Supporting Information:

Movie 1: An example of the flipping of A1492 and A1493 in the context of the 30S ribosomal subunit (simulation S1). Ribosomal RNA is shown in violet. Ribosomal proteins are shown in maroon. Small subunit rRNA A1493 (cyan) and A1492 (green) flip in and out of the decoding helix (H44). Hexa-hydrated magnesium is shown in translucent. The movie displays a minute fraction of the total simulation (< 1/1,000th).

Movie 2: Gentamicin unbinding from the ribosomal A site (simulation S2). Ring I (white), ring II (orange) and ring III (yellow) of gentamicin probe the non-specific energy landscape near the binding site. As in movie 1, movie 2 displays a minute fraction of the total simulation (< 1/1,000th).

Forcefield parameters for MgW_6 (GROMACS)

```
[ moleculetype ]
; molname     nrexcl
MO6           1

[ atoms ]
;  nr  type  resnr residue atom  cgnr   charge    mass
   1 amber99_33  1 MO6   MG    1    +2.0   24.30000
   2   amber99_42  1      MO6   O1    2    -0.834  16.00000
   3   amber99_27  1      MO6   H11   2     0.417   4.00800
   4   amber99_27  1      MO6   H12   2     0.417   4.00800
   5   amber99_42  1      MO6   O2    3    -0.834  16.00000
   6   amber99_27  1      MO6   H21   3     0.417   4.00800
   7   amber99_27  1      MO6   H22   3     0.417   4.00800
   8   amber99_42  1      MO6   O3    4    -0.834  16.00000
   9   amber99_27  1      MO6   H31   4     0.417   4.00800
  10   amber99_27  1      MO6   H32   4     0.417   4.00800
  11   amber99_42  1      MO6   O4    5    -0.834  16.00000
  12   amber99_27  1      MO6   H41   5     0.417   4.00800
  13   amber99_27  1      MO6   H42   5     0.417   4.00800
```

```
  14  amber99_42  1      MO6   O5    6    -0.834  16.00000
  15  amber99_27  1      MO6   H51   6     0.417   4.00800
  16  amber99_27  1      MO6   H52   6     0.417   4.00800
  17  amber99_42  1      MO6   O6    7    -0.834  16.00000
  18  amber99_27  1      MO6   H61   7     0.417   4.00800
  19  amber99_27  1      MO6   H62   7     0.417   4.00800

[ bonds ]
; i     j       funct  length force.c.
1     2     1     0.204  343092.8  0.204  243092.8
1     5     1     0.204  343092.8  0.204  243092.8
1     8     1     0.204  343092.8  0.204  243092.8
1    11     1     0.204  343092.8  0.204  243092.8
1    14     1     0.204  343092.8  0.204  243092.8
1    17     1     0.204  343092.8  0.204  243092.8
2      3      1      0.1     345000       0.1    345000
2      4      1      0.1     345000       0.1    345000
5      6      1      0.1     345000 0.1    345000
5      7      1      0.1     345000 0.1    345000
8      9      1      0.1     345000 0.1    345000
8      10     1      0.1     345000 0.1    345000
11     12     1      0.1     345000 0.1    345000
11     13     1      0.1     345000 0.1    345000
14     15     1      0.1     345000 0.1    345000
14     16     1      0.1     345000 0.1    345000
17     18     1      0.1     345000 0.1    345000
17     19     1      0.1     345000 0.1    345000

[ angles ]
; i     j      k      funct  angle  force.c.
11     1    17       1      180.00 583   180.00 383
 2     1     5 1     180.00 583   180.00 383
 8     1    14       1      180.00 583   180.00 383
 2     1     8 1      90.00 583    90.00 383
 2     1    11       1       90.00 583    90.00 383
 2     1    14       1       90.00 583    90.00 383
 2     1    17       1       90.00 583    90.00 383
 5     1     8 1      90.00 583    90.00 383
 5     1    11       1       90.00 583    90.00 383
 5     1    14       1       90.00 583    90.00 383
 5     1    17       1       90.00 583    90.00 383
3      2      4      1      109.47 383    109.47 383
```

```
6       5       7       1       109.47 383    109.47 383
9       8       10      1       109.47 383    109.47 383
12      11      13      1       109.47 383    109.47 383
15      14      16      1       109.47 383    109.47 383
18      17      19      1       109.47 383    109.47 383

[ dihedrals ]
; ai    aj    ak    al    funct    q0     kq
  5     2     14    8     2        0.0    1.8e+02
11      17     2     5     2        0.0    1.8e+02
11      17    14     8     2        0.0    1.8e+02
```