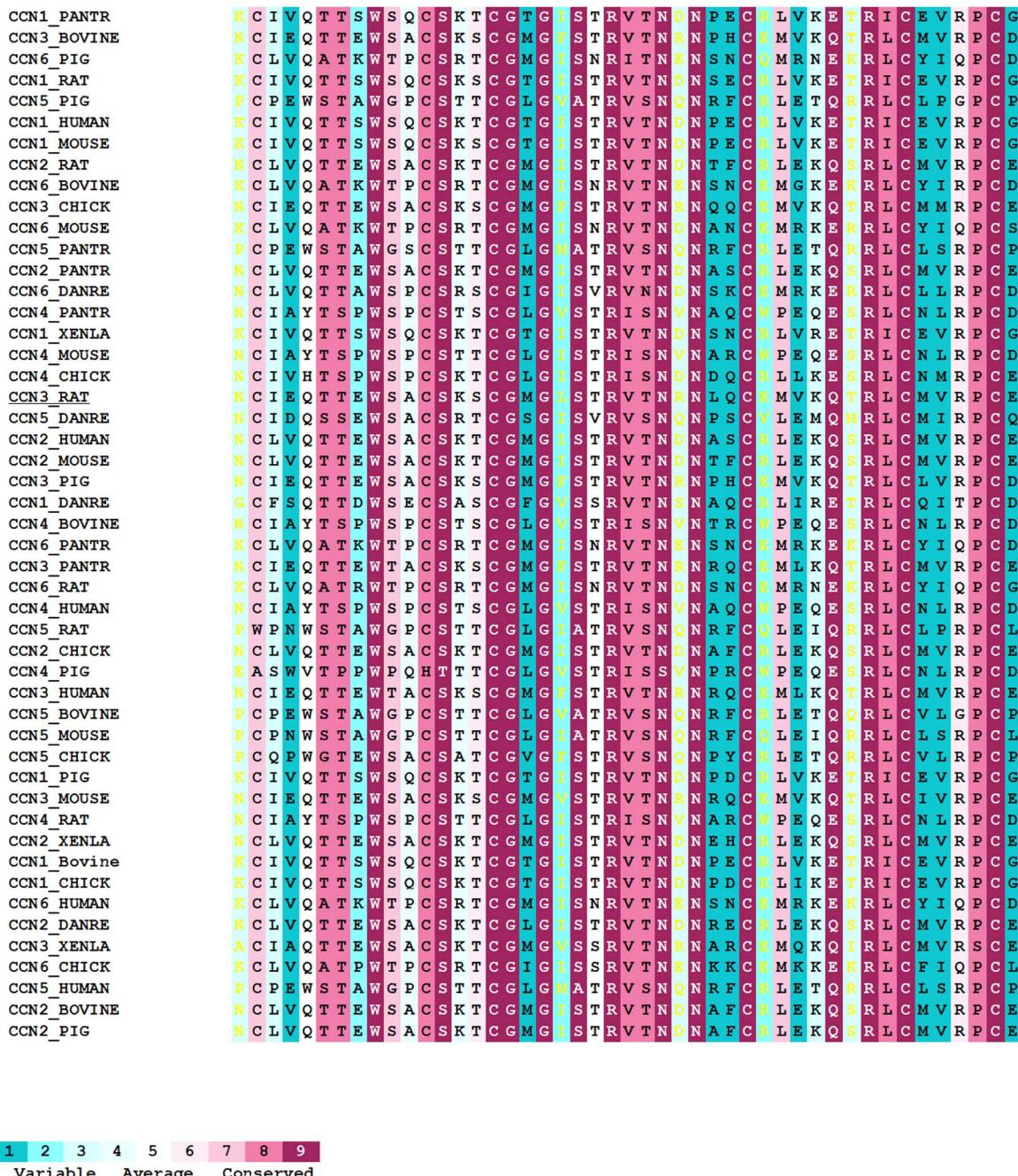


Figure S1 Sequence conservation analysis of the CCN proteins in a range of species generated by the ConSurf Server (<https://consurf.tau.ac.il>) (Ashkenazy *et al.*, 2010).

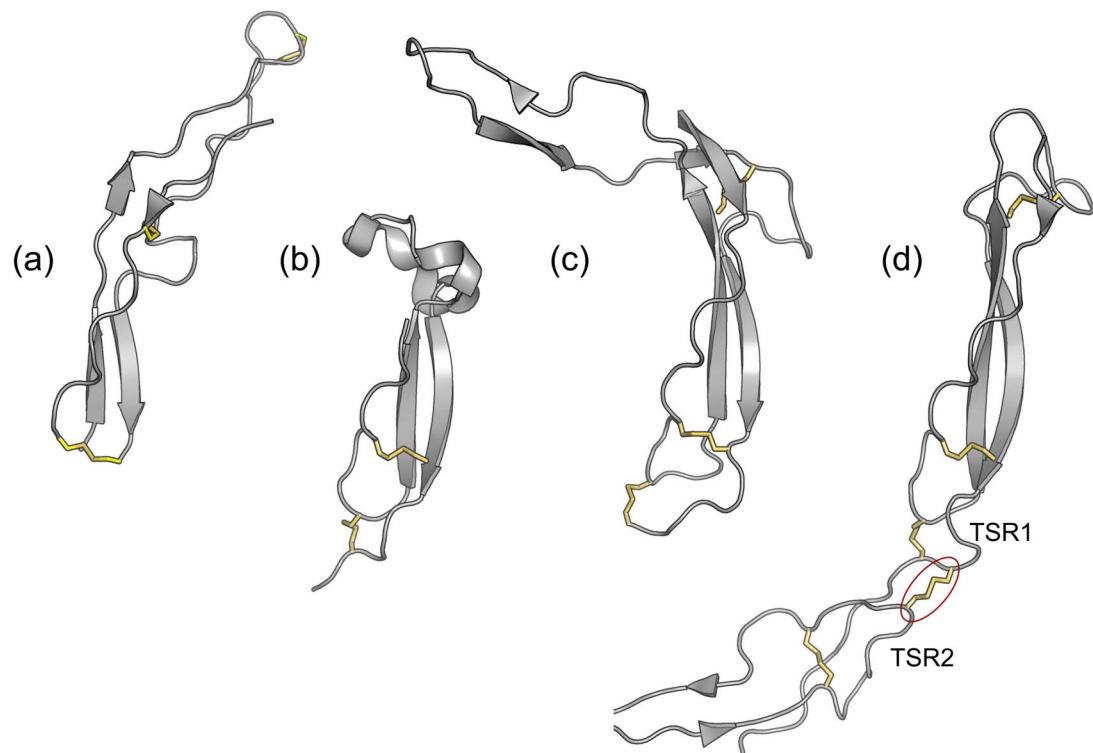


Figure S2 Structures of TSP1 domain from (a) circumsporozoite protein TSP1 domain (PDB 3vdl), (b) Micronemal protein 2 (PDB 4okr), (c) properdin 6th TSP1 (PDB 6s0a), and (d) 1st and 2nd TSP1s of properdin (PDB 6s0a) with their connecting disulfide highlighted by red ellipse.

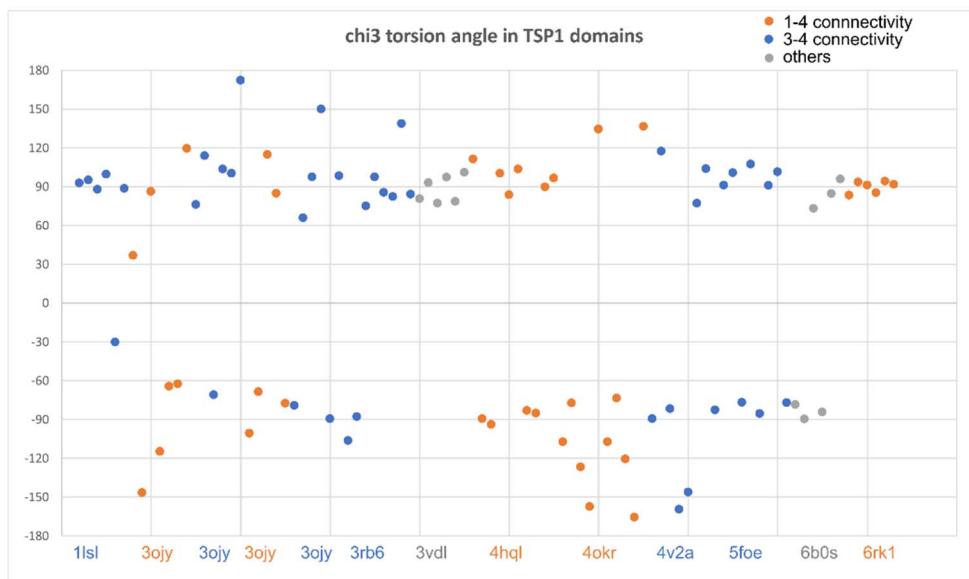


Figure S3 Distribution of disulfide chi3 angles. Selected crystal structures of TSP1 domain were analysed using CCP4 program geomcalc to calculate the torsion angle along the disulfide bond. The angles are plotted for the structures (labelled below) and the values coloured based on the domain connectivity with 1-4 connectivity in orange, 3-4 connectivity and the domains with other connectivity in gray.