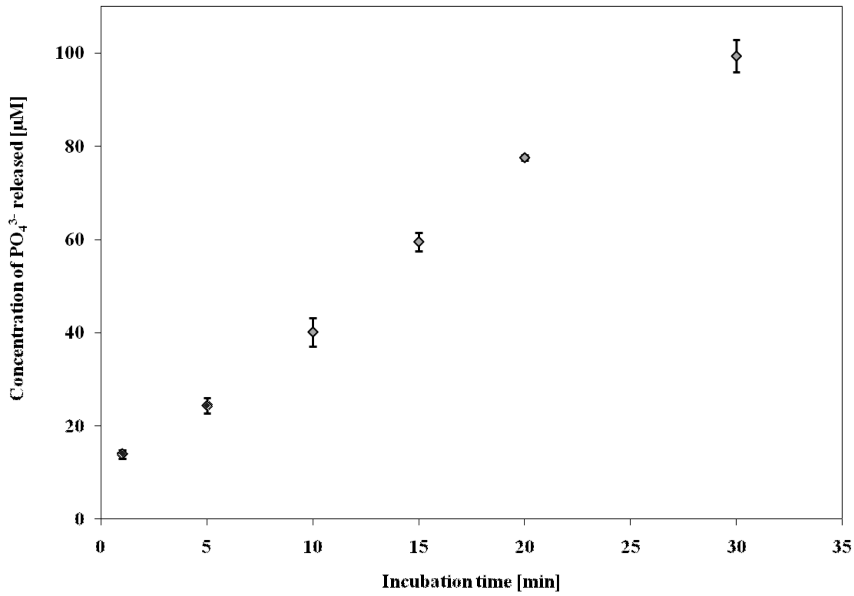
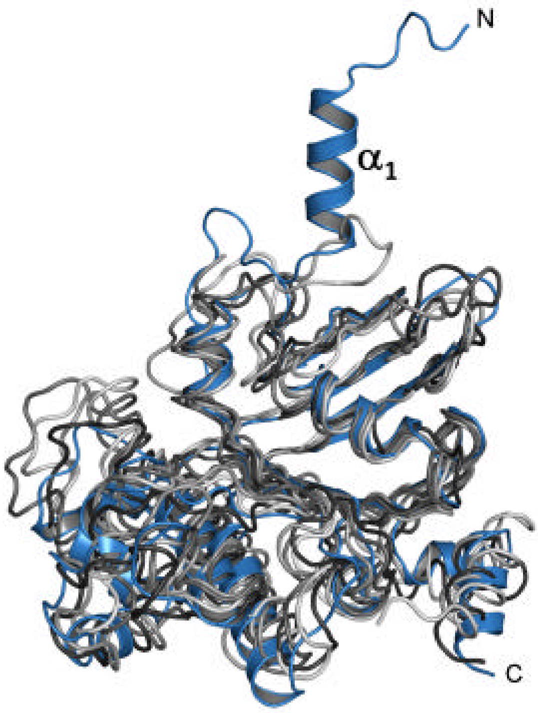


Supplementary Figure 1. ATPase activity assay. Reaction mixtures containing 100 µg ABCB6-NBD, 1 mM ATP and 5 mM $MgCl_2$ were incubated for 1, 5, 10, 15, 20 and 30 min, respectively. Error bars represent standard deviations from triplicates.

(*a*)



(*b*)

Supplementary Figure 2. Superposition of ABCB6-NBD with eight different NBDs. ABCB6-NBD is colored in blue and shown in cartoon representation. The other NBDs are shown as C_α traces and are colored in different grey scales. The structure were superimposed using the DaliLite Server (Holm *et al.*, 2000) *(a)* Superposition with PDB entries 1r0w (Z-score: 21.8; r.m.s.d.: 2.6 Å; sequence identity: 27%), 2cbz (Z-score: 23.6; r.m.s.d.: 2.4 Å; sequence identity: 30%), 2ixe (Z-score: 27.5; r.m.s.d.: 2.0 Å; sequence identity: 36%) and 2pze (Z-score 22.5; r.m.s.d.: 2.7 Å; sequence identity: 27%). (b) Superposition with PDB entries 1jj7 (Z-score: 27.1; r.m.s.d.: 2.2 Å; sequence identity: 34%), 1b0u (Z-Score: 23.2; r.m.s.d.: 2.5 Å; sequence identity: 24%), 1l2t (Z-score 21.2; r.m.s.d.: 2.6 Å; sequence identity: 26%) and 1mt0 (Z-score: 27.7; r.m.s.d.: 2.2 Å; sequence identity: 42%). The figures were prepared with *PyMOL* (DeLano, 2008)

Table 1 Known structures of NBDs.

PDB Entry	**Organism**	**Resolution [Å]**	**Ligands**	**Reference**
2CBZ	*H. sapiens*	1.50	ATP, Mg^{2+}	Ramaen *et al.*, 2006
1JJ7	*H. sapiens*	2.40	ADP, Mg^{2+}	Gaudet *et al.*, 2001
2IXE	*R. norvegicus*	2.00	ATP, Mg^{2+}, (D645N)	Procko *et al.*, 2001
2IXF	*R. norvegicus*	2.00	ATP, Mg^{2+}, (D645N, Q678H)	Procko *et al.*, 2001
2IXG	*R. norvegicus*	2.70	ATP, (S621A, G622V, D645N)	Procko *et al.*, 2001
1XMI	*H. sapiens*	2.25	ATP, Mg^{2+}, (F508A)	Lewis *et al.*, 2005
1XMJ	*H. sapiens*	2.30	ATP, Mg^{2+}, (ΔF508A)	Lewis *et al.*, 2005
2PZE	*H. sapiens*	1.70	ATP, $Mg^{2+,}$ (Δ405-436)	Atwell *et al.*, 2007
2PZF	*H. sapiens*	2.00	ATP, Mg^{2+} (Δ405-436, delF508)	Atwell *et al.*, 2007
2PZG	*H. sapiens*	1.80	ATP Mg^{2+} (Δ405-436)	Atwell *et al.*, 2007
2BBO	*H. sapiens*	2.55	ATP Mg^{2+} (F409L, F429S, F433L, G550E, R553Q, R555K, H667R)	Lewis *et al.*, unpublished
2BBS	*H. sapiens*	2.05	ATP Mg^{2+} (F429S, F494N, Q636R)	Lewis *et al.*, unpublished
2BBT	*H. sapiens*	2.30	ATP Mg^{2+} (F504N, Q646R)	Lewis *et al.*, unpublished
1R0W	*M. musculus*	2.20	-	Lewis *et al.*, 2004
1R0Y	*M. musculus*	2.55	ADP	Lewis *et al.*, 2004
1R0X	*M. musculus*	2.20	ATP, Mg^{2+}	Lewis *et al.*, 2004
1Q3H	*M. musculus*	2.50	ANP, Mg^{2+}	Lewis *et al.*, 2004
1XF9	*M. musculus*	2.70	ATP, Mg^{2+},(F508S)	Thibodeau *et al.*, 2005
1XFA	*M. musculus*	3.10	ATP, Mg^{2+}, (F508R)	Thibodeau *et al.*, 2005

1B0U	*S. typhimurium*	1.50	ATP	Hung *et al.*, 1998
1G29	*T. litoralis*	1.90	Mg^{2+}	Diederichs *et al.*, 2000
1F3O	*M. jannaschii*	2.70	ADP, Mg^{2+}	Yuan *et al.*, 2001
1L2T	*M. jannaschii*	1.90	ATP, (E171Q)	Smith *et al.*, 2002
1GAJ	*M. jannaschii*	2.50	-	Karpowich *et al.*, 2001
1G6H	*M. jannaschii*	1.60	ADP, Mg^{2+}	Karpowich *et al.*, 2001
1MT0	*E. coli*	2.60	-	Schmitt *et al.*, 2003
1XEF	*E. coli*	2.50	ATP, Mg^{2+} (H662A)	Zaitseva *et al.*, 2005
2FGK	*E. coli*	2.70	ATP, (E631Q)	Zaitseva *et al.*, 2006
2FGJ	*E. coli*	2.60	ATP, (H662A)	Zaitseva *et al.*, 2006
2FFB	*E. coli*	1.90	ADP, (E631Q)	Zaitseva *et al.*, 2006
2FFA	*E. coli*	1.70	ADP, (H662A)	Zaitseva *et al.*, 2006
2FF7	*E. coli*	1.60	ADP	Zaitseva *et al.*, 2006
3B5J	*E. coli*	2.00	TNP-ADP, (S504A)	Oswald *et al.*, 2008
2PMK	*E. coli*	1.60	TNP-ADP	Oswald *et al.*, 2008
1OXS	*S. solfataricus*	1.65	-	Verdon *et al.*, 2003
1OXT	*S. solfataricus*	2.10	-	Verdon *et al.*, 2003
1OXU	*S. solfataricus*	2.10	ADP, Mg^{2+}	Verdon *et al.*, 2003
1OXV	*S. solfataricus*	1.95	ANP, Mg^{2+}	Verdon *et al.*, 2003
1OXX	*S. solfataricus*	1.45	(G144A)	Verdon *et al.*, 2003
1Q1E	*E. coli*	2.90	-	Chen *et al.*, 2003
1Q1B	*E. coli*	2.80	-	Chen *et al.*, 2003
1Q12	*E. coli*	2.60	ATP	Chen *et al.*, 2003
1Z47	*A. acidocaldarius*	2.00	-	Scheffel *et al.*, 2005
1V43	*P. horikoshii*	2.20	-	Ose *et al.*, 2004
1VCI	*P. horikoshii*	2.90	ATP	Ose *et al.*, 2004
1MV5	*L. lactis*	3.10	ADP, ATP, Mg^{2+}	Yuan *et al.*, unpublished
1JIO	*T. maritima*	2.00	ATP	Zhang *et al.*, unpublished
3FVQ	*N. gonorrhoeae*	1.90	ATP	Newstead *et al.*, unpublished
3C41	*G. stearothermophilus*	2.25	ANP, Mg^{2+}	Thaben *et al.*, unpublished
3C4J	*G. stearothermophilus*	2.33	ATP, Mg^{2+}	Thaben *et al.*, unpublished
2OLJ	*G. stearothermophilus*	2.05	ADP, Mg^{2+}	Thaben *et al.*, unpublished
2OLK	*G. stearothermophilus*	2.00	ADP-β-S	Thaben *et al.*, unpublished
2OUK	*G. stearothermophilus*	2.15	-	Thaben *et al.*, unpublished
2GHI	*P. yoelii*	2.20		Vedadi *et al.*, 2007

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