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Supporting Information

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Molecular recognition of a three-way DNA junction by a metallo-supramolecular helicate

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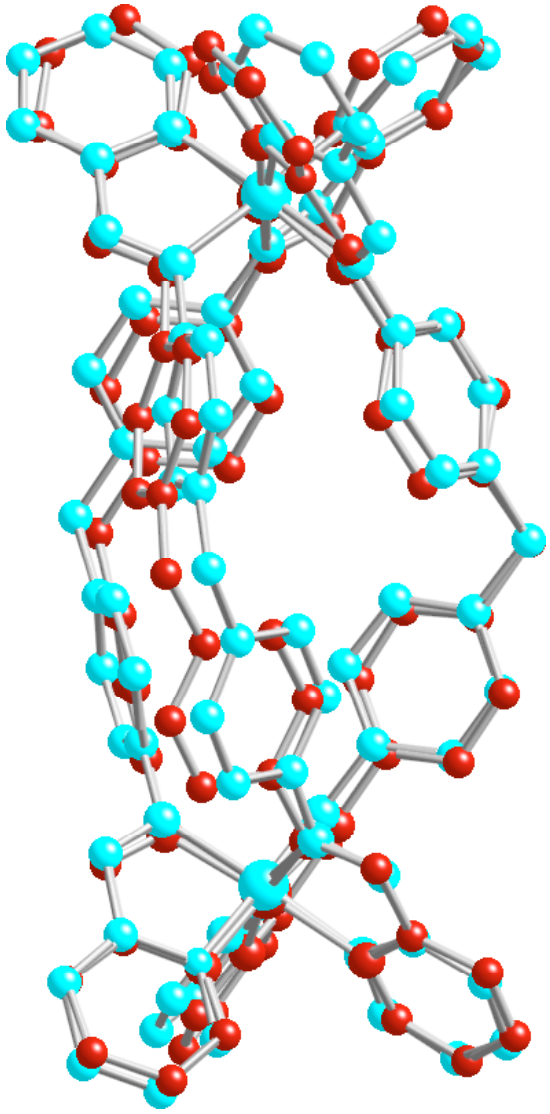

Fig. S1: Supermimposition of the free (blue; F. Tuna, M.J. Hannon and G.J. Clarkson, unpublished) and DNA-bound (red) structures of the supramolecular helicate $[Fe_2L_3]^{4+}$ ($L=C_{25}H_{20}N_4$).

Table S1. Data collection, phasing and refinement statistics

Data collection:				
Data set	Peak	Inflexion	Remote	High resolution
λ (Å) [a]	1.739	1.741	1.627	0.933
Space group	$P4_132$			
Unit cell parameters	a = b = c = 71.20 Å , $\alpha=\beta=\gamma= 90^o$			
Resolution range (Å)	30-2.6	30-2.6	30-2.8	22.5-1.7 (1.8-1.7)
Number of reflections:				
total	73,467	54,690	42,532	91,621
unique	3399	3407	2865	7,134
Completeness (%) [b]	99.3 (97.8)	99.5 (98.3)	99.7 (100)	99.2 (99.7)
$\langle I / \sigma(I) \rangle$ [b]	53.0 (11.4)	48.52 (9.3)	26.1 (5.5)	29.1 (8.8)
Average multiplicity	21.61	16.1	14.8	12.8
R_{sigma} [c,b]	4.7 (24.3)	3.9 (26.6)	9.8 (55.1)	2.4 (11.8)
Phasing:				
Connectivity [d]	0.90			
Contrast [e]	0.35			
Pseudo free CC [f]	62.9			
Map CC [g]	94			
Refinement:				
R_{factor} (free R_{factor}) [h]				24.9 (29.1)
r.m.s.deviation from target values				
Bond lengths (Å)				0.008
Bond angle distances (Å)				0.023
Average B-factors (Å^2)				
Fe^{2+}				17.1
Drug				18.0
DNA				22.6
Solvent				41.5
Number of Fe^{2+} [i]				2
Number of Drug atoms [i]				87
Number of DNA atoms [i]				180
Number of solvent molecules [i]				45

[a] The absorption peak dataset was taken as a reference.

[b] Outermost resolution shell values in parenthesis.

[c] $R_{sigma}= (\Sigma[\sigma(F_o^2)] / \Sigma[F_o^2]) \times 100$.

[d] The variance *V* of density on a spherical surface of radius 2.42 Å is calculated for each pixel in the map, and the pixels with the highest variances (*V*) are considered more likely to be atom positions. The *connectivity* is the fraction of adjacent pixels that are either both in the solvent or both in the macromolecular region(*22*).

[e] Contrast= The variance of *V* over all pixels(*22*).

[f] Pseudo free CC: CC (see g) calculated with 10% of the reflections omitted at random after performing one cycle of density modification(*22*).

[g] Map CC = $[N\Sigma|E_H| |E_A| - \Sigma |E_H| \Sigma|E_A|] / \{[N\Sigma|E_H|^2- (\Sigma|E_H|)^2] [N\Sigma|E_A|^2- (\Sigma|E_A|)^2]\}^{1/2} \times 100$ with E_H normalized structure factors derived from the calculated iron atom positions and E_A from the observed MAD F_A data(*22*).

[h] $R_{factor} =\{\Sigma_{hkl} ||F_o| - k |F_c|| / \Sigma_{hkl} |F_o|\} \times 100$, with F_o and F_c as the observed and calculated structure factor amplitudes; free R_{factor}, same for a test set of reflections not used during refinement.

[i] Per asymmetric unit.

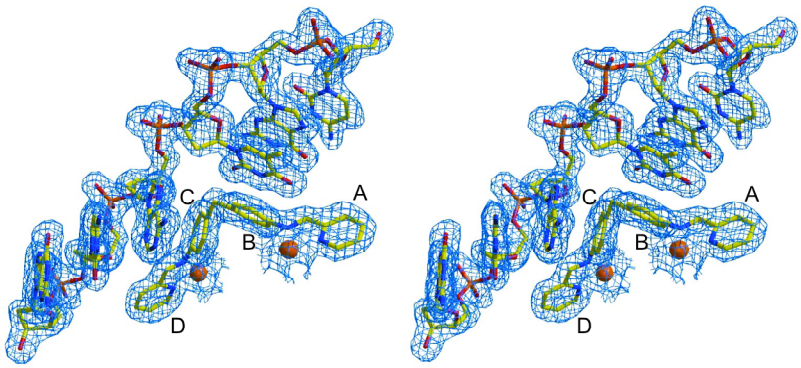

Fig. S2: Stereo plot of a σ_A-weighted Fourier map calculated with coefficients 2Fo-Fc and contoured at the 1σ level showing part of the refined DNA and drug molecules fitted in the electron density. The two Fe^{2+} ions are represented as spheres; pyridine rings: A, D; phenyl rings: B, C.