Supplementary Information

A glutamine amide flip elicits long distance allosteric responses in the LOV protein Vivid

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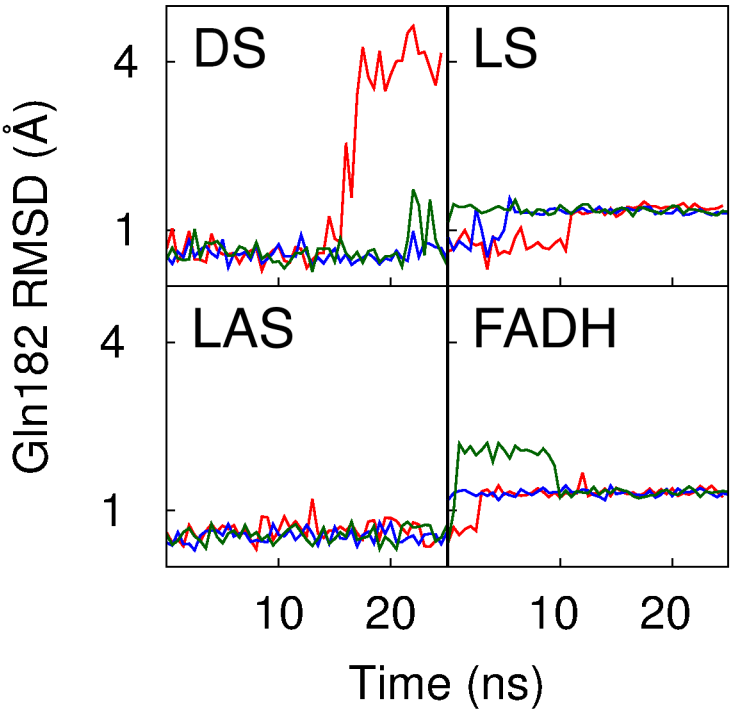

Figure S1. RMSDs of Gln182 with respect to the crystal structure in various VVD states during MD simulations. Plots are shown for DS, LS, LAS, and FADH, with red, blue, and green lines corresponding to independent MD trajectories. In DS, the RMSD fluctuates but remains less than 1 Å for major parts of the MD simulations indicating that Gln182 is somewhat flexible but remains mostly close to the crystal conformation facing FAD with its amide; in the later stage of one trajectory (red) the Gln182 rotates out of the active site away from the FAD. In LS and FADH the RMSDs stabilizes at a value slightly greater than 1 Å, in a conformation in which the residue faces FAD with its carbonyl. In LAS, Gln182 faces FAD with its carbonyl already in the crystal structure, and the RMSD remains close to zero suggesting that in this state the Gln182 is stable in the crystal conformation.

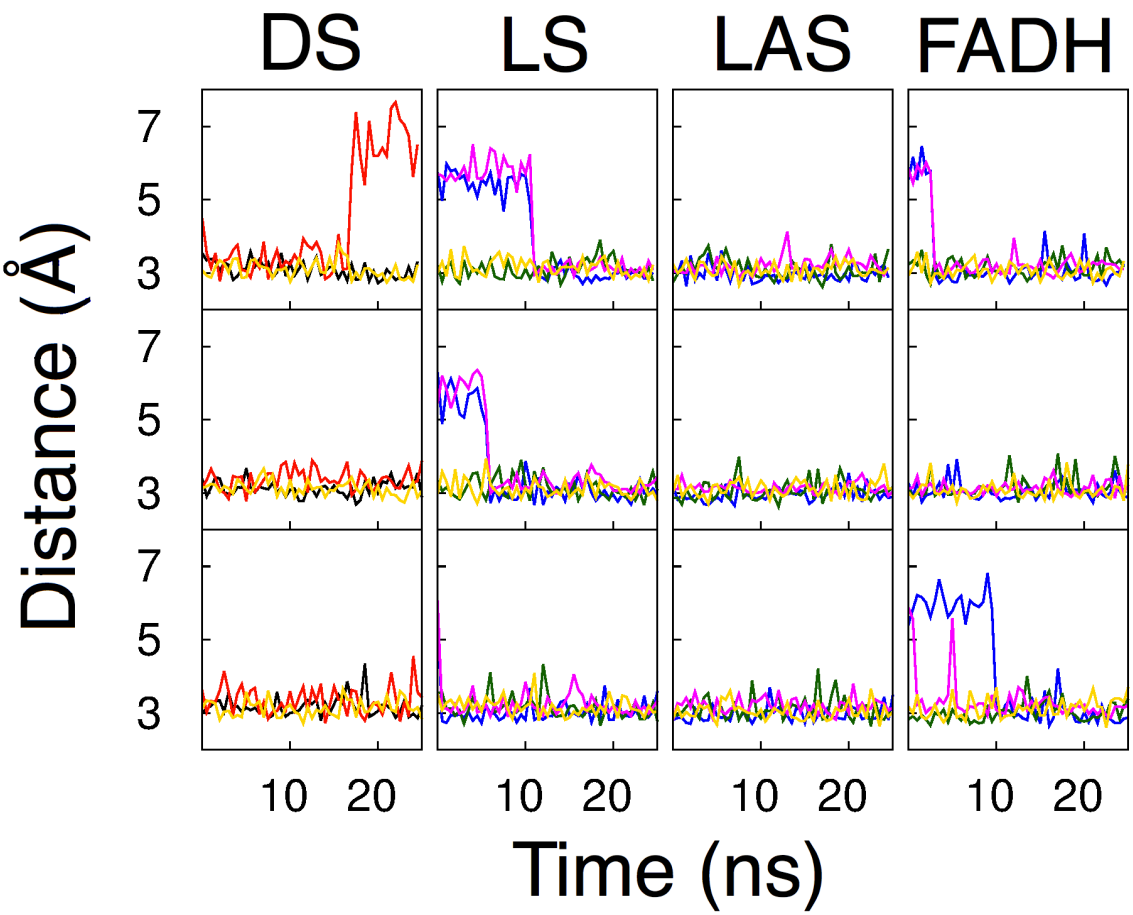

Figure S2. Hydrogen bonding pattern in the active site of the LOV domain in various VVD states during MD simulations. Key hydrogen bonding interactions of the active site are illustrated for VVD in DS, LS, LAS, and FADH (columns 1-4). The three rows refer to three independent MD trajectories. The following hydrogen bond distances are plotted: for DS, NE2(Gln182)-O4(FAD) (red), N(Gln182)-O(Ala72) (black), and N(Asn161)-O4(FAD) (gold); for LS, LAS, and FADH, OE1(Gln182)-N5(FAD) (purple), NE2(Gln182)-O(Ala72) (blue), N(Gln182)-O(Ala72) (green), and N(Asn161)-O4(FAD) (gold). The following hydrogen bonds are stable during the MD simulations: in DS, N(Gln182)-O(Ala72) (black) and N(Asn161)-O4(FAD) (gold); in LS, LAS, and FADH, OE1(Gln182)-N5(FAD) (purple), NE2(Gln182)-O(Ala72) (blue), and N(Gln182)-O(Ala72) (green). Note that in one trajectory of FADH, the Gln182 transition occurs within the equilibration stage of the simulation.

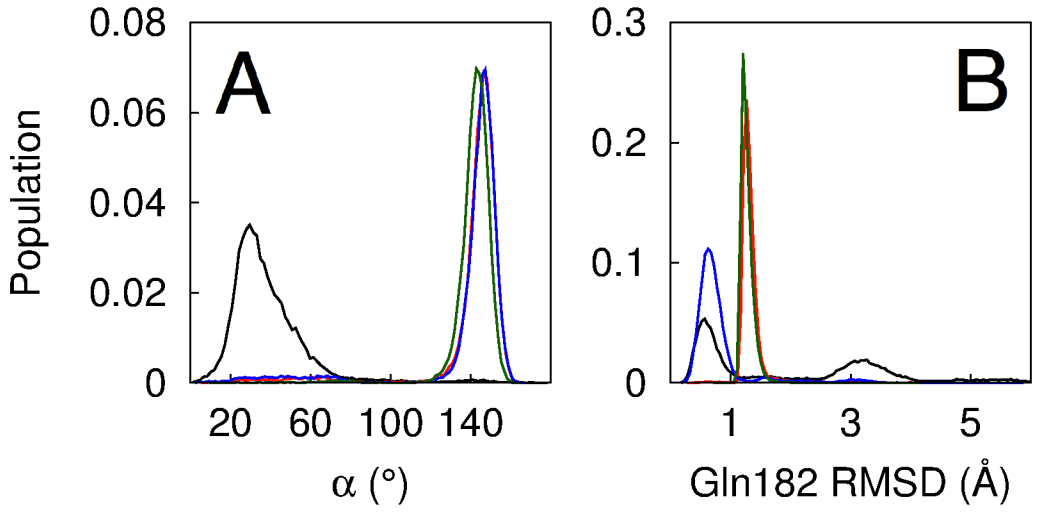

Figure S3. Conformation of Gln182 in various VVD states obtained from REMD simulations. (A) Distribution of angle α (defined in Figure 2A of the main paper) in DS (black), LS (red), LAS (blue), and FADH (green). (B) Distribution of RMSDs of Gln182 in DS (black), LS (red), LAS (blue), and FADH (green). In DS, Gln182 is flexible but mostly faces FAD with its amine and remains close to its crystal conformation as indicated by a broad distribution of α centered around 30° (A, black) and a small RMSD peak at less than 1 Å (B, black) (see Figure 2H of the main paper); a second smaller RMSD peak at ~ 3 Å represents configurations in which Gln182 rotates out of the active site (see Figure 2G of the main paper). In LS and FADH, Gln182 predominantly faces FAD with its carbonyl and mostly remains in this conformation as illustrated by a sharp α peak at ~ 150° (A, red, green) and a single sharp RMSD peak at values slightly higher than 1 Å (B, red, green). In LAS, Gln182 also predominantly faces FAD with its carbonyl (sharp α peak at ~ 150°; A, blue) but is somewhat more flexible than in LS and FADH as suggested by a comparatively low RMSD peak at less than 1 Å (B, blue).

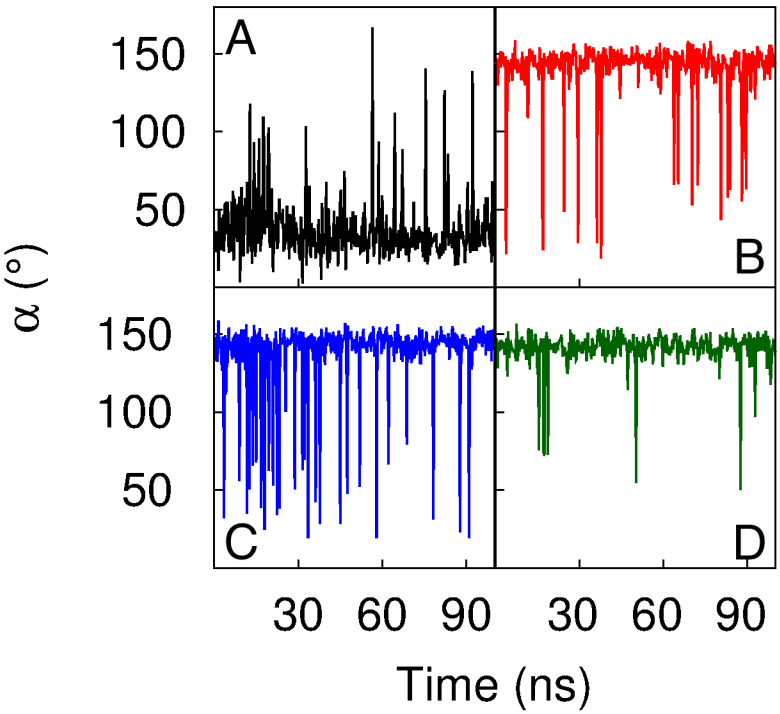

Figure S4. Conformation of Gln182 in various VVD states obtained from REMD simulations. Angle α (defined in Figure 2A of the main paper) is plotted for the lowest temperature ensemble of the REMD simulations for DS (black), LS (red), LAS (blue), and FADH (green). In each case, the peaks correspond to transitions of Gln182 between two conformations: facing FAD with its amine (α ~ 50°) and facing FAD with its carbonyl (α ~ 150°).

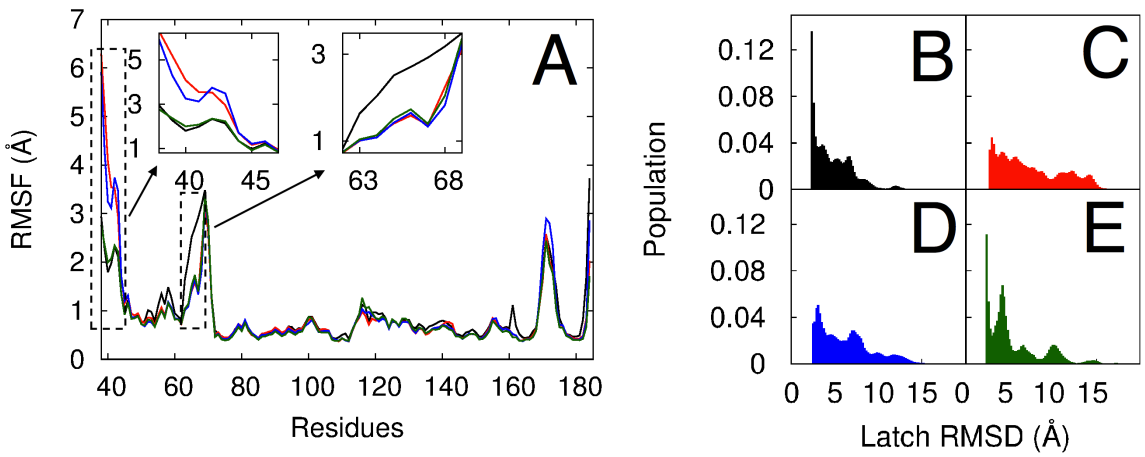

Figure S5. Dynamics of the N-terminal latch in various VVD states obtained from REMD simulations. (A) RMSFs of residues in DS (black), LS (red), LAS (blue), and FADH (green); those of residues in the N-terminal latch (residues 38-45) and the bβ region (residues 62-69) are highlighted in the insets. (B-E) Distribution of RMSDs of the N-terminal latch with respect to the crystal conformation in DS (B), LS (C), LAS (D), and FADH (E). In DS, VVD has low latch flexibility and high bβ flexibility as indicated by the RMSFs of the corresponding regions (A, black); the rigidity of the latch in DS is reflected in the latch RMSD distribution (B) that exhibits a sharp peak close to 3 Å and a negligible population beyond 10 Å. In LS and LAS, VVD has high latch flexibility and low bβ flexibility (A, red, blue); the corresponding latch RMSD distribution has significant population (beyond 10 Å) of configurations in which the latch has been released. In FADH, both the latch and the bβ region have low flexibility (A, green); however, in the corresponding latch RMSD distribution, there is a significant population of configurations with the latch released (E).

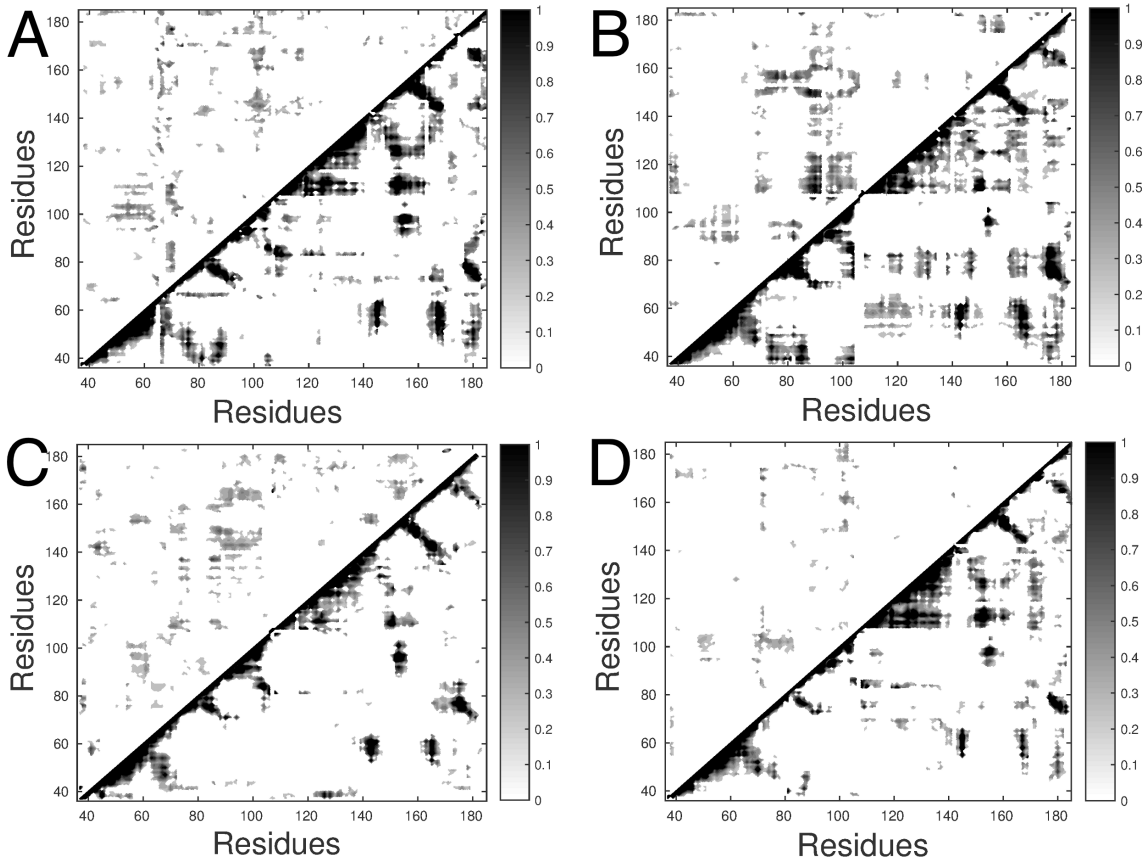

Figure S6. Correlated motions in VVD. DCCMS are constructed from MD simulations for VVD in DS (A), LS (B), LAS (C), FADH (D). In each case, the DCCMs are obtained from a single trajectory obtained by concatenating the various independent trajectories for that case. DCCMs obtained from individual MD trajectories were qualitatively similar. The upper triangle corresponds to positive correlations and the lower triangle corresponds to negative correlations.

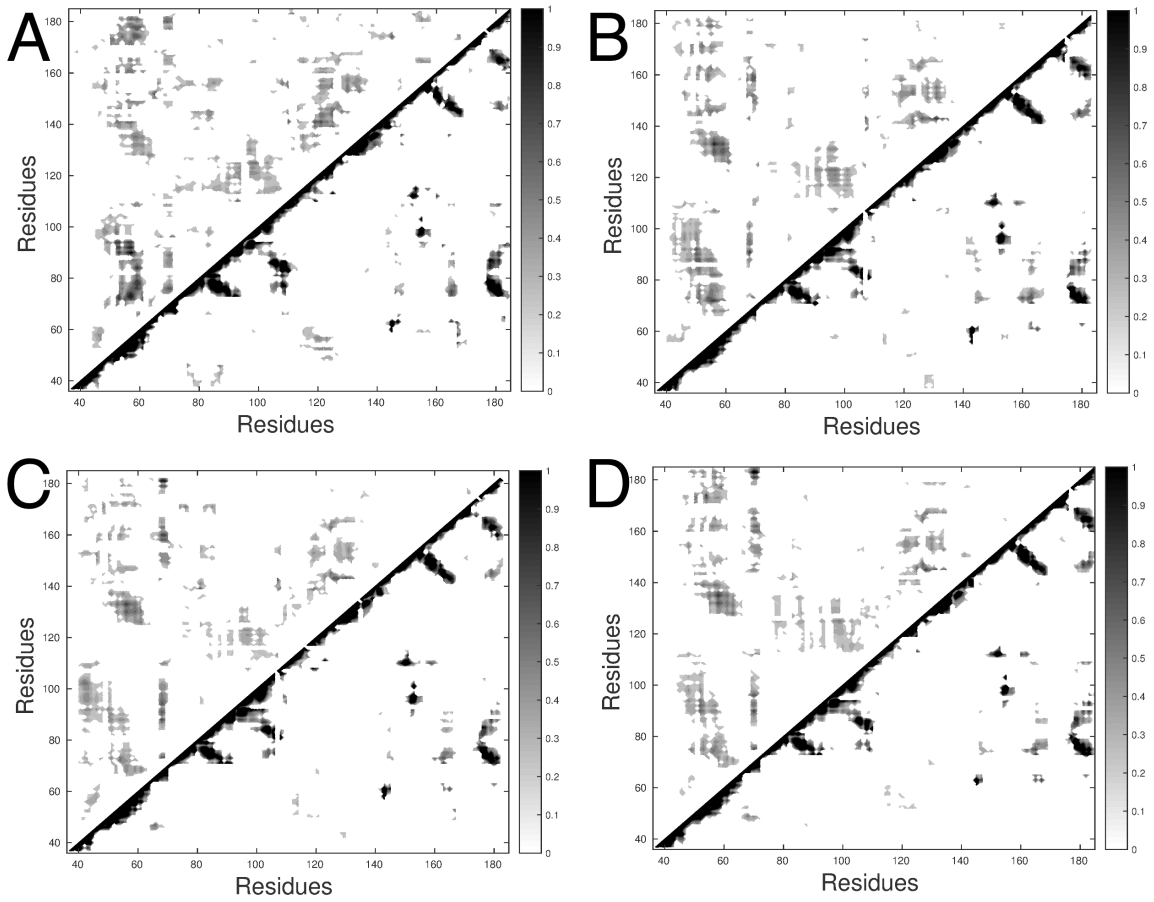

Figure S7. Correlated motions in VVD. DCCMS are constructed from REMD simulations for VVD in DS (A), LS (B), LAS (C), FADH (D). The upper triangle corresponds to positive correlations and the lower triangle corresponds to negative correlations.

Hinge-bβ residues	DS		LS		LAS		FADH	
	MD	REMD	MD	REMD	MD	REMD	MD	REMD
62	0.19	0.26	0.03	0.31	0.06	0.36	0.11	0.25
63	0.27	0.24	0.00	0.24	0.00	0.32	0.12	0.21
64	0.10	0.18	0.00	0.24	0.05	0.35	0.17	0.21
65	0.0	0.09	0.00	0.28	0.17	0.35	0.10	0.16
66	0.02	0.13	0.00	0.29	0.20	0.41	0.25	0.18
67	0.13	0.15	0.00	0.25	0.16	0.33	0.20	0.20
68	0.04	0.06	0.00	0.31	0.26	0.27	0.08	0.18
69	0.0	0.02	0.08	0.18	0.12	0.22	0.03	0.09
70	0.02	0.04	0.12	0.24	0.23	0.20	0.06	0.10
71	0.06	0.10	0.07	0.16	0.00	0.04	0.32	0.11

Table S1. Absolute correlations of the hinge-bβ residues to the latch obtained from the various MD and REMD simulations. Correlations from MD trajectories are calculated after concatenating all independent trajectories for each case into a single trajectory. The reported values correspond to the average correlation of each residue to the latch residues (residues 1-12).

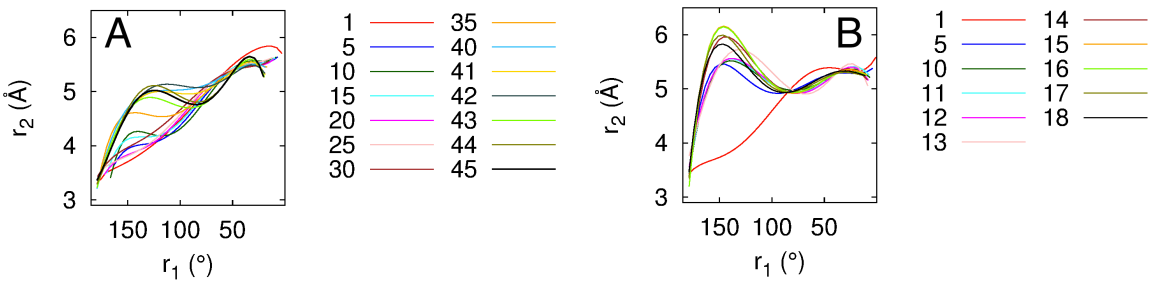

Figure S8. Convergence of the string simulations. Strings from various iterations of the simulations of VVD in DS (A) and LS (B) are plotted in the 2D space of the reaction coordinates r_1 and r_2 defined in Figure 5 of the main paper; iterations are color coded. During the final stages there are only small string displacements between consecutive iterations suggesting that the string has converged in the 2D space. For DS (A), the string was updated after 100 ps of MD on each image and was considered converged after 40 iterations. For LS (B), the string was updated after 500 ps of MD on each image and was considered converged after 18 iterations.

Flavin force field parameters used in the study

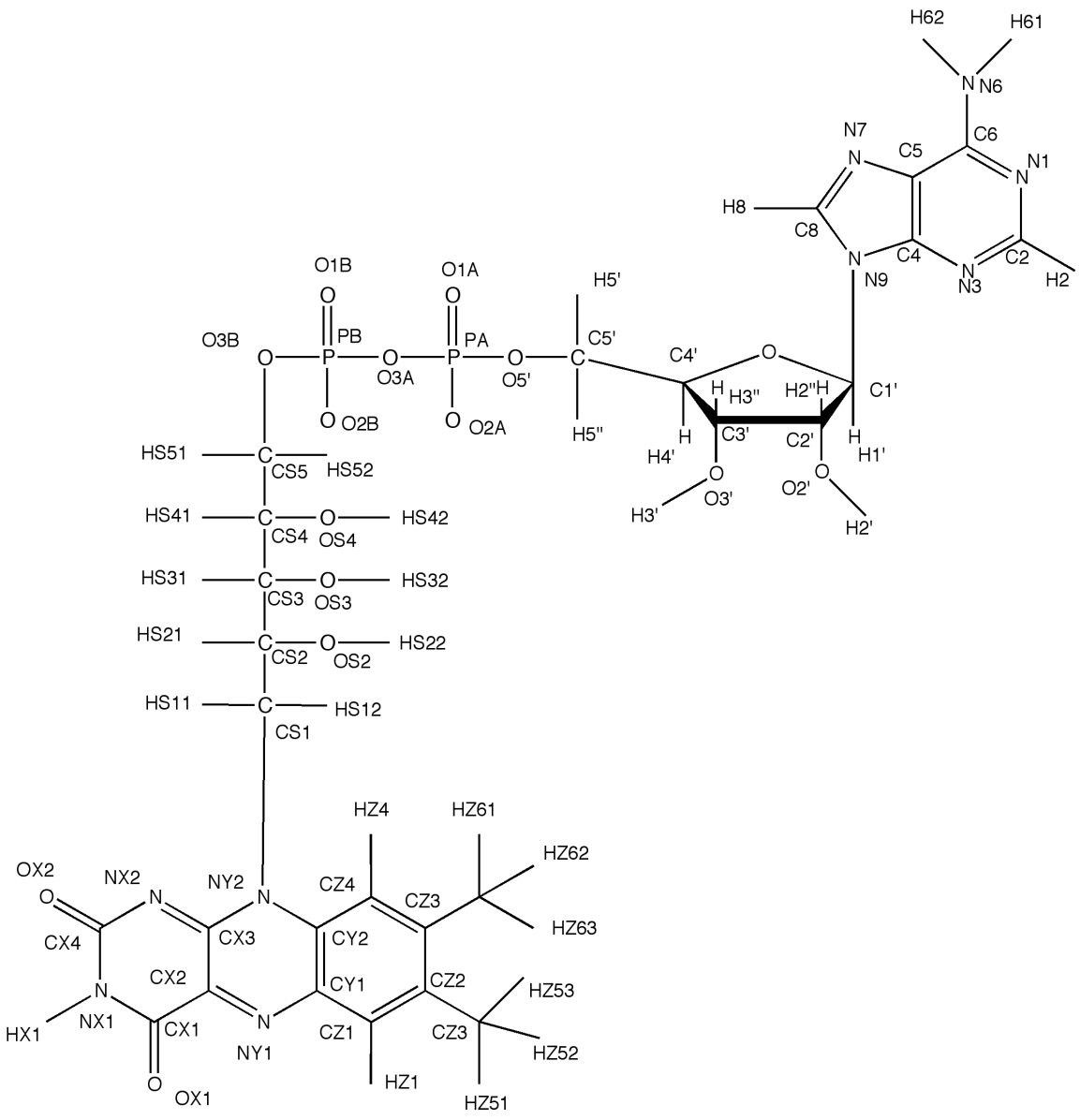

Figure S9. Chemdraw figure of flavin with atom names for reference

Flavin in neutral semiquinone state

```
ATOM C4'  CN7     0.16
ATOM H4'  HN7     0.09
ATOM O4'  ON6B   -0.50
ATOM C1'  CN7B    0.16
ATOM H1'  HN7     0.09
ATOM C5   CN5     0.28
ATOM N7   NN4    -0.71
ATOM C8   CN4     0.34
ATOM H8   HN3     0.12
ATOM N9   NN2    -0.05
ATOM N1   NN3A   -0.74
ATOM C2   CN4     0.50
ATOM H2   HN3     0.13
ATOM N3   NN3A   -0.75
ATOM C4   CN5     0.43
ATOM C6   CN2     0.46
ATOM N6   NN1    -0.77
ATOM H61  HN1     0.38
ATOM H62  HN1     0.38
ATOM C2'  CN7     0.14
ATOM H2'' HN7     0.09
ATOM O2'  ON5    -0.66
ATOM H2'  HN5     0.43
ATOM C3'  CN7     0.14
ATOM H3'  HN7     0.09
ATOM O3'  ON5    -0.66
ATOM H3T  HN5     0.43
ATOM C5'  CN8    -0.08
ATOM H5'  HN8     0.09
ATOM H5'' HN8     0.09
ATOM O5'  ON2    -0.62
ATOM PA   P       1.50
ATOM O1A  ON3    -0.82
ATOM O2A  ON3    -0.82
ATOM O3A  ON2    -0.74
ATOM PB   P       1.50
ATOM O1B  ON3    -0.90
ATOM O2B  ON3    -0.90
ATOM O3B  ON2    -0.74
ATOM CS1  CT2     0.21
ATOM HS11 HA      0.09
ATOM HS12 HA      0.09
ATOM CS2  CT1     0.17
ATOM HS21 HA      0.09
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```
ATOM OS2  OH1    -0.66
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ATOM CS3  CT1     0.17
ATOM HS31 HA      0.09
ATOM OS3  OH1    -0.66
ATOM HS32 H       0.43
ATOM CS4  CT1     0.17
ATOM HS41 HA      0.09
ATOM OS4  OH1    -0.66
ATOM HS42 H       0.43
ATOM CS5  CT2     0.22
ATOM HS51 HA      0.09
ATOM HS52 HA      0.09
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ATOM CX1  CX1     0.82
ATOM OX1  OX1    -0.61
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ATOM CX3  CX3     0.37
ATOM NX2  NX2    -0.81
ATOM CX4  CX4     1.09
ATOM OX2  OX2    -0.66
ATOM NY1  NY1    -0.60
ATOM CY1  CY1     0.60
ATOM CY2  CY2    -0.30
ATOM NY2  NY2     0.20
ATOM CZ1  CZ1    -0.46
ATOM HZ1  HZ1     0.24
ATOM CZ2  CZ2     0.19
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ATOM HZ52 HA      0.09
ATOM HZ53 HA      0.09
ATOM CZ3  CZ3     0.18
ATOM CZ6  CT3    -0.48
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ATOM HZ62 HA      0.09
ATOM HZ63 HA      0.09
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ATOM HZ4  HZ4     0.19
```

Cysteinyl flavin adduct

```
ATOM C    C       0.51
ATOM O    O      -0.51
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB      0.09
ATOM CB   CT2    -0.181
ATOM HB1  HA      0.115
ATOM HB2  HA      0.115
ATOM SG   S      -0.141
ATOM C4'  CN7     0.16
ATOM H4'  HN7     0.09
ATOM O4'  ON6B   -0.50
ATOM C1'  CN7B    0.16
ATOM H1'  HN7     0.09
ATOM C5   CN5     0.28
ATOM N7   NN4    -0.71
ATOM C8   CN4     0.34
ATOM H8   HN3     0.12
ATOM N9   NN2    -0.05
ATOM N1   NN3A   -0.74
ATOM C2   CN4     0.50
ATOM H2   HN3     0.13
ATOM N3   NN3A   -0.75
ATOM C4   CN5     0.43
ATOM C6   CN2     0.46
ATOM N6   NN1    -0.77
ATOM H61  HN1     0.38
ATOM H62  HN1     0.38
ATOM C2'  CN7     0.14
ATOM H2'' HN7     0.09
ATOM O2'  ON5    -0.66
ATOM H2'  HN5     0.43
ATOM C3'  CN7     0.14
ATOM H3'  HN7     0.09
ATOM O3'  ON5    -0.66
ATOM H3T  HN5     0.43
ATOM C5'  CN8    -0.08
ATOM H5'  HN8     0.09
ATOM H5'' HN8     0.09
ATOM O5'  ON2    -0.62
ATOM PA   P       1.50
ATOM O1A  ON3    -0.82
ATOM O2A  ON3    -0.82
```

```
ATOM O3A  ON2    -0.74
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ATOM O2B  ON3    -0.90
ATOM O3B  ON2    -0.74
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ATOM OS2  OH1    -0.66
ATOM HS22 H       0.43
ATOM CS3  CT1     0.17
ATOM HS31 HA      0.09
ATOM OS3  OH1    -0.66
ATOM HS32 H       0.43
ATOM CS4  CT1     0.17
ATOM HS41 HA      0.09
ATOM OS4  OH1    -0.66
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ATOM HS51 HA      0.09
ATOM HS52 HA      0.09
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ATOM CX3  CX3     0.586
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ATOM NY1  NY1    -0.436
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ATOM CY1  CY1     0.075
ATOM CY2  CY2     0.054
ATOM NY2  NY2    -0.110
ATOM CZ1  CZ1    -0.291
ATOM HZ1  HZ1     0.191
ATOM CZ2  CZ2     0.078
ATOM CZ5  CT3    -0.218
ATOM HZ51 HA      0.077
ATOM HZ52 HA      0.077
ATOM HZ53 HA      0.077
ATOM CZ3  CZ3     0.098
ATOM CZ6  CT3    -0.254
```

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ATOM HZ61 HA      0.083
ATOM HZ62 HA      0.083
ATOM HZ63 HA      0.083
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ATOM HZ4  HZ4     0.150
```

Flavin in neutral semiquinone radical state

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ATOM C4'  CN7     0.16
ATOM H4'  HN7     0.09
ATOM O4'  ON6B   -0.50
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ATOM C5   CN5     0.28
ATOM N7   NN4    -0.71
ATOM C8   CN4     0.34
ATOM H8   HN3     0.12
ATOM N9   NN2    -0.05
ATOM N1   NN3A   -0.74
ATOM C2   CN4     0.50
ATOM H2   HN3     0.13
ATOM N3   NN3A   -0.75
ATOM C4   CN5     0.43
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ATOM N6   NN1    -0.77
ATOM H61  HN1     0.38
ATOM H62  HN1     0.38
ATOM C2'  CN7     0.14
ATOM H2'' HN7     0.09
ATOM O2'  ON5    -0.66
ATOM H2'  HN5     0.43
ATOM C3'  CN7     0.14
ATOM H3'  HN7     0.09
ATOM O3'  ON5    -0.66
ATOM H3T  HN5     0.43
ATOM C5'  CN8    -0.08
ATOM H5'  HN8     0.09
ATOM H5'' HN8     0.09
ATOM O5'  ON2    -0.62
ATOM PA   P       1.50
ATOM O1A  ON3    -0.82
ATOM O2A  ON3    -0.82
ATOM O3A  ON2    -0.74
ATOM PB   P       1.50
ATOM O1B  ON3    -0.90
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ATOM O2B  ON3    -0.90
ATOM O3B  ON2    -0.74
ATOM CS1  CT2    -0.056
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ATOM HS12 HA      0.070
ATOM CS2  CT1     0.17
ATOM HS21 HA      0.09
ATOM OS2  OH1    -0.66
ATOM HS22 H       0.43
ATOM CS3  CT1     0.17
ATOM HS31 HA      0.09
ATOM OS3  OH1    -0.66
ATOM HS32 H       0.43
ATOM CS4  CT1     0.17
ATOM HS41 HA      0.09
ATOM OS4  OH1    -0.66
ATOM HS42 H       0.43
ATOM CS5  CT2     0.22
ATOM HS51 HA      0.09
ATOM HS52 HA      0.09
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ATOM CX3  CX3     0.360
ATOM NX2  NX2    -0.590
ATOM CX4  CX4     0.717
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ATOM HZ52 HA      0.072
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ATOM CZ4 CZ4 -0.251
ATOM HZ4 HZ4 0.166

Bonded parameters

CX4	NX2	350.000	1.3700
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CX4	OX2	640.000	1.1900
NX2	CX3	350.000	1.2900
CX3	CX2	282.000	1.4700
CX3	CXA	282.000	1.5200
CX2	CX1	282.000	1.5000
CXA	CX1	282.000	1.5200
CX3	NY2	350.000	1.3600
CX2	NY1	350.000	1.2700
CXA	NY1	350.000	1.4300
CX1	OX1	640.000	1.1900
CX1	NX1	350.000	1.3600
NX1	HX1	465.600	1.0000
NY2	CT2	310.000	1.4600
NY2	CY2	390.000	1.3900
CY2	CZ4	440.000	1.4000
CY2	CY1	440.000	1.4000
CY1	NY1	390.000	1.3700
CY1	CZ1	440.000	1.4000
CZ4	HZ4	370.000	1.0700
CZ4	CZ3	440.000	1.3800
CZ3	CZ2	440.000	1.4100
CZ2	CZ1	440.000	1.3700
CZ1	HZ1	370.000	1.0700
CZ2	CT3	345.000	1.5100
CZ3	CT3	345.000	1.5100
CT2	ON2	340.000	1.4400
NX2	HX2	465.600	1.0000
NY1	HY1	465.600	1.0000
NY1	HX1	465.600	1.0000
S	CXA	214.000	1.880

OX2	CX4	NX1	98.00	118.6
OX2	CX4	NX2	98.00	123.1
NX1	CX4	NX2	70.00	118.3
CX3	NX2	CX4	60.00	120.5
NX2	CX3	CX2	65.00	124.1
NX2	CX3	CXA	65.00	124.1
NX2	CX3	NY2	90.00	120.1

CX2	CX3	NY2	65.00	115.8
CXA	CX3	NY2	65.00	115.8
CX1	CX2	CX3	65.00	116.8
CX1	CXA	CX3	65.00	111.0
CX1	CX2	NY1	65.00	119.1
CX1	CXA	NY1	65.00	108.0
CX3	CX2	NY1	65.00	124.1
CX3	CXA	NY1	65.00	109.0
CX2	CX1	OX1	80.00	124.0
CXA	CX1	OX1	80.00	121.0
CX2	CX1	NX1	65.00	112.9
CXA	CX1	NX1	65.00	112.9
NX1	CX1	OX1	98.00	123.2
CX1	NX1	HX1	18.00	117.0
CX4	NX1	CX1	60.00	127.4
CX4	NX1	HX1	18.00	117.0
CX3	NY2	CT2	44.00	119.5
CT2	NY2	CY2	80.00	119.6
CX3	NY2	CY2	60.00	120.9
NY2	CY2	CZ4	65.00	122.7
NY2	CY2	CY1	65.00	118.9
CZ4	CY2	CY1	70.00	118.4
CY2	CY1	NY1	65.00	121.2
CY2	CY1	CZ1	70.00	120.1
NY1	CY1	CZ1	65.00	118.7
CY1	NY1	CX2	60.00	119.2
CY1	NY1	CXA	60.00	119.2
CY2	CZ4	HZ4	31.00	120.2
CZ3	CZ4	HZ4	31.00	118.6
CY2	CZ4	CZ3	70.00	121.1
CZ4	CZ3	CZ2	70.00	120.5
CZ4	CZ3	CT3	70.00	119.3
CZ2	CZ3	CT3	70.00	120.2
CZ1	CZ2	CZ3	70.00	118.1
CZ3	CZ2	CT3	70.00	121.2
CZ1	CZ2	CT3	70.00	120.7
CZ2	CZ1	CY1	70.00	121.8
CZ2	CZ1	HZ1	31.00	121.2
CY1	CZ1	HZ1	31.00	117.1
CZ2	CT3	HA	35.00	115.0
CZ3	CT3	HA	35.00	115.0
NY2	CT2	HA	46.50	106.2
NY2	CT2	CT1	65.00	109.5
CN8	CN7	ON6B	110.00	109.0
ON6B	CN7B	CN7	110.00	105.0
NN2	CN7B	CN7	70.00	113.7

```
CN7  CN7  CN7     53.35    111.0  8.0   2.561
CN7  CN8  ON2     75.70    110.1
P    ON2  CT2     20.0     120.0  35.   2.33
CT2  CT1  OH1     75.700   110.10
ON2  CT2  CT1     75.700   110.10
ON2  CT2  HA      45.900   108.89
CX3  NX2  HX2     18.00    117.0
CX4  NX2  HX2     18.00    117.0
CZ3  CT3  S       35.00    115.0
CX1  CXA  S       35.00    103.0
CX3  CXA  S       35.00    111.0
NY1  CXA  S       35.00    115.0
HY1  NY1  CY1     35.00    116.0
HX1  NY1  CX2     35.00    116.0
HX1  NY1  CY1     35.00    116.0
HY1  NY1  CXA     35.00    113.0
HX1  NY1  CXA     35.00    113.0
CT2  S    CXA     35.00    107.0


ON3  P    ON2  CT2      0.10    3      0.0
X    CX4  NX2  X        2.05    2     180.0
X    NX2  CX3  X        2.05    2     180.0
X    CX2  CX3  X        0.50    2     180.0
X    CXA  CX3  X        0.50    2     180.0
X    CX1  CX2  X        0.50    2     180.0
X    CX1  CXA  X        0.50    2     180.0
X    CX1  NX1  X        2.05    2     180.0
X    CX4  NX1  X        2.05    2     180.0
X    CX3  NY2  X        2.05    2     180.0
X    CY2  NY2  X        2.05    2     180.0
X    CY1  CY2  X        3.10    2     180.0
X    NY1  CY1  X        2.05    2     180.0
X    NY1  CX2  X        2.05    2     180.0
X    NY1  CXA  X        2.05    2     180.0
X    CY2  CZ4  X        3.10    2     180.0
X    CZ4  CZ3  X        3.10    2     180.0
X    CZ2  CZ3  X        3.10    2     180.0
X    CZ1  CZ2  X        3.10    2     180.0
X    CY1  CZ1  X        3.10    2     180.0
X    CZ2  CT3  X        0.10    3      0.0
X    CZ3  CT3  X        0.10    3      0.0
X    CT2  NY2  X        0.01    3      0.0
X    CN7  CN7  X        0.15    3      0.0
X    CT2  ON2  X        0.25    3      0.0
X    ON6B CN7B X        0.10    3      0.0
```

X CN7 CN8 X 0.200 3 0.0
X CN7 CN7B X 0.15 3 0.0
X CN7 ON6B X 0.10 3 0.0
X CN8 ON2 X -0.10 3 0.0
ON2 P ON2 CT2 0.95 2 0.0
X CX3 NX2 X 2.05 2 180.0
X CX4 NX2 X 2.05 2 180.0
CT3 S CT2 CT1 0.2400 1 0.00
CT3 S CT2 CT1 0.1500 2 0.00
CT3 S CT2 CT1 0.2700 3 0.00
CZ3 CT3 S CT2 0.2800 3 0.00
CXA S CT2 CT1 0.1000 3 0.00
X S CXA X 0.1000 3 0.00
HA CT2 S CXA 0.1000 3 0.00

Non bonded parameters

CX1 0.000000 -0.141000 1.870000
CX2 0.000000 -0.141000 1.870000
CXA 0.000000 -0.141000 1.870000
CX3 0.000000 -0.141000 1.870000
CX4 0.000000 -0.141000 1.870000
CY1 0.000000 -0.141000 1.870000
CY2 0.000000 -0.141000 1.870000
CZ1 0.000000 -0.141000 1.870000
CZ2 0.000000 -0.141000 1.870000
CZ3 0.000000 -0.141000 1.870000
CZ4 0.000000 -0.141000 1.870000
HX1 0.000000 -0.049800 0.800000
HZ1 0.000000 -0.042000 1.330000
HZ4 0.000000 -0.042000 1.330000
NX1 0.000000 -0.090000 1.830000
NX2 0.000000 -0.090000 1.830000
NY1 0.000000 -0.090000 1.830000
NY2 0.000000 -0.090000 1.830000
OX1 0.000000 -0.120000 1.700000
OX2 0.000000 -0.120000 1.700000
HX2 0.000000 -0.049800 0.800000
HY1 0.000000 -0.049800 0.800000