Table S1 The spin-spin coupling constants ($^3J_{HN\alpha}$) of SBP-W2DP6V.

Residue	$^3J_{HN\alpha}$ (HZ)
Met3	6.76
Thr4	7.09
Thr5	7.61
Val6	6.95
Trp7	7.09
Gly8	6.29
Phe9	6.79
Leu10	7.18
His11	7.69

Table S2 ^{1}H chemical shift assignment (in ppm) for SBP-W2DP6V at 298 K and pH 6.1.

Residue	NH	α-CH	β-CH	γ-CH	δ-CH	others	α protons [a]	Chemical shift index
Ser1		4.15	3.98, 3.99				4.50 ± 0.1	-1
Asp2	8.80	4.71	2.68, 2.78				4.76 ± 0.1	0
Met3	8.58	4,53	1.99, 2.11	2.53, 2.61		ε-CH3 2.01	4.52 ± 0.1	0
Thr4	8.30	4.29	4.23			γ-CH3 1.19	4.35 ± 0.1	0
Thr5	8.07	4.29	4.15			γ-CH3 1.08	4.35 ± 0.1	0
Val6	7.98	4.04	2.01			γ-CH3 0.84, 0.86	3.95 ± 0.1	0
Trp7	8.22	4.56	3.25, 3.25			2H 7.23, 4H 7.59, 5H 7.15, 6H 7.21, 7H 7.41	4.70 ± 0.1	-1
Gly8	8.21	3.76, 3.86					3.97 ± 0.1	-1
Phe9	7.85	4.54	3.05, 3.12			2,6H 7.22; 3,5H 7.33; 4H 7.25	4.66 ± 0.1	-1
Leu10	7.94	4.19	1.33, 1.52	1.48		δ-CH3 0.82, 0.88	4.17 ± 0.1	0
His11	8.19	4.89	2.89, 3.11			2H 8.42; 4H 7.03	4.63 ± 0.1	1
Pro12		4.39	1.95, 2.27	1.97, 1.98	3.52, 3.57	-NH2 7.05, 7.73	4.44 ± 0.1	0

[a], standard chemical shift values of α-protons (26)

Table S3 NMR structural statistics

Experimental restraints	Number
Seqential backbone NOEs (i, i+1)	17
Seqential non backbone NOEs (i, i+1)	40
Inter-residue NOEs (i, i+2-4)	30
Average energy	299 kcal/mol
NOE constraints	31 Kcal/mol
Rmsd from backbone (3-11)	0.26±0.11Å
Nonhydrogen heavy atoms (residues3-11)	0.99±0.19 Å
Rachandran statistics from PROCHECK-NMR	
Most favored regions, %	66.0
Additional allowed regions, %	31.1
Generously allowed regions, %	0
Disallowed regions, %	2.9

Figure legend

Fig.S1 Binding of SBP-W2DP6V to the GroEL apical domain. **A)** Titration of fluoresceinated peptides with the apical domain monitored by fluorescence polarization. f_B is the fraction of the apical domain-bound peptide. The average values and the derived errors from two measurements were shown, along with the fitting curve. Circles, SBP-P6VW2D; triangles, SBP-P6V; squares, SBP. **B)** One-dimensional proton NMR spectra of SBP-W2DP6V in the absence (2 mM, bottom panel) and presence of the MBP-apical domain (50 μM, top panel). The buffer was 50 mM potassium phosphate pH 6.1.

Fig.S2 Effects of the peptide binding on the ^{1}H-^{15}N HSQC spectrum of the GroEL apical domain. Shown here is a selected region of the overlaid ^{1}H-^{15}N HSQC spectra of the apical domain in isolation (black，0.28mM) and with the peptide (red) (protein 0.28mM, peptide 0.56mM).

Fig.S3 Circular dichroism spectrum of SBP-W2DP6V (150 μM) in 10 mM sodium phosphate (pH6.1) and 10 mM NaCl at 25 ^{o}C. Shown here is the average of three measurements.

Fig.S4 2D NOESY spectra of SBP-W2DP6V (2 mM) in presence of tetradecameric GroEL (1.4 μM).

Fig.S5 Model of SBP-W2DP6V bound to the GroEL apical domain.

Fig.S1

A)

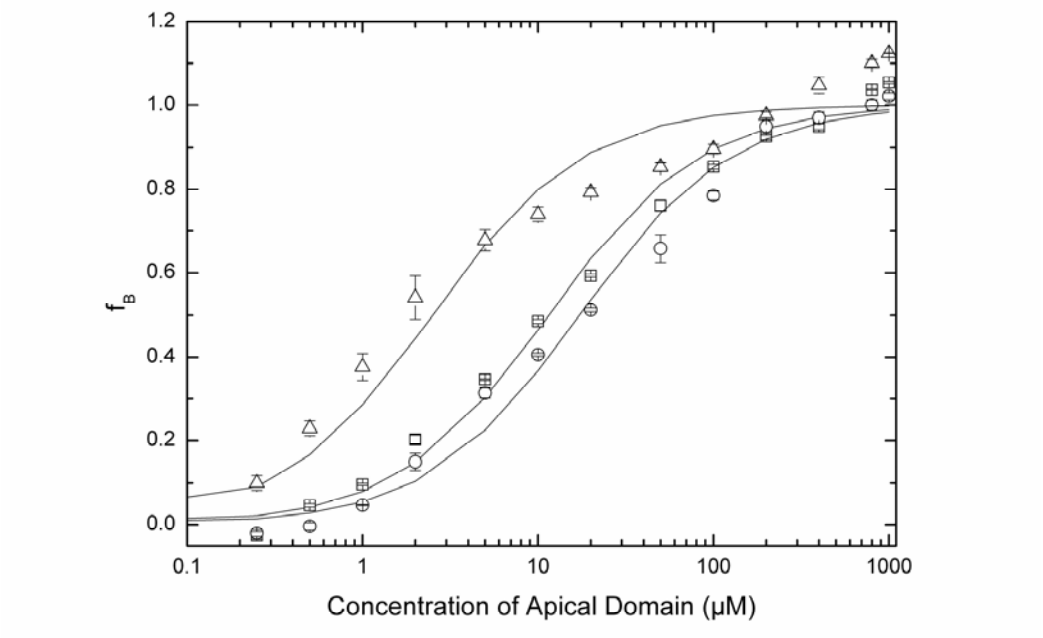
1.2
1.0
0.8
0.6
0.4
0.2
0.0
f_B
0.1
1
10
100
1000
Concentration of Apical Domain (μM)

Fig.S1

B)

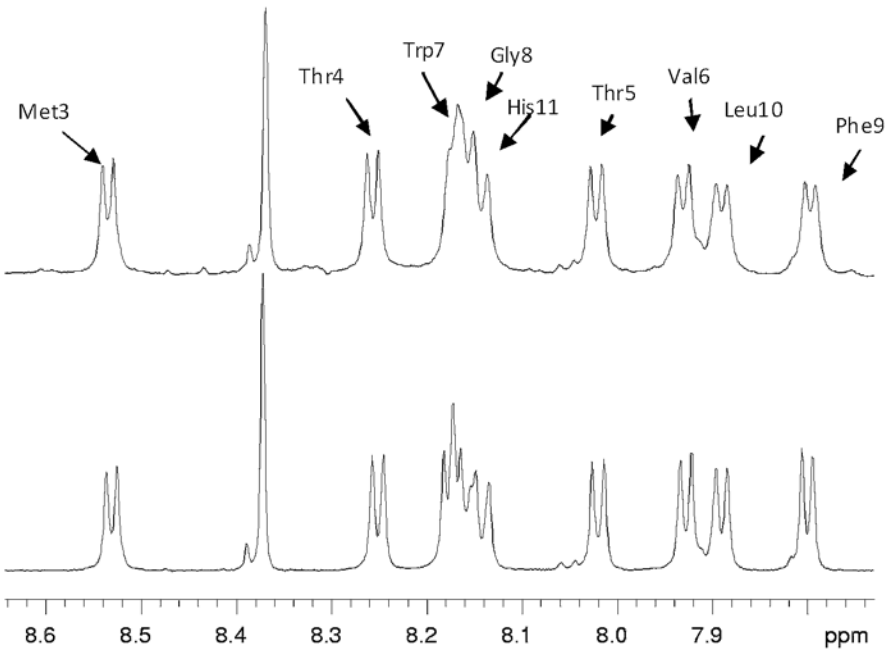
Met3
Thr4
Trp7
Gly8
His11
Thr5
Val6
Leu10
Phe9
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
ppm

Fig.S2

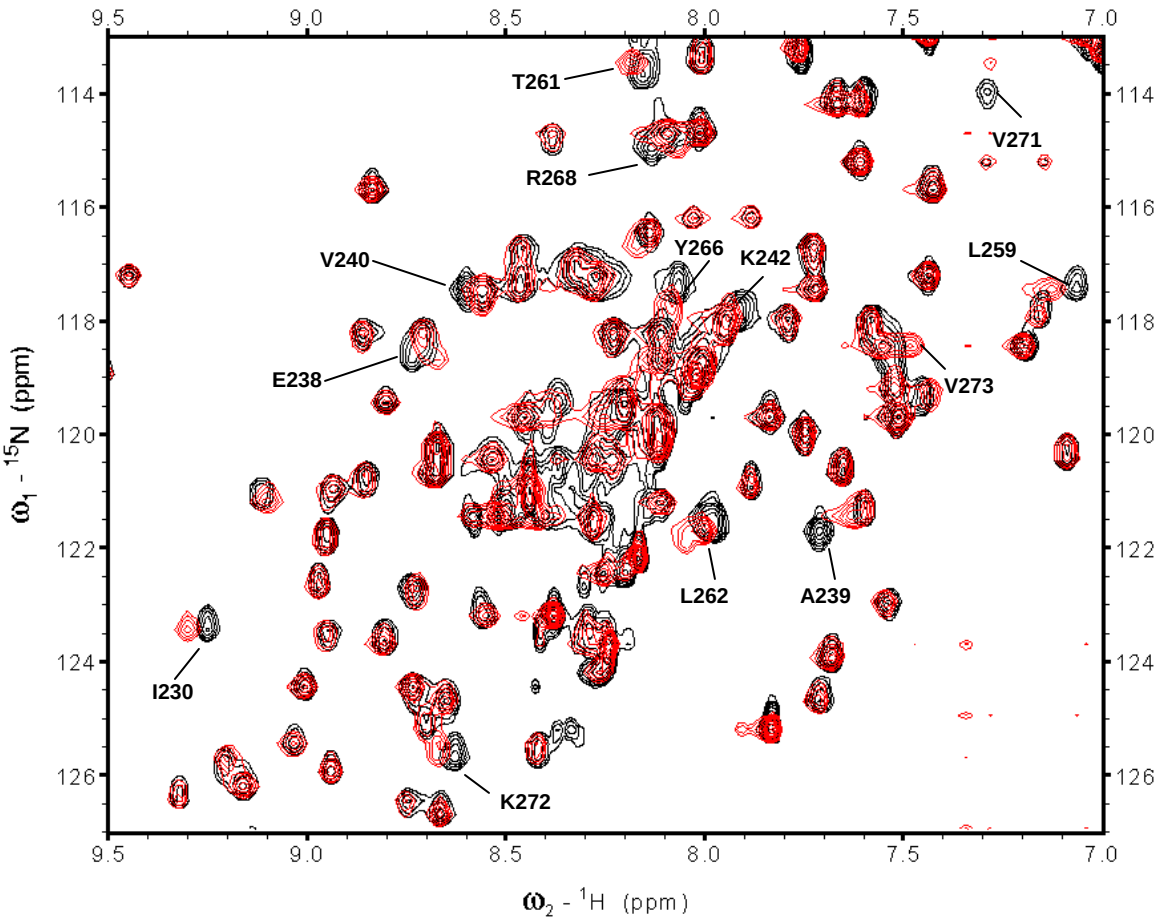
T261
R268
V271
V240
Y266
K242
L259
E238
V273
L262
A239
I230
K272
9.5
9.0
8.5
8.0
7.5
7.0
114
116
118
120
122
124
126
ω1 - 15N (ppm)
ω2 - 1H (ppm)

Fig.S3

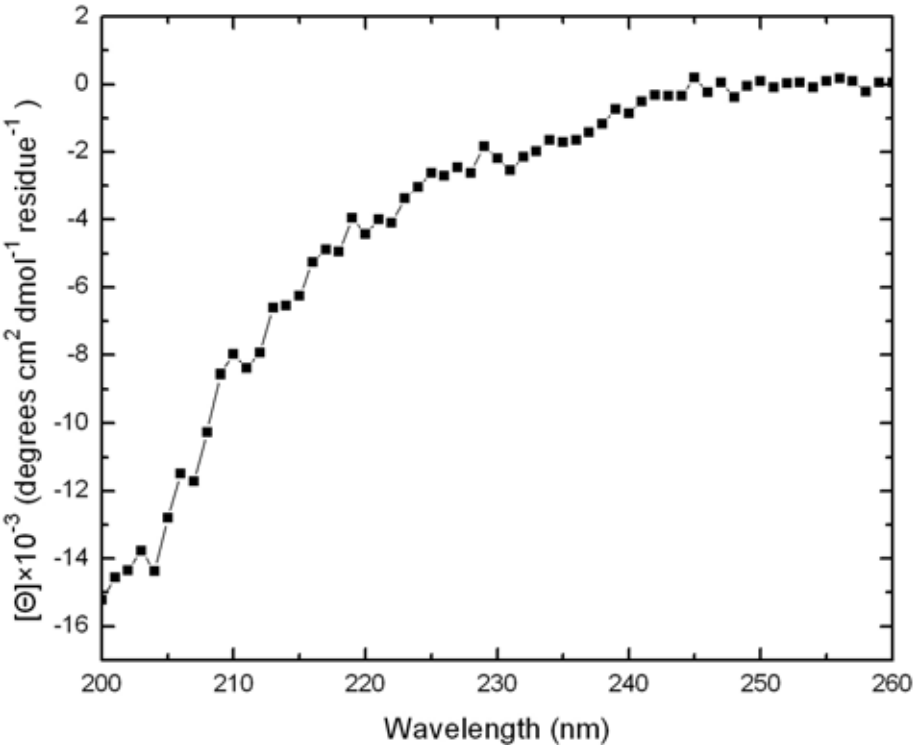
2
0
-2
-4
-6
-8
-10
-12
-14
-16
200
210
220
230
240
250
260
Wavelength (nm)
[Θ]×10^-3 (degrees cm^2 dmol^-1 residue^-1)

Fig.S4

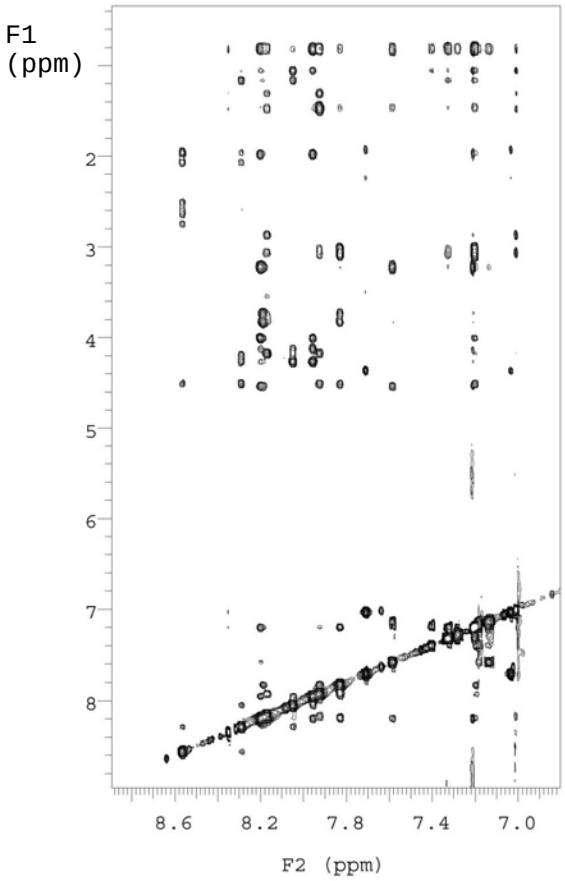

Fig.S5