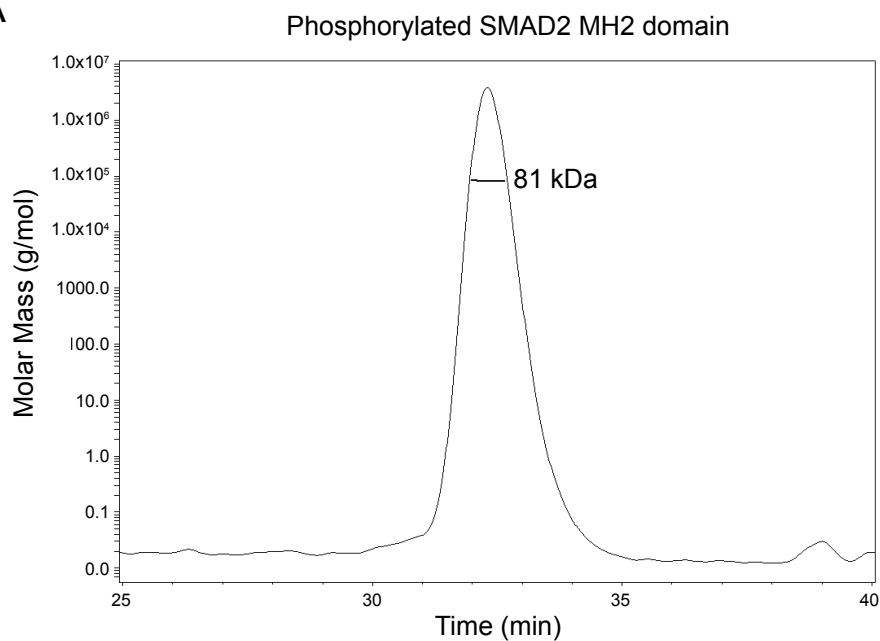
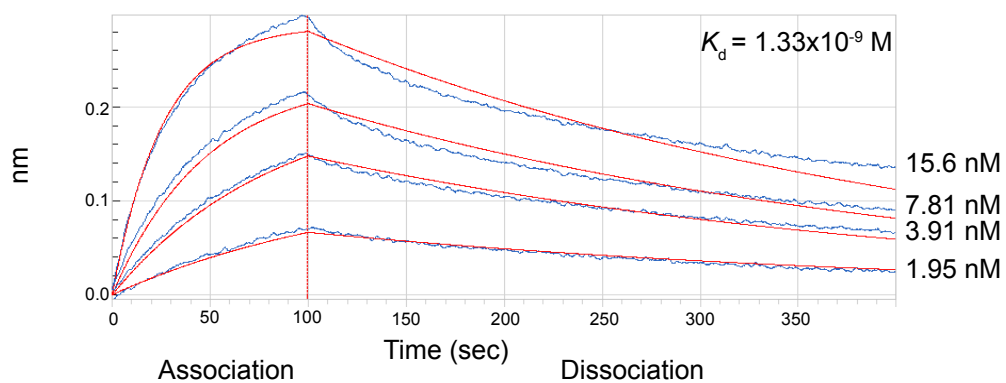


A



B



C

Data collection and refinement statistics	
Wavelength (Å)	0.9686
Resolution range (Å)	56.91 - 2.031 (2.104 - 2.031)
Space group	I 2 ₁ 3
Unit cell (Å)	113.82, 113.82, 113.82, 90, 90, 90
Total reflections	159694 (15932)
Unique reflections	15983 (1565)
Multiplicity	10.0 (10.1)
Completeness (%)	99.95 (100.00)
Mean I/sigma(I)	12.24 (1.89)
Wilson B-factor	37.09
R-merge	0.125 (1.469)
R-meas	0.1319 (1.547)
R-pim	0.04167 (0.4846)
CC1/2	0.998 (0.635)
CC*	1 (0.881)
Reflections used in refinement	15980 (1573)
Reflections used for R-free	744 (63)
R-work	0.1641 (0.2697)
R-free	0.2101 (0.2817)
CC(work)	0.972 (0.842)
CC(free)	0.952 (0.824)
Number of non-hydrogen atoms	1943
Macromolecules	1779
Ligands	88