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**Supporting information for article:**

# The putative role of some conserved water molecules in the structure and function of human transthyretin

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**Table S1** Free energy (kcal/mole) contribution of the water-clusters in the different X-ray and neutron - diffraction structures.

| | 1F41 | 3CFM | 3U2I | 3I9P | 4PVM | 3U2J | Avg | % |
|---|---|---|---|---|---|---|---|---|
| ΔG (Cryst) | -31.86 | -20.48 | -16.87 | -38.78 | -10.65 | -14.83 | -22.25 | |
| ΔG (Cryst wow) | -28.33 | -15.29 | -14.68 | -33.43 | -8.43 | -12.92 | -18.82 | |
| ΔG (Cryst WC-A) | -31.60 | -20.18 | -16.59 | -38.56 | -10.42 | -14.60 | -21.99 | |
| ΔG (Cryst WC-B) | -30.95 | -19.35 | -16.25 | -37.59 | -10.14 | -14.56 | -21.47 | |
| ΔG (Cryst WC-C) | -31.43 | -20.05 | -16.61 | -38.34 | -10.50 | -14.43 | -21.90 | |
| ΔG (Cryst WC-D) | -31.42 | -19.91 | -16.46 | -38.31 | -10.23 | -14.40 | -21.79 | |
| ΔG (Cryst WC-E) | -31.73 | -20.31 | -16.87 | -38.41 | -10.62 | -14.70 | -22.11 | |
| ΔΔG Wcryst | -3.53 | -5.18 | -2.19 | -5.35 | -2.22 | -1.90 | -3.40 | 100.00 |
| ΔΔG WC-A | -0.26 | -0.29 | -0.29 | -0.22 | -0.23 | -0.23 | -0.25 | 7.46 |
| ΔΔG WC-B | -0.91 | -1.13 | -0.63 | -1.20 | -0.51 | -0.27 | -0.78 | 22.81 |
| ΔΔG WC-C | -0.43 | -0.43 | -0.26 | -0.44 | -0.15 | -0.39 | -0.35 | 10.29 |
| ΔΔG WC-D | -0.44 | -0.57 | -0.42 | -0.47 | -0.42 | -0.42 | -0.46 | 13.44 |
| ΔΔG WC-E | -0.13 | -0.16 | 0.00 | -0.37 | -0.03 | -0.13 | -0.14 | 4.04 |
| | | | | | | | | |

Note:

WC-A: water cluster formed by W9, W10, W11, W25, W34, W35, W36 and W42.

WC-B: water cluster formed by W5, W6, W7, W8, W30, W31, W32 and W33.

WC-C: water cluster formed by W12, W20, W22 and W41.

WC-D: water cluster formed by W13, W16, W17, W37, W39 and W40.

ΔG (Cryst): Stability free energy of the dimeric Crystal Structure with all water molecules; ΔG (Cryst wow): stability free energy of the dimeric Crystal Structure without the water molecules.

ΔΔG Wcryst: contribution of all the water molecules towards stability free energy of the dimeric crystal.

ΔG (Cryst WC-i): stability free energy of the dimeric Crystal Structure without i-th water cluster.

ΔΔG WC-i: contribution of i-th water cluster towards stability free energy of the dimeric crystal.

Avg: Average of all the crystal structures taken for free energy calculation.