Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Structure and dynamics of solvent molecules inside Polytheonamide B channel in different environments: A molecular dynamics study

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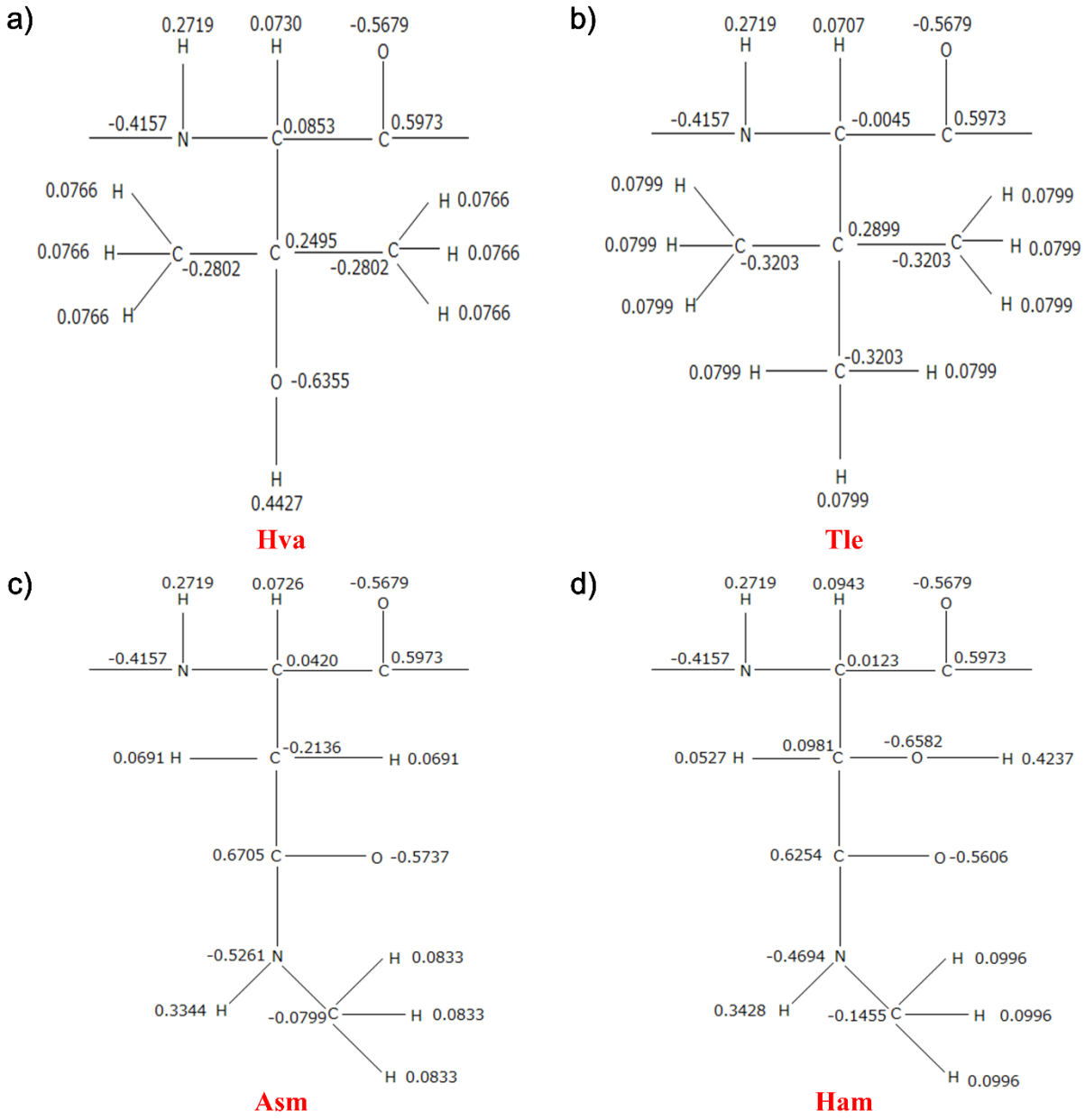


**Figure S1:** Point charges for the non-standard groups in pTB. **(a)** β-hydroxyvaline (Hva). **(b)** *tert*-leucine (Tle). **(c)** γ-N-methylasparagine (Asm). **(d)** γ-N-methyl-*threo*-β-hydroxyasparagine (Ham).

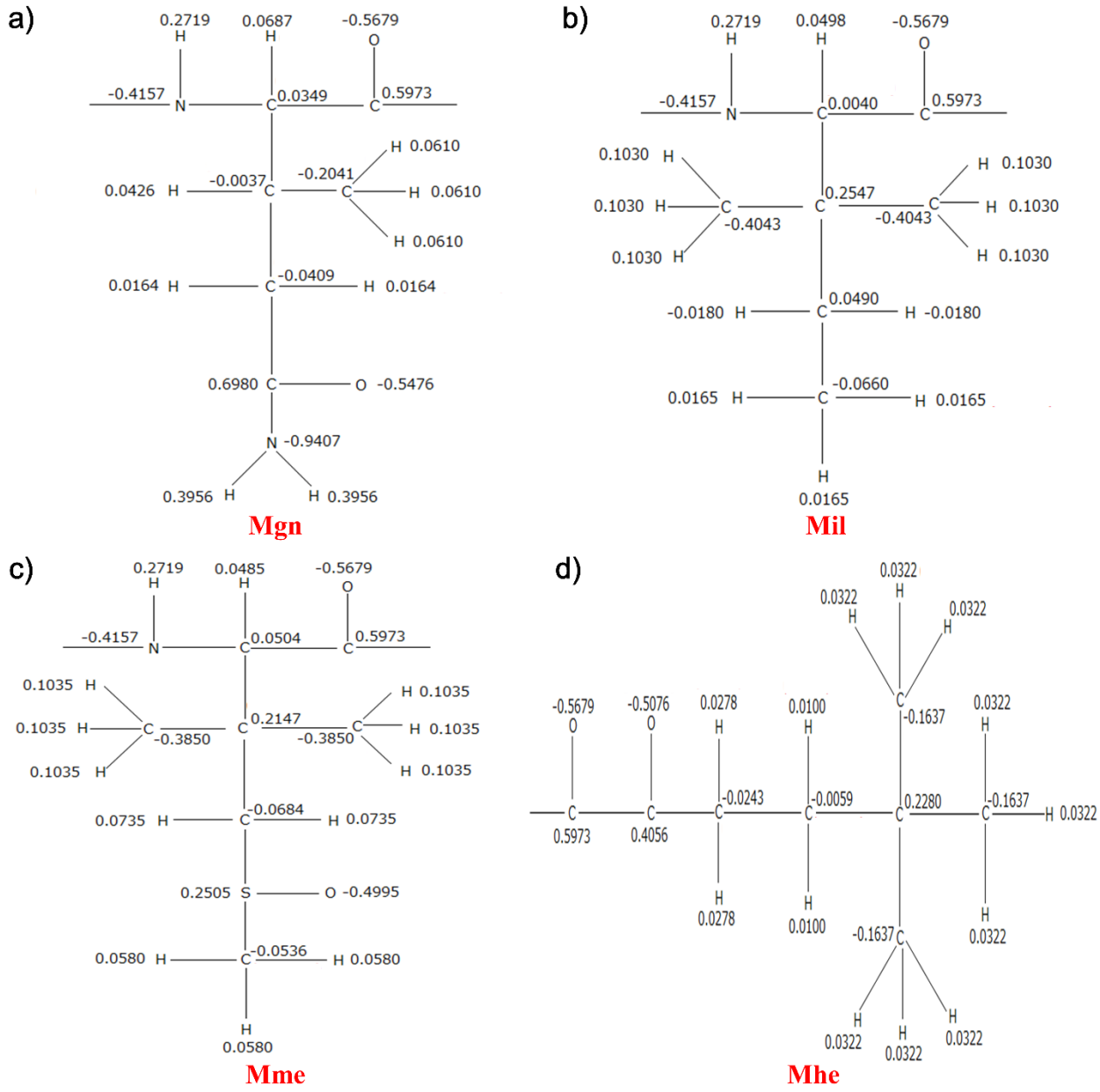


**Figure S2:** Point charges for the non-standard groups in pTB. **(a)** β-methylglutamine (Mgn). **(b)** β-methylisoleucine (Mil). **(c)** β,β-dimethylmethionine sulphoxide (Mme). **(d)** 5,5-dimethyl-2-oxo-hexanoyl (Mhe).

**Table S1:** Probabilities of zero and double occupancies, and average number of molecules at sites 2-11 for water molecules inside the pore in water, calculated from 1.5 μs data.

| Site Number | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| P(n=0) | 0.0662 | 0.0657 | 0.0760 | 0.0402 | 0.0134 | 0.0154 | 0.0068 | 0.0261 | 0.0160 | 0.0728 |
| P(n=2) | 0.2804 | 0.0204 | 0.0255 | 0.0205 | 0.0769 | 0.0430 | 0.0320 | 0.0068 | 0.0179 | 0.0080 |
| <n> | 1.2146 | 0.9547 | 0.9495 | 0.9803 | 1.0635 | 1.0277 | 1.0251 | 0.9807 | 1.0019 | 0.9351 |

**Table S2:** Probabilities of zero and double occupancies, and average number of molecules at sites 2-11 for water molecules inside the pore in POPC bilayer, calculated from 2 μs data.

| Site Number | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| P(n=0) | 0.0022 | 0.0069 | 0.0032 | 0.0033 | 0.0076 | 0.0249 | 0.0008 | 0.0133 | 0.0386 | 0.0659 |
| P(n=2) | 0.0228 | 0.0125 | 0.0057 | 0.0050 | 0.0084 | 0.0099 | 0.2572 | 0.0497 | 0.0155 | 0.0086 |
| <n> | 1.0206 | 1.0056 | 1.0025 | 1.0017 | 1.0008 | 0.9850 | 1.2564 | 1.0364 | 0.9769 | 0.9427 |

**Table S3:** Probabilities of zero and double occupancies, and average number of molecules at sites 2-7 for methanol molecules inside the pore in 1:1 chloroform/methanol mixture, calculated from 2 μs data.

| Site Number | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|
| P(n=0) | 0.0854 | 0.0569 | 0.0505 | 0.0709 | 0.0409 | 0.0824 |
| P(n=2) | 0.0275 | 0.0640 | 0.0520 | 0.0508 | 0.0712 | 0.0167 |
| <n> | 0.9421 | 1.0071 | 1.0015 | 0.9800 | 1.0303 | 0.9342 |