Structural basis for telomeric G-quadruplex targeting by naphthalene diimide ligands

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1) Supplementary Figures

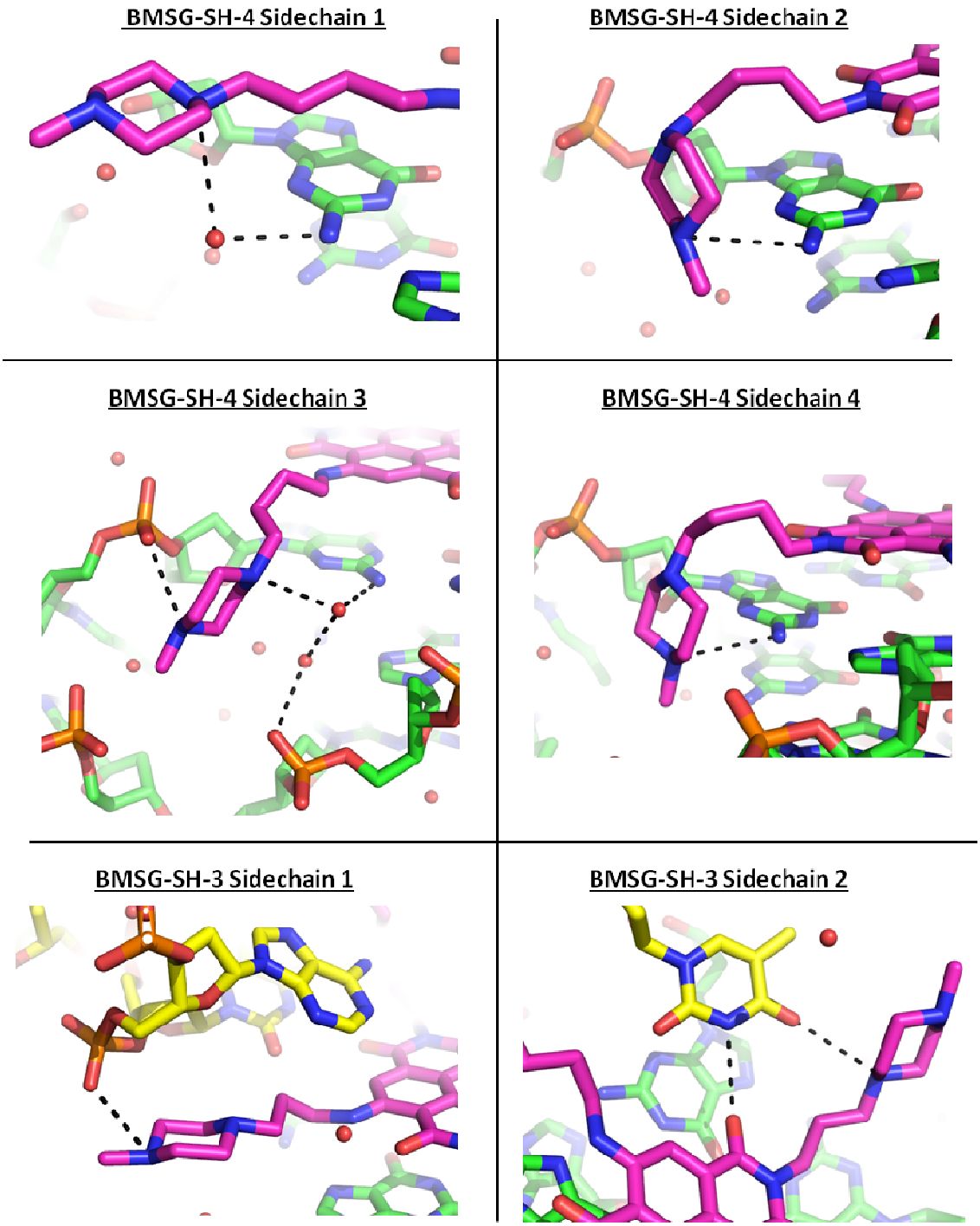

Figure S1: Contacts are highlighted for all the key ligand and quadruplex groove interactions. Dashed lines represent contact < 3.4 Å.

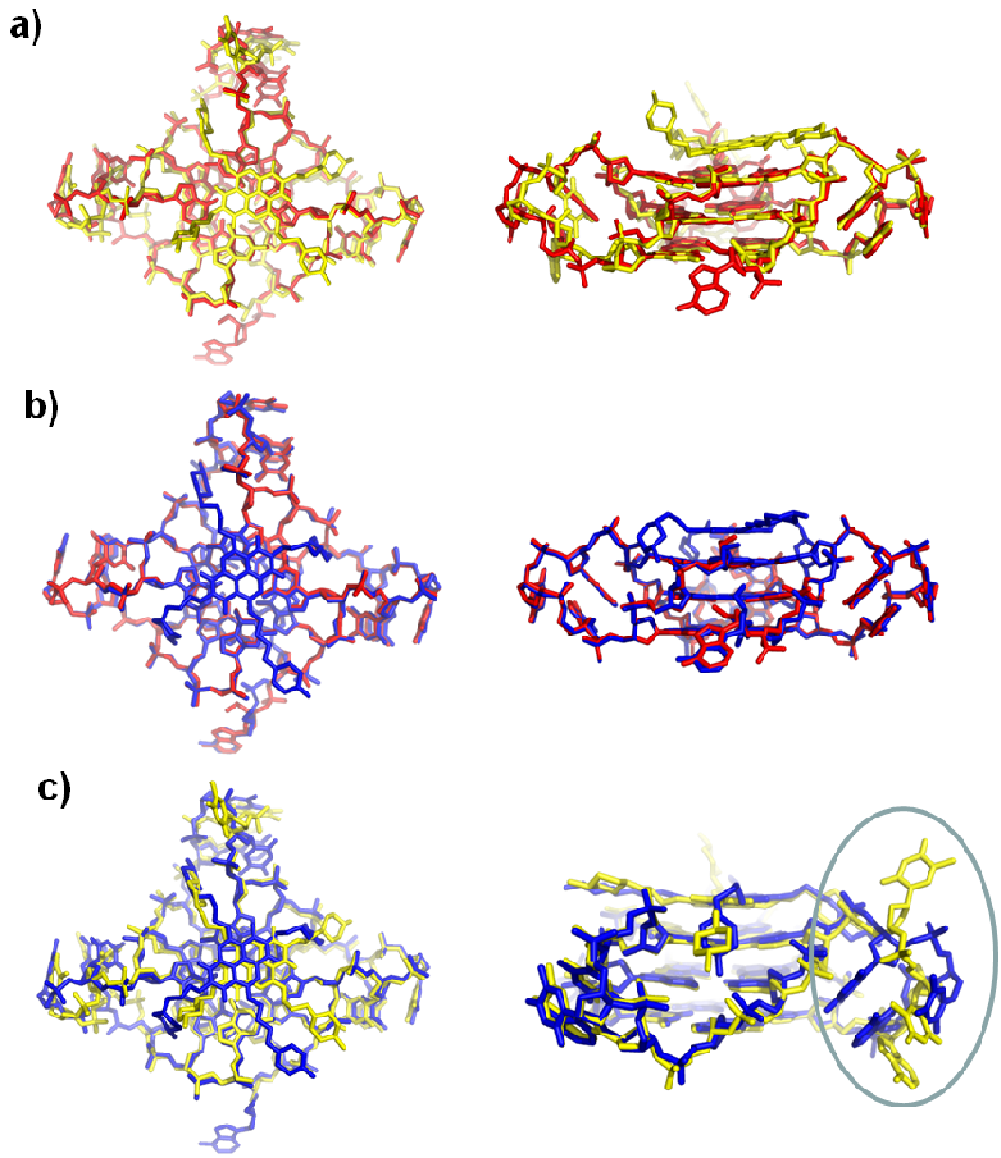

Figure S2: a) Structural alignment of the native human 22-mer G-quadruplex 1KF1 (red) and the 22-mer-BMSG-SH-3 complex (yellow). RMSD (root mean square deviation) = 2.235 (450 to 450 atoms). b) Structural alignment of the native human 22-mer G-quadruplex 1KF1 (red) and the 22-mer-BMSG-SH-4 complex (blue). RMSD = 0.540 (468 to 468 atoms). c) Structural alignment of the 22-mer-BMSG-SH-3 complex (yellow) and the 22-mer-BMSG-SH-4 complex (blue). RMSD3 = 2.186 (447 to 447 atoms). The main region of structural deviation is circled in blue. RMSDs calculated using PyMol. The low RMSD of (b) highlights the complete absence of conformational changes induced by BMSG-SH-4. The higher RMSDs of (a) and (c) are due largely to the rearrangement of one propeller-loop in the BMSG-SH-3 complex compared to the native and BSMG-SH-4 structures. This loop rearrangement plays a major role in crystal packing stabilisation (i.e. in crystal growth) but is not significantly involved in ligand binding.

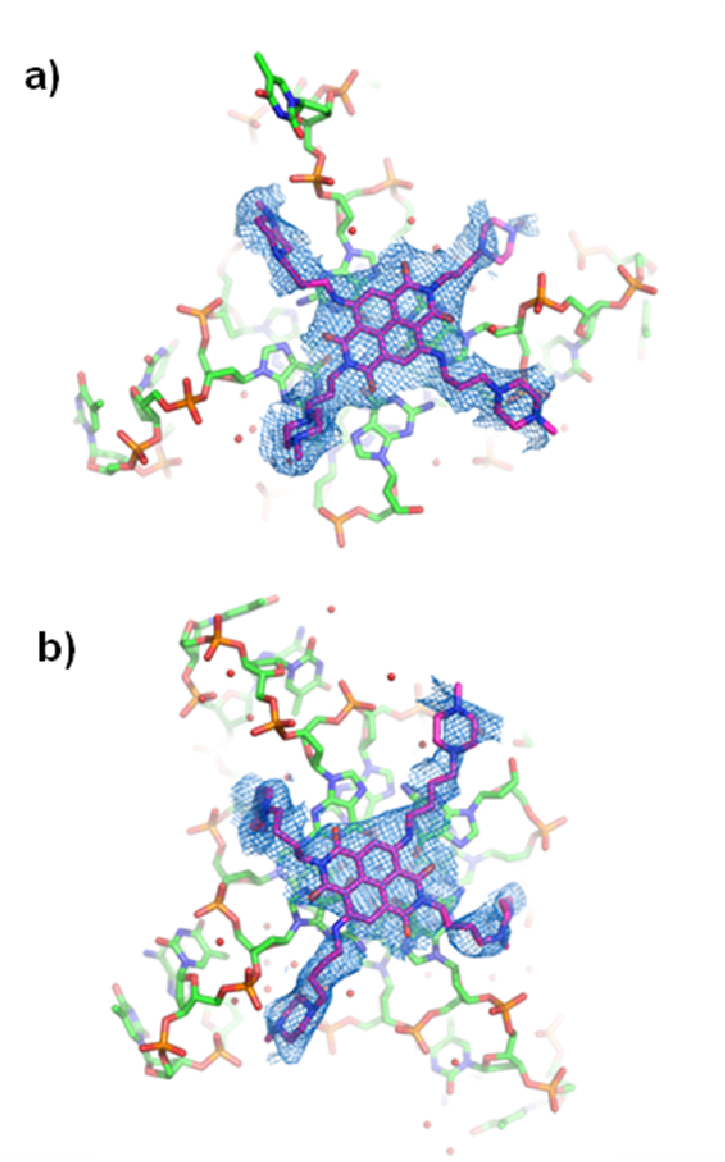

Figure S3: Ligand omit maps for BMSG-SH-3 (A) and BMSG-SH-4 (B) complexes sigma levels 0.9 and 0.8 for (a) and (b), respectively.

2) REFERENCE

10d. Salvati, E.; Leonetti, C.; Rizzo, A.; Scarsella, M.; Mottolese, M.; Galati, R.; Sperduti, I.; Stevens, M. F. G.; D'Incalci, M.; Blasco, M.; Chiorino, G.; Bauwens, S.; Horard, B.; Gilson, E.; Stoppacciaro, A.; Zupi, G.; Biroccio, A. *J. Clin. Investig*. **2007**, *117*, 3236-3247.