1 Supporting Information: How cysteine oxidation affects protein stability and binding studied by free energy calculations

1.1 Methods

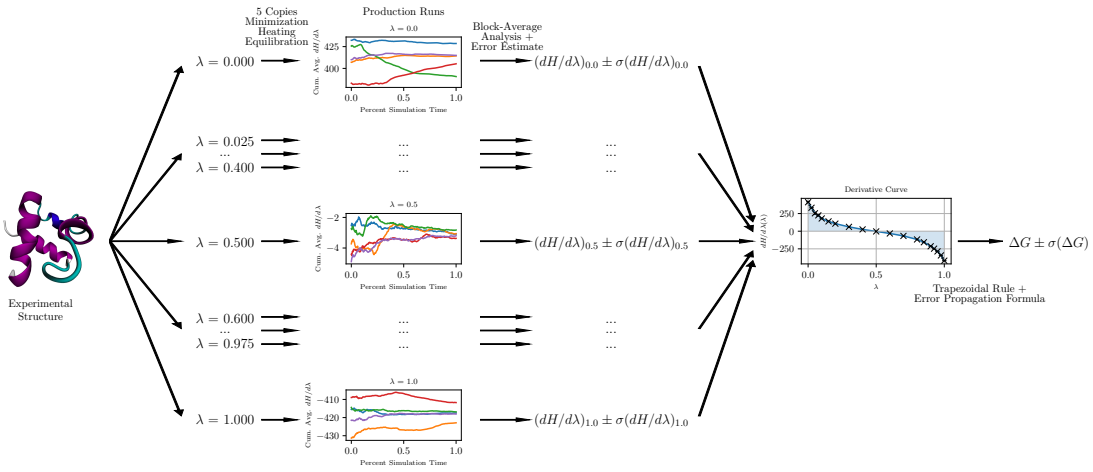

Figure S1: Schematic representation of the workflow conducted for the evaluation of the free energy difference ΔG^{MUT} of an alchemical transformation using thermodynamic integration. It is important to note that all simulations are performed independently and multiple times allowing to extract mean free energy changes and errors of the mean.

1.2 Correction for deprotonation effect (DJ-1)

Due to the protein residues surrounding CYS-106 in the DJ-1 protein, its pKa is reduced to 5.4. Hence, the deprotonated form is dominating substantially over the protonated one at physiological pH [11]. In our computational model, the deprotonated form of CYS was therefore chosen as the starting configuration of the alchemical transformations to the respective oxidized forms. In consequence, the raw results of the model record the change in folding free energy due to oxidation between the an unfolded protein chain and the folded state both with a deprotonated residue at position 106. This is appropriate for the folded states due to the protein environment as discussed in the main text. In the unfolded states, this is, however, only reasonable for the oxidized states of CYS due to their low intrinsic pKa. Native CYS featuring only solvent interaction should be protonated at pH=7. In fact, free energy is needed to deprotonated the residue under these conditions. In consequence, the measured stability of the native state is overestimated as the reference state, being a protein chain with a deprotonated CYS residue, is artificially high in free energy. This leads to the following correction term, setting the correct reference state, that will also occur in experiments.

$$\begin{aligned}\Delta\Delta G^{WT\to OX}_{Exp} &= \Delta G^{OX}_{Fold(Exp)} - \Delta G^{WT}_{Fold(Exp)} \\ &= \Delta G^{OX}_{Fold(Model)} - \left(\Delta G^{WT}_{Fold(Model)} + \Delta G^{WT}_{Deprotonation(Unfolded)}\right) \\ &= \Delta\Delta G^{WT\to OX}_{Model} - \Delta G^{WT}_{Deprotonation(Unfolded)}\end{aligned}$$

This correction can be calculated based in ambient pH and pKa of solvent exposed cysteine.

$$\Delta G^{WT}_{Deprotonation(Unfolded)} = 2.303RT(pKa - pH) \tag{1}$$

This yields a correction of 1.77 kcal/mol.

1.3 URN1-FF domain protein

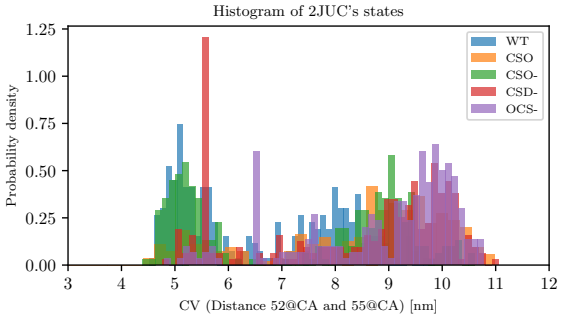

Figure S2: Histogram of CA-CA distance between TRP-52 (actual 56) and GLU-55 (actual 59) sampled from 1 μs long simulations for all CYS oxidation states of URN1-FF. Two regimes can be distinguished in the diagram, representing the folded and partly unfolded state of the C-terminal segment of URN1-FF.

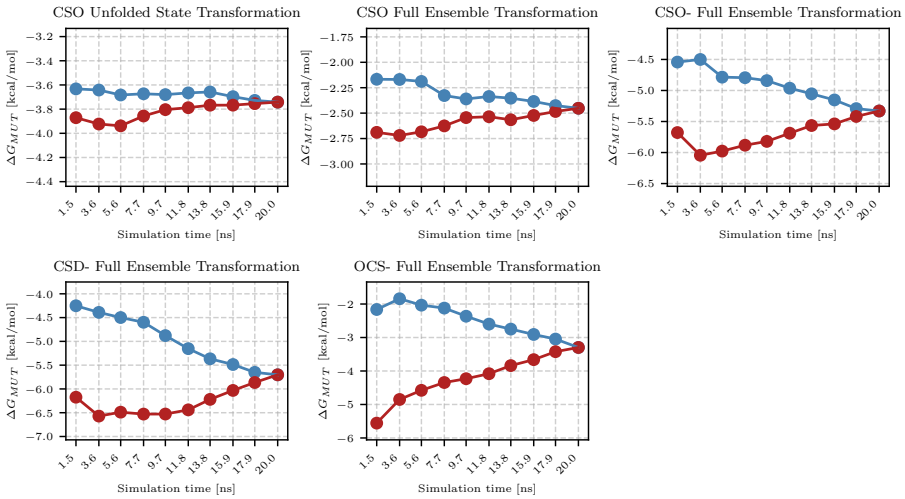

Figure S3: Convergence of the alchemical transformations studied by considering alchemical forward (blue dots) and backward (red dots) transformations for the URN1-FF system vs. simulation time per lambda window (taking consecutively more data into account) following the method by A. Mey et Al. [36]. Close final proximity of both curves indicates convergence.

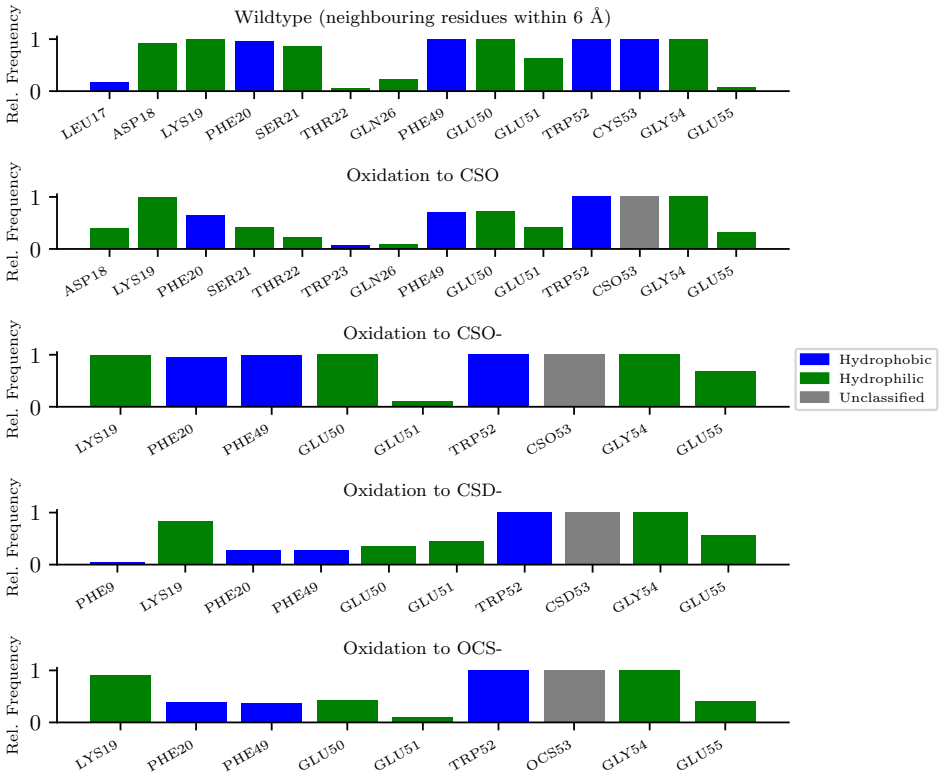

Figure S4: Neighborhood analysis of the oxidized residue. All residues within 6A of the central sulfur atom were considered a neighboring residue. The analysis was conducted using the *pytraj* package. Color coding for hydrophobic and hydrophilic residues was added to classify the environment. Note that the numbering of the residues is shifted here by -4 relative to the original sequence. This is due to the first N-terminal 4 residues not having been resolved in the crystal structure.

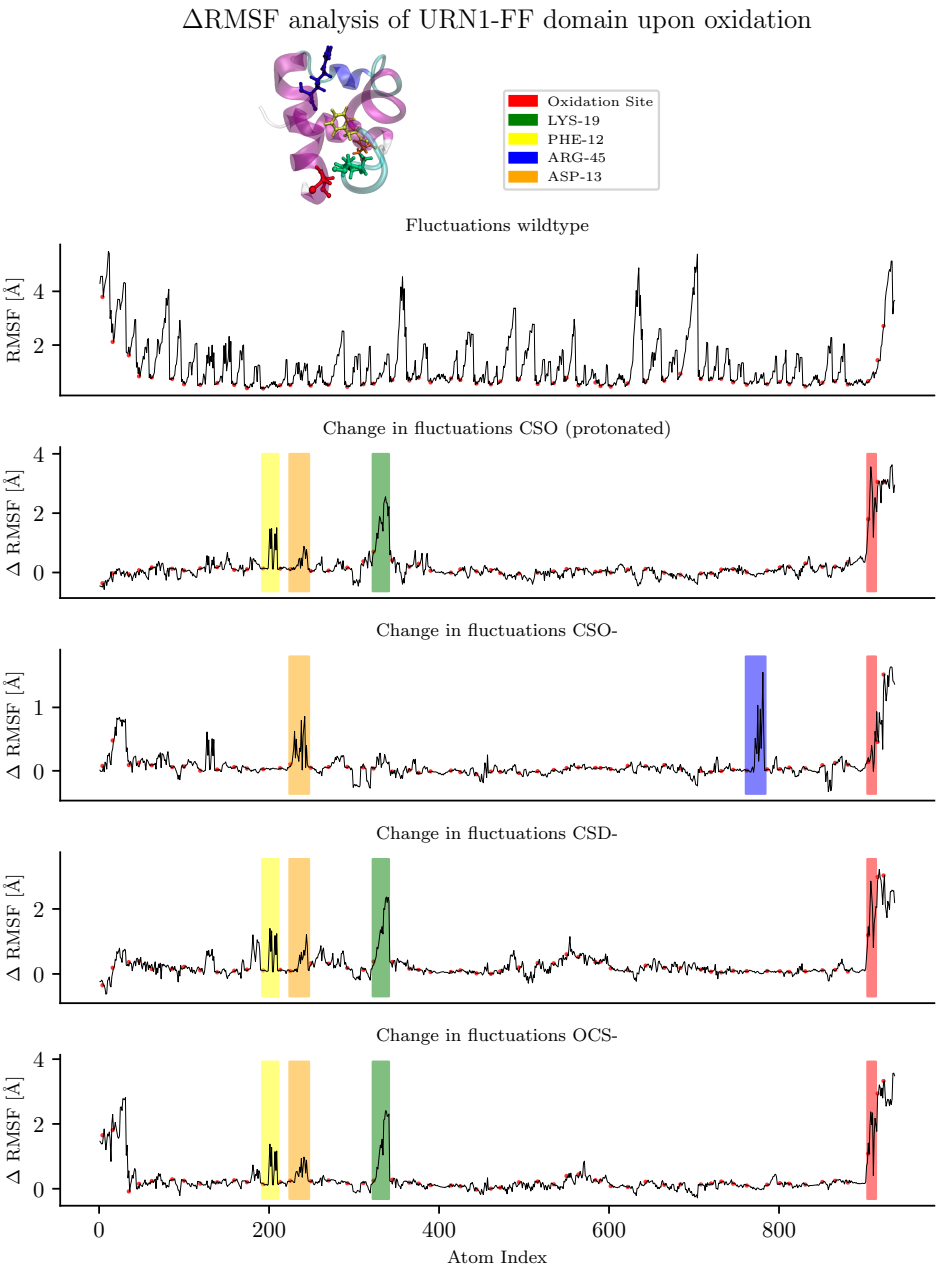

Figure S5: ΔRoot-Mean-Square-Fluctuation (RMSF) analysis of the oxidized states of the URN1-FF protein (all atom RMSF). The graphs for the oxidized states show the respective difference in the RMSF for all atoms with backbone CA atoms marked as red dots. Important residues were highlighted and can be located in the above illustration of the protein. Note that the numbering of the residues is shifted here by -4. This is due to the first four residues not having been resolved in the crystal structure.

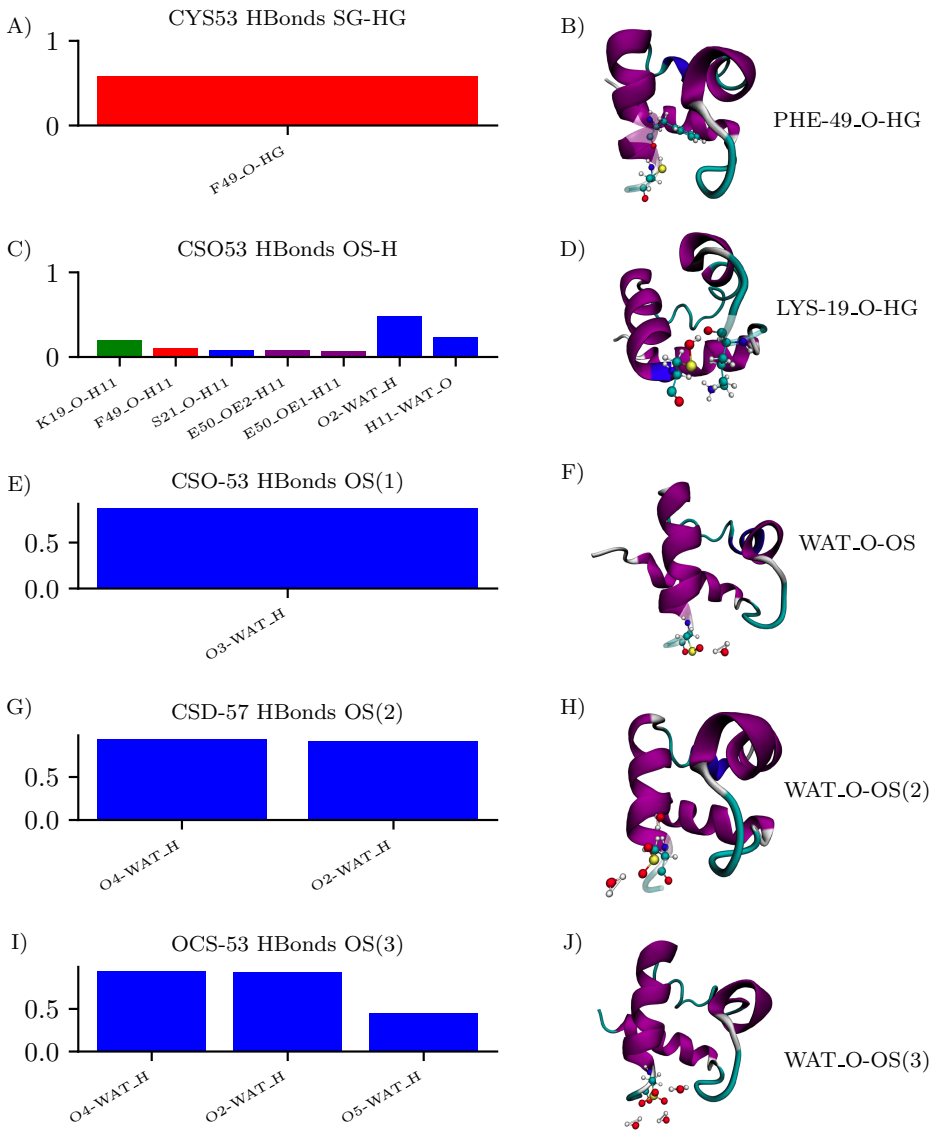

Figure S6: Hydrogen bond analysis of the side chain of the oxidized residue (position 53) in URN1-FF protein. The analysis was conducted using *pytraj*'s searchhbond function. The bar plots indicate the fraction of frames, the respective interaction was observed. The right side shows illustrations of the respective interactions. Interactions observed in less than 5% of frames are not shown. Note that the numbering of the residues is shifted here by -4. This is due to the first four residues not having been resolved in the crystal structure.

1.4 DJ-1 Homodimer system

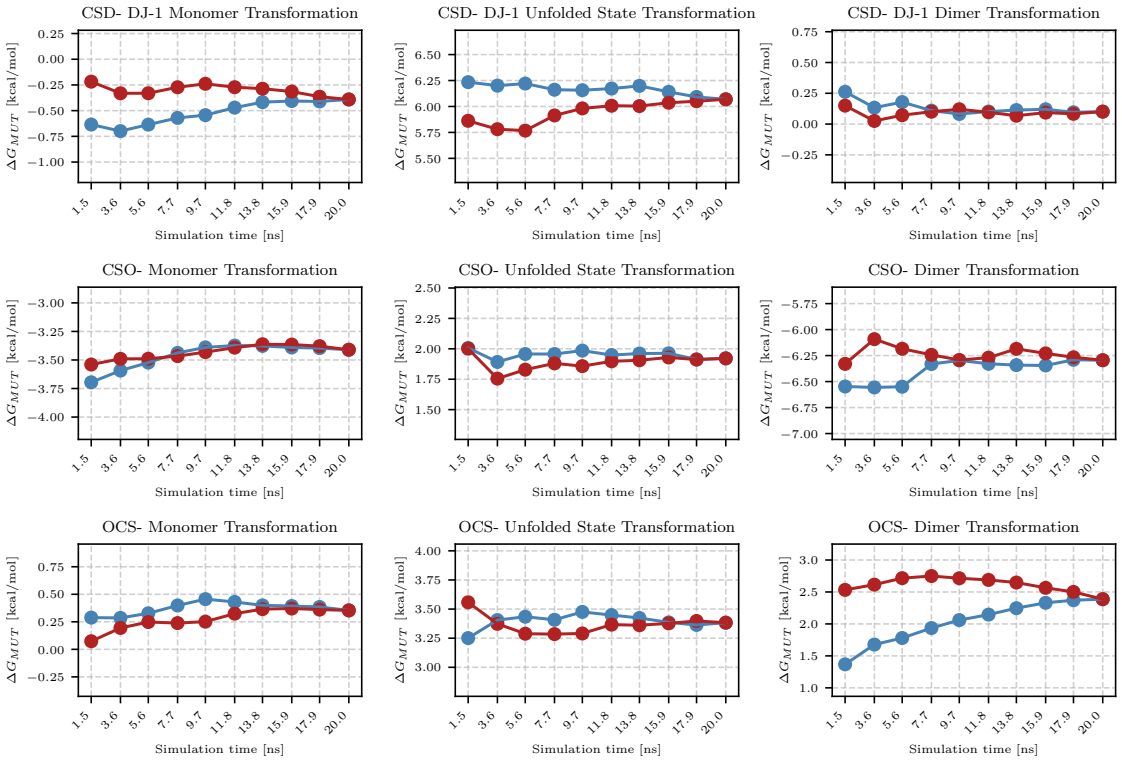

Figure S7: Convergence of the alchemical transformations studied by considering alchemical forward (blue dots) and backward (red dots) transformations for the DJ-1 dimer system vs. simulation time per lambda window (taking consecutively more data into account) following the method by A. Mey et Al. [36]. Close final proximity of both curves indicates convergence.

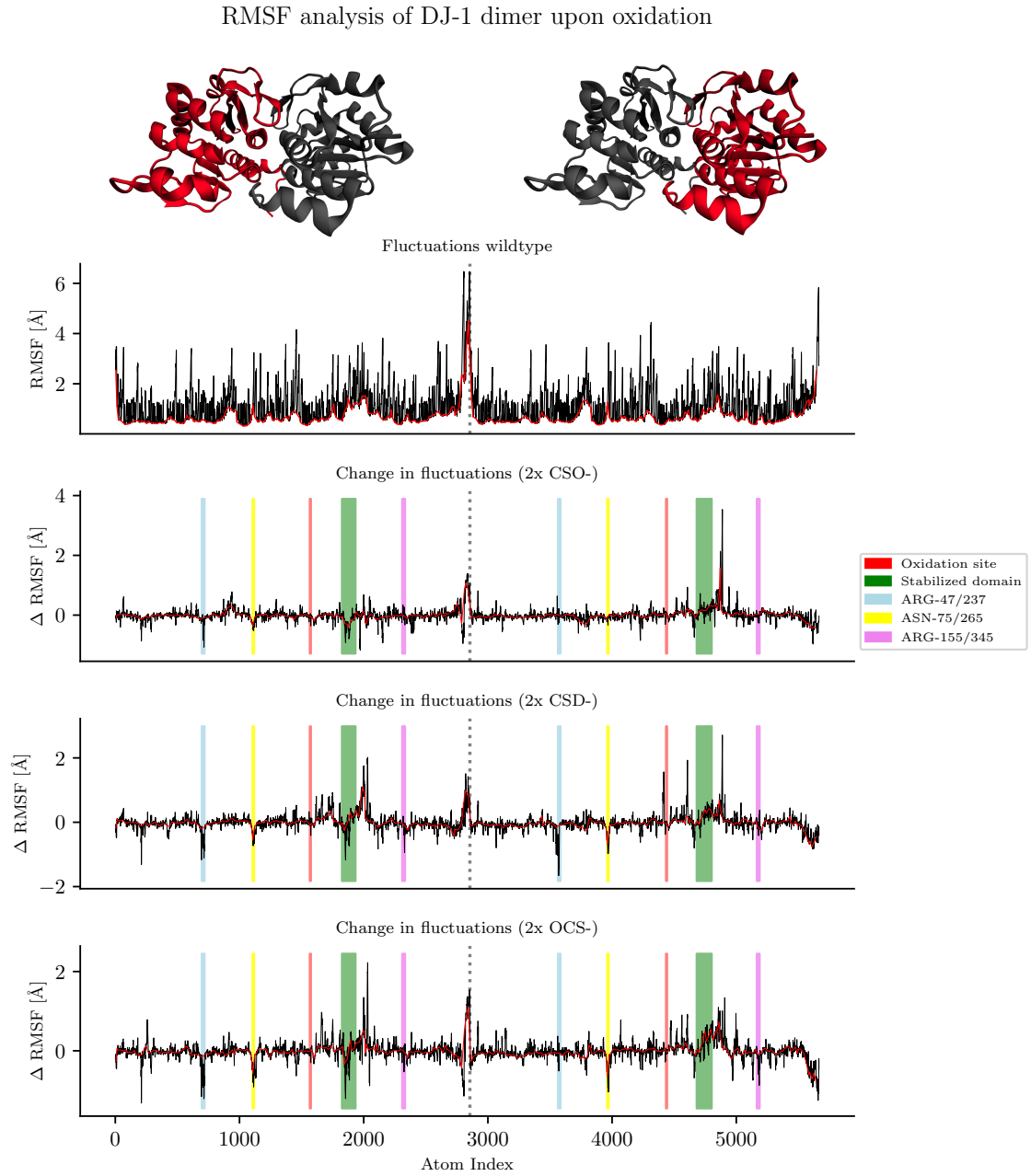

Figure S8: ΔRoot Mean Square Fluctuation (RMSF) analysis of the DJ-1 dimer (all atom RMSF). The graphs for the oxidized states show the respective difference in the RMSF for all atoms with backbone CA atoms marked as red dots. The results belonging to different monomers are separated by a dotted line, with the illustrations indicating the respective protein. For general assessment, the wild type's absolute fluctuations are shown first. To highlight the effects of the oxidations, the respective graphs show the changes in RMSF. Important regions are marked in the graphs.

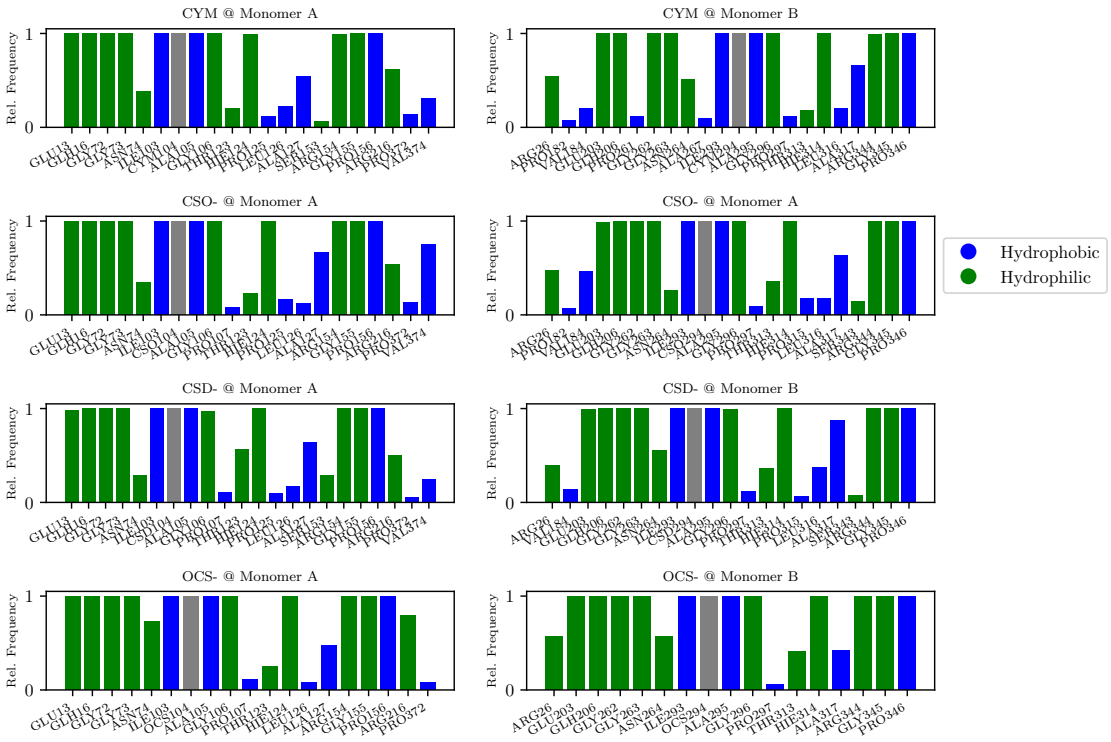

Figure S9: Neighbouring residues of the residue 106 (oxidation site) in DJ-1 protein. On the left, the results for the first monomer are presented and on the right for the second monomer. Interactions observed in less than 5% of the frames are not shown. Analysis conducted using *pytraj*'s searchneighbours function [40]. Note that the numbering of the residues is shifted here by -2. This is due to the first four residues not having been resolved in the crystal structure.

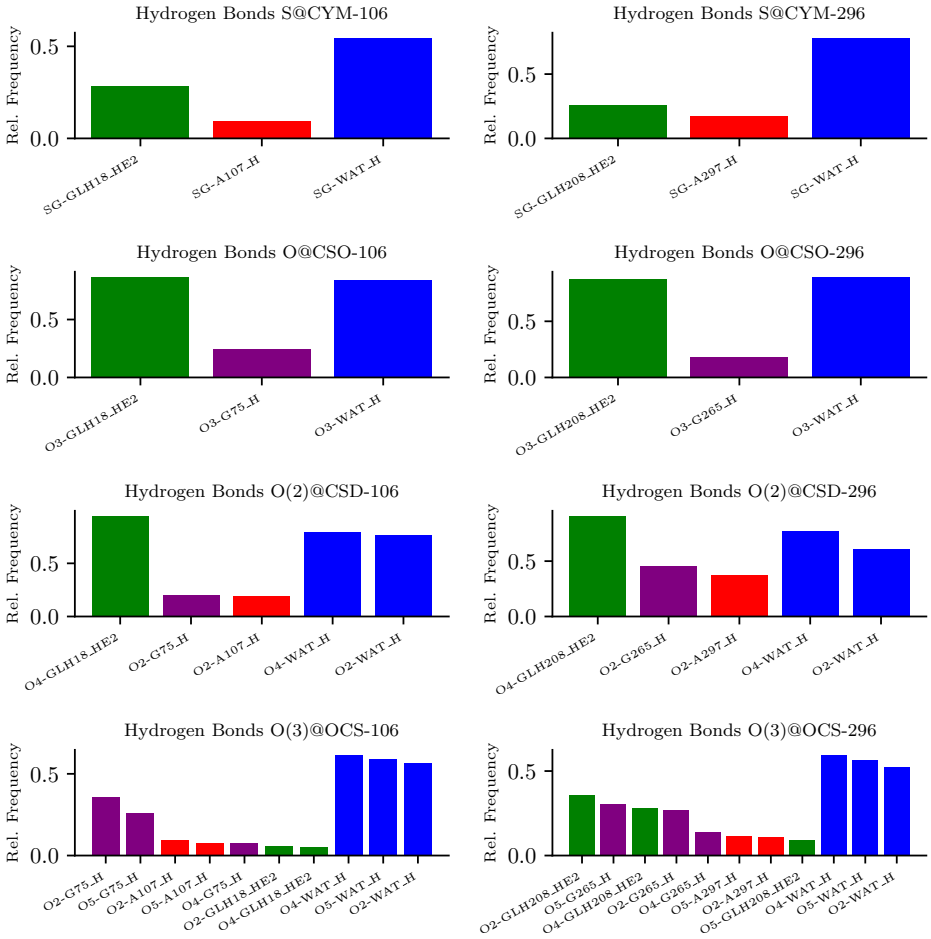

Figure S10: Hydrogen bond analysis of CYS-106 and CYS-296 for all three oxidation states. Hydrogen bonds were detected using *pytraj*'s searchhbonds function. Note that the detection algorithm is based on a cutoff distance and angle between the donor and acceptor atom. Due to this it can happen that more than one hydrogen bond exists in one frame. In consequence, the frequencies shown should be treated more as a general measure. Note that the numbering of the residues is shifted here by -2. This is due to the first four residues not having been resolved in the crystal structure.

1.5 Force field parameters

CSO.prepin

```
    0    0    2

Cysteine sulfenic acid (protonated/neutral) by T.Mauck and M.Zacharias
molecule.res
CSO    INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1   DUMM   DU     M     0   -1   -2      0.000       .0        .0       .00000
   2   DUMM   DU     M     1    0   -1      1.449       .0        .0       .00000
   3   DUMM   DU     M     2    1    0      1.523    111.21       .0       .00000
   4   N      N      M     3    2    1      1.540    111.208   -180.000  -0.415700
   5   H      H      E     4    3    2      1.015    139.534     65.031   0.271900
   6   CA     CT     M     4    3    2      1.460     95.148    -74.769   0.079652
   7   CB     CT     3     6    4    3      1.538    111.215    163.166  -0.045783
   8   S      S      S     7    6    4      1.826    115.027    -56.813  -0.037190
   9   OS     OH     S     8    7    6      1.694    101.408    -53.406  -0.475221
  10   HOS    HO     E     9    8    7      0.973    106.884    -88.482   0.387275
  11   HB1    H1     E     7    6    4      1.092    108.009    178.602   0.076982
  12   HB2    H1     E     7    6    4      1.099    110.964     60.630   0.076982
  13   HA     H1     E     6    4    3      1.095    109.369     43.052   0.051803
  14   C      C      M     6    4    3      1.544    114.924    -75.109   0.597200
  15   O      O      E    14    6    4      1.227    119.192    170.912  -0.567900
```

```
LOOP

IMPROPER
   -M   CA    N    H
   CA   +M    C    O

DONE
STOP
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frcmod1.CSO

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AMBER-Parameters for Cysteine sulfenic acid (protonated) by T.Mauck and M.Zacharias
MASS
N  14.010         0.530
H  1.008          0.161
CT 12.010         0.878
S  32.060         2.900
OH 16.000         0.465
HO 1.008          0.135
H1 1.008          0.135
C  12.010         0.616
O  16.000         0.434

BOND
H -N   403.20   1.013
CT-N   328.70   1.462
CT-CT  300.90   1.538
CT-H1  330.60   1.097
C -CT  313.00   1.524
CT-S   215.90   1.839
OH-S   261.40   1.688
HO-OH  371.40   0.973
C -O   637.70   1.218

ANGLE
CT-CT-N    65.900     111.610
H1-CT-N    49.800     108.880
C -CT-N    67.000     109.060
CT-N -H    45.800     117.680
CT-CT-S    61.300     110.270
CT-CT-H1   46.400     109.560
CT-C -O    67.400     123.200
C -CT-CT   63.300     111.040
CT-S -OH   64.800      98.280
H1-CT-S    42.100     108.760
HO-OH-S    42.900     107.110
H1-CT-H1   39.200     108.460
C -CT-H1   47.000     108.220

DIHE
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H1-CT-CT-N    9    1.400         0.000          3.000
O -C -CT-N    6    0.000       180.000          2.000
CT-CT-N -H    6    0.000         0.000          2.000
H1-CT-N -H    6    0.000         0.000          2.000
C -CT-N -H    6    0.000         0.000          2.000
CT-CT-S -OH   3    1.000         0.000          3.000
O -C -CT-CT   6    0.000       180.000          2.000
HO-OH-S -CT   1    2.400         0.000          2.000
H1-CT-S -OH   3    1.000         0.000          3.000
H1-CT-CT-S    9    1.400         0.000          3.000
H1-CT-CT-H1   9    1.400         0.000          3.000
O -C -CT-H1   1    0.800         0.000         -1.000
O -C -CT-H1   1    0.000         0.000         -2.000
O -C -CT-H1   1    0.080       180.000          3.000
C -CT-CT-S    9    1.400         0.000          3.000
C -CT-CT-H1   9    1.400         0.000          3.000

IMPROPER

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  H           0.6000  0.0157
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  OH          1.7210  0.2104
  HO          0.0000  0.0000
  H1          1.3870  0.0157
  C           1.9080  0.0860
  O           1.6612  0.2100
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frcmod2.CSO

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GAFF-Parameters for Cysteine sulfenic acid (protonated) by T.Mauck and M.Zacharias
MASS
N  14.010        0.530
H  1.008         0.161
CT 12.010        0.878
S  32.060        2.900
OH 16.000        0.465
HO 1.008         0.135
H1 1.008         0.135
C  12.010        0.616
O  16.000        0.434

BOND
H -N   403.20   1.013
CT-N   328.70   1.462
CT-CT  300.90   1.538
CT-H1  330.60   1.097
C -CT  313.00   1.524
CT-S   215.90   1.839
OH-S   261.40   1.688
HO-OH  371.40   0.973
C -O   637.70   1.218

ANGLE
CT-CT-N    65.900     111.610
H1-CT-N    49.800     108.880
C -CT-N    67.000     109.060
CT-N -H    45.800     117.680
CT-CT-S    61.300     110.270
CT-CT-H1   46.400     109.560
CT-C -O    67.400     123.200
C -CT-CT   63.300     111.040
CT-S -OH   64.800      98.280
H1-CT-S    42.100     108.760
HO-OH-S    42.900     107.110
H1-CT-H1   39.200     108.460
C -CT-H1   47.000     108.220

DIHE
N -CT-CT-S    9    1.400         0.000          3.000
H1-CT-CT-N    9    1.400         0.000          3.000
O -C -CT-N    6    0.000       180.000          2.000
CT-CT-N -H    6    0.000         0.000          2.000
H1-CT-N -H    6    0.000         0.000          2.000
C -CT-N -H    6    0.000         0.000          2.000
CT-CT-S -OH   3    1.000         0.000          3.000
O -C -CT-CT   6    0.000       180.000          2.000
HO-OH-S -CT   1    2.400         0.000          2.000
H1-CT-S -OH   3    1.000         0.000          3.000
H1-CT-CT-S    9    1.400         0.000          3.000
H1-CT-CT-H1   9    1.400         0.000          3.000
O -C -CT-H1   1    0.800         0.000         -1.000
O -C -CT-H1   1    0.000         0.000         -2.000
O -C -CT-H1   1    0.080       180.000          3.000
C -CT-CT-S    9    1.400         0.000          3.000
C -CT-CT-H1   9    1.400         0.000          3.000

IMPROPER

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  CT          1.9080  0.1094            same as c3
  S           2.0000  0.2500            same as ss
  OH          1.7210  0.2104            same as oh
  HO          0.0000  0.0000            same as ho
  H1          1.3870  0.0157            same as h1
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  O           1.6612  0.2100             same as o
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CSO-.prepin

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Cysteine sulfinic acid (deprotonated) by T.Mauck and M.Zacharias
molecule.res
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CORRECT     OMIT DU   BEG
  0.0000
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   3   DUMM   DU     M     2    1    0      1.523    111.21        .0       .00000
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  11   HB2    H1     E     7    6    4      1.100    109.982     68.141   0.098871
  12   HA     H1     E     6    4    3      1.096    110.381    -67.522   0.114025
  13   C      C      M     6    4    3      1.524    113.797    171.289   0.536600
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LOOP

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STOP
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frcmod1.CSO-

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AMBER14-Parameters for Cysteine sulfenic acid (deprotonated) by T.Mauck and M.Zacharias
MASS
N  14.010         0.530
H  1.008          0.161
CT 12.010         0.878
S  32.060         2.900
O  16.000         0.434
H1 1.008          0.135
C  12.010         0.616

BOND
H -N    434.00    1.010
CT-N    337.00    1.449
CT-CT   310.00    1.526
CT-H1   340.00    1.090
C -CT   317.00    1.522
CT-S    227.00    1.810
C -O    570.00    1.229

ANGLE
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C -CT-N     63.000      110.100
CT-N -H     50.000      118.040
CT-CT-S     50.000      114.700
CT-CT-H1    50.000      109.500
CT-C -O     80.000      120.400
C -CT-CT    63.000      111.100
H1-CT-S     50.000      109.500
H1-CT-H1    35.000      109.500
C -CT-H1    50.000      109.500

DIHE
N -CT-CT-S     9    1.400          0.000           3.000
H1-CT-CT-N     9    1.400          0.000           3.000
O -C -CT-N     6    0.000          0.000           2.000
CT-CT-N -H     6    0.000          0.000           2.000
H1-CT-N -H     6    0.000          0.000           2.000
```

```
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O -C -CT-CT    6     0.000          0.000            2.000
H1-CT-S -O     3     1.000          0.000            3.000
H1-CT-CT-S     9     1.400          0.000            3.000
H1-CT-CT-H1    9     1.400          0.000            3.000
O -C -CT-H1    1     0.800          0.000           -1.000
O -C -CT-H1    1     0.000          0.000           -2.000
O -C -CT-H1    1     0.080        180.000            3.000
C -CT-CT-S     9     1.400          0.000            3.000
C -CT-CT-H1    9     1.400          0.000            3.000

IMPROPER

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  H           0.6000  0.0157
  CT          1.9080  0.1094
  S           2.0000  0.2500
  O           1.6612  0.2100
  H1          1.3870  0.0157
  C           1.9080  0.0860
```

frcmod2.CSO-

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MASS
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H  1.008          0.161
CT 12.010         0.878
S  32.060         2.900
O  16.000         0.434
H1 1.008          0.135
C  12.010         0.616

BOND
H -N    403.20    1.013
CT-N    328.70    1.462
CT-CT   300.90    1.538
CT-H1   330.60    1.097
C -CT   313.00    1.524
CT-S    215.90    1.839
O -S    435.70    1.507
C -O    637.70    1.218

ANGLE
CT-CT-N     65.900      111.610
H1-CT-N     49.800      108.880
C -CT-N     67.000      109.060
CT-N -H     45.800      117.680
CT-CT-S     61.300      110.270
CT-CT-H1    46.400      109.560
CT-C -O     67.400      123.200
C -CT-CT    63.300      111.040
CT-S -O     64.400      106.990
H1-CT-S     42.100      108.760
H1-CT-H1    39.200      108.460
C -CT-H1    47.000      108.220

DIHE
N -CT-CT-S     9     1.400          0.000            3.000
H1-CT-CT-N     9     1.400          0.000            3.000
O -C -CT-N     6     0.000        180.000            2.000
CT-CT-N -H     6     0.000          0.000            2.000
H1-CT-N -H     6     0.000          0.000            2.000
C -CT-N -H     6     0.000          0.000            2.000
CT-CT-S -O     3     1.000          0.000            3.000
O -C -CT-CT    6     0.000        180.000            2.000
H1-CT-S -O     3     1.000          0.000            3.000
H1-CT-CT-S     9     1.400          0.000            3.000
H1-CT-CT-H1    9     1.400          0.000            3.000
O -C -CT-H1    1     0.800          0.000           -1.000
O -C -CT-H1    1     0.000          0.000           -2.000
O -C -CT-H1    1     0.080        180.000            3.000
C -CT-CT-S     9     1.400          0.000            3.000
C -CT-CT-H1    9     1.400          0.000            3.000
```

```
IMPROPER

NONBON
  N           1.8240  0.1700            same as n
  H           0.6000  0.0157            same as hn
  CT          1.9080  0.1094            same as c3
  S           2.0000  0.2500            same as ss
  O           1.6612  0.2100            same as o
  H1          1.3870  0.0157            same as h1
  C           1.9080  0.0860            same as c
```

CSD-.prepin

```
    0    0    2

Cysteine sulfinic acid (deprotonated) by T.Mauck and M.Zacharias
molecule.res
CSD   INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0      .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0      .00000
   3  DUMM  DU    M    2   1   0     1.523   111.21       .0      .00000
   4  N     n     M    3   2   1     1.540   111.208  -180.000 -0.516300
   5  H     hn    E    4   3   2     1.047    25.193    81.870  0.293600
   6  CA    c3    M    4   3   2     1.478   103.255   -28.560 -0.025473
   7  CB    c3    3    6   4   3     1.525   108.523    35.550 -0.074089
   8  SG    s4    B    7   6   4     1.895   111.980   -51.896  0.164280
   9  OS1   o     E    8   7   6     1.558    98.938    70.130 -0.517771
  10  OS2   o     E    8   7   6     1.523   101.999   -46.205 -0.517771
  11  HB1   h1    E    7   6   4     1.094   111.359    68.225  0.080403
  12  HB2   h1    E    7   6   4     1.095   109.410  -172.038  0.080403
  13  HA    h1    E    6   4   3     1.099   107.364   -81.427  0.078018
  14  C     c     M    6   4   3     1.551   113.028   159.622  0.536600
  15  O     o     E   14   6   4     1.232   122.842  -121.642 -0.581900


LOOP

IMPROPER
   -M   CA   N    H
   CA   +M   C    O

DONE
STOP
```

frcmod1.CSD-

```
GAFF-Parameters (+ GAFF/AMBER junctions) for Cysteine sulfinic acid (deprotonated) by T.Mauck and M.Z
MASS
n  14.010        0.530              same as n

BOND
hn-n   403.20   1.013
c3-n   328.70   1.462
c -N   490.00   1.335
C -n   490.00   1.335

ANGLE
c3-c3-n    80.000     109.700
h1-c3-n    50.000     109.500
c -c3-n    63.000     110.100
c3-n -hn   50.000     118.040
c3-c -N    70.000     116.600
c -N -H    50.000     120.000
c -N -CX   50.000     121.900
o -c -N    80.000     122.900
CX-C -n    70.000     116.600
C -n -hn   50.000     120.000
C -n -c3   50.000     121.900
O -C -n    80.000     122.900

DIHE
c3-c3-n -hn   6    0.000         0.000          2.000
h1-c3-n -hn   6    0.000         0.000          2.000
c -c3-n -hn   6    0.000         0.000          2.000
```

```
c3-c -N -H     4    10.000        180.000            2.000
c3-c -N -CX    4    10.000        180.000            2.000
o -c -N -H     1     2.500        180.000           -2.000
o -c -N -H     1     2.000          0.000            1.000
CX-C -n -hn    4    10.000        180.000            2.000
CX-C -n -c3    4    10.000        180.000            2.000
C -n -c3-c3    1     0.000          0.000           -4.000
C -n -c3-c3    1     0.400          0.000           -3.000
C -n -c3-c3    1     2.000          0.000           -2.000
C -n -c3-c3    1     2.000          0.000            1.000
C -n -c3-h1    6     0.000          0.000            2.000
c -c3-n -C     6     0.000          0.000            2.000
O -C -n -hn    1     2.000          0.000            1.000
O -C -n -hn    1     2.500        180.000           -2.000
o -C -n -c3    4    10.000        180.000            2.000
o -c -N -CX    4    10.000        180.000            2.000
O -C -n -c3    4    10.000        180.000            2.000

IMPROPER
c -c3-n -hn          1.1          180.0          2.0
o -c -N -CX         10.5          180.0          2.0

NONBON
  ns           1.8240   0.1700              same as n
```

OCS-.prepin

```
    0    0    2

Cysteine sulfonic acid (deprotonated) by T.Mauck and M.Zacharias
molecule.res
OCS     INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0       .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0       .00000
   3  DUMM  DU    M    2   1   0     1.523   111.21       .0       .00000
   4  N     N     M    3   2   1     1.540   111.208  -180.000 -0.516300
   5  H     H     E    4   3   2     1.036    32.297   130.826  0.293600
   6  CA    CT    M    4   3   2     1.465    82.902   -30.376  0.047695
   7  CB    CT    3    6   4   3     1.539   109.776    -4.451 -0.055004
   8  SG    SO    3    7   6   4     1.845   116.054    43.514  1.061279
   9  OS1   O     E    8   7   6     1.513   102.853   -62.056 -0.650854
  10  OS2   O     E    8   7   6     1.482   106.066    56.899 -0.650854
  11  OS3   O     E    8   7   6     1.482   103.652   179.857 -0.650854
  12  HB1   H1    E    7   6   4     1.091   108.491   163.727  0.051984
  13  HB2   H1    E    7   6   4     1.093   110.313   -76.184  0.051984
  14  HA    H1    E    6   4   3     1.101   107.141  -121.533  0.062624
  15  C     C     M    6   4   3     1.554   116.220   123.216  0.536600
  16  O     O     E   15   6   4     1.227   121.632  -152.218 -0.581900


LOOP

IMPROPER
   -M   CA   N    H
   CA   +M   C    O

DONE
STOP
```

frcmod1.OCS-

```
AMBER-Parameters for Cysteine sulfonic acid (deprotonated) by T.Mauck and M.Zacharias
MASS
N  14.010         0.530
H  1.008          0.161
CT 12.010         0.878
O  16.000         0.434
H1 1.008          0.135
C  12.010         0.616

BOND
H -N    434.00    1.010
CT-N    337.00    1.449
CT-CT   310.00    1.526
CT-H1   340.00    1.090
```

```
C -CT  317.00   1.522
C -O   570.00   1.229

ANGLE
CT-CT-N    80.000     109.700
H1-CT-N    50.000     109.500
C -CT-N    63.000     110.100
CT-N -H    50.000     118.040
CT-CT-H1   50.000     109.500
CT-C -O    80.000     120.400
C -CT-CT   63.000     111.100
H1-CT-H1   35.000     109.500
C -CT-H1   50.000     109.500

DIHE
N -CT-CT-SO   9    1.400         0.000          3.000
H1-CT-CT-N    9    1.400         0.000          3.000
O -C -CT-N    6    0.000         0.000          2.000
CT-CT-N -H    6    0.000         0.000          2.000
H1-CT-N -H    6    0.000         0.000          2.000
C -CT-N -H    6    0.000         0.000          2.000
CT-CT-SO-O    0    0.000         0.000          0.000
O -C -CT-CT   6    0.000         0.000          2.000
H1-CT-SO-O    0    0.000         0.000          0.000
H1-CT-CT-SO   9    1.400         0.000          3.000
H1-CT-CT-H1   9    1.400         0.000          3.000
O -C -CT-H1   1    0.800         0.000         -1.000
O -C -CT-H1   1    0.000         0.000         -2.000
O -C -CT-H1   1    0.080       180.000          3.000
C -CT-CT-SO   9    1.400         0.000          3.000
C -CT-CT-H1   9    1.400         0.000          3.000

IMPROPER

NONBON
  N           1.8240  0.1700
  H           0.6000  0.0157
  CT          1.9080  0.1094
  O           1.6612  0.2100
  H1          1.3870  0.0157
  C           1.9080  0.0860
```

frcmod2.OCS-

```
GAFF-Parameters for Cysteine sulfonic acid (deprotonated) by T.Mauck and M.Zacharias
MASS
N  14.010        0.530
H  1.008         0.161
CT 12.010        0.878
SO 32.060        2.900
O  16.000        0.434
H1 1.008         0.135
C  12.010        0.616

BOND
H -N   403.20   1.013
CT-N   328.70   1.462
CT-CT  300.90   1.538
CT-H1  330.60   1.097
C -CT  313.00   1.524
CT-SO  233.50   1.808
O -SO  512.70   1.453
C -O   637.70   1.218

ANGLE
CT-CT-N    65.900     111.610
H1-CT-N    49.800     108.880
C -CT-N    67.000     109.060
CT-N -H    45.800     117.680
CT-CT-SO   62.100     110.220
CT-CT-H1   46.400     109.560
CT-C -O    67.400     123.200
C -CT-CT   63.300     111.040
CT-SO-O    65.400     108.610
H1-CT-SO   43.200     107.150
O -SO-O    73.600     120.050
```

```
H1-CT-H1    39.200      108.460
C -CT-H1    47.000      108.220

DIHE
N -CT-CT-SO    9     1.400          0.000          3.000
H1-CT-CT-N     9     1.400          0.000          3.000
O -C -CT-N     6     0.000        180.000          2.000
CT-CT-N -H     6     0.000          0.000          2.000
H1-CT-N -H     6     0.000          0.000          2.000
C -CT-N -H     6     0.000          0.000          2.000
CT-CT-SO-O     9     1.300          0.000          3.000
O -C -CT-CT    6     0.000        180.000          2.000
H1-CT-SO-O     9     1.300          0.000          3.000
H1-CT-CT-SO    9     1.400          0.000          3.000
H1-CT-CT-H1    9     1.400          0.000          3.000
O -C -CT-H1    1     0.800          0.000         -1.000
O -C -CT-H1    1     0.000          0.000         -2.000
O -C -CT-H1    1     0.080        180.000          3.000
C -CT-CT-SO    9     1.400          0.000          3.000
C -CT-CT-H1    9     1.400          0.000          3.000

IMPROPER

NONBON
  N           1.8240  0.1700            same as n
  H           0.6000  0.0157            same as hn
  CT          1.9080  0.1094            same as c3
  SO          2.0000  0.2500            same as s6
  O           1.6612  0.2100            same as o
  H1          1.3870  0.0157            same as h1
  C           1.9080  0.0860            same as c
```