Supporting Information

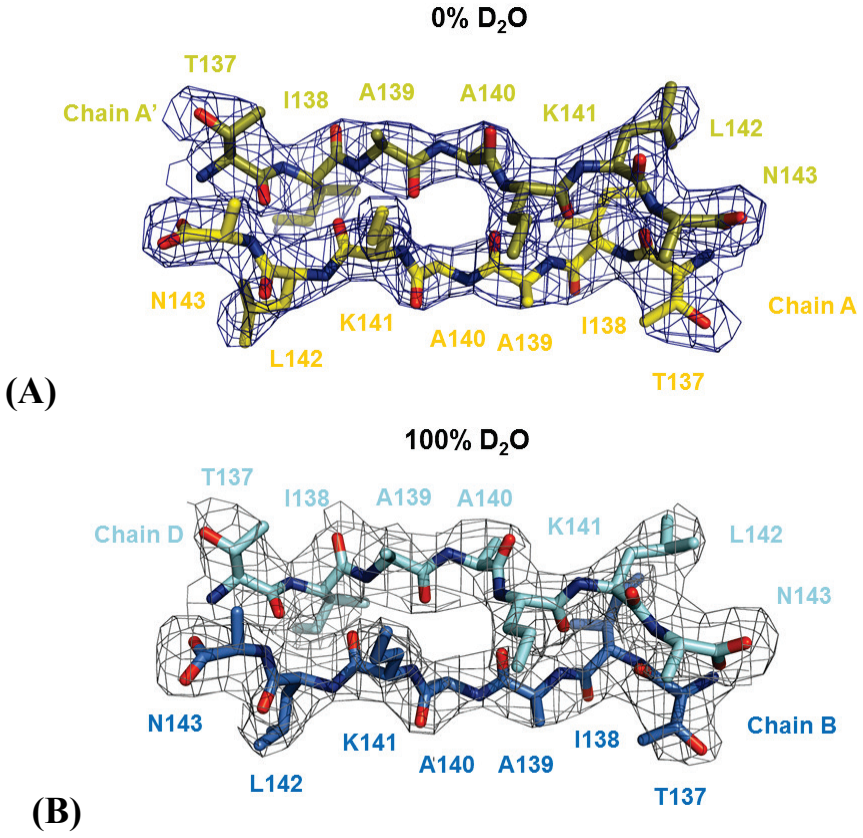
Promoting Crystallization using Deuterium Oxide

Bing Liu[a‡], *James. A. Garnett*[a‡], *Wei-chao Lee*[a], *Jing Lin*[a], *Paula Salgado*[a], *Jonathan Taylor*[a], *Yingqi Xu*[a], *Sebastian Lambert*[a], *Ernesto Cota*[a] *and Steve Matthews*[a]*

[a]Centre for Structural Biology & Division of Molecular Biosciences, Imperial College London, South Kensington, London, SW7 2AZ, UK

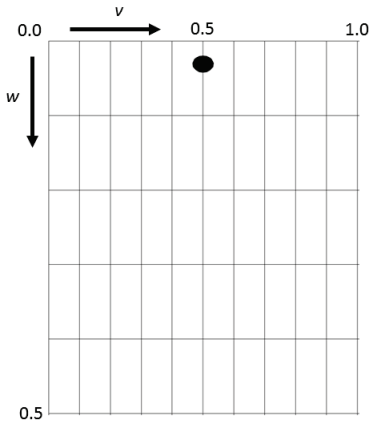
*Corresponding author.
Email address: s.j.matthews@imperial.ac.uk
Telephone: +44(0)20 7594 5315
Fax: +44(0)20 7594 3057

‡These authors contributed equally

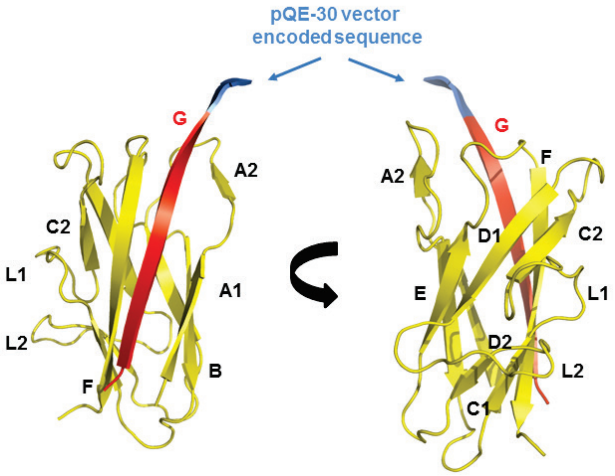


Supplementary Figure 1: An example of the electron density quality of the $SefD_{dscA}$ crystal structures. Residues T137-N143 of (A) chain A and its symmetry mate, chain A', from crystals obtained with 0% D_2O, and (B) chain B and D from crystals obtained from 100%

D_2O are shown as sticks with sigma-A weighted $2F_o$-F_c maps contoured at 1.0 r.m.s electron density.

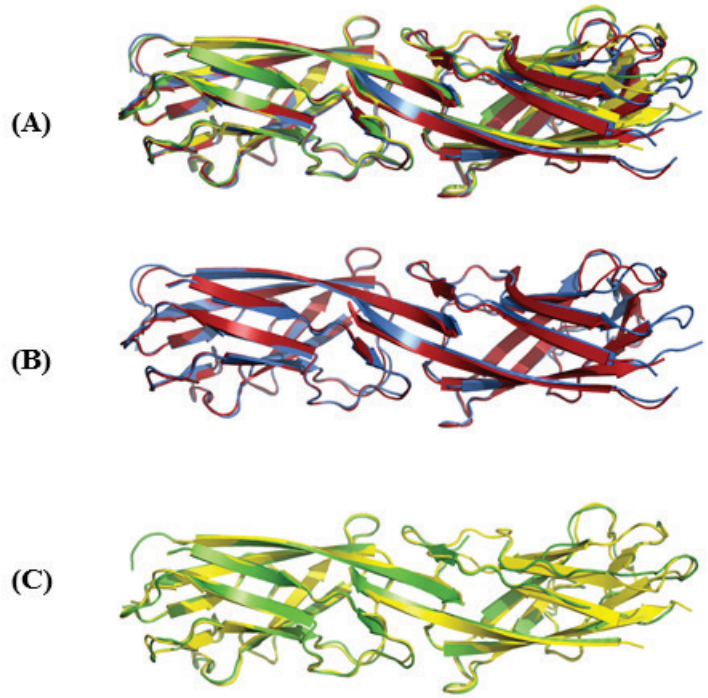


Supplementary Figure 2: Plot of the *u*=0.5 section of a native Patterson map of the $SefD_{dscA}$ crystal in 100% D_2O indicating translational pseudo-symmetry with a peak at *v*=0.5, *w*=0.031 with a total height of 38.8% of the origin peak (the origin peak has not been plotted).

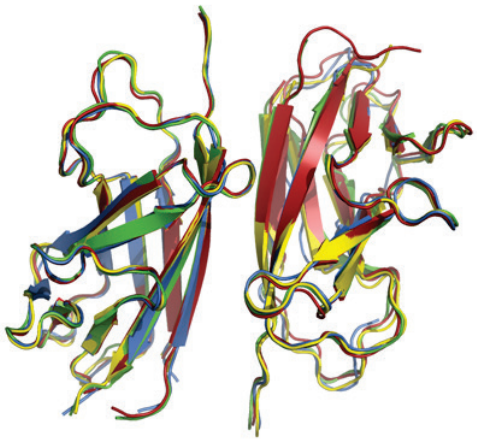


Supplementary Figure 3: Crystal structure of $SefD_{dscA}$ in 0% D_2O with β-sheets labelled A1-G and loops labelled L1-L2. The N-terminal extension from SefA (G-strand), which donor strand complements SefD to form a stable homogeneous reagent, is coloured red. The three vector encoded residues (Lys141, Leu142 and Asn143) which contribute to the domain-swapped dimer stability are coloured blue.

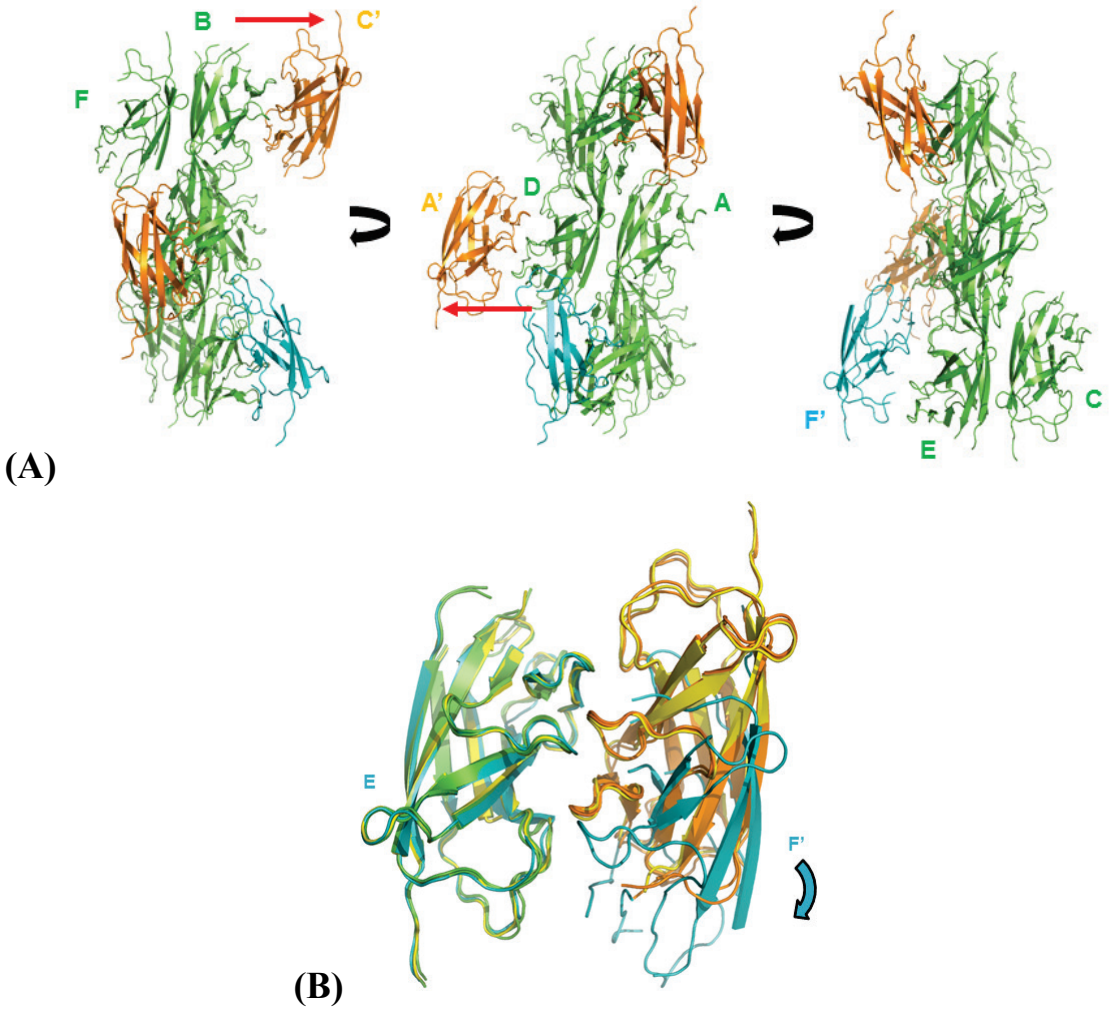
Supplementary Figure 4: Overlay of $SefD_{dscA}$ in 0% D_2O (yellow) with the six molecules of $SefD_{dscA}$ in 100% D_2O (rmsd 0.37-0.56 Å).



Supplementary Figure 5: Overlay of the domain-swapped dimers of $SefD_{dscA}$ from crystals grown in 0% and 100% D_2O. (A) Superimposition of chains A, D and C from the three dimers of the 100% D_2O crystal (chains AE: red; chains DB blue; chains CF: green) with chain A of the 0% D_2O crystal (chains AA': yellow). Chains A, D and C (100% D_2O) overlay very well with chain A (0% D_2O), whilst the other molecules of the chain AE and DB dimers (100% D_2O) are shifted due to an increased twist within the inter-domain beta sheets. (B) Whilst the chain AE and DB dimers superimpose very well with each other, (C) the chain CF dimer is not affected by D_2O and has the same conformation as the 0% D_2O form.



Supplementary Figure 6: Overlay of the 'back-to-back' dimers of $SefD_{dscA}$ from crystals grown in 0% and 100% D_2O. Superimposition of chains A, B and C from the three dimers of the 100% D_2O crystal (chains AE: red; chains BD blue; chains CF: green) with chain A of the 0% D_2O crystal (chains AA': yellow).



Supplementary Figure 7: Non-crystallographic relationship within the 'face-to-face' dimers of $SefD_{dscA}$ in the 100% D_2O crystal. (A) The asymmetric unit is coloured green and shown in three orientations. Symmetry related molecules with are related by the pseudo-translational vector (0.5,0.5,0.031) are coloured orange and indicated by a red arrow (chains B and C'; chains D and A'). Chains E and F' (coloured teal) are not related by this pseudo-translation vector and do not possess any intermolecular interactions. (B) Superimposition of chains A, C (green) and E (cyan) of the 100% D_2O 'face-to-face' dimers on the 0% D_2O dimer (yellow). Whilst chains A to D (yellow and green) from the 100% D_2O dimers contain the same conformation as the 0% D_2O dimer, the E and F' subunits are substantially shifted and do not form any interface.