Electronic Supplementary Material (ESI) for Chemical Science.

Re-pairing DNA: Binding of a ruthenium phi complex to a double mismatch

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Figure S1 – Perspective view of the unit cell from the crystal structure of *rac*-[Ru(phen)$_2$phi]$^{2+}$ with DNA mismatch, illustrating the solvent channels.

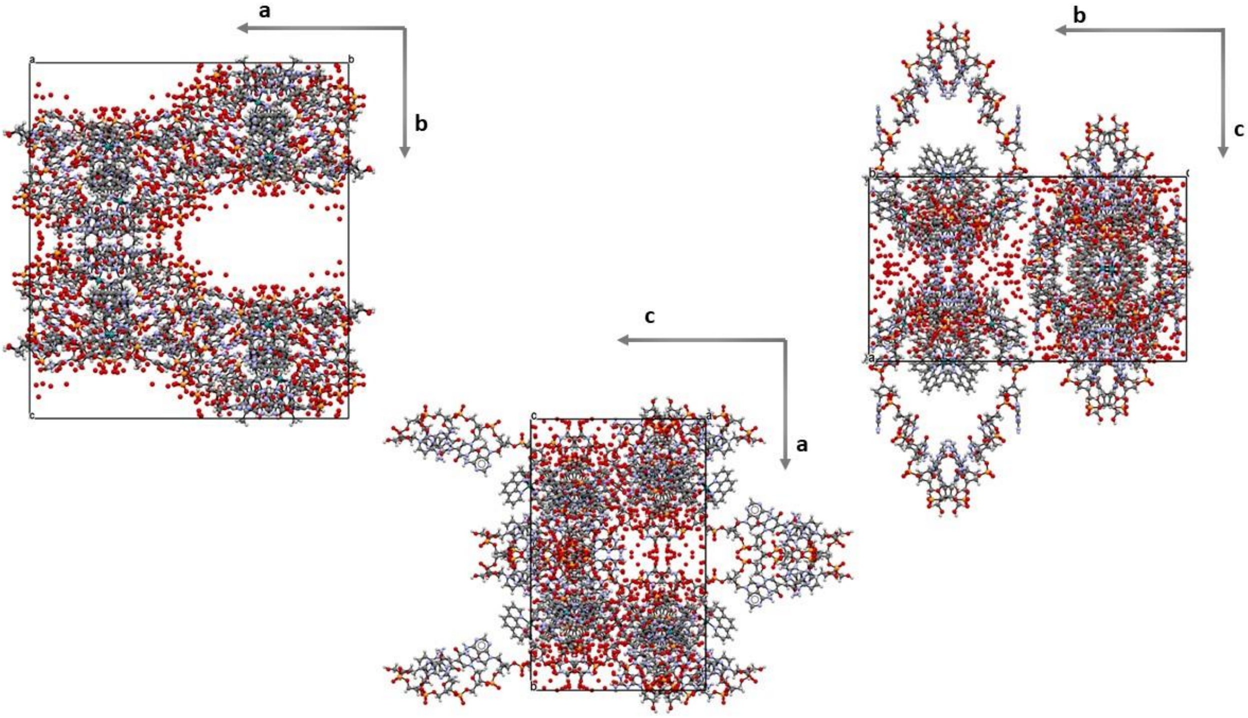

Figure S2 – Electron density around a) [Ru(phen)2phi]2+, and b) guanine-cytosine base pair, showing the high-quality data of this crystal structure. Map contouring level 0.8800 e/Å^3 (1.5σ).

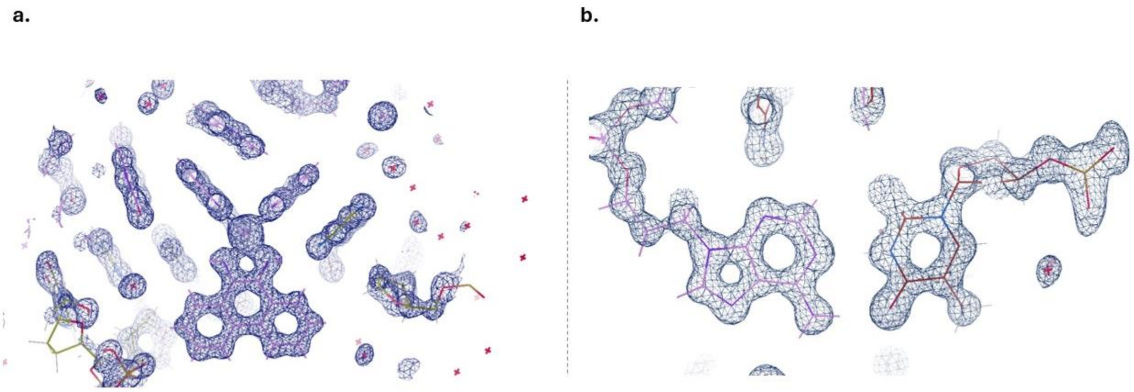

Figure S3. The location of 69 water molecules (red spheres) in this structure (8CMM), shown from both sides of the DNA backbone. The asymmetric unit, shown as spheres. Nucleic acid component – grey; ruthenium complexes – pink. K^+ and Li+ shown as small spheres for clarity.

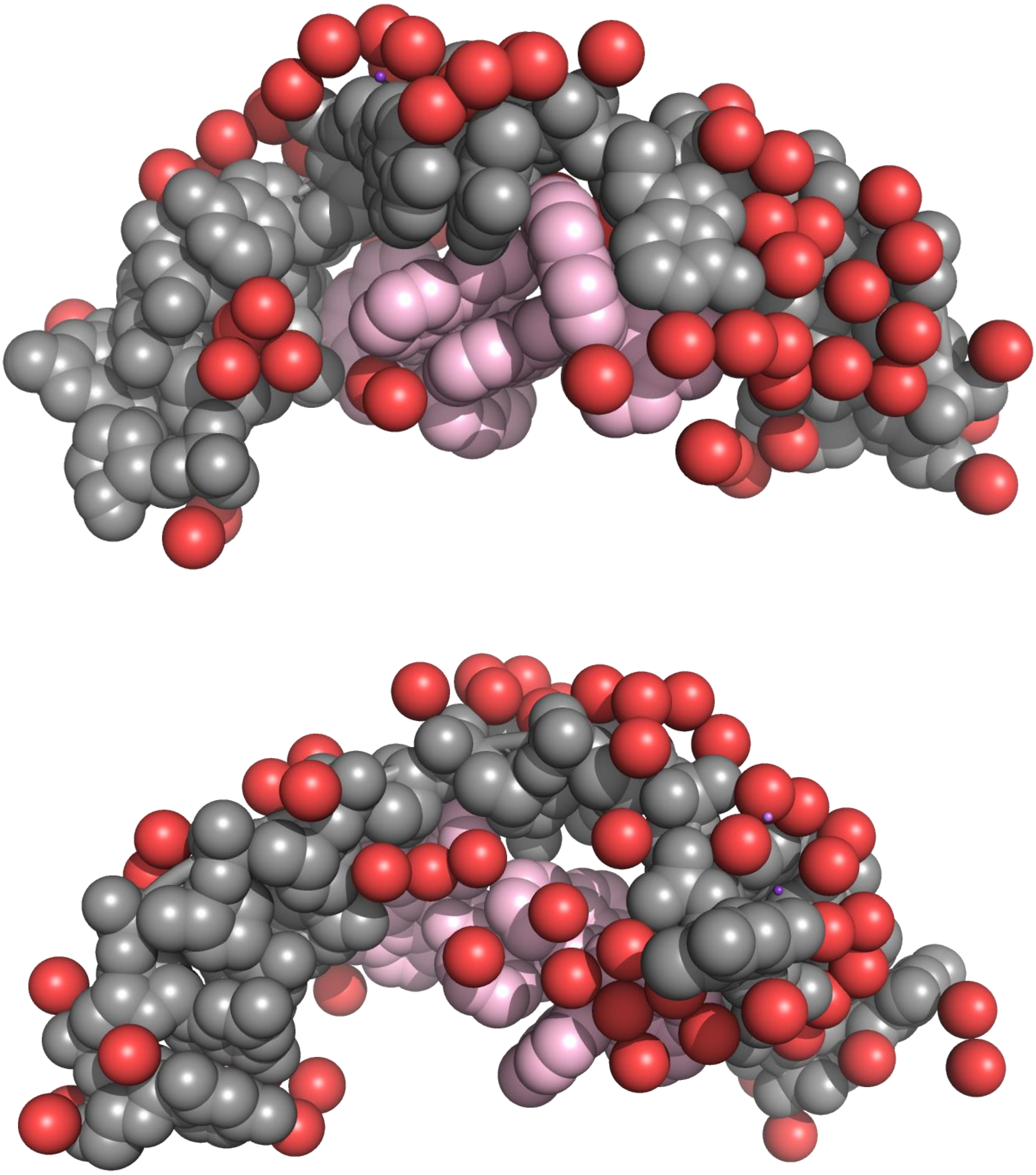

Table S1 – Summary, data collection and refinement statistics.

Data collection

Space group	$I2_12_12_1$
Resolution (Å)	36.20 – 0.90
Data collection temperature (K)	100
R_{merge}	0.044
R_{pim}	0.013
R_{meas}	0.046
Anisotropy	0.492
F_o, F_c correlation	0.98
I/σI	1.00 (at 0.90 Å)
$CC_{1/2}$	0.999
Completeness for range %	92.47
Data redundancy	12.1
Wilson B factor (Å^2)	10.08
Total number of atoms	447
Average B, all atoms (Å^2)	13.0

Refinement

N_o reflections measured	27375
R_{work}/R_{free}	0.1359/0.1594
Data cutoff (sigma(F))	NONE
Free R value test set count	1425
Mean B value (overall A^2)	11.224
PDB ID	**8CMM**

Table S2. Conformational analysis- The list of parameters given below correspond to the 5´ to the 3´ direction of strand I, and 3´ to 5´ direction of strand II.

```
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 C-G       0.35     -0.21      0.18      7.69    -15.86     -0.85
    2 G-C       0.03     -0.15      0.01      3.21    -18.73      2.98
    3 C-G       0.21     -0.16      0.09      3.42    -10.57     -1.01
    4 T-A      -0.16     -0.09     -0.32     13.17     -5.09      4.75
    5 T-A       0.05     -0.17      0.26    -18.22     15.64     -1.79
    6 A-T      -0.05     -0.17      0.26     18.22     15.64     -1.79
    7 A-T       0.16     -0.09     -0.32    -13.17     -5.09      4.75
    8 G-C      -0.21     -0.16      0.09     -3.42    -10.57     -1.01
    9 C-G      -0.03     -0.15      0.01     -3.21    -18.73      2.98
   10 G-C      -0.35     -0.21      0.18     -7.69    -15.86     -0.85
   11 G-G      -0.00     -8.41      2.09      0.00    -33.00   -157.99
   12 C-G       0.35     -0.21      0.18      7.69    -15.86     -0.85
   13 G-C       0.03     -0.15      0.01      3.21    -18.73      2.98
   14 C-G       0.21     -0.16      0.09      3.42    -10.57     -1.01
   15 T-A      -0.16     -0.09     -0.32     13.17     -5.09      4.75
   16 T-A       0.05     -0.17      0.26    -18.22     15.64     -1.79
   17 A-T      -0.05     -0.17      0.26     18.22     15.64     -1.79
   18 A-T       0.16     -0.09     -0.32    -13.17     -5.09      4.75
   19 G-C      -0.21     -0.16      0.09     -3.42    -10.57     -1.01
   20 C-G      -0.03     -0.15      0.01     -3.21    -18.73      2.98
   21 G-C      -0.35     -0.21      0.18     -7.69    -15.86     -0.85
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      0.00     -0.55      0.14     -0.00     -8.17     -6.75
      s.d.      0.20      1.80      0.49     10.83     13.47     34.75
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Local base-pair step parameters
      step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 CG/CG        0.27      0.45      3.52      3.40      7.19     32.54
   2 GC/GC        0.72     -0.69      3.23     -2.86     -0.91     38.15
   3 CT/AG       -0.94     -0.86      3.08      2.33      2.45     19.43
   4 TT/AA        ----      ----      ----      ----      ----      ----
   5 TA/TA       -0.00      2.66      2.58     -0.00      4.83      2.86
   6 AA/TT        ----      ----      ----      ----      ----      ----
   7 AG/CT        0.94     -0.86      3.08     -2.33      2.45     19.43
   8 GC/GC       -0.72     -0.69      3.23      2.86     -0.91     38.15
   9 CG/CG       -0.27      0.45      3.52     -3.40      7.19     32.54
  10 GG/GC        ----      ----      ----      ----      ----      ----
  11 GC/GG        ----      ----      ----      ----      ----      ----
  12 CG/CG        0.27      0.45      3.52      3.40      7.19     32.54
  13 GC/GC        0.72     -0.69      3.23     -2.86     -0.91     38.15
  14 CT/AG       -0.94     -0.86      3.08      2.33      2.45     19.43
  15 TT/AA        ----      ----      ----      ----      ----      ----
  16 TA/TA        0.00      2.66      2.58     -0.00      4.83      2.86
  17 AA/TT        ----      ----      ----      ----      ----      ----
  18 AG/CT        0.94     -0.86      3.08     -2.33      2.45     19.43
  19 GC/GC       -0.72     -0.69      3.23      2.86     -0.91     38.15
  20 CG/CG       -0.27      0.45      3.52     -3.40      7.19     32.54
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
        ave.      0.00      0.07      3.18     -0.00      3.18     26.16
        s.d.      0.68      1.23      0.31      2.78      3.27     12.42
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Local base-pair helical parameters
      step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 CG/CG       -0.51      0.14      3.55     12.60     -5.95     33.47
   2 GC/GC       -0.94     -1.45      3.19     -1.39      4.36     38.26
   3 CT/AG       -3.58      3.77      2.81      7.18     -6.85     19.72
   4 TT/AA        ----      ----      ----      ----      ----      ----
   5 TA/TA       -8.79     -0.00      3.60     59.34      0.00      5.61
   6 AA/TT        ----      ----      ----      ----      ----      ----
   7 AG/CT       -3.58     -3.77      2.81      7.18      6.85     19.72
   8 GC/GC       -0.94      1.45      3.19     -1.39     -4.36     38.26
   9 CG/CG       -0.51     -0.14      3.55     12.60      5.95     33.47
  10 GG/GC        ----      ----      ----      ----      ----      ----
  11 GC/GG        ----      ----      ----      ----      ----      ----
  12 CG/CG       -0.51      0.14      3.55     12.60     -5.95     33.47
  13 GC/GC       -0.94     -1.45      3.19     -1.39      4.36     38.26
  14 CT/AG       -3.58      3.77      2.81      7.18     -6.85     19.72
  15 TT/AA        ----      ----      ----      ----      ----      ----
  16 TA/TA       -8.79     -0.00      3.60     59.34      0.00      5.61
  17 AA/TT        ----      ----      ----      ----      ----      ----
  18 AG/CT       -3.58     -3.77      2.81      7.18      6.85     19.72
  19 GC/GC       -0.94      1.45      3.19     -1.39     -4.36     38.26
  20 CG/CG       -0.51     -0.14      3.55     12.60      5.95     33.47
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
        ave.     -2.69     -0.00      3.24     13.73      0.00     26.93
        s.d.      2.89      2.24      0.33     20.10      5.58     11.77
```