

Supplementary Information for Sources of non-Arrhenius electron transport in bacterial nanowires

Kiriko Terai^{1,2}, Peng Zhang¹, and David N. Beratan^{1,3,4,*}

¹Department of Chemistry, Duke University, Durham, NC 27708, USA

²Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

³Department of Physics, Duke University, Durham, NC, 27708 USA

⁴Department of Biochemistry, Duke University, Durham, NC 27710, USA

*Correspondence: david.beratan@duke.edu

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1 Reorganization energies computed with different dielectric constants for water-accessible protein cavities

Dielectric constants for the internal water-accessible cavities (ϵ_c) were estimated using:[1]

$$\Phi_M(R) = \frac{(\epsilon - 1)}{9\epsilon(\epsilon + 2)} \left[(\epsilon + 2)(2\epsilon + 1) - 2(\epsilon - 1)^2 \left(\frac{R}{R_c} \right)^3 \right] \quad (1)$$

where R_c is the cavity radius, R is the radius of a sphere within the cavity. The quantity $\Phi_M(R)$ varies approximately between 2 to 12.[1] Setting $R/R_c = 0.5$ and solving for the dielectric constant, ϵ , gives $\epsilon \approx 10, 20, 40$, and 60 for $\Phi_M(R) = 2, 4, 8$, and 12, respectively. We thus assess the sensitivity of the reorganization energies to the choice of ϵ_c , by testing $\epsilon_c = 10, 20, 40$, and 60.

Table S1 compares the reorganization energies computed with these different values of ϵ_c , based on a single molecular dynamics snapshot at 300 K. The calculation is performed for the nearest-neighbor hemes in monomer unit 3 of the OmcS heptamer (see Fig. 1 in the main text). The computed reorganization energies vary by at most ~ 0.02 eV across the different ϵ_c values, showing no substantial dependence on ϵ_c . This small variation indicates that the calculation is robust with respect to the choice of this parameter.

Table S1: Computed reorganization energies for electron transfer between nearest-neighbor heme pairs $i - j$ with different static dielectric constants of the internal water accessible cavities in the protein (ϵ_c). ϵ_w and ϵ_p are the static dielectric constants of bulk water and protein, respectively.

$\epsilon_p=4, \epsilon_c=20, \epsilon_w=77.70$		λ_{ij} (eV)				
Temperature (K)	1-2	2-3	3-4	4-5	5-6	6-1s
$\epsilon_c=20$	0.848	0.765	0.803	0.775	0.849	0.804
$\epsilon_c=10$	0.837	0.759	0.796	0.767	0.839	0.796
$\epsilon_c=40$	0.859	0.770	0.809	0.784	0.858	0.812
$\epsilon_c=60$	0.864	0.773	0.813	0.788	0.862	0.816

2 Computed electron transfer parameters for units 1, 2, 4, and 5 of the OmcS heptamer

Figs. S1, S2, S3, and S4 show the electron transfer parameters computed for nearest-neighbor heme pairs in units 1, 2, 4, and 5 of the OmcS heptamer. Main text includes the results for unit 3.

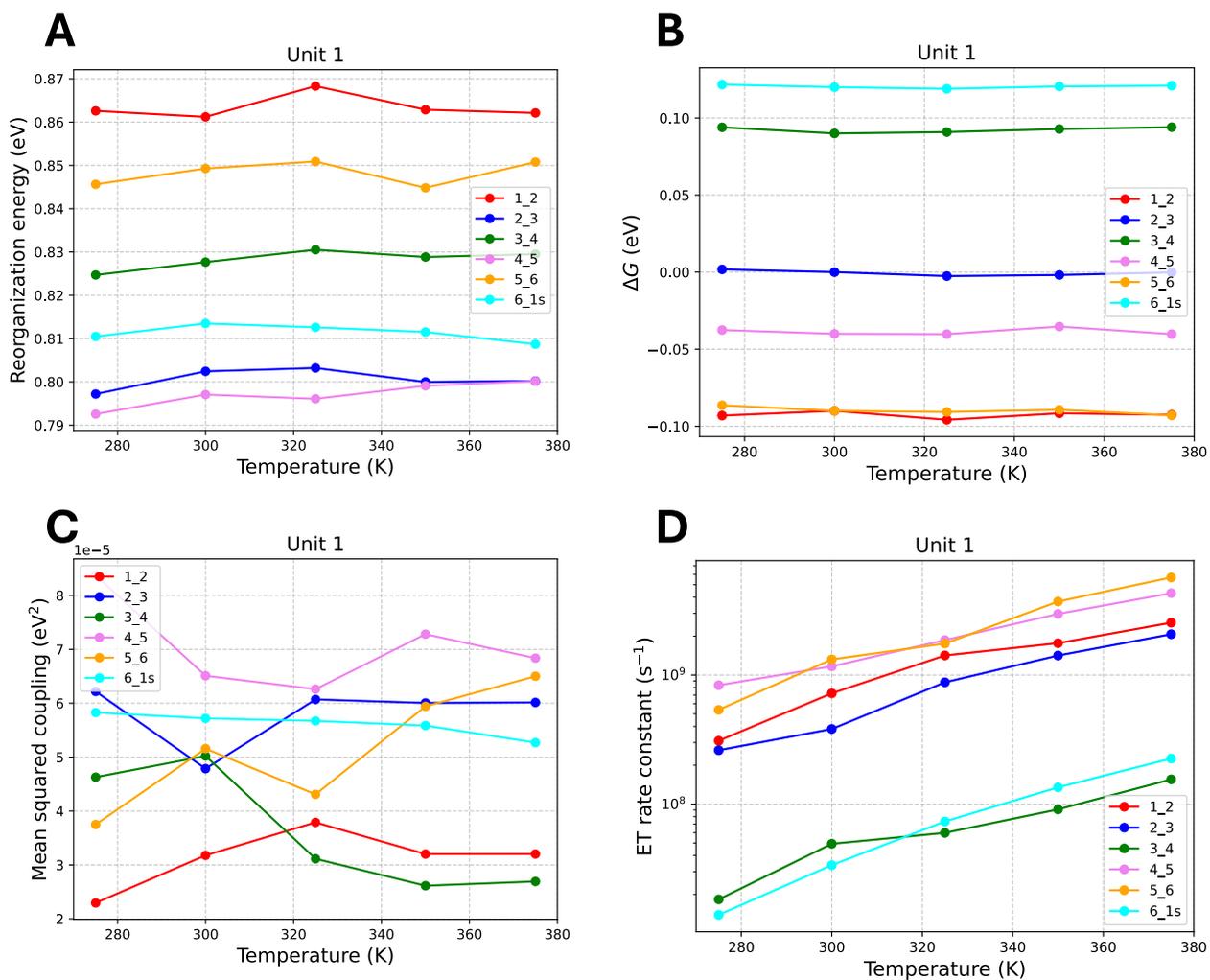


Figure S1: Computed temperature dependent electron transfer parameters and the resulting electron transfer rate constants for $i - j$ heme pairs in unit 1 of the OmcS heptamer.

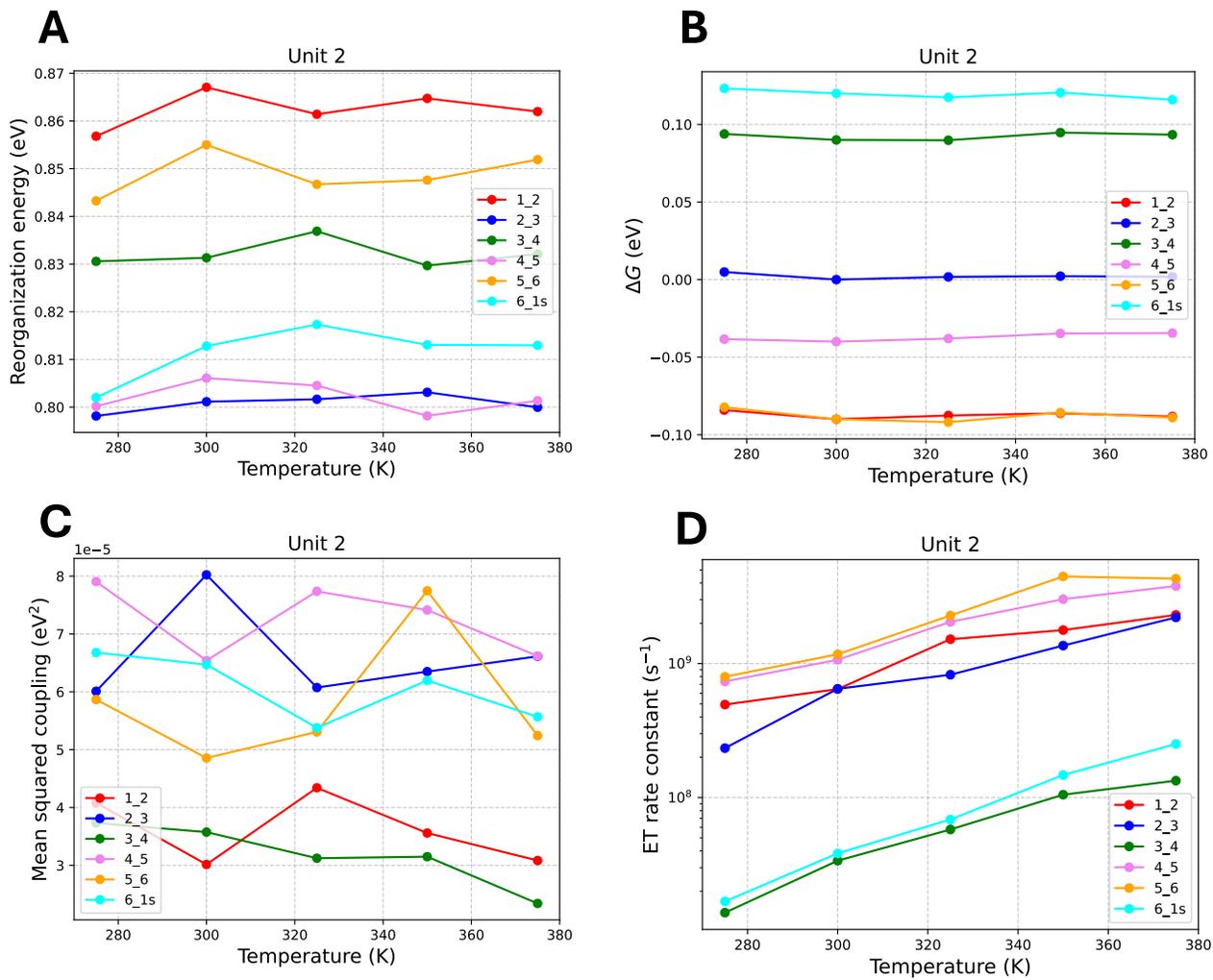


Figure S2: Computed temperature dependent electron-transfer parameters and electron transfer rate constants for $i - j$ heme pairs in unit 2 of the OmcS heptamer.

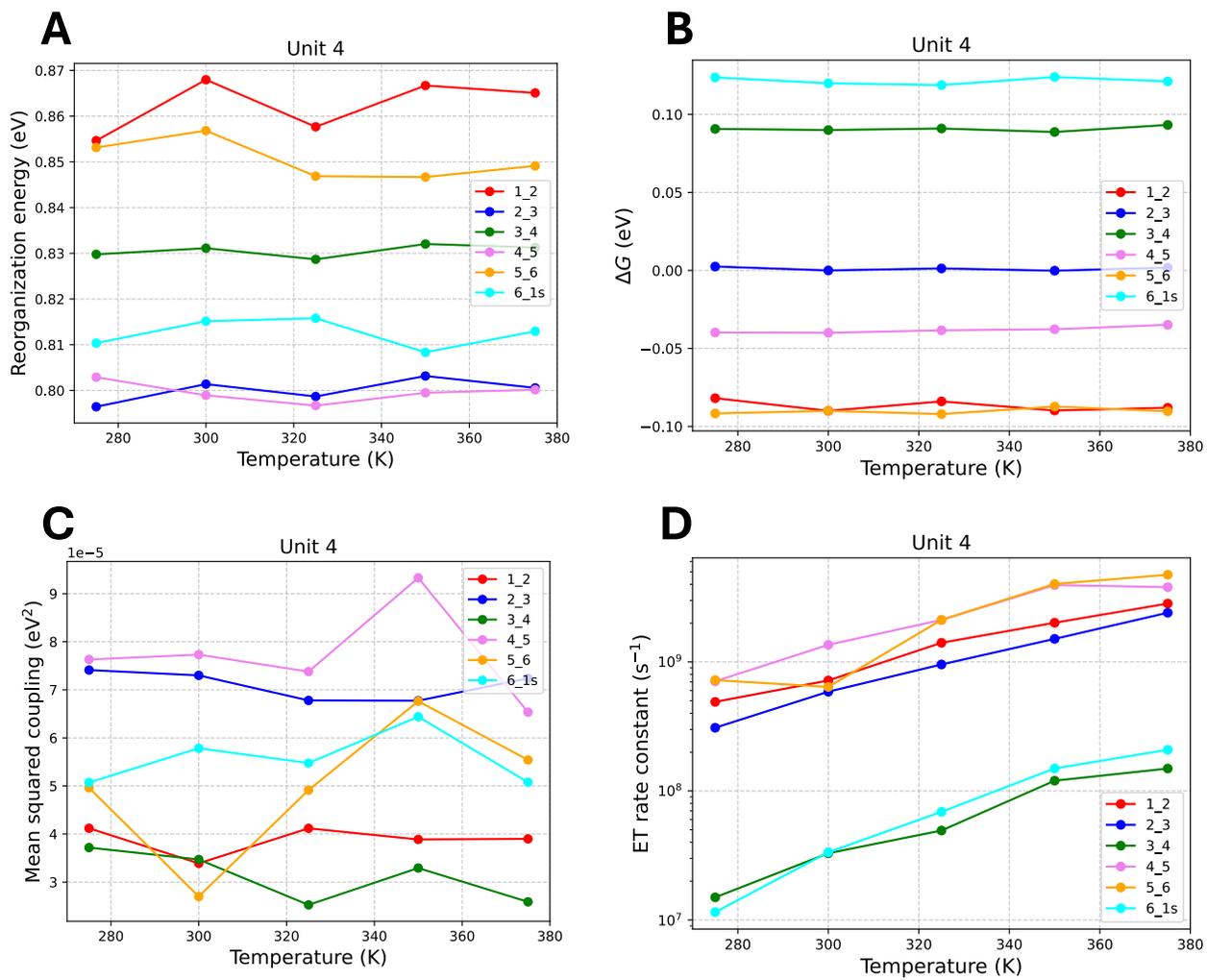


Figure S3: Computed temperature dependent electron transfer parameters and electron transfer rate constants for $i - j$ heme pairs in unit 4 of the OmcS heptamer.

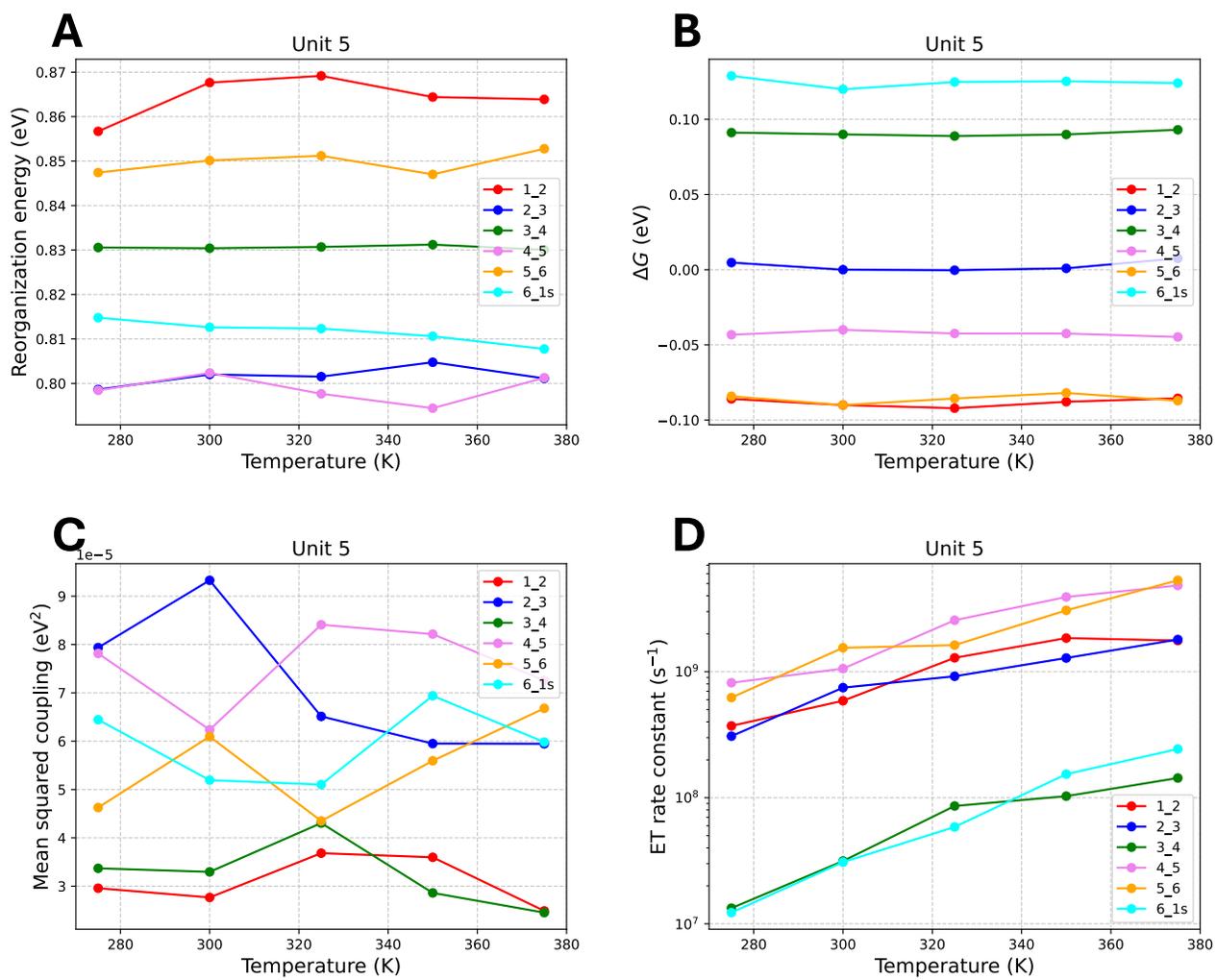


Figure S4: Computed temperature dependent electron transfer parameters and electron transfer rate constants for $i - j$ heme pairs in unit 5 of the OmcS heptamer.

3 Edge-to-edge distances between nearest-neighbor heme pairs

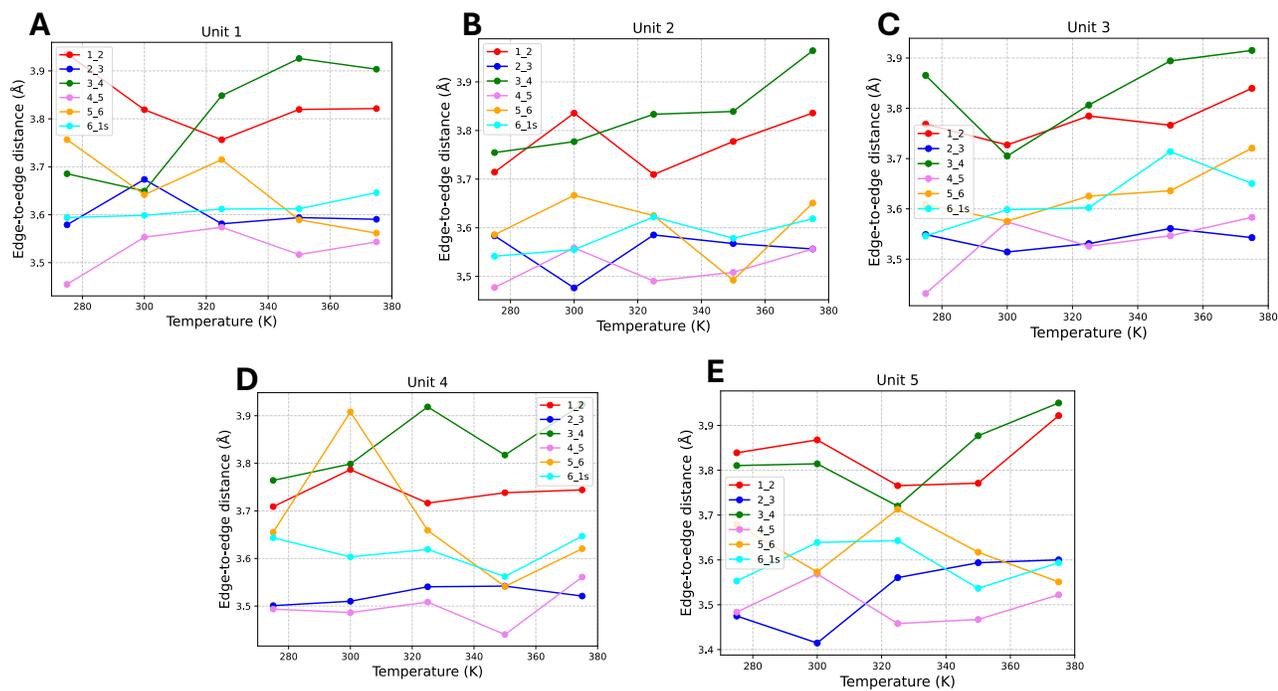


Figure S5: Edge-to-edge distances between heavy atoms of the $i - j$ heme pairs in each unit of the OmcS heptamer. Standard deviations are reported in Table S2.

Table S2: Standard deviations of the edge-to-edge distances between heavy atoms of the $i - j$ heme pairs in each unit of the OmcS heptamer.

Unit	T (K)	1_2	2_3	3_4	4_5	5_6	6_1s
1	275	0.1666	0.1762	0.1747	0.1352	0.1647	0.1544
1	300	0.1704	0.1756	0.1589	0.1547	0.1655	0.1494
1	325	0.1722	0.1600	0.2158	0.1704	0.1857	0.1732
1	350	0.1791	0.1820	0.2408	0.1663	0.1622	0.1628
1	375	0.1832	0.1748	0.2214	0.1761	0.1735	0.1911
2	275	0.1342	0.1565	0.1563	0.1386	0.1406	0.1490
2	300	0.1638	0.1492	0.1719	0.1728	0.1746	0.1517
2	325	0.1730	0.1713	0.1882	0.1529	0.1496	0.1538
2	350	0.1684	0.1656	0.2054	0.1612	0.1594	0.1669
2	375	0.1834	0.1752	0.2379	0.1775	0.1990	0.1765
3	275	0.1477	0.1499	0.2089	0.1313	0.1512	0.1381
3	300	0.1417	0.1537	0.1784	0.1836	0.1396	0.1639
3	325	0.1580	0.1588	0.1885	0.1745	0.1678	0.1679
3	350	0.1677	0.1733	0.2119	0.1696	0.1708	0.1800
3	375	0.1781	0.1784	0.2214	0.1794	0.2080	0.1833
4	275	0.1283	0.1389	0.1735	0.1494	0.1629	0.1525
4	300	0.1477	0.1496	0.1945	0.1427	0.2322	0.1671
4	325	0.1493	0.1587	0.2051	0.1571	0.1653	0.1626
4	350	0.1501	0.1621	0.1955	0.1821	0.1581	0.1669
4	375	0.1676	0.1708	0.2347	0.1783	0.1780	0.1629
5	275	0.1555	0.1360	0.1975	0.1474	0.1619	0.1422
5	300	0.1655	0.1318	0.1889	0.1560	0.1451	0.1646
5	325	0.1697	0.1746	0.1926	0.1495	0.1875	0.1577
5	350	0.1635	0.1732	0.2116	0.1511	0.1777	0.1697
5	375	0.2021	0.1879	0.2447	0.1772	0.1725	0.1794

3.1 Edge-to-edge distance distributions for unit 3 of the OmcS heptamer for MD snapshots used in electron transfer parameter calculations

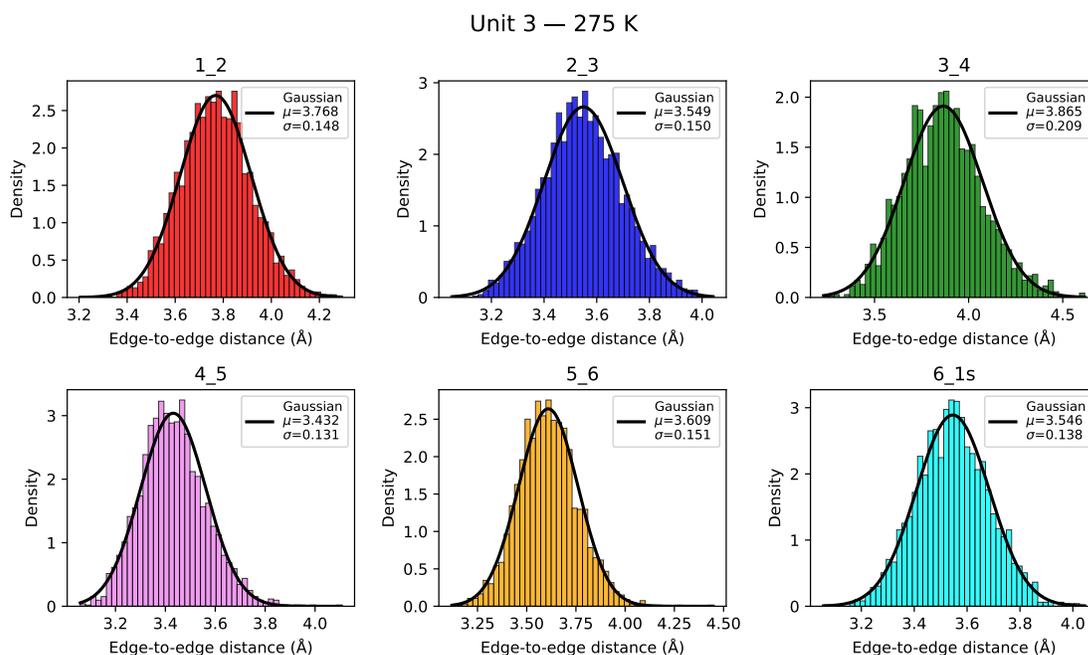


Figure S6: Edge-to-edge distance distributions at 275 K obtained from MD snapshots sampled over the 50–75 ns time window.

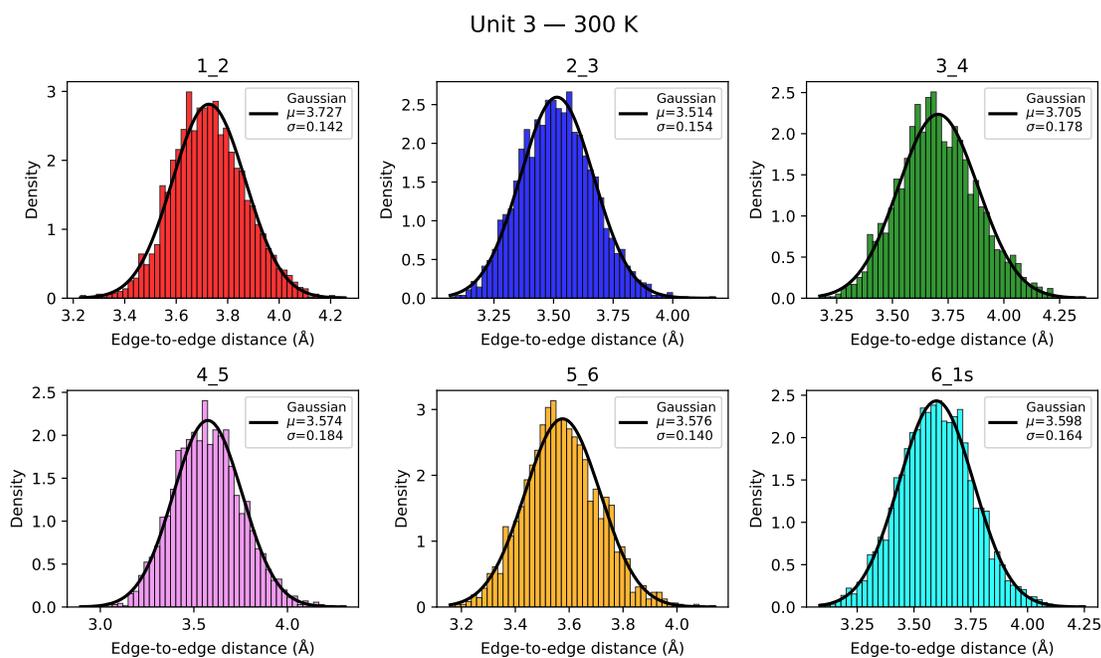


Figure S7: Edge-to-edge distance distributions at 300 K obtained from MD snapshots sampled over the 50–75 ns time window.

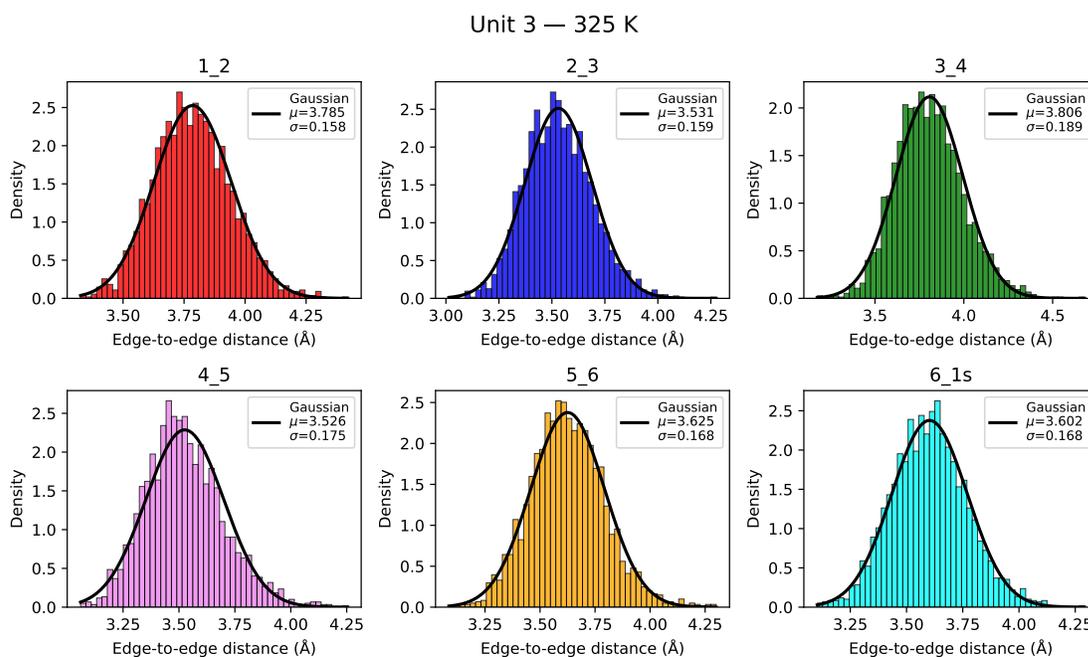


Figure S8: Edge-to-edge distance distributions at 325 K obtained from MD snapshots sampled over the 50–75 ns time window.

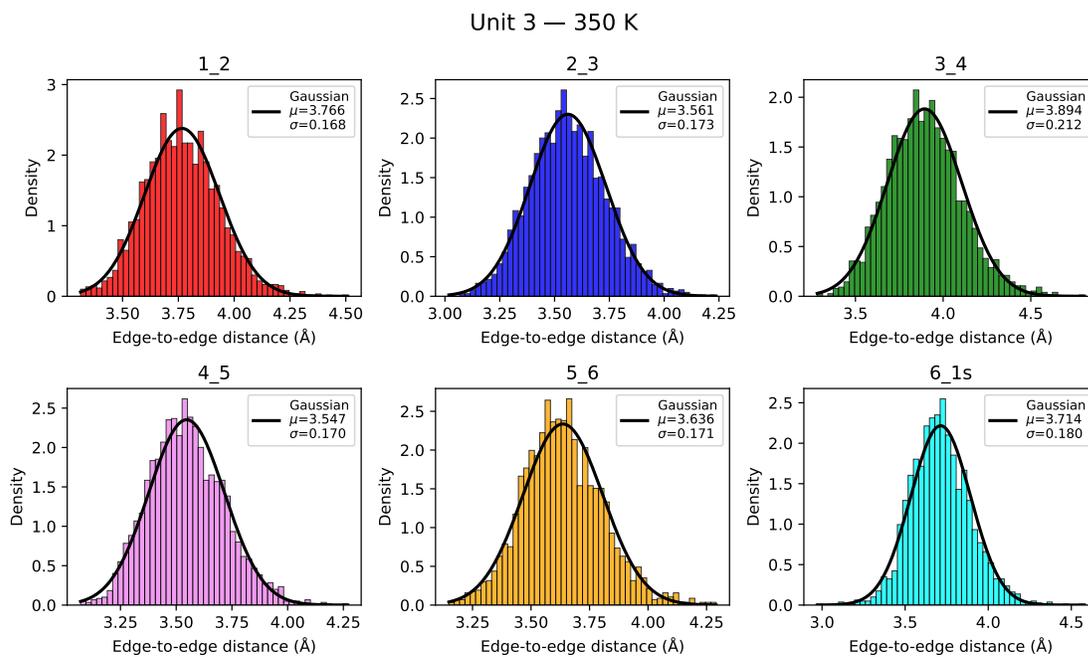


Figure S9: Edge-to-edge distance distributions at 350 K obtained from MD snapshots sampled over the 50–75 ns time window.

Unit 3 — 375 K

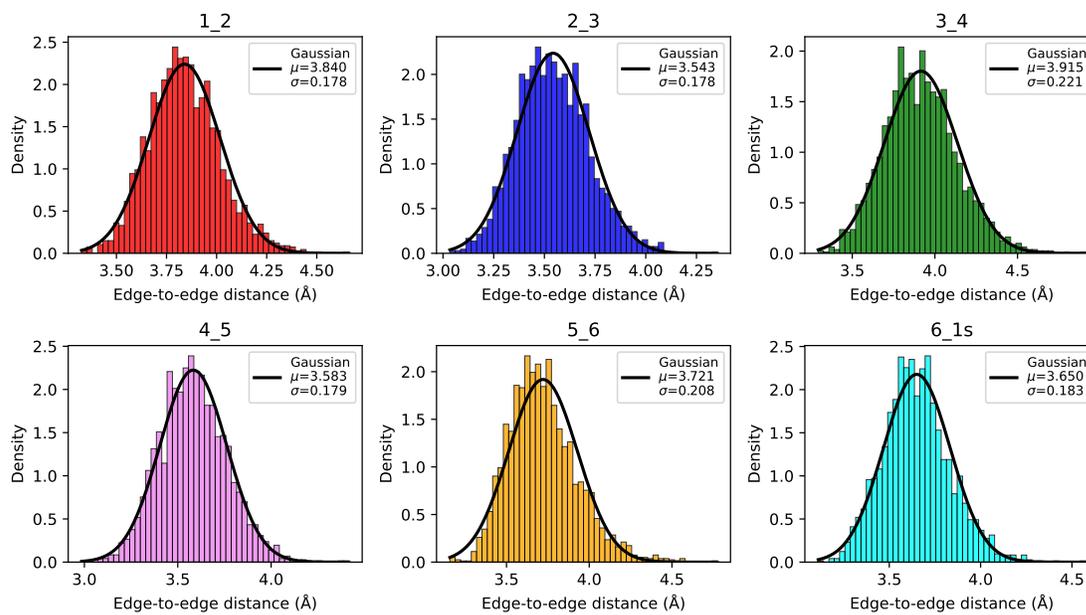


Figure S10: Edge-to-edge distance distributions at 375 K obtained from MD snapshots sampled over the 125–150 ns time window.

4 Computed effective electron transport rates for units 1, 2, 3, 4, and 5 of the OmcS heptamer

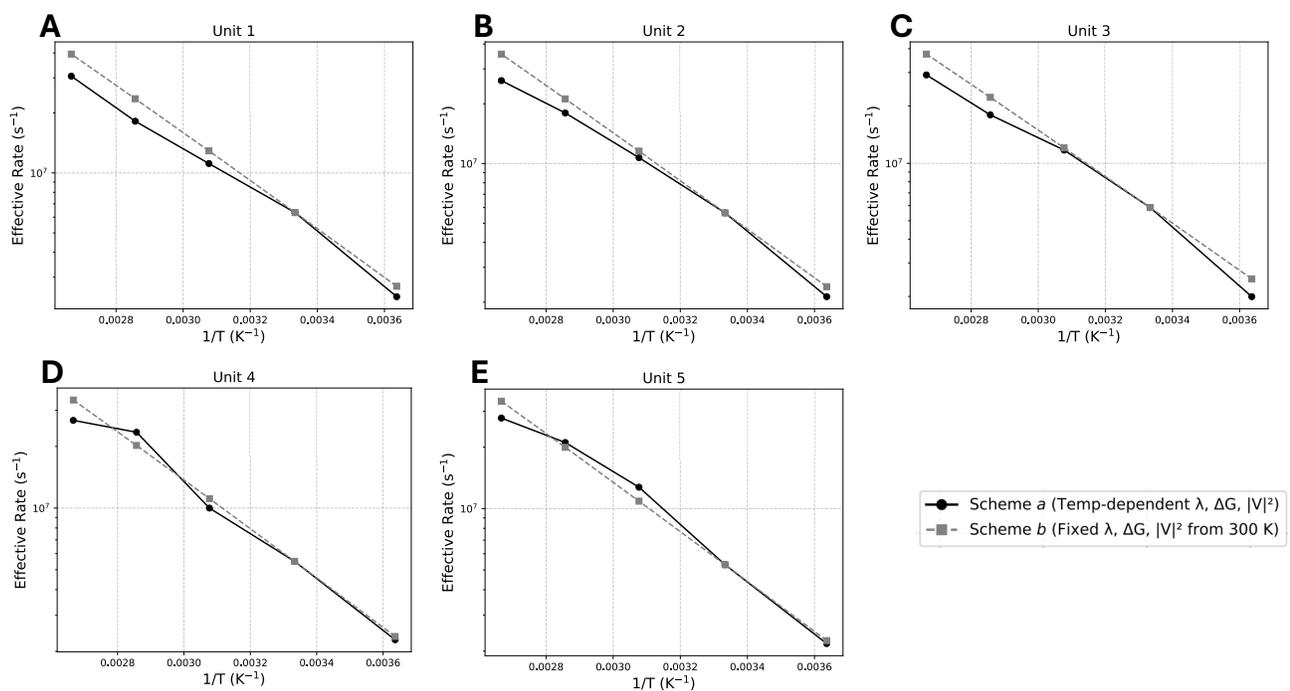


Figure S11: Computed effective electron transport rate to traverse each unit of the OmcS heptamer.

5 Comparison of computed electron transfer parameters with those of previous studies

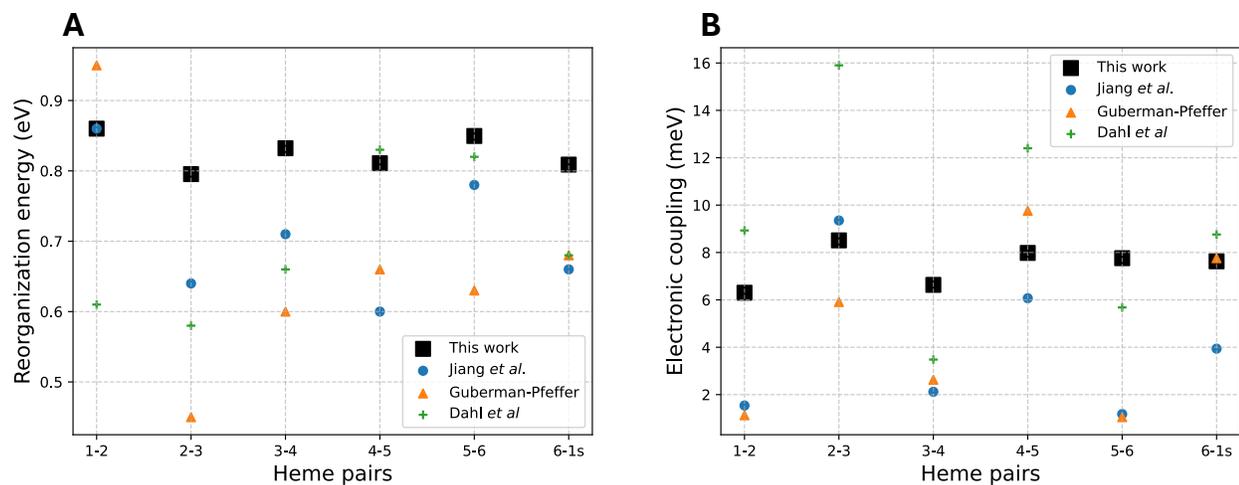


Figure S12: Computed electron transfer parameters at 300 K for heme pairs in unit 3 of the OmcS heptamer compared with results of Jiang *et al.*[2], Guberman-Pfeffer [3], and Dahl *et al.*[4] Note that values by Dahl *et al.* are at 310 K.

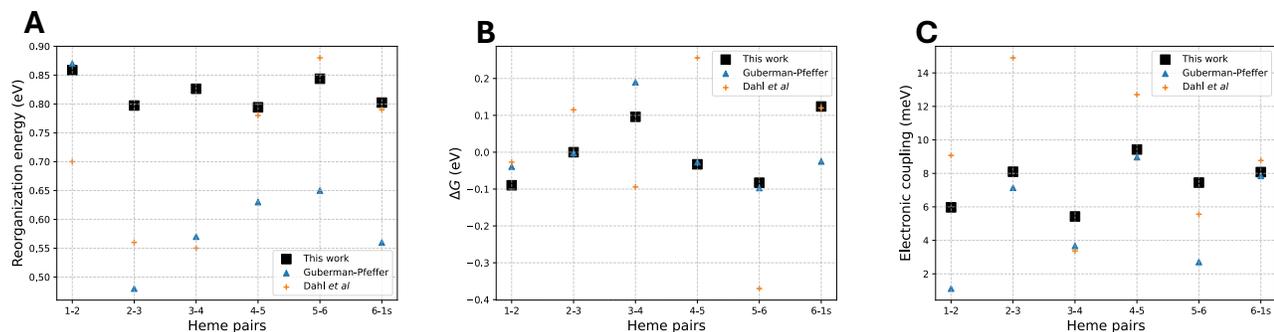


Figure S13: Computed electron transfer parameters at 275 K for heme pairs in unit 3 of the OmcS heptamer compared with results of Guberman-Pfeffer [3] and Dahl *et al.*[4] Note that values by Guberman-Pfeffer and Dahl *et al.* are at 270 K.

6 Protein backbone RMSD analysis of MD trajectories

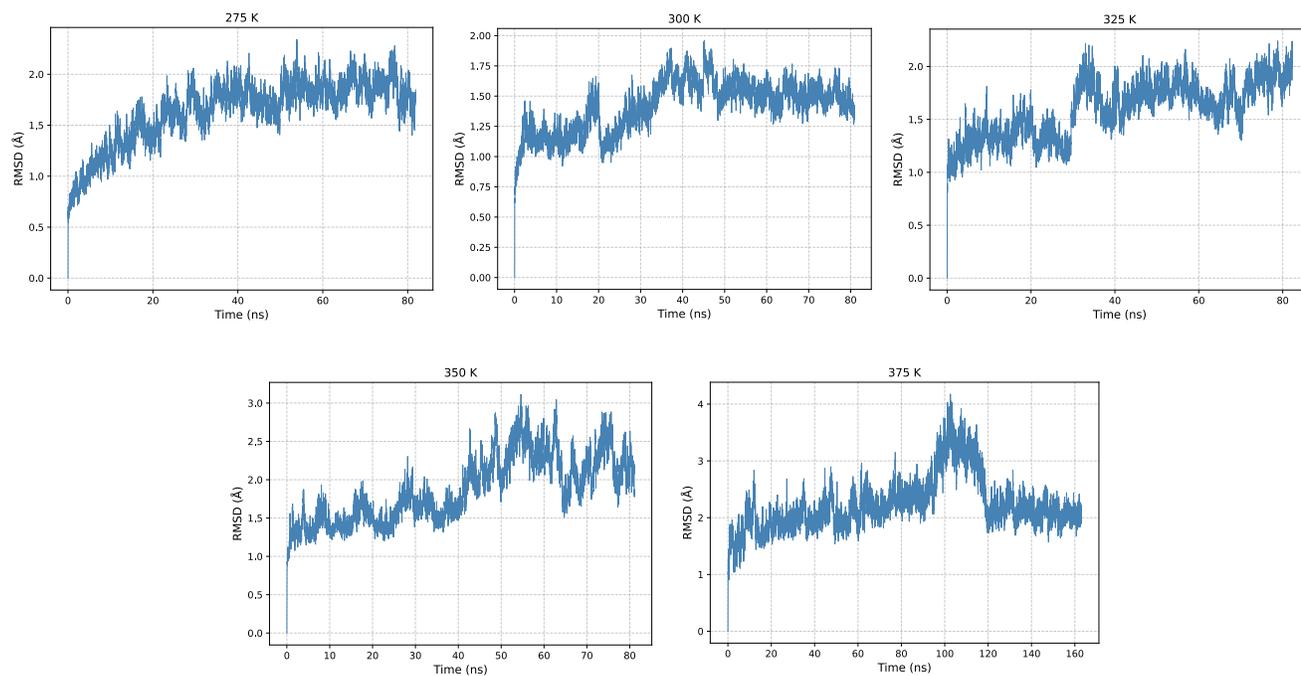


Figure S14: Protein backbone RMSD of the OmcS heptamer relative to the starting structure for MD trajectories at 275, 300, 325, 350, and 375 K.

References

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