

Dataset S2. Amino acids close to the PCB chromophore (within the region of ~ 3.5 Å). The signals labeled with the Latin capitals A to O in Fig. 2 correspond to intermolecular ^1H correlations of the uniformly ^{13}C -labeled chromophore (acquired with a relatively short LG-CP contact time of 900 μs).

Labels	Proton contact	Pr				Pfr			
		σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [6]	σ^{proton} (ppm)	Cofactor carbon	σ^{carbon} (ppm) [3, 4]	XRD distance (Å) [14]
A	Tyr-257 N	9.8	8 ³	180.1	3.69	-	-	-	-
B	Thr-274 OG1	10.7	12 ³	179.0	3.14	-	-	-	-
C	Arg-222 NH1	-	-	-	-	11.5	8 ³	180.5	3.16
D	Thr-274 OG1	-	-	-	-	10.6	12 ³	175.3	-
E	His-290 NE2 (Pr-II)	12.7	19	172.7	3.87	-	-	-	-
F	Tyr-263 CE1	-	-	-	-	9.2	19	169.0	4.30
G	His-260 CE1	-	-	-	-	10.1	9/11	131.0	3.52/3.26
H	His-260 CE1	10.0	11	127.9	3.25	-	-	-	-
I	His-260 CE1	10.0	10	112.8	3.54	-	-	-	-
J	His-260 ND1-I	12.3	10	112.8	3.39	-	-	-	-
K	His-260 NE2	-	-	-	-	13.1	10	112.4	3.94
L	Thr-274 OG1	10.7	12 ²	38.1	3.14	-	-	-	-
M	Tyr-198 CD2	9.7	18 ²	13.2	3.46	-	-	-	-
N	Tyr-257 CD2	9.6	7 ¹	9.3	3.34	-	-	-	-
O	Tyr-203 CD1	-	-	-	-	10.1	17 ¹	9.2	5.98