Incorrect dvdlambda : posres() in gmxlib/bondfree.c (4.6.* & 4.5.2+)

I think I found a simple (three year old) BUG in the line 2290 of gmxlib/bondfree.c (ver 4.6.5),

```
-fm*dpdl[m];
```

which should be

```
+fm*dpdl[m];
```

if I understand correctly the notation etc.

Comparing this code, which calculates dvdlambda, with the code at the line 431 of the same file,

```
dvdlambda = half*(kB-kA)*dx2 + (xA-xB)*kk*dx;
```

which is inside the real function hamonic(), one may notice the inconsistency.

(c.f. fm=-kk*dx[m], dpdl[posB - posA])
- Target version changed from 4.6.x to 4.6.6

Sorry, I missed that the force fm also had a minus sign in it. So indeed the sign is incorrect!

#4 - 06/18/2014 09:00 AM - Berk Hess
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 2394f4f4e359533215d7c2c1815e5385751686.

#5 - 06/18/2014 10:13 AM - Erik Lindahl
- Status changed from Resolved to Closed