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Supplementary Materials for

Fast iodide-SAD phasing for high-throughput membrane protein structure determination

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This PDF file includes:

Supplementary Materials

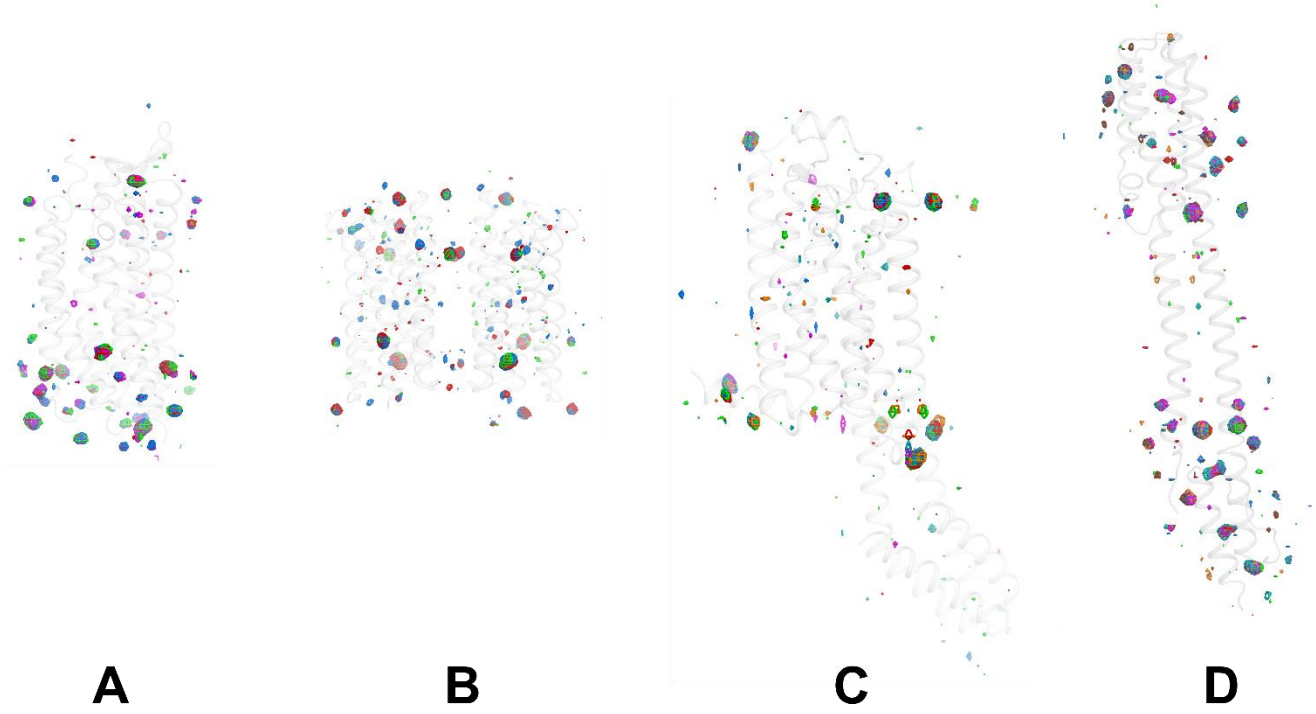

fig. S1. Comparison of peaks in anomalous difference Fourier maps calculated from individual data sets in I-SAD experiment. Only the regions close to the proteins are shown and the maps are contoured at the 3.5 x r.m.s. (root mean square) level. Each individual data set (see Table 1) is represented by its individual color (red, green, marine, teal, orange, magenta, firebrick, skyblue) for each of the structures displayed: (**A**) KR2, (**B**) MACR, (**C**) A_{2A}AR-BRIL-ΔC, (**D**) NarQ.

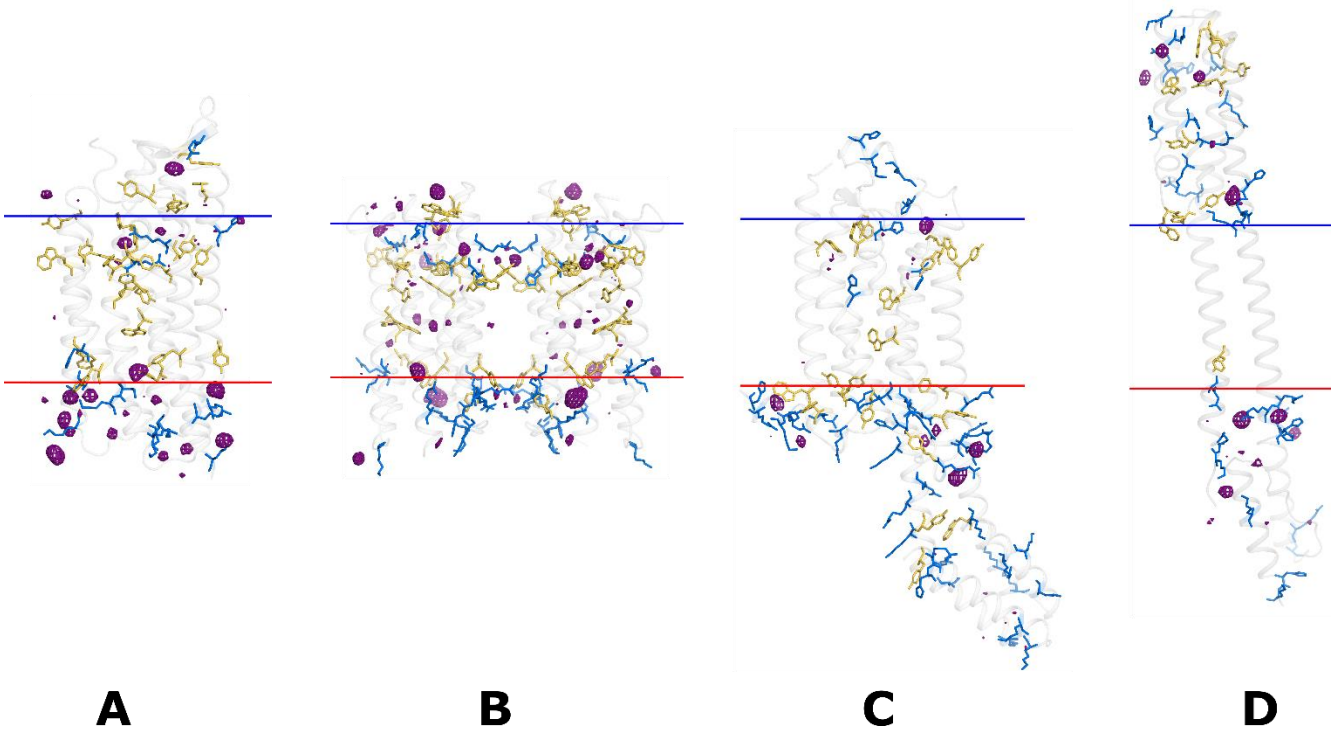

fig. S2. The distribution of positively charged and aromatic residues in the crystal structures obtained in I-SAD experiment. Positively charged protein residues (Arg, Lys, His) are represented as blue sticks, aromatic residues (Trp, Tyr) are represented as yellow sticks. The anomalous difference Fourier maps from I-SAD experiment (purple chicken wire, calculated from highest-resolution I-SAD data sets for each target (Table 1), contoured at 3.5 x r.m.s. level) are shown superposed on the structures of KR2 (**A**), MACR (**B**), A_{2A}AR-BRIL-ΔC (**C**), NarQ (**D**). The blue and red lines represent outer and inner lipidic membrane surfaces, respectively.

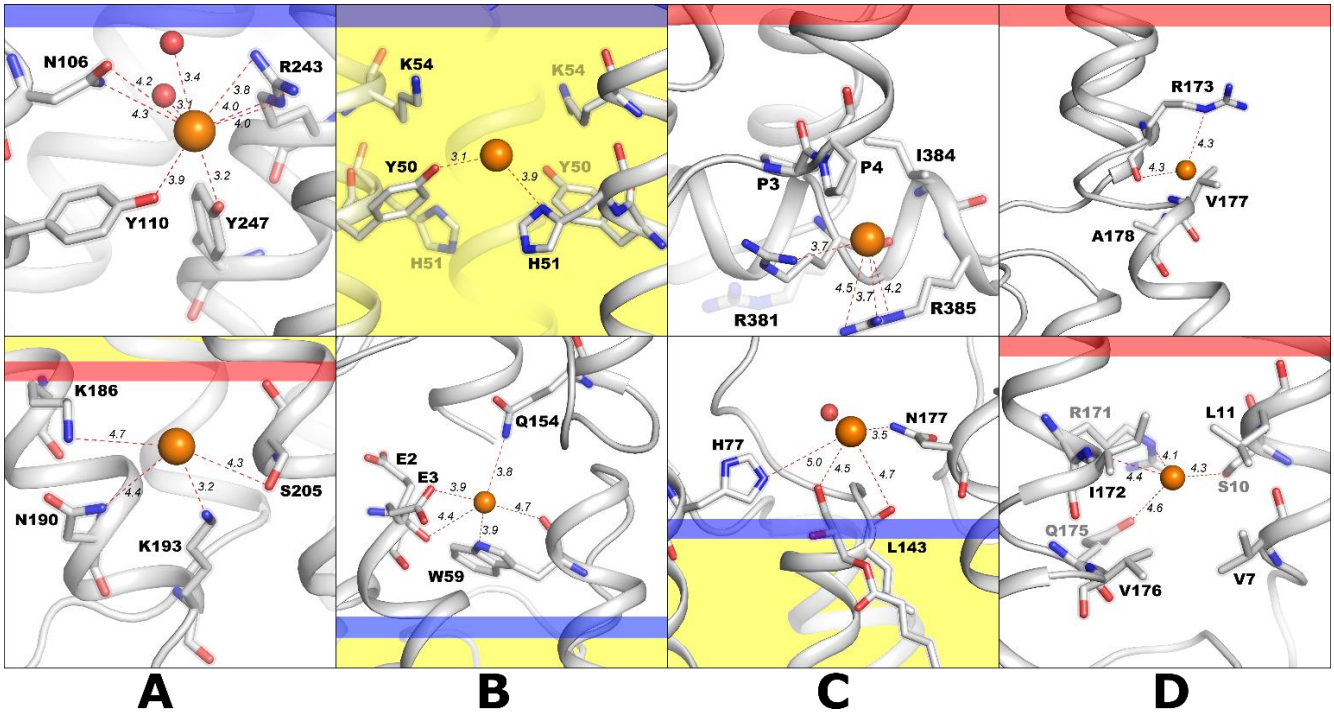

fig. S3. The bound iodide ions and their environment. Two figures (top and bottom) illustrating iodide environment at different binding sites are shown for each of the proteins investigated: (**A**) KR2, (**B**) MACR, (**C**) A_{2A}AR-BRIL-ΔC, (**D**) NarQ. The blue and red stripes represent outer and inner lipidic membrane surfaces respectively with the hydrophobic region of the lipidic membrane represented in yellow. Iodide ions are shown as orange spheres. Water molecules are shown as red spheres.