nonbonded weight

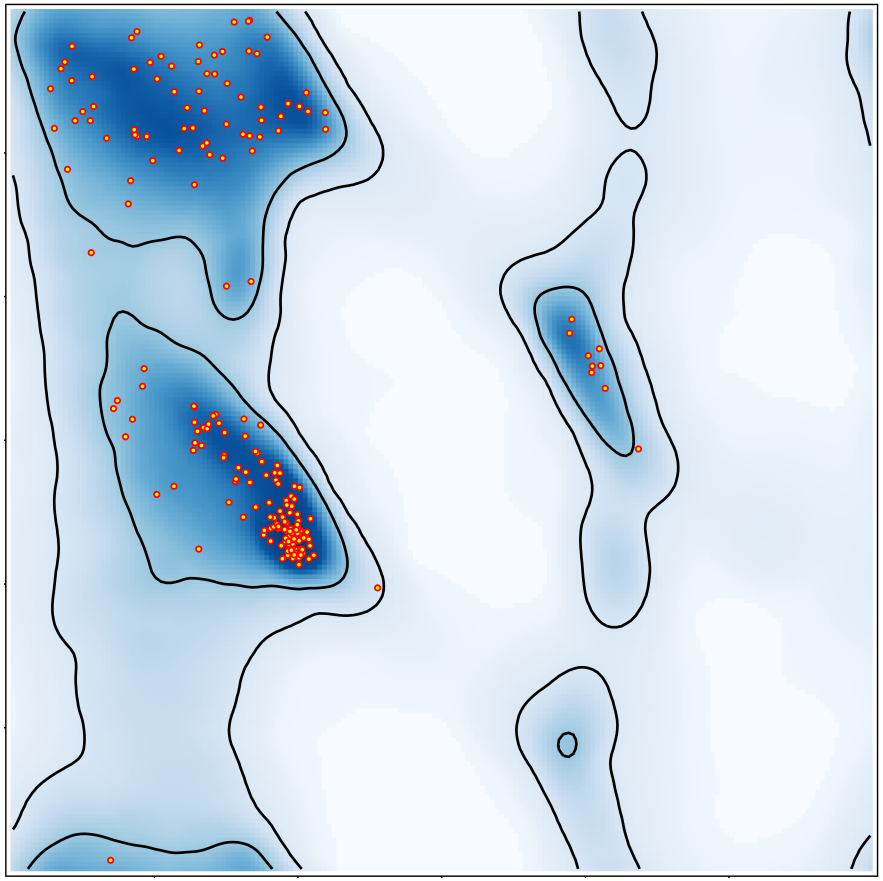
Ramachandran plot options and nonbonded weight

- Numerical test setup
  - Consider two extreme examples
    - Perfect ultra-high resolution model (1US0; 0.66 Å resolution)
    - Low-resolution model with poor geometry (3ZX0; 17 Å resolution)
  - Do pure geometry optimization, varying following options:
    - H present / absent
    - Non-bonded weight = 1, 16, 100, 1000
    - Ramachandran plot restraints:
      - No
      - Yes; type:
        - Emsley
        - Oldfied
    - See effect of adding secondary structure restraints
    - *Optimization* uses basic restraints (bonds, angles, planes, chirals, torsions, nonbonded) with no any extras, 50 cycles of 500 iterations. Any additions are specified in the title of each slide.

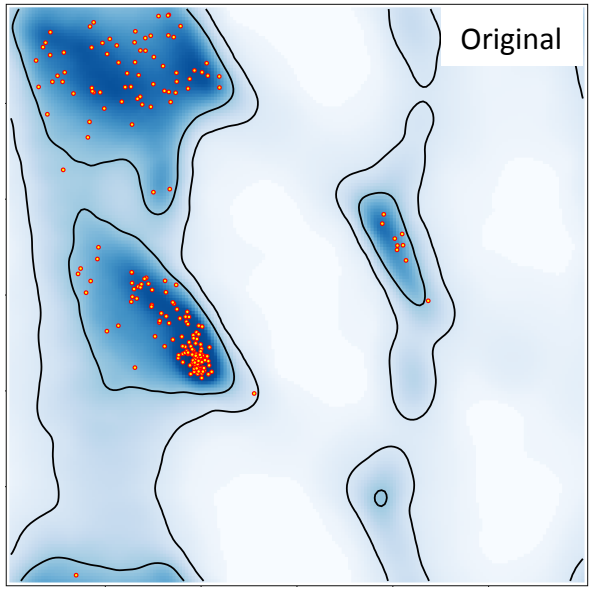
Test model – good high-resolution model

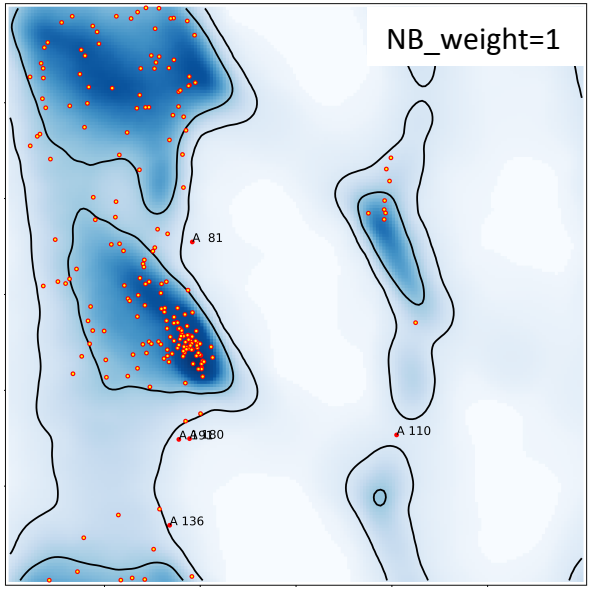
Aldose reductase, 1US0, resolution = 0.66 Å

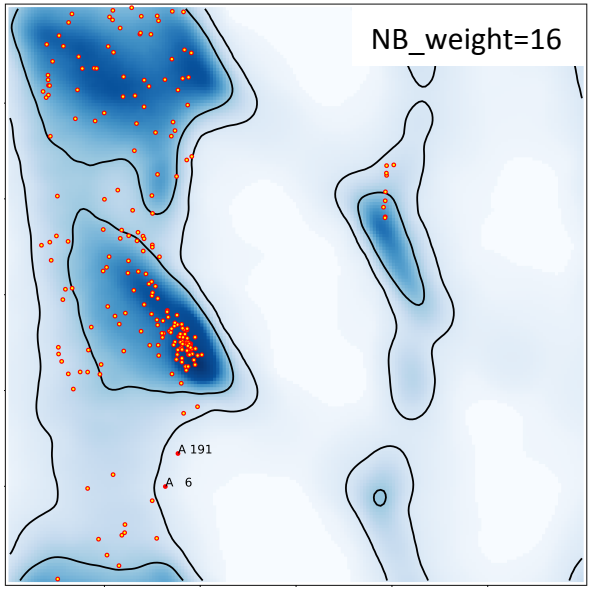
```
DEVIATIONS FROM IDEAL VALUES.
  BOND      :  0.017
  ANGLE     :  1.956
  CHIRALITY :  0.111
  PLANARITY :  0.013
  DIHEDRAL  : 11.999

MOLPROBITY STATISTICS.
  ALL-ATOM CLASHSCORE : 1.40
  RAMACHANDRAN PLOT:
    OUTLIERS : 0.00  %
    ALLOWED  : 1.29  %
    FAVORED  : 98.71 %
  ROTAMER OUTLIERS : 0.72 %
  CBETA DEVIATIONS : 0
  PEPTIDE PLANE:
    CIS-PROLINE     : 0.0
    CIS-GENERAL     : 0.0
    TWISTED PROLINE : 0.0
    TWISTED GENERAL : 0.0
```

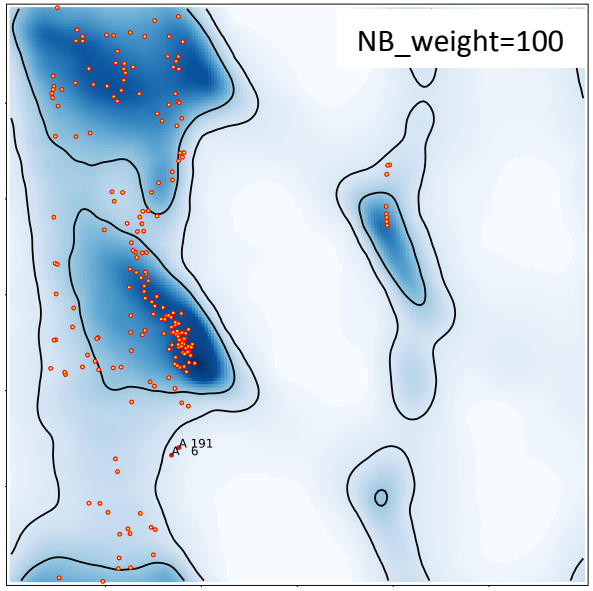


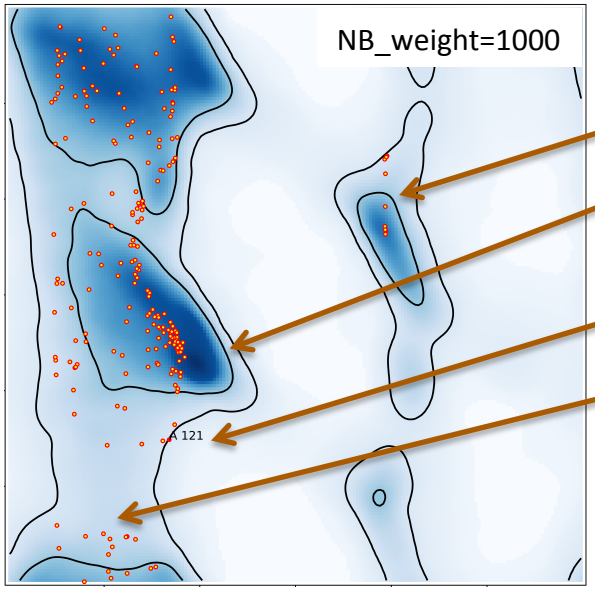
Optimization, no H





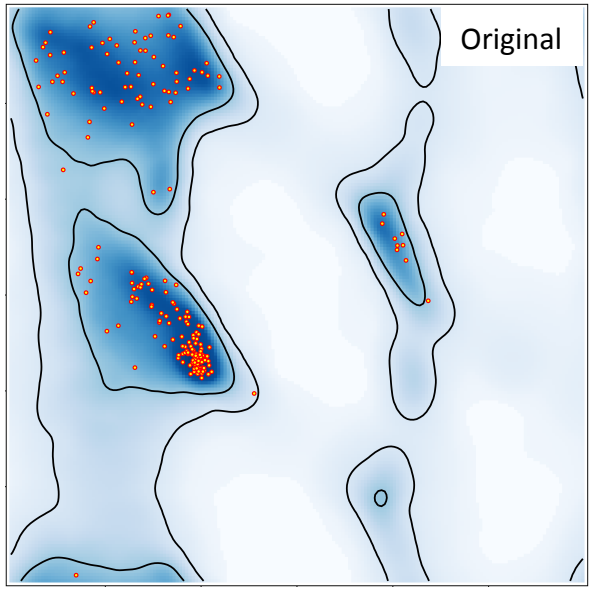


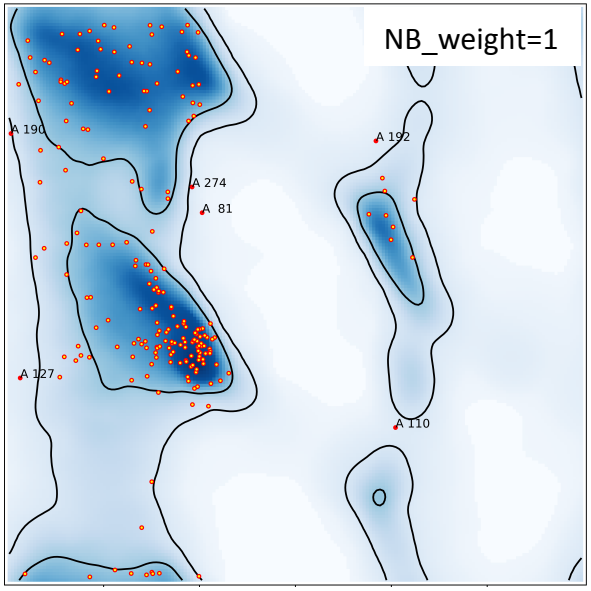


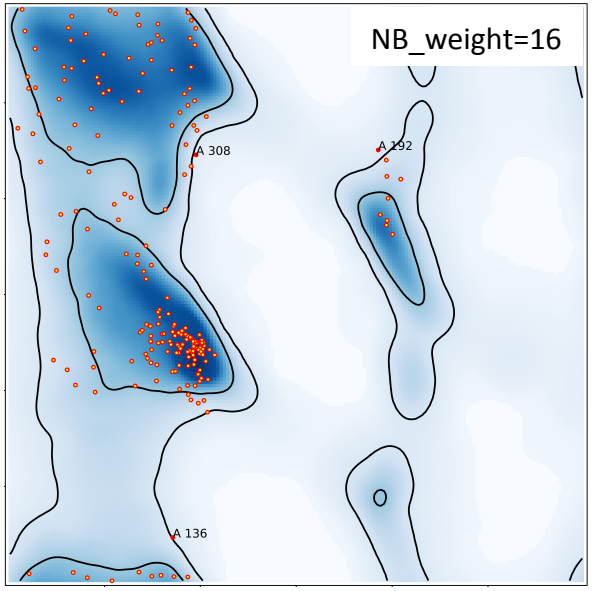


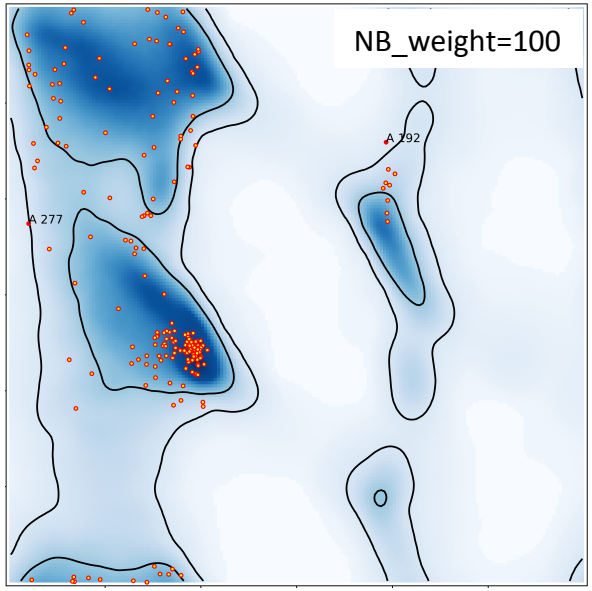
- Vertical line in all cases
- Skewed distribution in all cases, except w=1
- Outliers in all cases
- Residues migrate from favored to allowed

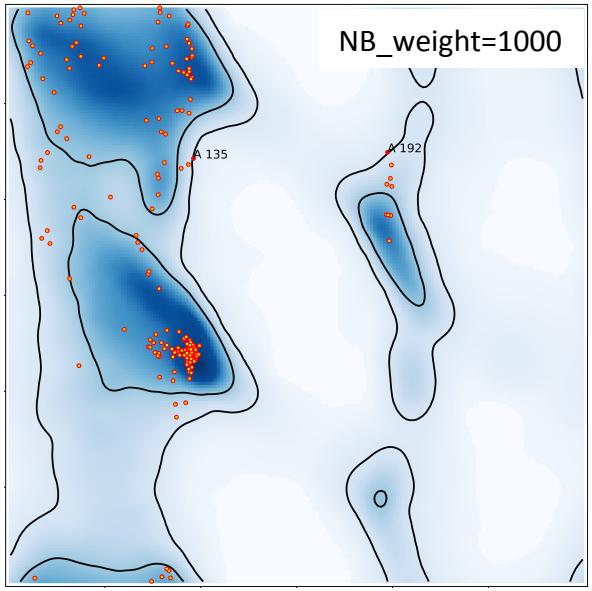
Optimization, H added





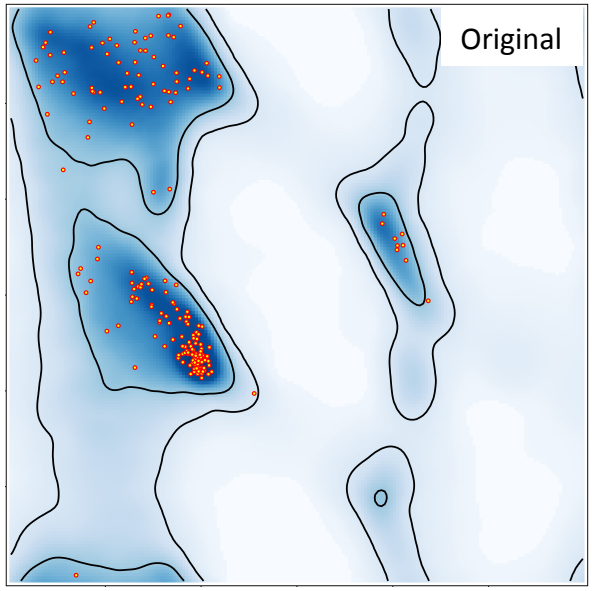


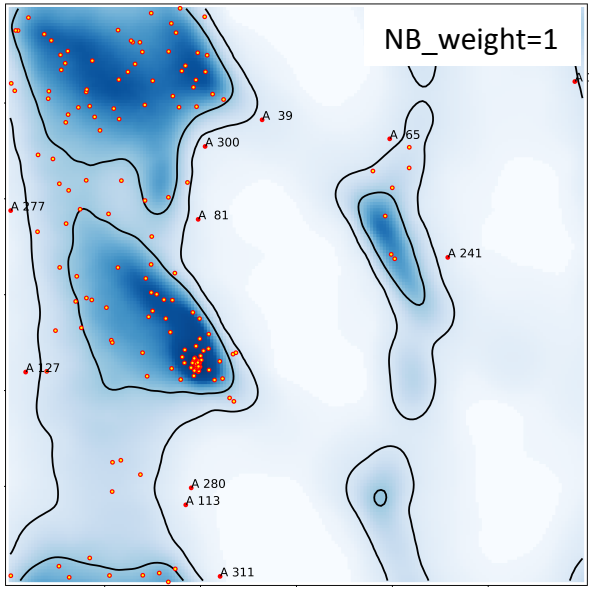


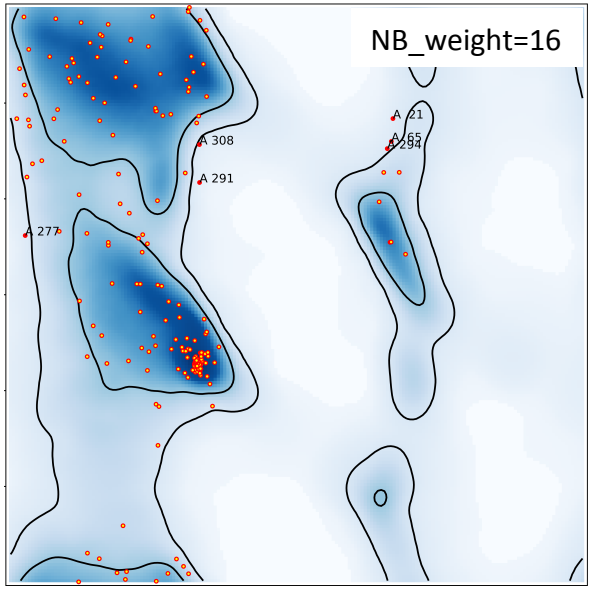


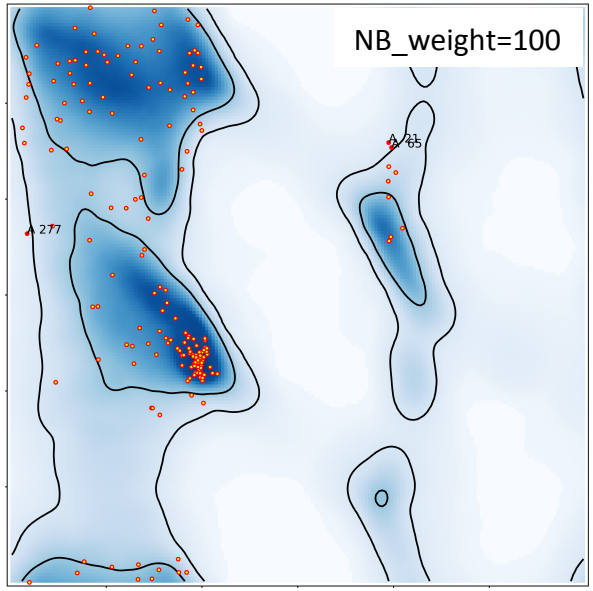
- Vertical line remains in all cases
- Distribution is different from “no H” case and seems somewhat better, but still odd.
- Less outliers
- Residues still migrate from favored to allowed regions

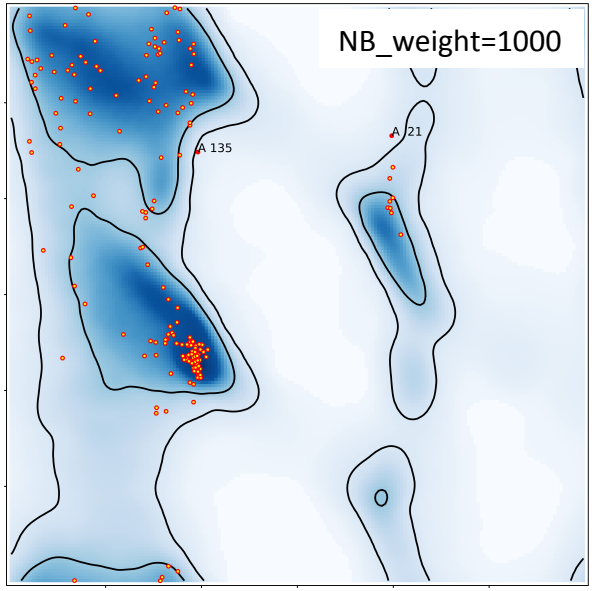
Optimization, H added, use SS restraints





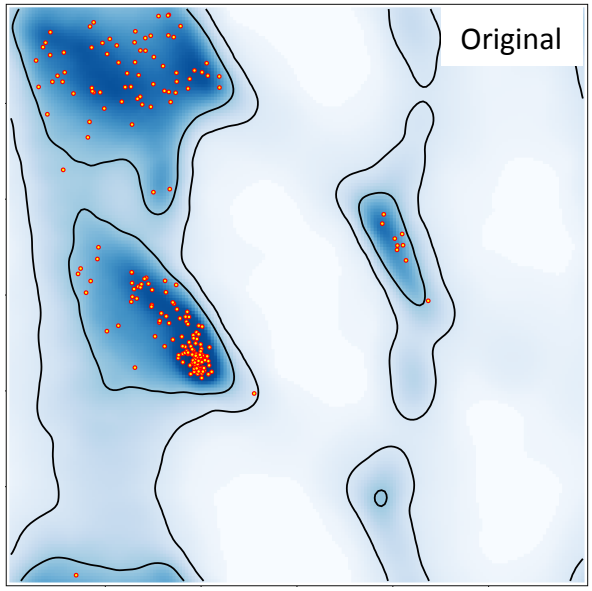


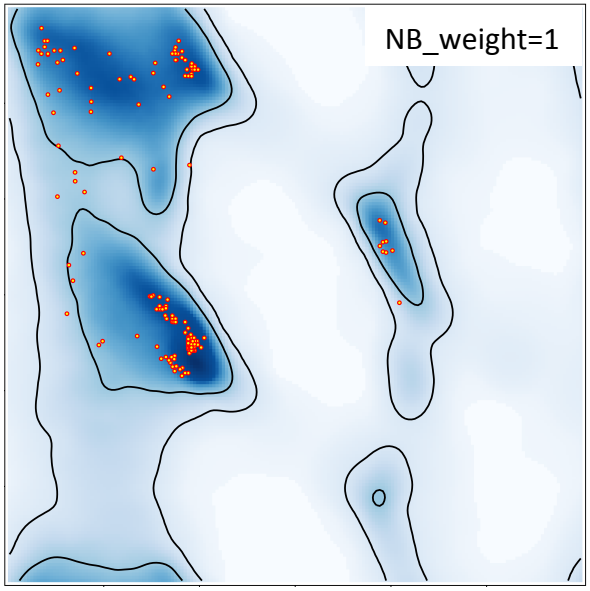


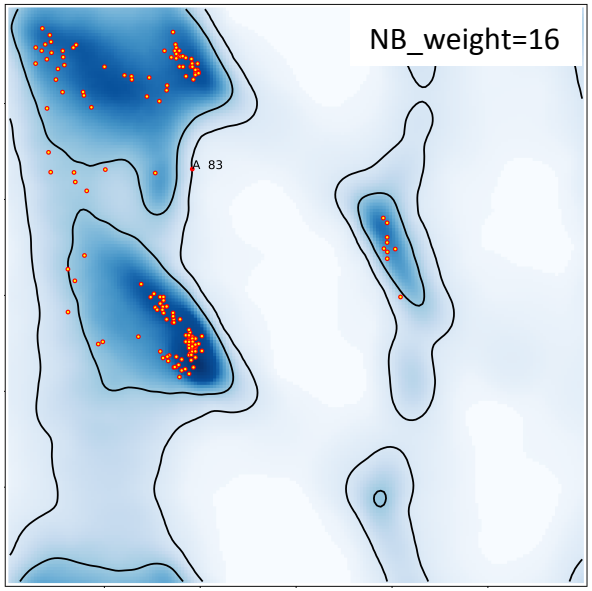


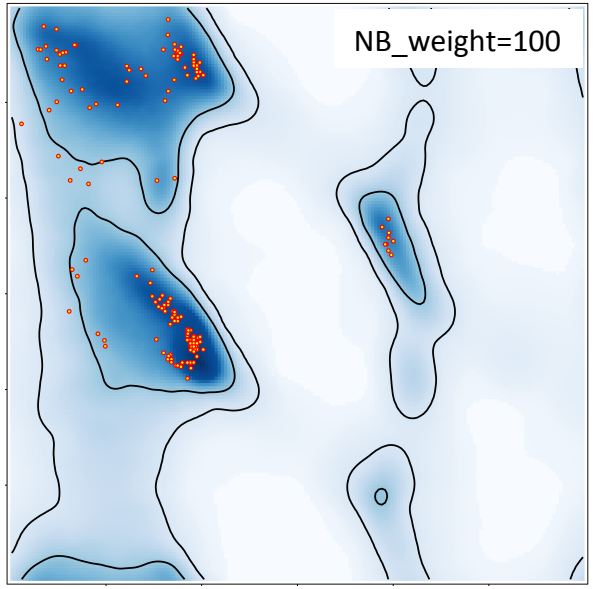
- Adding SS restraints does not make any visible changes

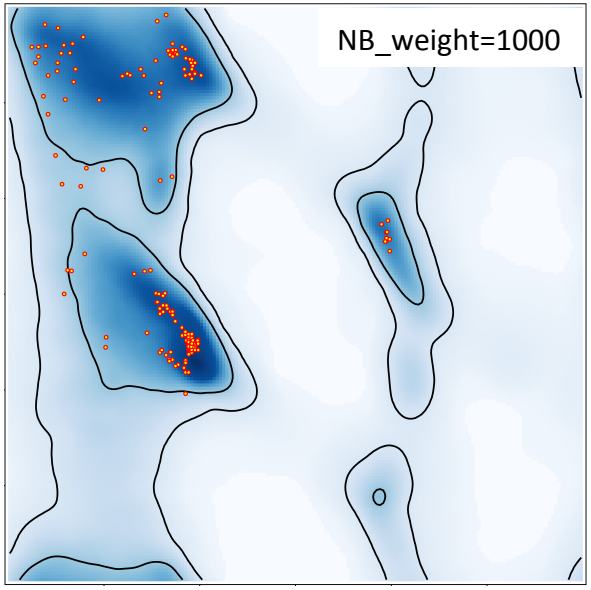
Optimization, H added, Ramachandran restraints (Emsley)





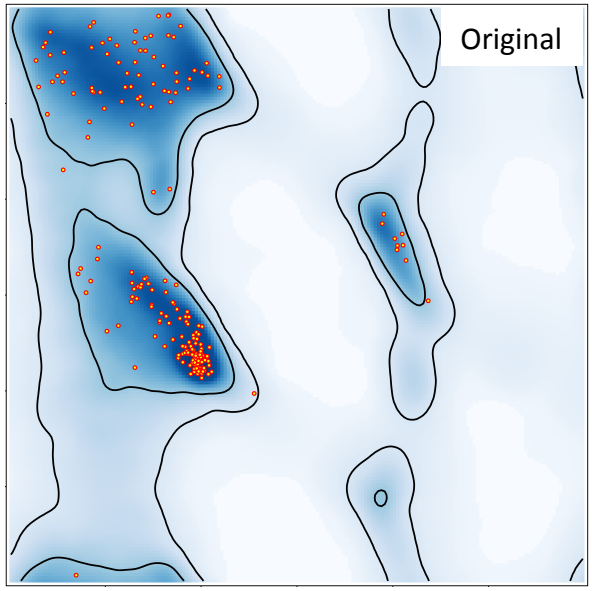


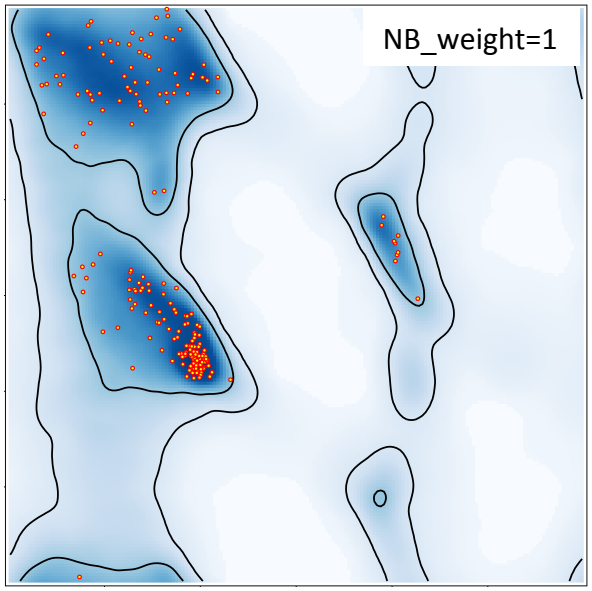


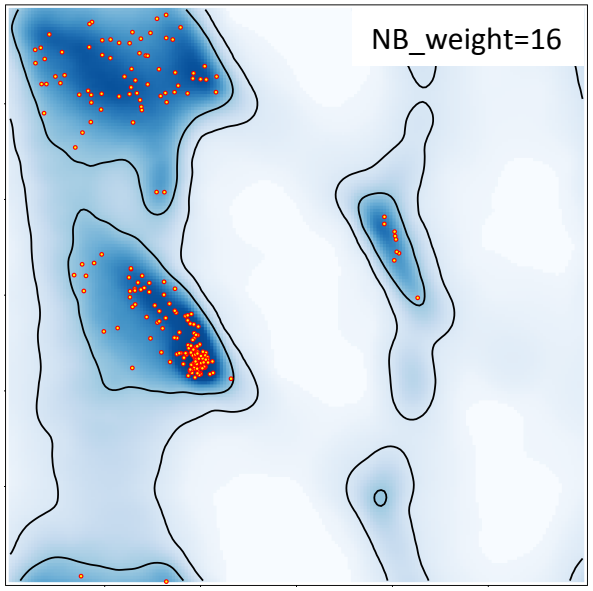


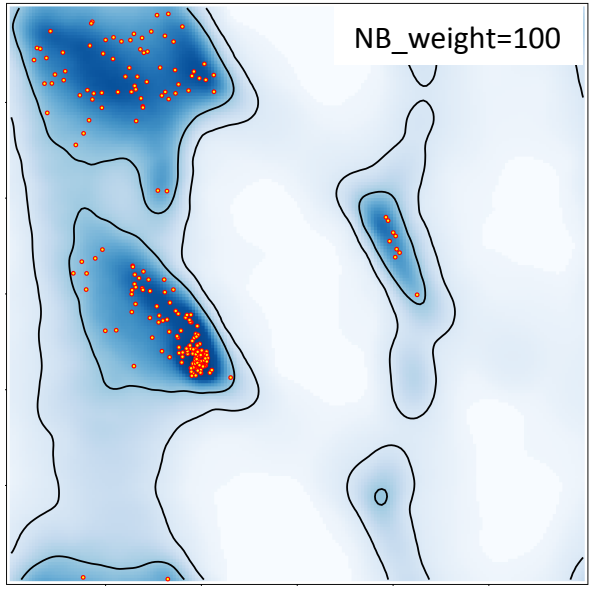
- Much less outliers
- No vertical line
- Less residues migrated from favored to allowed
- Distribution in favored regions is different from original

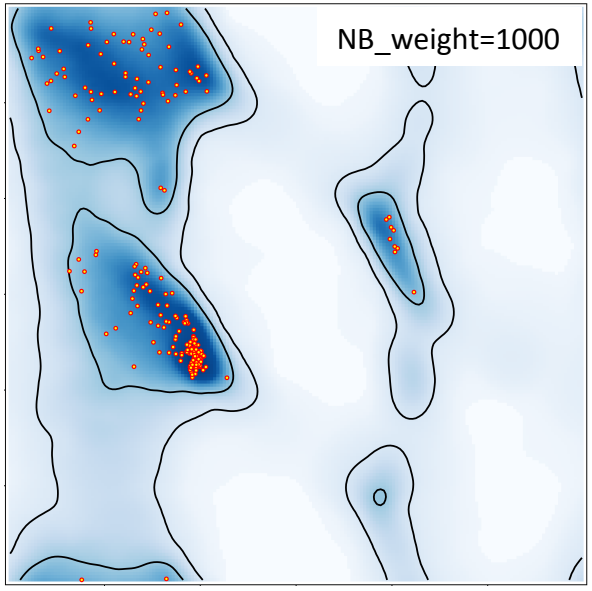
Optimization, H added, Ramachandran restraints (Oldfield)







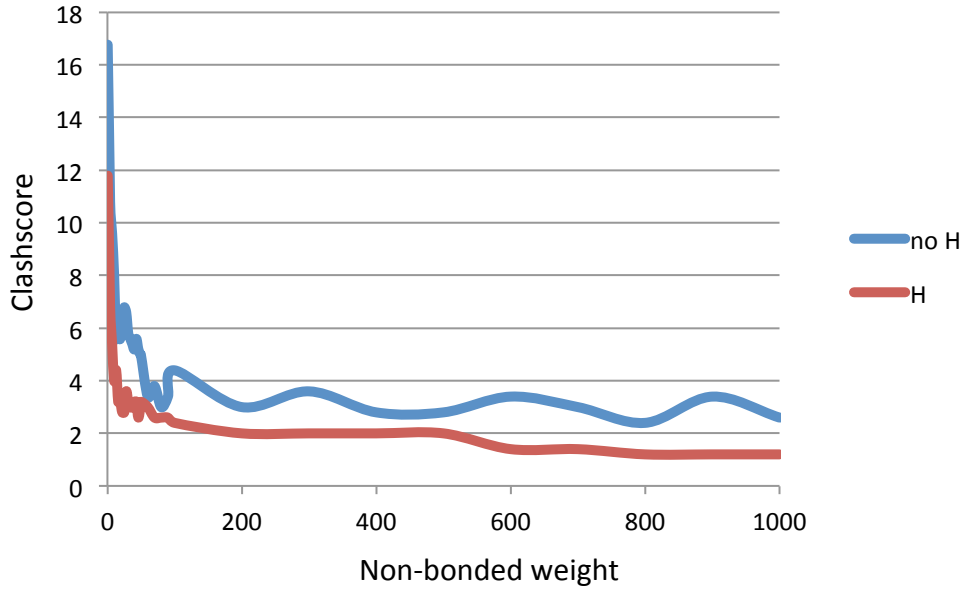




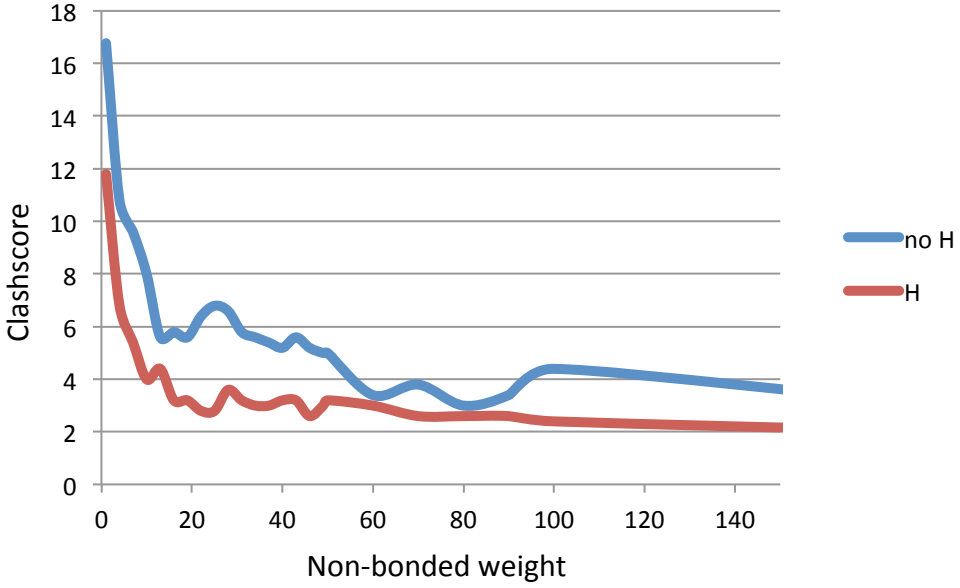
- No outliers
- No vertical line
- No residues migrated from favored to allowed
- Distribution in favored regions is very similar to original
- Overall, this function seems to perform best for preserving initially good plot
- Residues are likely to migrate from allowed to favored, which may not always be desirable

Effect of non-bonded weight on clashscore

Each data point is a result of 50x500 pure optimization using only basic restraints



Same plot as above, zoom on smaller weights

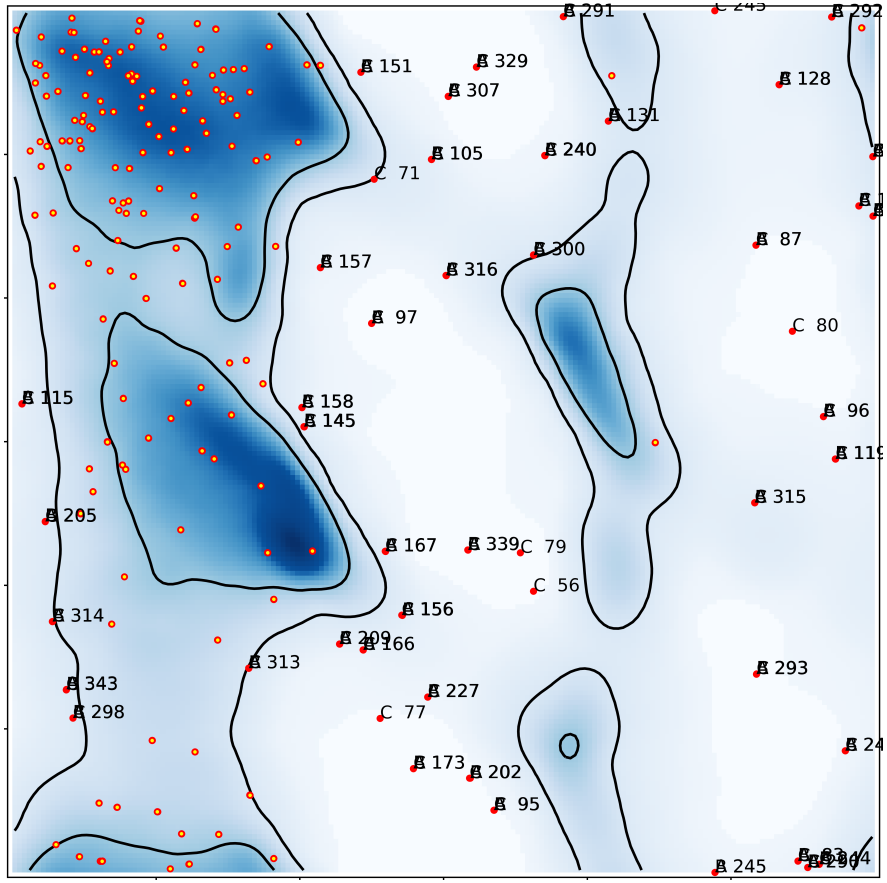


Clashscore stops changing at around 100 non-bonded weight

Test model – geometrically poor model

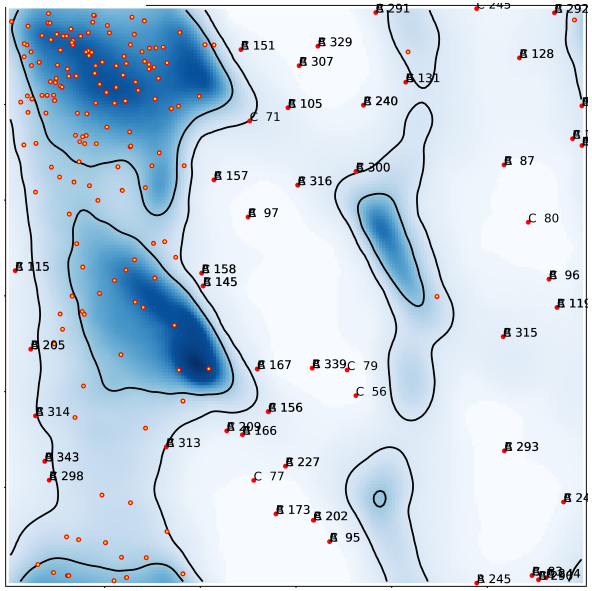
Aldose reductase, 3zx9, resolution = 17 Å

```
DEVIATIONS FROM IDEAL VALUES.
  BOND      :   0.052
  ANGLE     :   4.651
  CHIRALITY :   0.167
  PLANARITY :   0.022
  DIHEDRAL  :  15.640

MOLPROBITY STATISTICS.
  ALL-ATOM CLASHSCORE : 244.84
  RAMACHANDRAN PLOT:
    OUTLIERS : 22.52 %
    ALLOWED  : 22.52 %
    FAVORED  : 54.96 %
  ROTAMER OUTLIERS : 15.57 %
  CBETA DEVIATIONS : 6
  PEPTIDE PLANE:
    CIS-PROLINE     : 0.0
    CIS-GENERAL     : 0.0
    TWISTED PROLINE : 0.0
    TWISTED GENERAL : 1.156
```

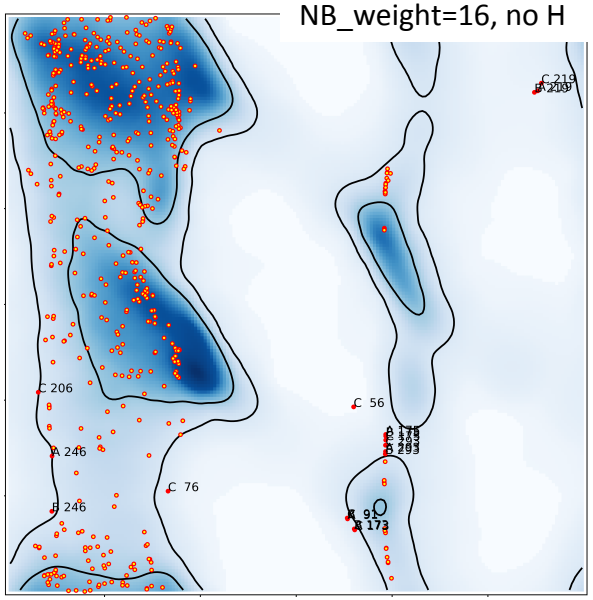


Test model – very bad model

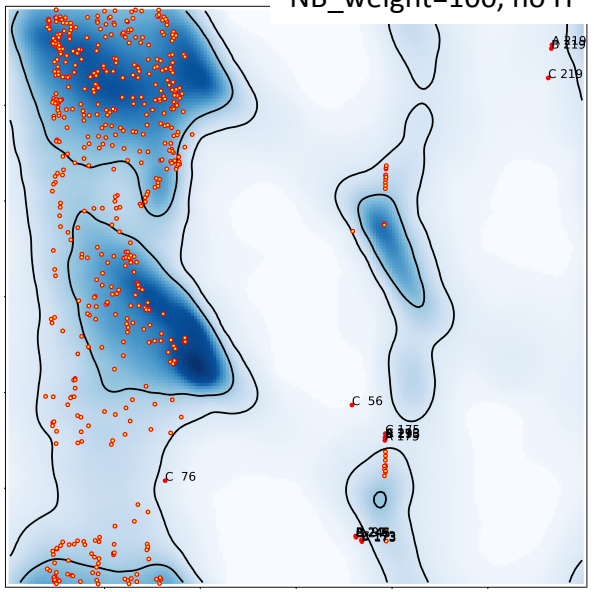
Original



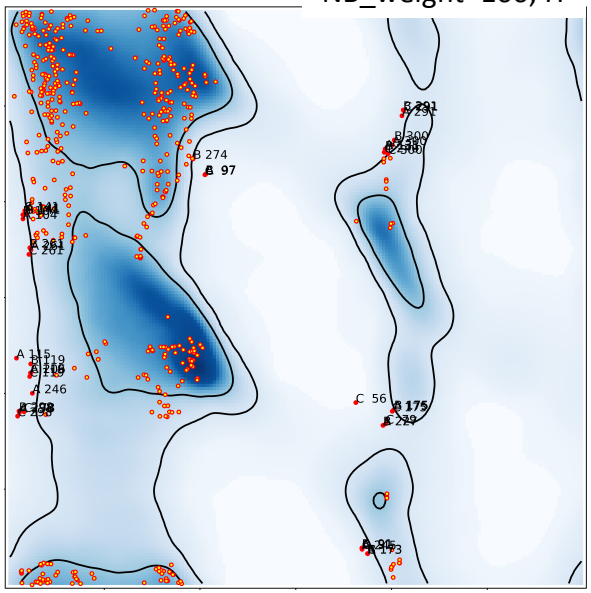
NB_weight=16, no H



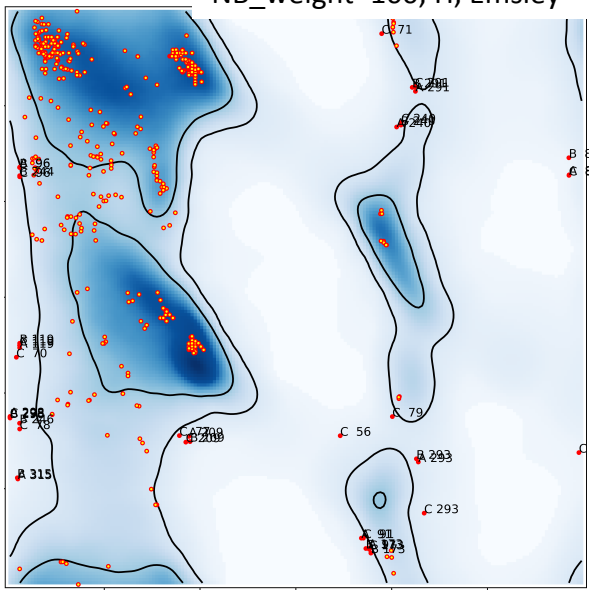
NB_weight=100, no H



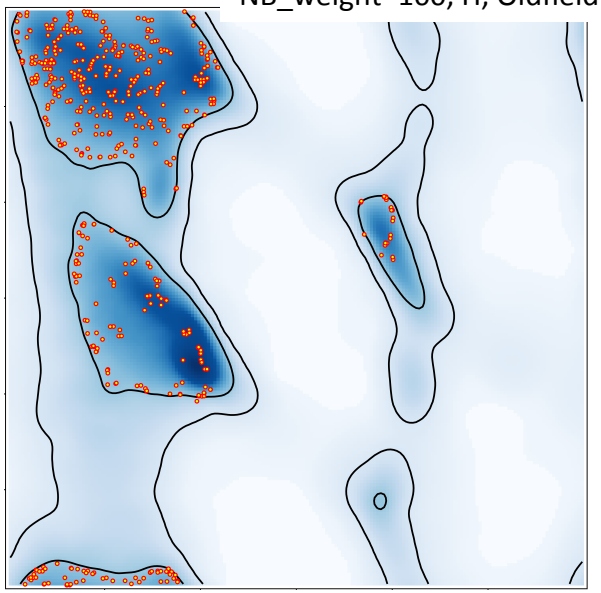
NB_weight=100, H



NB_weight=100, H, Emsley

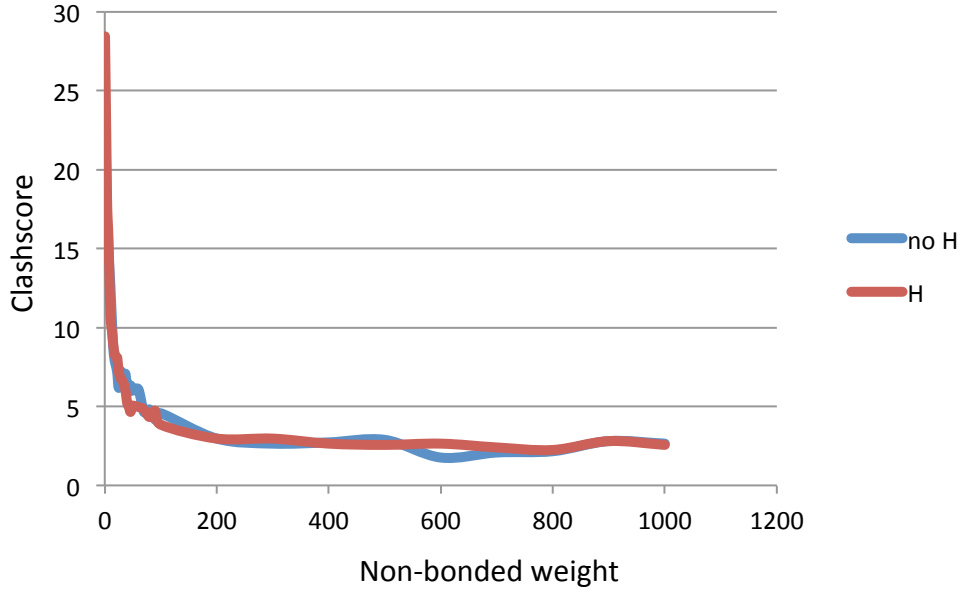


NB_weight=100, H, Oldfield

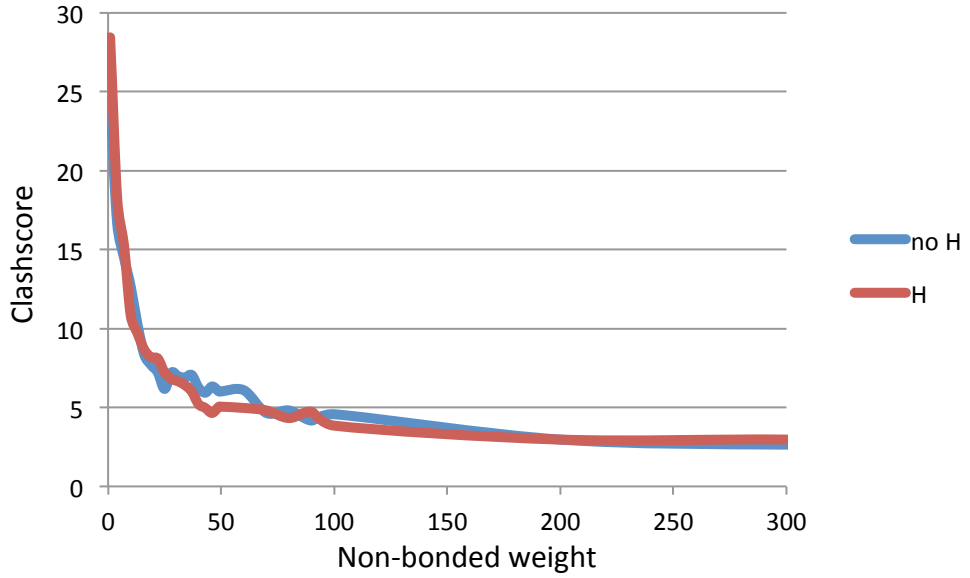


Effect of non-bonded weight on clashscore

Each data point is a result of 50x500 pure optimization using only basic restraints



Same plot as above, zoom on smaller weights



Clashscore stops changing at around 200 non-bonded weight