

Results & Conclusion

- The BI/BII population of guanine is in good agreement with the results of Lavery. et. al [6].
- Comparison of Na⁺ distribution indicates different populations for 6MG and Guanine containing DNA which might be important for rapid indirect readout recognition (Fig 4).
- BP-REMD allows much more rapid identification of putative substates compared to cMD.
- In the case of 6MG new substates for the coupled ϵ/ζ -backbone dihedral angles have been observed (Fig 5)
- BDNA-models simulations shows comparable results to crystal structure MD Simulations
- 6MG has a strong influence to the conformations of his nearest neighbors

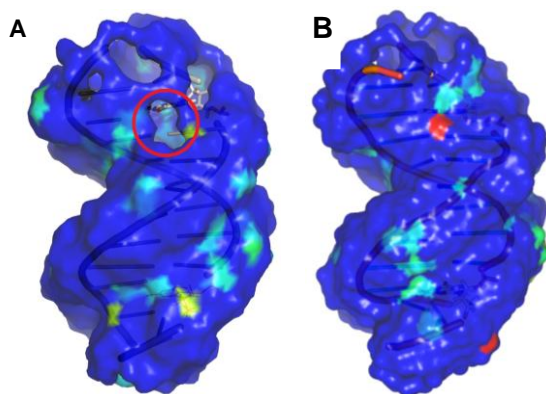


Fig 4: Comparison of Na⁺ distribution (A):6MG and

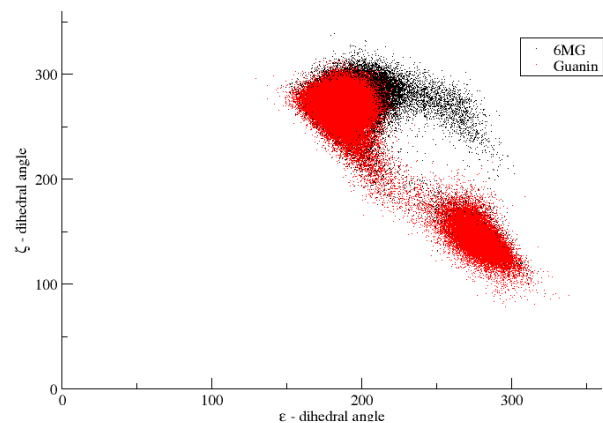


Fig 5: Sampling of ϵ/ζ backbone dihedral angles

References

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