Supplemental Materials

Table S1 Data collection*, phasing and refinement statistics for **MAD** (SeMet) structures

	L18-6 (Native)	32_4 (Se-Met)	F12 (Fab-free)	39_4 (Se-Met)	
Data collection					
Space group	P1	P1	P1	P1	
Cell dimensions					
a, *b*, *c* (Å)	79.7,104.1,154.0	79.8,102.8,154.0	82.2,112.2,113.8	80.0,103.7,153.5	80.1,104.1,154.1
α, β, γ (º)	82.0,75.9,73.7	82.3,75.5,73.6	80.2,74.9,69.5	82.2,76.2,73.4	82.2,76.2,73.4
				Peak	*Inflection*
Wavelength	1.006	0.97942	1.0809	0.97942	0.97969
Resolution (Å)	3.2	3.6	3.7	3.7	3.4
R_{sym} or R_{merge}	8.6 (86)	10.9 (62)	6.2 (52)	8.8 (38)	8.7 (59)
$I/\sigma I$	25 (2.2)	22 (3.0)	21 (2.4)	24 (1.8)	24 (1.8)
Completeness (%)	98 (99)	92 (70)	98 (97)	87 (56)	74 (28)
Redundancy	3.7	11.29	3.2	11.6	11.6
Refinement					
Resolution (Å)	3.2				
Completeness (%)	96				
No. reflections	79,849				
R_{work}/ R_{free}	29.5 / 32.4				
No. atoms					
Protein	18,826				
Ligand/ion	0				
Water	0				
Ramchandran Outliers (%)	1.9				
R.m.s deviations					
Bond length (Å)	0.015				
Bond angle (º)	12.1				

*Highest resolution shell is shown in parenthesis.
Data were collected at the following Beamlines : L18-6 (NSLS , Brookhaven National Labs X-29), 32-4 , 39-4 (Advanced Photon Source (APS) 23 ID-B),F12 (Advanced light source (ALS), Berkeley, 8.2.2)

Legend: Data were processed and scaled in HKL, Se sites were located in SHELX, and phases were determined in the CCP4 suite. The AdiC-FAB model was built in COOT with helical restraints for TM segments. The initial model was subject to simulated annealing refinement followed by several rounds of restrained refinement with a mlhl target using experimental phases in Phenix version 1.4. The final model was obtained following restrained positional, individual B-factor, and TLS refinement. Tight 4-fold NCS restraint for AdiC and tight 2-fold NCS restraint for FAB were applied throughout the refinement. Structure figures were composed in PyMol (DeLano Scientific LLC). Ramachandran outliers were identified in COOT.

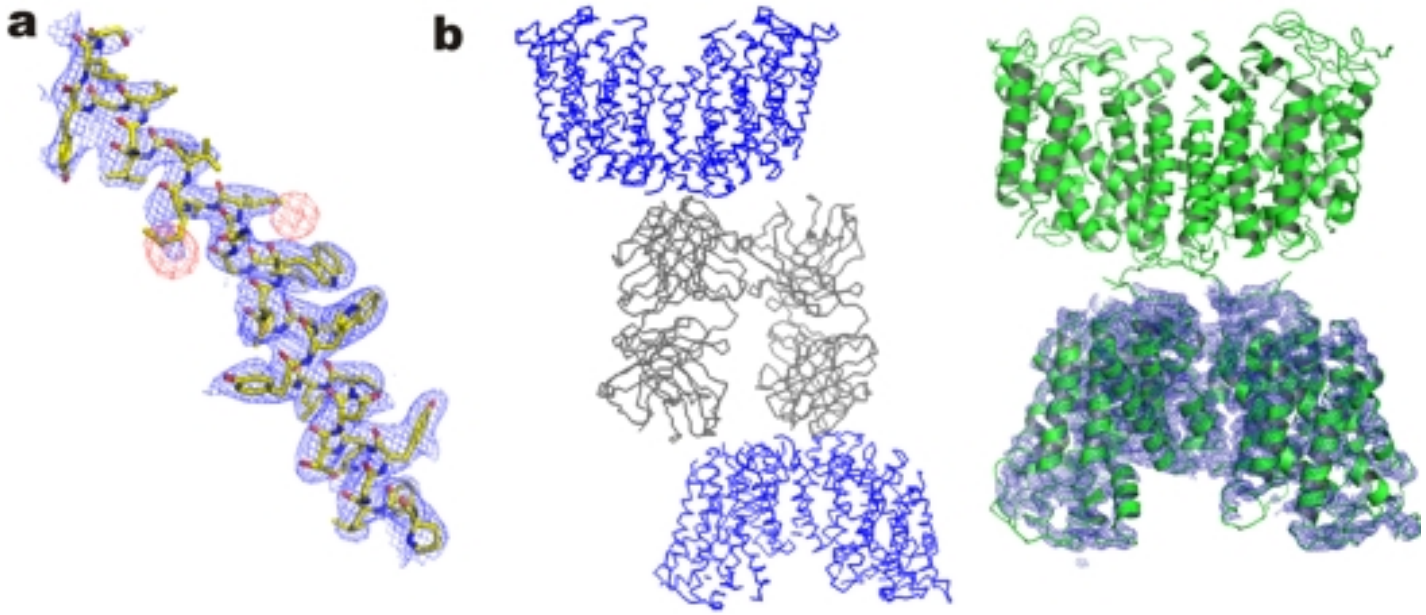

Fig S1. **Additional views of AdiC.**
a. Experimental electron density (blue, contour 1.5 σ) and Se anomalous difference (red, contour 7 σ) maps around TM3. b. Crystallographic arrangement of AdiC in P1 unit cell. Left panel, AdiC-F_{AB} complex; right panel, AdiC without F_{AB}, with 2Fo-Fc map calculated from phases determined by molecular replacement shown on lower subunit.

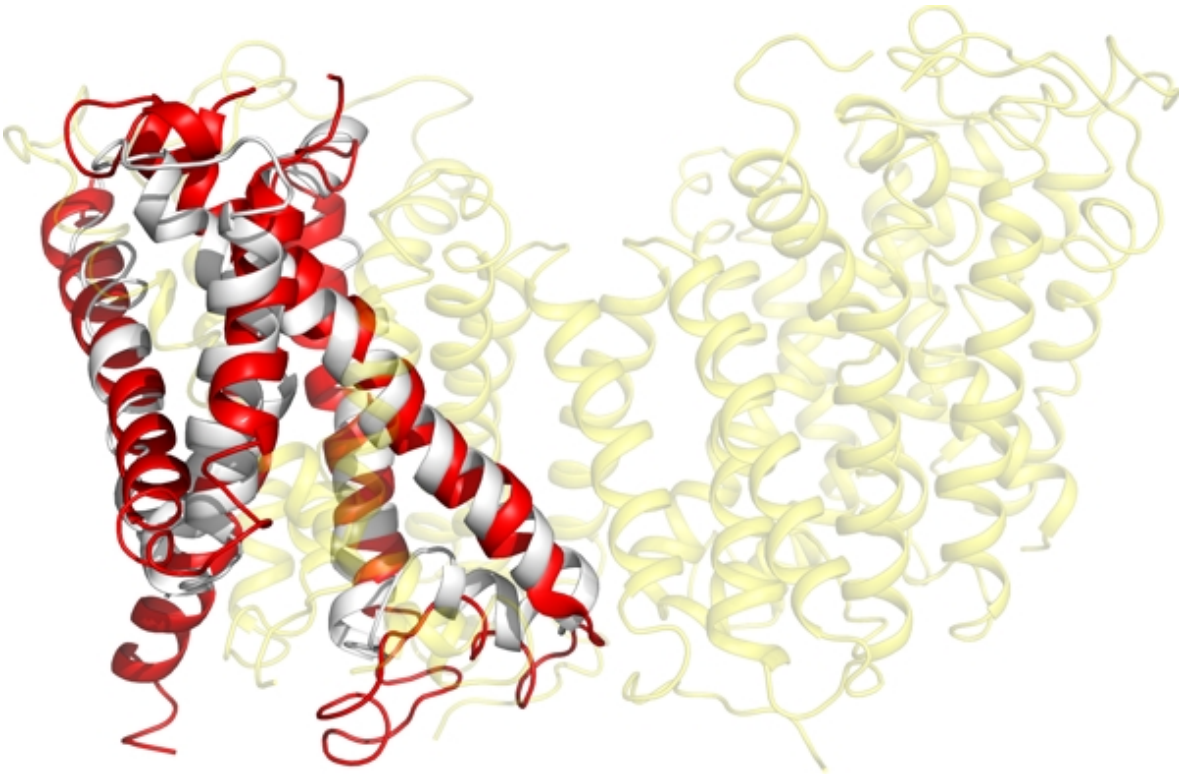

Fig. S2. **Inverted repeat within AdiC**. TMs 6-10 (red ribbons) are shown optimally aligned onto TM 1-5 (grey ribbons) by a pseudo-twofold rotation (175^{o} about an axis inclined 3^{o} to the membrane plane). Yellow ribbons lurking discretely in the background show orientation of homodimer.

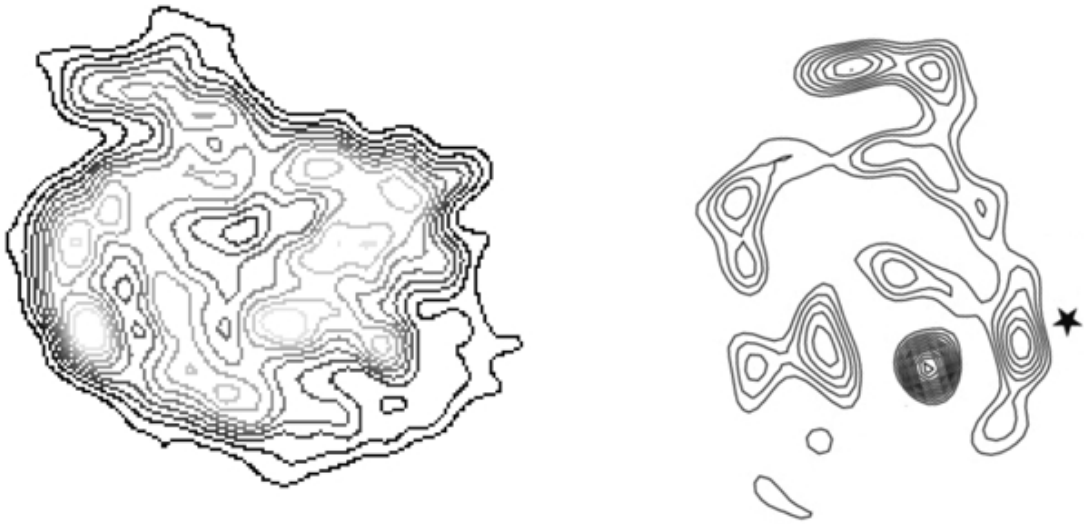

Fig S3. **Comparison of AdiC projections at 6.5 Å resolution**
Projections are shown for single subunit of AdiC calculated using EMAN from AdiC x-ray crystal structure (left panel) or measured by cryo-electronmicroscopy in 2-D crystals[7] (right panel). Both projections are parallel to homodimer 2-fold axis (marked by star on right), and hence normal to the membrane. Although the two projections cannot be compared quantitatively because of unknown absolute scales, it is clear that the strong helix perpendicular to the membrane apparent in the EM projection is absent in the x-ray structure. We thank Peter Moore for pointing out the scaling ambiguitiy and Wen Jiang for help making this figure.