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Supplemental Information

Phase Transition in Postsynaptic Densities Underlies Formation of Synaptic Complexes and Synaptic Plasticity

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Supplemental Table1. Data collection and refinement statistics of PSD-95 PDZ3-C/SynGAP PBM complex, related to Figure 1

Data collection and processing	
Source	SSRF-BL17U
Wavelength(Å)	0.9795
Space group	C 2 2 21
Unit cell(a,b,c,Å)	70.286,71.094,115.791
Unit cell(α,β,γ,。)	90,90,90
Resolution range (Å)	50.00–2.90 (2.98 -2.90)
No. of unique reflections	6482 (407)
Redundancy	7.0 (7.1)
I/σ(I)	43.3 (10.9)
Completeness (%)	99.2 (99.3)
R_{merge} (%)[a]	6.8 (26.1)
Structure refinement	
Resolution (Å)	35.55-2.90 (3.00-2.90)
R_{work}[b]/R_{free}[c] (%)	0.2397 (0.3196)/0.2866 (0.3946)
Rmsd bonds/angles (Å/ °)	0.017/1.87
Number of reflections	
Working set	6641 (659)
Test set	314 (36)
Number of Protein atoms	1777
Number of Water atoms	4
Average B factor ($Å^2$)	79.2
Ramachandran plot(%)	
Most favored regions	95.6
Additionally allowed	4.4
Generously allowed	0

Numbers in parentheses represent the value for the highest resolution shell.

[a] $R_{merge} = \sum|Ii - Im|/\sum Ii$, where Ii is the intensity of the measured reflection and Im is the mean intensity of all symmetry related reflections.

[b] $R_{cryst} = \Sigma||Fobs| - |Fcalc||/\Sigma|Fobs|$, where Fobs and Fcalc are observed and calculated structure factors.

[c] $R_{free} = \Sigma T||Fobs| - |Fcalc||/\Sigma T|Fobs|$, where T is a test data set of about 5% of the total reflections randomly chosen and set aside prior to refinement.

Supplemental Table 2. Data collection and refinement statistics of SynGAP coiled-coil domain, related to Figure 2

Data collection and processing				
Dataset	Native	SeMet		
Space group	p21	p21		
Unit cell (a,b,c,Å)	28.803, 236.664, 42.207	29.091, 230.209, 41.654		
Unit cell (α,β,γ,°)	90.000, 96.922, 90.000	90.000, 91.921, 90.000		
Wavelength (Å)	0.97886	0.97949	0.97930	0.91162
Resolution range (Å)	50.00-2.50 (2.54-2.50)	50.00-2.80 (2.85-2.80)	50.00-2.90 (2.95-2.90)	50.00-3.00 (3.05-3.00)
No. of unique reflections	19240(958)	13464(651)	11982(575)	10885(540)
Redundancy	3.8(3.8)	6.1(6.3)	5.9(6.2)	5.0(5.2)
I/σ	22.8(2.7)	36.5(4.7)	33.5(7.6)	31.6(4.6)
Completeness (%)	99.7(100.0)	99.8(100.0)	99.5(100.0)	99.8(100.0)
Rmerge (%) [a]	7.3(60.9)	7.6(48.5)	8.2(36.0)	7.8(48.8)
Structure refinement				
Resolution, Å	39.00-2.50(2.59-2.50)			
R_{work} [b]/R_{free} [c] (%)	0.2229 (0.2973)/0.3070 (0.3693)			
Rmsd bonds/angles (Å/ °)	0.008/0.97			
Average B factor (Å^2)	65.67			
No. of protein atoms	3804			
No. of water molecules	36			
No. of reflections				
Working set	19058 (1875)			
Test set	973 (100)			
Ramachandran plot (%)				
Favored regions	99.58			
Allowed regions	0.42			
Outliers	0			

Numbers in parentheses represent the value for the highest resolution shell.

[a] $R_{merge} = \sum|Ii - Im|/\sum Ii$, where Ii is the intensity of the measured reflection and Im is the mean intensity of all symmetry related reflections.

[b] $R_{cryst} = \Sigma||Fobs| - |Fcalc||/\Sigma|Fobs|$, where Fobs and Fcalc are observed and calculated structure factors.

[c] $R_{free} = \Sigma T||Fobs| - |Fcalc||/\Sigma T|Fobs|$, where T is a test data set of about 5% of the total reflections randomly chosen and set aside prior to refinement.