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Supporting information for article:

A radical approach to radicals

Youjia Liu, Małgorzata Biczysko and Nigel W. Moriarty

Table S1 List of excluded proteins along with the criteria to discard.

| Criteria | PDB code |
|-------------------------------------|--|
| Model and Polder map correspondence | 1ZYT 2CUU 2OU8 2OU9 2Q9D 2W8H 3G3V 3G3W 3G3X 3M8B 3M8D 3RGM 3RGN 5BMG 5UUI |
| Incomplete MTN structure | 3IFX 3V3X |
| NMR experiment | 1RF8 2JXN 2K3M 2KSQ 2N2K 2VER |

Table S2 Model and model-to-data fit statistics for the original and refined structures.

| | | 2IGC | 2NTH | 2Q9E | 2XGA | 2XIU | 3MPN |
|---------------------------------------|---------|--------|--------|--------|--------|--------|--------|
| Z-score | initial | 0.65 | 0.19 | -0.38 | -0.28 | -0.21 | -1.93 |
| | refine | 0.83 | 0.01 | -0.83 | -0.54 | 0.11 | -1.68 |
| Ramanchandran plot(%) | | | | | | | |
| Outliers | initial | 0 | 0 | 0 | 0 | 0 | 0.2 |
| | refine | 0 | 0 | 0 | 0 | 0 | 0.2 |
| Favored | initial | 98.15 | 97.53 | 98.35 | 99.6 | 100 | 97.21 |
| | refine | 98.15 | 98.15 | 98.35 | 98.79 | 100 | 97.6 |
| Rotamer outliers (%) | initial | 0 | 2.19 | 1.47 | 0.84 | 2.36 | 4.39 |
| | refine | 0 | 1.46 | 0.25 | 1.69 | 1.57 | 2.2 |
| C ^β deviations | initial | 0 | 0 | 0 | 0 | 0 | 3 |
| | refine | 0 | 0 | 0 | 0 | 1 | 0 |
| Clashscore | initial | 6.75 | 9.02 | 10.55 | 13.25 | 6.14 | 6.40 |
| | refine | 2.25 | 4.51 | 6.46 | 10.36 | 5.32 | 6.76 |
| R.m.s.d. | | | | | | | |
| Bonds (Å) | initial | 0.1270 | 0.0111 | 0.0111 | 0.0088 | 0.0347 | 0.0229 |
| | refine | 0.0080 | 0.0091 | 0.0123 | 0.0134 | 0.0106 | 0.0131 |
| Angles (°) | initial | 2.19 | 1.39 | 1.41 | 1.20 | 2.40 | 1.79 |
| | refine | 0.94 | 0.98 | 1.21 | 1.28 | 1.29 | 1.30 |
| Molprobity score | initial | 1.37 | 1.84 | 1.67 | 1.63 | 1.62 | 1.99 |
| | refine | 1.00 | 1.35 | 1.36 | 1.71 | 1.44 | 1.72 |
| resolution | | 1.4 | 1.8 | 2.1 | 2.3 | 1.5 | 2.25 |
| | | | | | | | |
| R factors (%) | | | | | | | |
| R _{work} | initial | 0.1530 | 0.1830 | 0.2020 | 0.2237 | 0.1420 | 0.1730 |
| | refine | 0.1394 | 0.1726 | 0.1923 | 0.1864 | 0.1303 | 0.1635 |
| R _{free} | initial | 0.1980 | 0.2120 | 0.2500 | 0.2637 | 0.1970 | 0.2140 |
| | refine | 0.1725 | 0.2138 | 0.2457 | 0.2596 | 0.1652 | 0.2070 |
| R _{free} - R _{work} | initial | 0.045 | 0.029 | 0.048 | 0.040 | 0.055 | 0.041 |
| | refine | 0.033 | 0.041 | 0.053 | 0.073 | 0.035 | 0.044 |
| | | 3MPQ | 3STZ | 4EK1 | 4WWL | 5BMH | 5BMI |
| Z-score | initial | -1.7 | -2.32 | -0.97 | 0.16 | 0.23 | -2.1 |
| | refine | -1.75 | -2.24 | -0.92 | -0.14 | 0.19 | -2.96 |
| Ramanchandran plot(%) | | | | | | | |
| Outliers | initial | 0 | 0.95 | 0 | 0.19 | 0 | 0 |
| | refine | 0 | 0.57 | 0 | 0 | 0 | 0 |
| Favored | initial | 97.31 | 93.17 | 97.26 | 96.75 | 98.15 | 98.15 |
| | refine | 97.31 | 94.88 | 97.26 | 96.75 | 98.15 | 94.44 |
| Rotamer outliers (%) | initial | 3.54 | 2.46 | 0.71 | 0.46 | 2.08 | 0 |

| | | | | | | | |
|---------------------------------------|---------|--------|--------|--------|--------|--------|--------|
| | refine | 0.76 | 0.89 | 0.14 | 0.23 | 0 | 2.17 |
| C ^β deviations | initial | 2 | 0 | 2 | 8 | 0 | 0 |
| | refine | 0 | 0 | 0 | 0 | 0 | 0 |
| Clashscore | initial | 4.96 | 14.42 | 3.74 | 0.97 | 0 | 2.27 |
| | refine | 4.59 | 9.94 | 3.66 | 4.13 | 4.31 | 9.08 |
| R.m.s.d. | | | | | | | |
| Bonds (Å) | initial | 0.0228 | 0.0076 | 0.0130 | 0.0138 | 0.0149 | 0.0057 |
| | refine | 0.0124 | 0.0143 | 0.0118 | 0.0119 | 0.0124 | 0.0153 |
| Angles (°) | initial | 1.73 | 1.45 | 1.36 | 1.65 | 1.42 | 0.81 |
| | refine | 1.23 | 1.43 | 1.24 | 1.09 | 1.20 | 1.61 |
| Molprobity score | initial | 1.81 | 2.40 | 1.30 | 0.99 | 0.74 | 1.00 |
| | refine | 1.36 | 1.87 | 1.29 | 1.40 | 1.21 | 2.12 |
| resolution | | 2.25 | 2.5 | 1.97 | 2.23 | 1.6 | 2.5 |
| | | | | | | | |
| R factors (%) | | | | | | | |
| R _{work} | initial | 0.1850 | 0.2460 | 0.2040 | 0.1550 | 0.1550 | 0.2350 |
| | refine | 0.1742 | 0.2241 | 0.1631 | 0.1475 | 0.1592 | 0.1724 |
| R _{free} | initial | 0.2230 | 0.2850 | 0.2530 | 0.1870 | 0.1750 | 0.2510 |
| | refine | 0.2204 | 0.2671 | 0.2266 | 0.1895 | 0.1852 | 0.2935 |
| R _{free} - R _{work} | initial | 0.038 | 0.039 | 0.049 | 0.032 | 0.020 | 0.016 |
| | refine | 0.046 | 0.043 | 0.064 | 0.042 | 0.026 | 0.121 |
| | | 5G27 | 5JDT | 6N87 | 6PGY | 6PGZ | |
| Z-score | initial | -0.12 | 0 | 0.06 | 0.02 | -0.68 | |
| | refine | 0.02 | 0.10 | 0.12 | -0.19 | -2.03 | |
| Ramanchandran plot(%) | | | | | | | |
| Outliers | initial | 0.62 | 0 | 0 | 0 | 0 | |
| | refine | 0.62 | 0 | 0 | 0 | 0 | |
| Favored | initial | 97.53 | 98.77 | 97.46 | 99.38 | 98.76 | |
| | refine | 98.77 | 98.15 | 97.46 | 99.38 | 97.2 | |
| Rotamer outliers (%) | initial | 0 | 0.57 | 0 | 0 | 0 | |
| | refine | 0 | 0.57 | 0.73 | 0 | 0.37 | |
| C ^β deviations | initial | 0 | 0 | 0 | 0 | 0 | |
| | refine | 0 | 0 | 0 | 0 | 0 | |
| Clashscore | initial | 1.37 | 2.61 | 3.40 | 0 | 5.66 | |
| | refine | 2.24 | 1.16 | 3.00 | 0.37 | 12.65 | |
| R.m.s.d. | | | | | | | |
| Bonds (Å) | initial | 0.0158 | 0.0174 | 0.0165 | 0.0074 | 0.0070 | |
| | refine | 0.0099 | 0.0075 | 0.0086 | 0.0108 | 0.0131 | |
| Angles (°) | initial | 1.59 | 1.68 | 1.66 | 0.98 | 0.94 | |
| | refine | 1.06 | 1.06 | 1.00 | 1.04 | 1.26 | |
| Molprobity score | initial | 0.96 | 1.05 | 1.24 | 0.50 | 1.31 | |

| | refine | 1.00 | 0.83 | 1.20 | 0.63 | 1.76 |
|---------------------------------------|---------|--------|--------|--------|--------|--------|
| resolution | | 1.61 | 1 | 1.59 | 2 | 2 |
| R factors (%) | | | | | | |
| R _{work} | initial | 0.1505 | 0.1150 | 0.1600 | 0.1580 | 0.2530 |
| | refine | 0.1657 | 0.1177 | 0.1610 | 0.1523 | 0.2298 |
| R _{free} | initial | 0.1691 | 0.1300 | 0.1880 | 0.1820 | 0.2910 |
| | refine | 0.1839 | 0.1310 | 0.1892 | 0.1876 | 0.2961 |
| R _{free} - R _{work} | initial | 0.019 | 0.015 | 0.028 | 0.024 | 0.038 |
| | refine | 0.018 | 0.013 | 0.028 | 0.035 | 0.066 |

Table S3 Deviations of bond length, bond angle and dihedral angle: Δ_{initial} (initial value – ideal value) & Δ_{refine} (refined value – ideal value) .

Bond lengths are in ångströms, angles and dihedrals are in degrees.

| | Resolu- | N–O | | N–C | | C–N–C | | O–N–C | | O–N–C–C | |
|---|---------|--------|---------------------------|--------------------------|---------------------------|--------------------------|---------------------------|--------------------------|---------------------------|--------------------------|--------|
| | | tion | Δ_{initial} | Δ_{refine} | Δ_{initial} | Δ_{refine} | Δ_{initial} | Δ_{refine} | Δ_{initial} | Δ_{refine} | |
| 2IGC - chain A and resseq 200 | 1.4 | -0.054 | -0.001 | 0.014 | -0.001 | 0.93 | -0.07 | -0.66 | 0.33 | -0.82 | -0.53 |
| 5JDI - chain A and resseq 201 and altloc B | 1 | 0.053 | 0.005 | -0.018 | 0.005 | -4.90 | -0.36 | -2.54 | -0.17 | -28.05 | -10.37 |
| 5JDI - chain A and resseq 201 and altloc A | 1 | 0.078 | 0.008 | -0.008 | 0.000 | -1.35 | -0.98 | -4.30 | -0.23 | -18.91 | -11.09 |
| 2XIU - chain A and resseq 1055 | 1.5 | -0.038 | -0.004 | -0.024 | 0.000 | -1.44 | -0.01 | 1.02 | 0.28 | -6.13 | -0.11 |
| 2XIU - chain B and resseq 1055 | 1.5 | -0.033 | 0.003 | -0.029 | -0.005 | -2.57 | -0.43 | 1.58 | 0.42 | -2.36 | -3.23 |
| 6N87 - chain C and resseq 101 | 1.59 | -0.170 | 0.003 | -0.011 | -0.001 | -8.63 | 0.19 | -7.22 | 0.16 | -30.10 | -0.09 |
| 5BMH - chain A and resseq 101 and altloc A | 1.6 | -0.030 | 0.000 | -0.019 | 0.002 | -0.16 | -0.19 | 0.26 | 0.39 | -1.05 | -3.69 |
| 5BMH - chain A and resseq 101 and altloc B | 1.6 | -0.024 | 0.004 | -0.019 | 0.003 | 0.00 | -0.29 | 0.23 | 0.45 | -0.92 | -1.69 |
| 5G27 - chain A and resseq 501 | 1.61 | 0.190 | 0.005 | 0.046 | 0.002 | -2.96 | -1.37 | -7.80 | 0.39 | -28.33 | -9.24 |
| 2NTH - chain A and resseq 200 | 1.8 | -0.046 | 0.006 | 0.036 | 0.010 | -0.27 | -0.20 | -0.10 | 0.17 | -2.26 | -5.65 |
| 4EK1 - chain A and resseq 504 | 1.97 | 0.123 | -0.026 | -0.029 | -0.006 | -0.95 | -0.29 | 0.78 | 0.45 | -3.63 | -0.47 |
| 4EK1 - chain A and resseq 505 | 1.97 | 0.134 | 0.001 | -0.019 | 0.014 | -0.97 | 0.03 | 0.79 | 0.20 | -7.50 | -7.02 |
| 4EK1 - chain B and resseq 504 | 1.97 | 0.123 | -0.020 | -0.023 | 0.000 | -0.46 | 0.57 | 0.53 | -0.61 | -7.10 | -14.70 |
| 6PGY - chain A and resseq 203 | 2 | 0.205 | -0.002 | -0.006 | 0.002 | -4.32 | 0.04 | 2.46 | -0.23 | -14.69 | -14.14 |
| 6PGZ - chain A and resseq 201 | 2 | 0.205 | 0.003 | -0.006 | -0.006 | -4.17 | -1.99 | 2.39 | 1.27 | -8.87 | -1.30 |
| 6PGZ - chain B and resseq 300 | 2 | 0.205 | 0.000 | -0.005 | -0.002 | -3.93 | 0.03 | 2.27 | -0.64 | -1.66 | -15.17 |
| 2Q9E - chain A and resseq 844 | 2.1 | -0.052 | 0.018 | 0.033 | 0.001 | 0.01 | -0.92 | -1.21 | -0.52 | -16.82 | -15.05 |
| 2Q9E - chain B and resseq 844 | 2.1 | -0.067 | -0.003 | 0.040 | -0.005 | 0.49 | 0.44 | -0.26 | -0.30 | -6.97 | -8.32 |
| 2Q9E - chain C and resseq 844 | 2.1 | -0.078 | 0.003 | 0.039 | 0.006 | 0.17 | 0.30 | 0.21 | 0.03 | -0.82 | -6.39 |
| 4WWL - chain A and resseq 601 | 2.23 | 0.135 | 0.002 | -0.016 | 0.004 | -0.80 | -0.50 | 0.70 | 0.55 | -7.07 | -3.39 |
| 3MPN - chain A and resseq 801 | 2.25 | 0.142 | 0.000 | -0.006 | 0.001 | -3.14 | 0.51 | 1.71 | 0.02 | -3.34 | -0.70 |
| 3MPQ - chain A and resseq 801 | 2.25 | 0.131 | -0.002 | 0.020 | 0.009 | -1.70 | 0.29 | 1.12 | 0.14 | -0.72 | -2.01 |
| 2XGA - chain A and resseq 1019 | 2.3 | -0.013 | -0.002 | -0.007 | -0.005 | -0.11 | -0.15 | 0.36 | 0.21 | -4.74 | -8.17 |
| 2XGA - chain B and resseq 1019 | 2.3 | -0.008 | 0.020 | -0.003 | -0.004 | -0.53 | -1.06 | 0.57 | 0.81 | -9.76 | -4.47 |
| 3STZ - chain C and resseq 201 | 2.5 | -0.032 | -0.014 | 0.025 | -0.001 | -3.09 | 1.33 | 1.86 | -0.80 | -0.11 | -10.86 |
| 5BM - chain A and resseq 101 | 2.5 | -0.037 | -0.015 | -0.025 | -0.004 | -1.50 | -0.09 | 1.05 | -0.16 | -0.19 | -7.54 |

Table S4 Electron populations of some relevant ELF basins for MTN from 6N87 and 6PGZ proteins.

| Basin | 6N87 (Initial/Refine) El. Pop | 6PGZ (Initial/Refine) El. Pop |
|------------------------|----------------------------------|----------------------------------|
| V ₁ (O) | 2.69/2.91 | 3.03/2.87 |
| V ₂ (O) | 2.69/2.90 | 3.04/2.91 |
| V ₁ (N) | 1.65/1.31 | 1.12/1.27 |
| V ₂ (N) | -/0.60 | 1.08/0.67 |
| V(N,O) | 1.87/1.23 | 0.78/1.25 |
| V(N,C1) | 1.80/1.76 | 1.77/1.78 |
| V(N,C5) | 1.80/1.74 | 1.76/1.77 |
| V ₁ (C2,C3) | 1.70/1.75 | 1.78/1.73 |
| V ₂ (C2,C3) | 1.70/1.75 | 1.74/1.76 |
| V ₁ (S1) | 2.19/2.21 | 2.19/2.21 |
| V ₂ (S1) | 2.21/2.24 | 2.42/2.35 |
| V(S1,C4) | 1.52/1.43 | 1.47/1.45 |

| | |
|--|--|
| T1 *CONN NFRAG -99 AT1 N 3 T3 :XY 251 206 AT2 C 4 T4 :XY 202 242 AT3 C 2 T3 :XY 221 299 AT4 C 2 T3 :XY 281 299 AT5 C 4 T4 :XY 299 242 AT6 O 1 T1 :XY 251 147 AT7 C 1 :XY 357 258 AT8 C 1 :XY 342 200 AT9 C 1 :XY 160 200 AT10 C 1 :XY 150 272 BO 1 6 1 BO 2 10 1 BO 5 1 1 BO 5 8 1 BO 3 4 2 BO 2 3 1 BO 5 7 1 BO 2 9 1 BO 4 5 1 BO 1 2 1 GEOM DEFINE DIST1 6 1 DEFINE DIST2 1 2 DEFINE DIST3 1 5 DEFINE DIST4 2 3 DEFINE DIST5 5 4 DEFINE DIST6 3 4 DEFINE ANG1 6 1 2 DEFINE ANG2 6 1 5 DEFINE ANG3 2 1 5 DEFINE ANG4 1 2 3 DEFINE ANG5 1 5 4 DEFINE ANG6 2 3 4 DEFINE ANG7 5 4 3 DEFINE TOR1 6 1 2 3 DEFINE TOR2 6 1 5 4 SYMCHK ON ENANT NORMAL END | <p>Filters Advanced Options</p> <p><input checked="" type="checkbox"/> 3D coordinates determined</p> <p><input checked="" type="checkbox"/> R factor <input type="radio"/> <= 0.05 <input type="radio"/> <= 0.075 <input checked="" type="radio"/> <= 0.1</p> <p><input type="checkbox"/> Only <input checked="" type="radio"/> Non-disordered <input type="radio"/> Disordered</p> <p><input type="checkbox"/> No errors</p> <p><input type="checkbox"/> Not polymeric</p> <p><input type="checkbox"/> No ions</p> <p><input type="checkbox"/> Only <input checked="" type="radio"/> Single crystal structures <input type="radio"/> Powder structures</p> <p><input type="checkbox"/> Only <input checked="" type="radio"/> Organics <input type="radio"/> Organometallic</p> |
|--|--|

Figure S1 CSD query

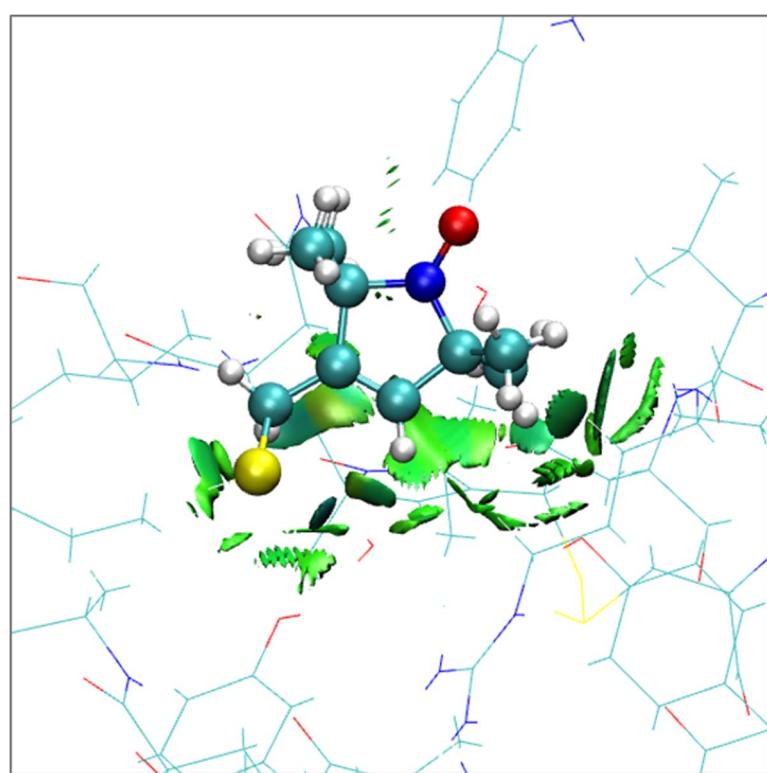


Figure S2 Non-covalent interactions of 6PGZ MTN ligand with its surroundings, RDG isosurface at 0.300 a.u.