

Table S1. Analysis of open and locked core buried surface areas, related to figure 4

Buried surface areas (to nearest 10 Å²)

<i>Contact</i>		<i>locked</i>	<i>open</i>
α	$\sigma 2$	2300	2670
$\beta 2$	N- $\mu 2$	2430	2370
α	$\beta 2$	1740	1850
α	N- $\mu 2$	170	200
$\sigma 2$	N- $\mu 2$	80	80
$\sigma 2$	$\beta 2$	630 (430*)	310
C- $\mu 2$	N- $\mu 2$	380	360
C- $\mu 2$	$\sigma 2$	510	0
C- $\mu 2$	α	960	0
C- $\mu 2$	$\beta 2$	840	1560

* The number in brackets is the contribution from the $\beta 2$ N-terminal residues 4-12 conformation: the figure for the open conformation excludes the pseudo-acidic dileucine sequence. Buried interaction surfaces were calculated and analysed in PISA (Krissinel and Henrick, 2005)

Table S2. Crystallographic data for the open form of AP2, related to Experimental

Procedures

Compound	Native	TaBr	Xe1	Xe2
Resolution range Å (outer bin)	64 – 3.1 (3.27 – 3.10)	46 – 5.0 (5.27 – 5.0)	75 – 3.5 (3.69 – 3.5)	74 – 3.5 (3.69 – 3.5)
Beamline	ESRF ID29	ESRF ID29	ESRF ID29	Diamond I02
Number of crystals	1	3	3	1
Wavelength Å	0.873	1.254	1.800	1.771
R_{merge}	0.195 (1.15)	0.223 (0.85)	0.331 (1.8)	0.128 (0.81)
R_{merge} (top intensity bin)	0.075	0.118	0.180	0.046
R_{meas} (within I+/-)	0.214 (1.26)	0.239 (0.90)	0.351 (1.9)	0.171 (1.08)
R_{pim} (within I+/-)	0.087 (0.52)	0.084 (0.31)	0.118 (0.64)	0.112 (0.71)
$\langle I \rangle / \sigma(\langle I \rangle)$	5.7 (1.3)	9.6 (3.4)	5.9 (1.7)	3.6 (0.9)
Completeness %	96.7 (97.7)	99.8 (100)	100 (100)	93.0 (88.4)
Multiplicity	5.5 (5.5)	16.2 (16.5)	17.5 (17.6)	2.4 (2.3)
Anomalous completeness %	-	99.8 (100)	100 (100)	45.6 (36.7)
Anomalous multiplicity	-	8.0 (8.2)	8.5 (8.4)	1.5 (1.5)
Δ_{anom} correlation (half-datasets)	-	0.484 (0.0)	-0.28 (-0.04)	0.120 (0.08)
Anomalous normal probability slope	-	1.21	0.922	0.916
Anisotropy ΔB Å ²	42	25	23	15
Phasing (1)				
Phasing power (Isomorphous/Anomalous)		0.41 / 0.71	0.40 / 0.22	–
Mean Figure of merit (inner resolution bin)	0.10 (0.84)	–	–	–
$\langle \text{FoM} \rangle$ after solvent flattening (68%)	0.82			
Phasing (2)				
Phasing power (Isomorphous/Anomalous)		0.38 / 0.67	0.56 / 0.22	0.36 / 0.20
Mean Figure of merit (inner resolution bin)	0.16 (0.83)	–	–	–
$\langle \text{FoM} \rangle$ after solvent flattening (68%)	0.86			
Refinement				
Number of reflections (free set)	63145 (3376)			
R / R_{free}	0.197 / 0.264			
Number of atoms	14153			
$\langle B \rangle$ Å ²	140			
RMS bond length deviation Å (angles °)	0.022 (1.9)			

$$R_{\text{merge}} = \frac{\sum_{\mathbf{h}} |I_{\mathbf{h}} - \langle I_{\mathbf{h}} \rangle|}{\sum_{\mathbf{h}} \langle I_{\mathbf{h}} \rangle}; R_{\text{meas}} = \frac{\sum_{\mathbf{h}} [n_{\mathbf{h}} / (n_{\mathbf{h}} - 1)]^{1/2} |I_{\mathbf{h}} - \langle I_{\mathbf{h}} \rangle|}{\sum_{\mathbf{h}} \langle I_{\mathbf{h}} \rangle}$$

$$R_{\text{pim}} = \frac{\sum_{\mathbf{h}} [1 / (n_{\mathbf{h}} - 1)]^{1/2} |I_{\mathbf{h}} - \langle I_{\mathbf{h}} \rangle|}{\sum_{\mathbf{h}} \langle I_{\mathbf{h}} \rangle} \text{ where } n_{\mathbf{h}} \text{ is the number of observations of reflection } \mathbf{h}.$$

Δ_{anom} correlation is the correlation coefficient between anomalous differences calculated for random half-datasets.