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Supporting information for article:

A scalable strategy to solve structures of PDZ domains and their complexes

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Table S1, 48-well ANXA2 crystallization screen				
No.	**Precipitant**	**Buffer (pH)**	**Salts**	**Others**
1	15% PEG 1000			
2	25% PEG 1000	0.1M HEPES pH 7.5		
3	20% PEG 3350	0.1M tri-Sodium citrate pH 5.5		
4	20% PEG 3350	0.1M BIS-TRIS pH 5.5		
5	25% PEG 3350	0.1M Bis-TRIS pH 5.5	0.2M Lithium sulfate	
6	25% PEG 3350	0.1M Bis-TRIS pH 5.5	0.2M Ammonium sulfate	
7	25% PEG 3350	0.1M BIS-TRIS pH 6.5		
8	25% PEG 3350	0.1M TRIS pH 8.5		
9	20% PEG 3350		0.2M Calcium acetate	
10	20% PEG 3350		0.2M Calcium chloride	
11	20% PEG 3350		0.2M Potassium nitrate	
12	20% PEG 3350		0.2M tri-Potassium citrate	
13	20% PEG 3350		0.2M Potassium Sodium tartrate	
14	20% PEG 3350		0.2M Lithium acetate	
15	10% PEG 3350		0.2M Ammonium chloride	
16	20% PEG 3350		0.2M Ammonium nitrate	
17	20% PEG 3350		0.2M tri-Ammonium citrate	
18	20% PEG 3350		0.2M di-Sodium malonate	
19	20% PEG 3350		0.2M Sodium iodide	
20	10% PEG 4000	0.1M Sodium acetate pH 4.6		
21	10% PEG 4000	0.1M HEPES pH 7.5	0.09M Potassium phosphate, 0.09M Ammonium sulfate	20% Glycerol
22	15% PEG 4000	0.1M TRIS pH 8.5	0.2M Ammonium sulfate	
23	10% PEG 4000	0.1M Bis-TRIS pH 6.5	0.2M Ammonium acetate	1.5% Glycerol
24	5% PEG 8000	0.1M Sodium cacodylate pH 6.5		40% MPD
25	15% PEG 8000	0.1M Sodium cacodylate pH 6.5	0.16M Calcium acetate,	20% glycerol
26	20% PEG 8000	0.1M MES pH 6.5	0.2M Calcium acetate,	
27	10% PEG 8000	0.1M HEPES pH 7.5	0.06M Magnesium chloride, 0.06M Calcium chloride,	20% Ethylene glycol
28	10% PEG 8000	0.1M HEPES pH 7.5		9% Ethylene glycol
29	20% PEG 8000	0.1M HEPES pH 7.5	50mM Magnesium acetate	
30	20% PEG 8000	0.1M HEPES pH 7.5		
31	10% PEG 8000	0.1M imidazole pH 8.0		
32	20% PEG 8000	0.1M TRIS pH 8.5	0.2M Magnesium chloride	
33	10% PEG 8000	0.1M TRIS pH 8.5	0.2M Lithium chloride	
34	20% PEG 8000	0.1M CHES pH 9.5	0.05M Magnesium acetate	
35	15% PEG 20,000	0.1M HEPES pH 7.5		
36	7% PEG 20,000, 20% PEG 550 MME	0.1M HEPES pH 7.5		
37	22% PEG Smear Broad	0.1M TRIS pH 8.5		
38	20% PEG Smear Broad	0.1M tri-Sodium citrate pH 5.5	0.15M Magnesium acetate	
39	15% PEG Smear Broad	0.1M MES pH6.5	0.15M Calcium chloride,	5% glycerol
40	25% PEG Smear Broad	0.1M HEPES pH 7.5	0.1M Ammonium sulfate, 0.1M Sodium formate	
41	20% PEG Smear High	0.1M TRIS pH 8.5		
42	12% PEG Smear High	0.1M MES pH 6.5	0.1M Sodium bromide, 0.1M Potassium thiocyanate	
43	18% PEG Smear High	0.1M Bis TRIS-propane pH 8.0	0.2M Ammonium nitrate	
44	12% PEG Smear High	0.1M MES pH 6.5	0.1M Potassium chloride, 0.1M Magnesium acetate	
45	20% PEG Smear High	0.1M HEPES pH 7.5	0.15M Lithium sulfate, 0.05M Magnesium chloride	
46	20% PEG Smear Medium	0.1M tri-Sodium citrate pH 5.5	0.1M Ammonium sulfate, 0.05M Magnesium sulfate	
47	12% PEG Smear Medium	0.1M HEPES pH 7.5	0.15M Magnesium sulfate, 0.05M Ammonium acetate,	
48			0.14M Calcium chloride, 0.07M Sodium acetate	30% Glycerol, 14% 2-Propanol

Table S2. Data collection and refinement statistics.

Fusion strategy	ANXA2^{short}	ANXA2^{short}	ANXA2^{short}	ANXA2^{short}	ANXA2^{long}	ANXA2^{long}	ANXA2^{long}	ANXA2^{long}	ANXA2^{long}	ANXA2^{long}
PDZ-domain	SNX27	SYNJ2BP	DLG1_2	SNTG2	SNTB1	SNTG1	SNTG1	SNTG1	PDZD7_3	LRRC7
PBM peptide	APO, (MERS-E)	HTLV1-TAX1	HTLV1-TAX1	RSK1_-3P	HTLV1-TAX1	RSK1_-3E	PTEN_-1Ac	TRPV3	EXOC4	APO, (HTLV1-TAX1)
Wavelength	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Resolution range	46.17 - 2.0 (2.05 - 2.0)	49.33 - 2.4 (2.46 - 2.4)	43.93 - 1.95 (2.0 - 1.95)	46.43 - 2.44 (2.5-2.44)	47.03 - 2.3 (2.36 - 2.3)	46.68 - 2.5 (2.56 - 2.5)	46.69 - 2.1 (2.15 - 2.1)	44.7 - 2.45 (2.51 – 2.45)	42.75 - 1.7 (1.74 - 1.7)	45.48 - 1.6 (1.64 – 1.6)
Space group	P 2 21 21	P 21 21 21	P 21 21 21	P 1 21 1	P 21 21 21	C 1 2 1	P 21 21 21	P 1 21 1	P 2 21 21	P 21 21 21
Unit cell [a, b, c (Å)]	53.68 59.21 180.96	59.99 99.85 173.34	55.67 61.32 143.05	97.46 60.55 135.21	54.27 61.73 145.25	226.58 59.82 125.21	60.31 61.74 285.39	59.83 132.44 63.66	54.11 60.35 181.68	59.78 70.08 102.44
[α, β, γ (°)]	90 90 90	90 90 90	90 90 90	90 92.421 90	90 90 90	90 117.841 90	90 90 90	90 100.769 90	90 90 90	90 90 90
Total reflections	522508 (37354)	556815 (42236)	485623 (36559)	402115 (27760)	293910 (22774)	352832 (25039)	849085 (65245)	238197 (17473)	885808 (67524)	759945 (55786)
Unique reflections	39829 (2885)	41356 (2991)	36311 (2616)	59163 (4350)	22343 (1644)	51681 (3761)	63552 (4649)	35752 (2621)	64942 (4670)	57570 (4207)
Multiplicity	13.1 (12.9)	13.5 (14.1)	13.3 (14.0)	6.8 (6.4)	13.2 (13.9)	6.8 (6.7)	13.3 (14.0)	6.7 (6.7)	13.6 (14.5)	13.2 (13.26)
Completeness (%)	99.6 (98.9)	99.3 (100)	99.2 (98.2)	99.9 (99.9)	99.4 (99.8)	99.5 (99.9)	100 (100)	99.8 (99.6)	97.6 (96.0)	100 (100)
Mean I/sigma(I)	17.70 (1.16)	8.93 (1.22)	12.58 (1.79)	11.30 (1.18)	16.58 (1.18)	9.56 (1.26)	14.38 (1.71)	8.22 (1.18)	16.64 (1.83)	18.28 (1.57)
Wilson B-factor	38.6	38.89	25.6	48.55	53.66	48.83	36.36	43.97	24.28	20.62
R-meas	12.5 (249)	31.6 (243)	17.8 (160)	14.7 (165.5)	11.2 (224)	19.8 (166)	14.8 (177)	22.2 (204,2)	10.1 (156)	10.6 (195.2)
CC1/2	99.9 (40.3)	99.5 (44.9)	99.8 (64.5)	99.8 (45.4)	99.9 (63.6)	99.5 (53.5)	99.9 (57.0)	99.6 (52.9)	99.9 (71.5)	100(57.2)
R-work	0.1898	0.2028	0.1715	0.1962	0.2049	0.2032	0.1854	0.2203	0.1665	0.1697
R-free	0.2065	0.2439	0.2016	0.2313	0.2603	0.2318	0.218	0.2637	0.1888	0.1983
Number of non-hydrogen atoms	3561	6854	3721	9838	3370	6914	6965	6870	3882	4021
macromolecules	3296	6481	3291	9583	3283	6648	6524	6641	3361	3494
ligands	11	10	33	32	13	45	36	15	17	28
solvent	254	363	397	223	74	221	405	214	504	499
Protein residues	415	822	412	1204	418	836	812	838	411	413
RMS(bonds)	0.002	0.003	0.003	0.002	0.003	0.003	0.006	0.002	0.014	0.004
RMS(angles)	0.48	0.52	0.56	0.45	0.56	0.53	0.7	0.43	1.14	0.65
Ramachandran favored (%)	98.06	97.89	97.29	97.12	97.8	97.83	97.75	97.95	98.77	96.59
Ramachandran allowed (%)	1.69	1.87	2.46	2.63	1.96	1.81	2	1.69	0.99	3.16
Ramachandran outliers (%)	0.24	0.25	0.25	0.25	0.24	0.36	0.25	0.36	0.25	0.24
Rotamer outliers (%)	3.91	3.12	1.11	2.2	2.83	4.13	3.09	2.62	4.32	2.58
Clashscore	3.01	2.62	1.49	3.06	2.71	2.37	2.73	3.28	4.53	1.97
Average B-factor	55.23	53.87	30.79	66.75	71.83	61.69	56.4	63.17	40.4	28.31
macromolecules	55.62	54.27	29.5	67.03	72.07	61.99	56.76	63.67	39.95	26.73
ligands	44.5	67.33	44.41	67.16	75.45	63.02	56.09	66.38	36.44	26.7
solvent	50.55	46.36	40.38	54.54	60.33	52.36	50.56	47.23	43.59	39.49
Number of TLS groups	4	8	3	13	4	6	7	6	3	4
PDB ID	**7PCB**	**7PC9**	**7PC3**	**7QQN**	**7PC4**	**7PC8**	**7PC7**	**7QQL**	**7PC5**	**7QQM**

The PBM peptide that was used for crystallization is indicated in parantheses for APO structures. Note that structure solution revealed that the peptides were not bound to the PDZ domains in these crystals.
Statistics for the highest-resolution shell are shown in parentheses.