

Table S1. Crystallographic Data Collection and Refinement
(Data in parentheses are for the highest resolution shell)

Wavelength (Å)	0.97950
Resolution range (Å)	19.95 - 2.002 (2.073 - 2.002)
Space group	C 1 2 1
Unit cell	a = 130.28, b = 45.043, c = 87.574 $\alpha=90$ $\beta=90.85$ $\gamma=90$
Total reflections	
Unique reflections	34186 (3176)
Multiplicity	3.49
Completeness (%)	98.64 (93.19)
Mean I/sigma(I)	11.69 (6.39)
Wilson B-factor	23.44
R-merge	0.108
R-work	0.1701 (0.1662)
R-free	0.2171 (0.2121)
Number of atoms	7440
macromolecules	3393
ligands	277
water	204
Protein residues	477
RMS(bonds)	0.015
RMS(angles)	1.53
Ramachandran favored (%)	99
Ramachandran outliers (%)	0
Clashscore	8.71
Average B-factor	25.20
macromolecules	25.40
ligands	19.30
solvent	29.20

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      10          20          30          40          50
GDAAGKAK SVMCAACHGGA AGVSAVPTYP NLAGQKEAYL TKQLNDFKSG

      60          70          80          90          100
KRNDPTMKGM VMALSPADME NLAAYYANMK PGTKMIFAGI KKKTEREDLI

      109
AYLKKATNE

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Figure S1. Amino acid sequence of cytochrome c_{552} from *Colwellia psychrerythraea*, numbered to be consistent with cyt c_{552} from *Marinobacter hydrocarbonoclasticus*. Labeled in bold are the covalent heme attachments (Cys14 and Cys17) and the native axial metal-binding residues (His18 and Met57).

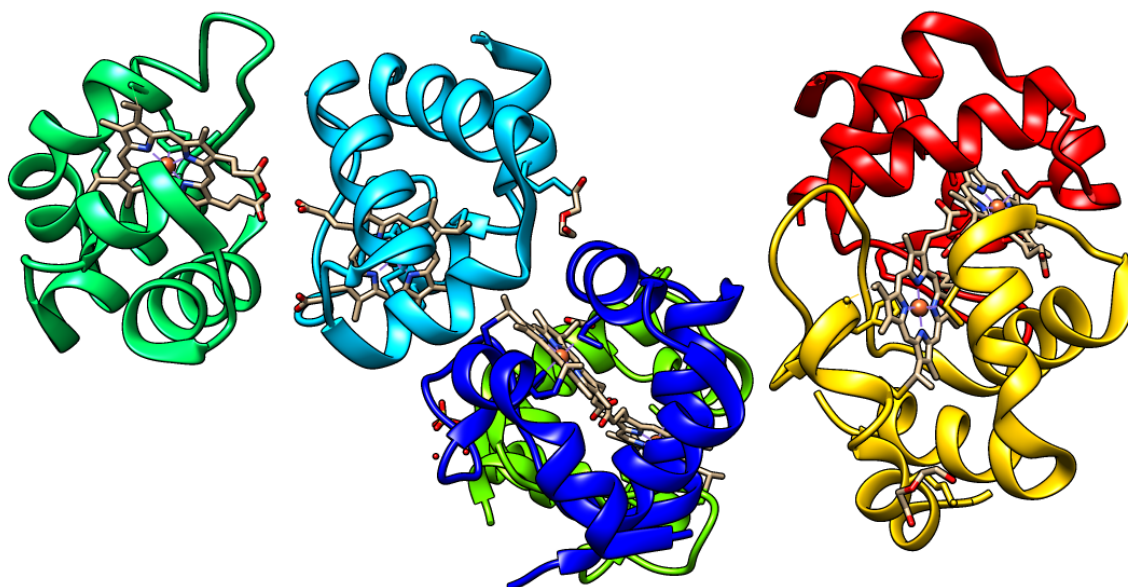


Figure S2. Molecular structure of *Cpcyt* c_{552} showing the three dimer pairs in the asymmetric unit.

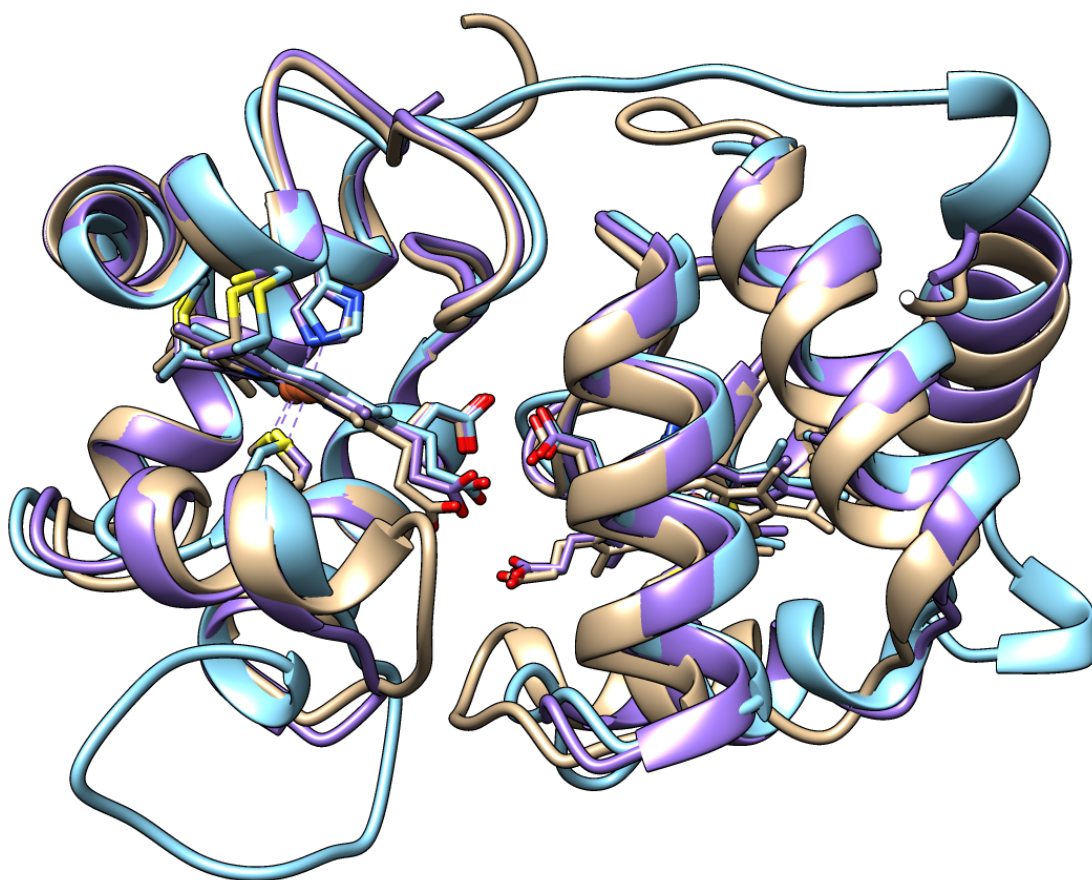


Figure S3. Superposition of the structures of a *Cpcyt c₅₅₂* dimer (4O1W, purple), a *Mhcyt c₅₅₂* dimer (1CNO, tan), and the two-heme *cyt c₄* from *Pseudomonas stutzerii* (1ETP, blue).

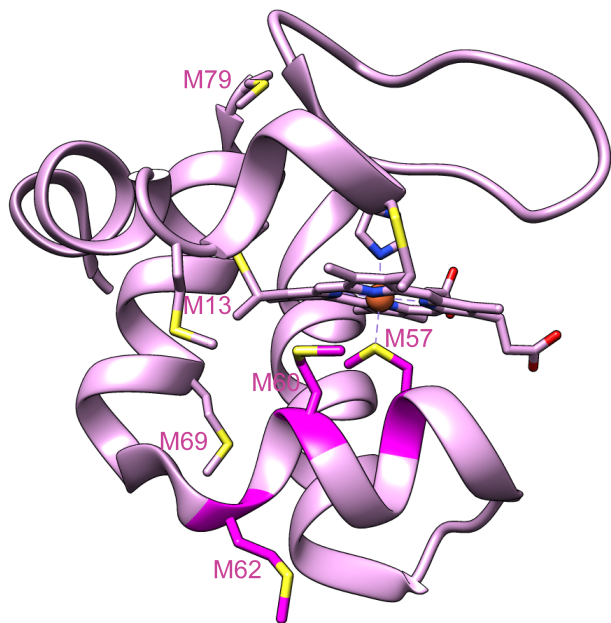


Figure S4. Structure of *Cpcyt c₅₅₂* monomer showing the position of the six methionine residues. Met57 (the axial methionine), Met60, and Met 62 are shown in darker magenta and are highly conserved in psychrophilic cytochromes. Met13, Met69, and Met79 are shown in lighter pink and are conserved as hydrophobic amino acids but not specifically as methionine.

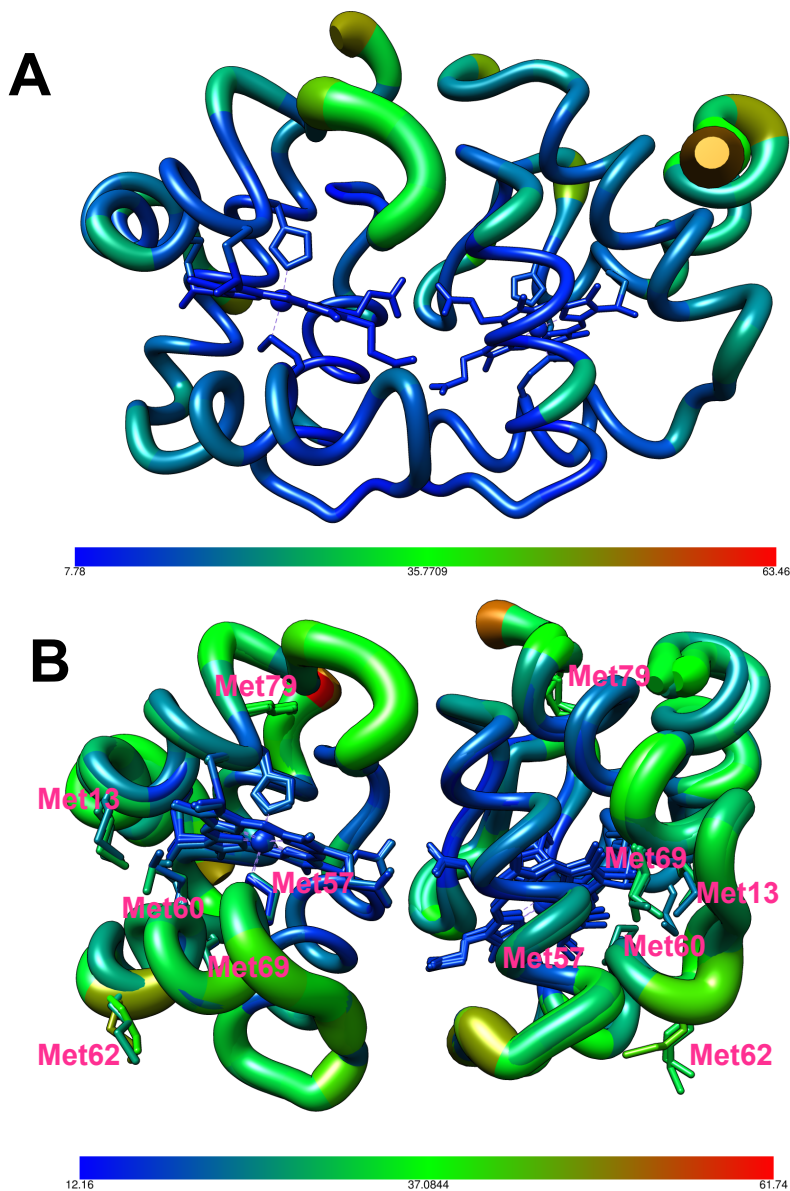


Figure S5. Structures of *cyt c₅₅₂* colored by residue-averaged B-factor. The structures are depicted using “worms,” with the diameter of the “worm” proportional to the B-factor. The greater average B-factors for the *Cpcyt c₅₅₂* (**B**) structure, particularly in the outer portions of the structure, are consistent with greater flexibility and dynamics than observed for the *Mhcyt c₅₅₂* structure (**A**).

A. Structure of *Mhcyt c₅₅₂* (PDB: 1CNO) **B.** Structure of *Cpcyt c₅₅₂* (PDB: 4O1W). The three dimers found in the asymmetric unit are superposed. Methionine residues are highlighted. Met62 in particular exhibits relatively high B-factors, consistent with high flexibility or dynamics.

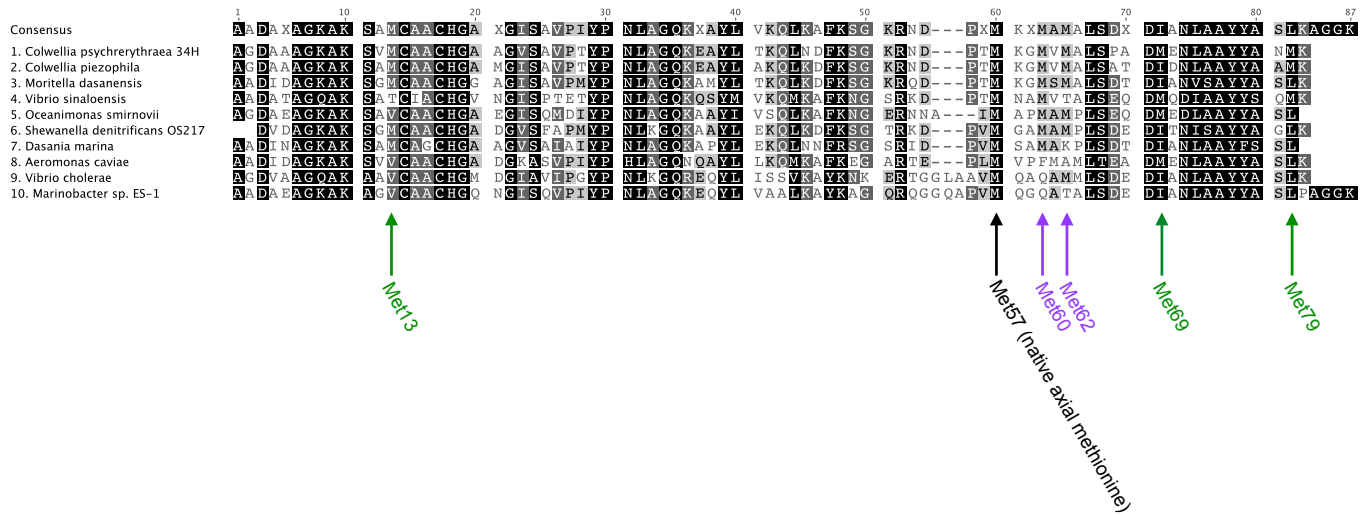


Figure S6. Sequence alignment of ten homologous cytochrome *c* sequences. Sequences 1-3 are from psychrophiles, sequences 4-7 are from psychrotolerant species, and sequences 8-10 are from mesophiles. Met60 and Met62 are highly conserved as methionines in psychrophiles, fairly well-conserved in psychrotolerant species, and not well-conserved in mesophiles. Met13, Met69 and Met79 are well conserved as hydrophobic residues (e.g., Met, Ile, Leu, Val) but not necessarily as methionine. The trends exemplified here are also observed in a larger sequence alignment that includes the top 100 sequences from a BLAST search of *Cpcyt c*₅₅₂ against the NCBI nr protein database.

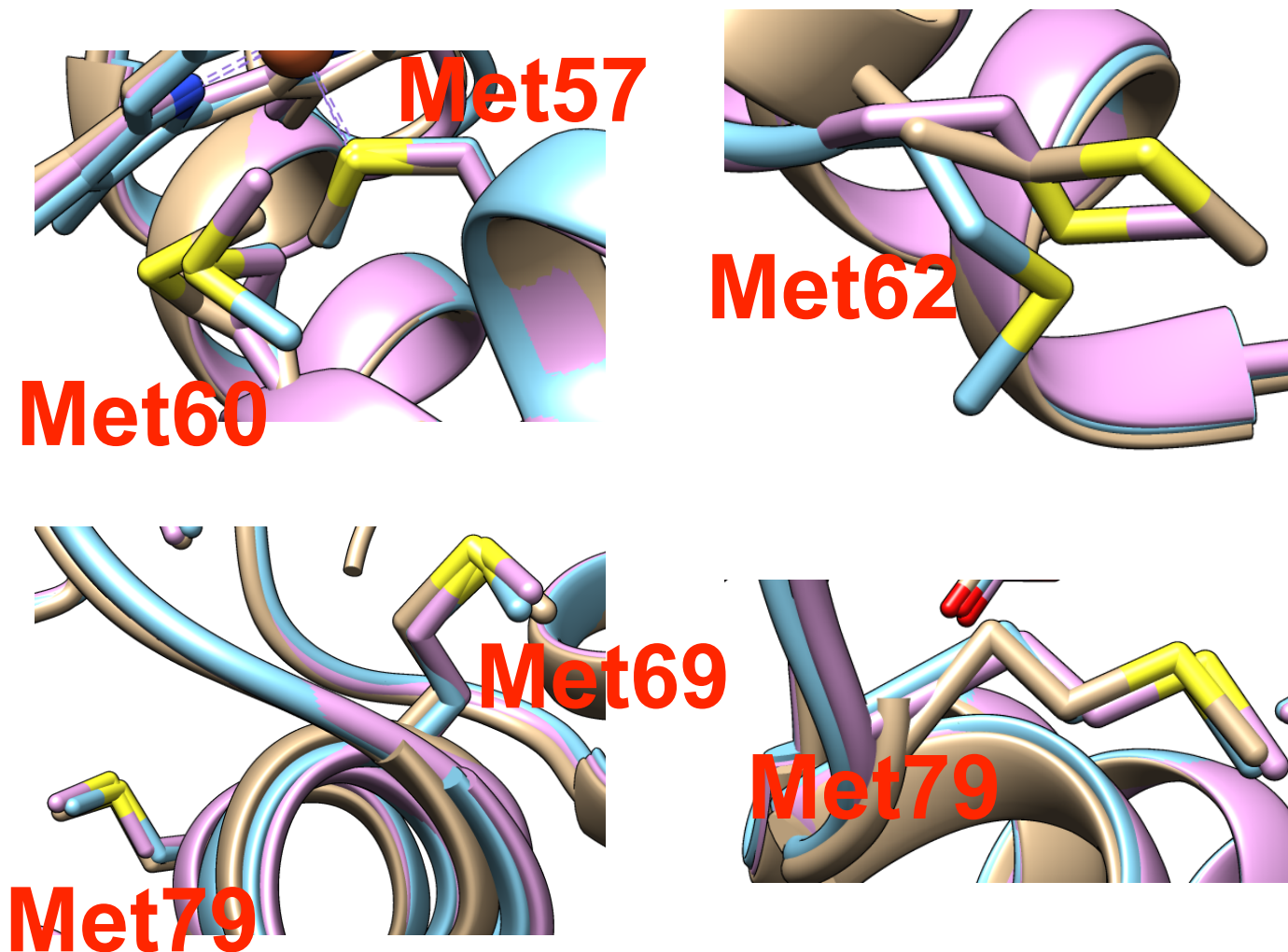


Figure S7. Superposition of the three dimers found in the *Cpcyt c552* asymmetric unit highlighting the methionine residues, with chain A in purple, chain C in blue, and chain E in tan. There are substantial differences in the positions of Met60 and Met62 in each of the three chains. By contrast, Met69, Met79, and Met57 (the axial methionine) from each chain are highly superposable.

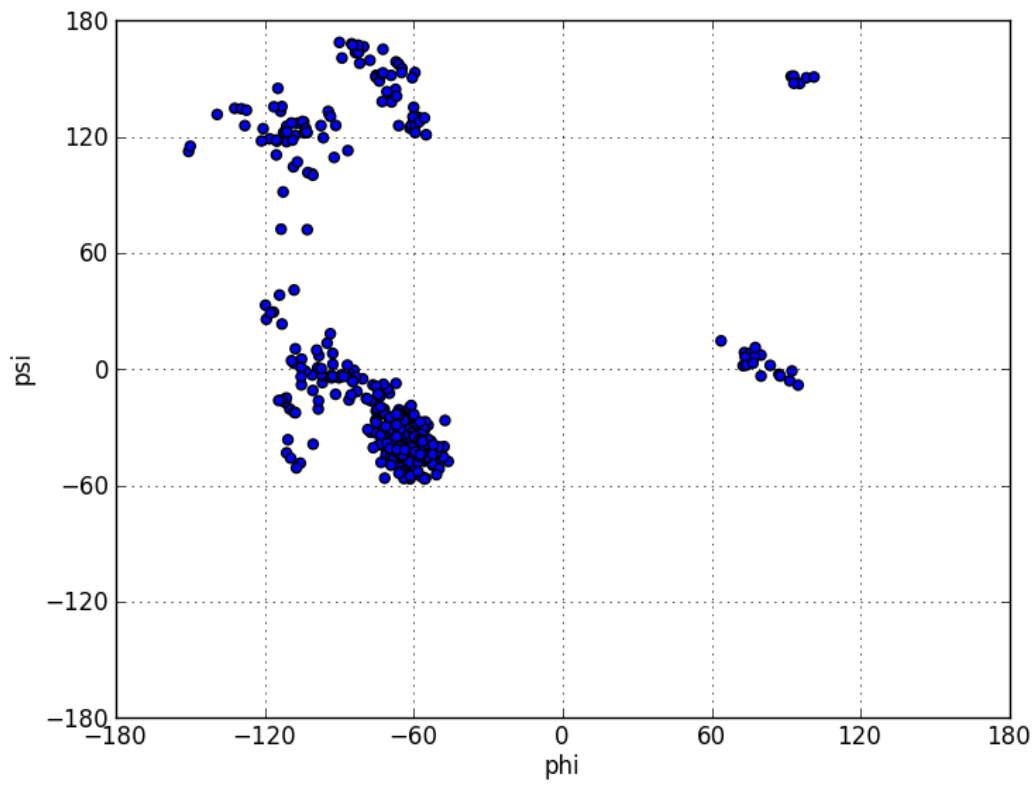


Figure S8. Ramachandran plot for *Cpcyt c₅₅₂*.