

Supplementary Information for :

Duplication of a single strand in a beta sheet can produce new switching function in a photosensory protein

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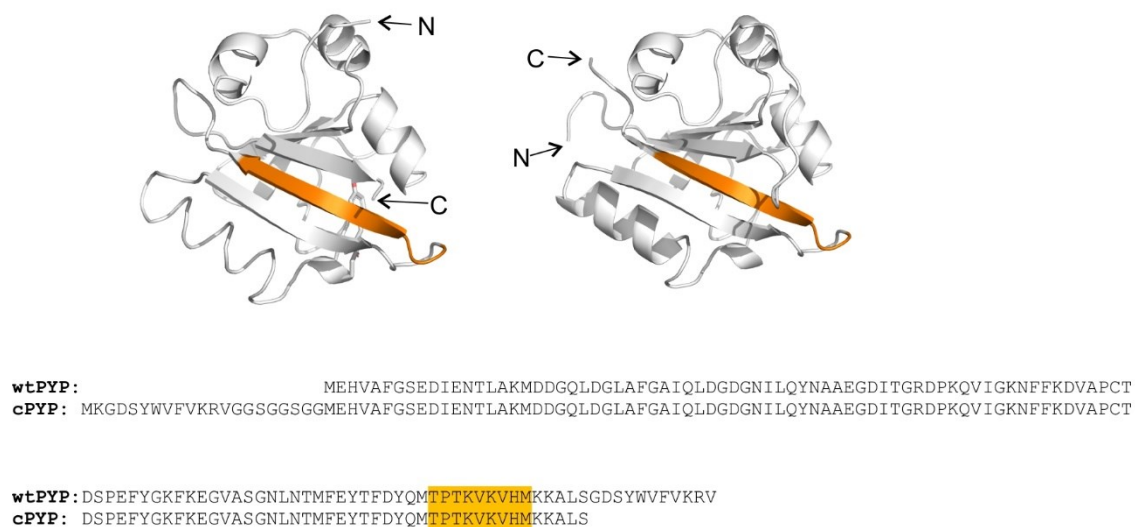


Figure S1. Models of wild-type PYP and the circular permutant (cPYP).¹ The strand that is duplicated in cPYP-dup is highlighted in orange. In wtPYP this is an internal strand; in cPYP it is the C-terminal strand.

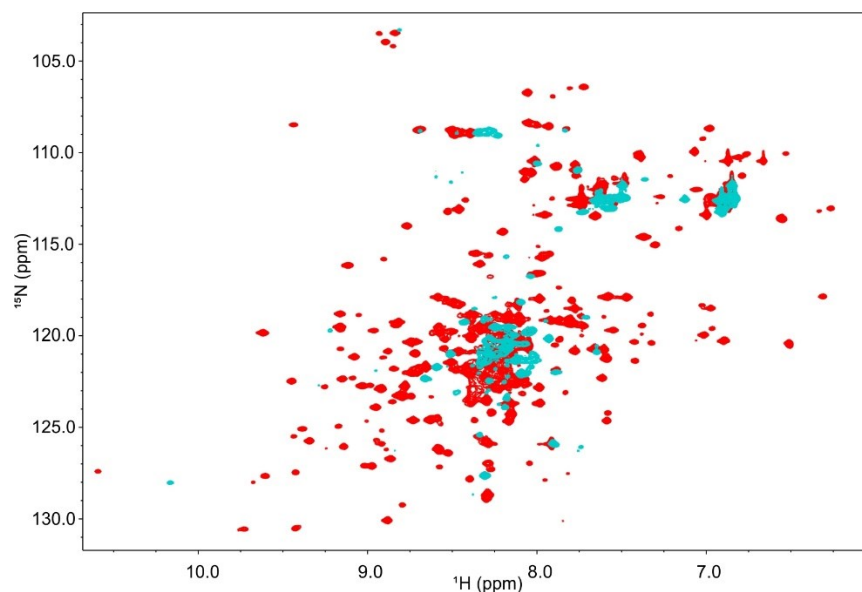


Figure S2. NH-HSQC spectra of cPYP-dup under continuous low intensity blue irradiation (red peaks) and under high intensity blue-light irradiation (blue peaks).

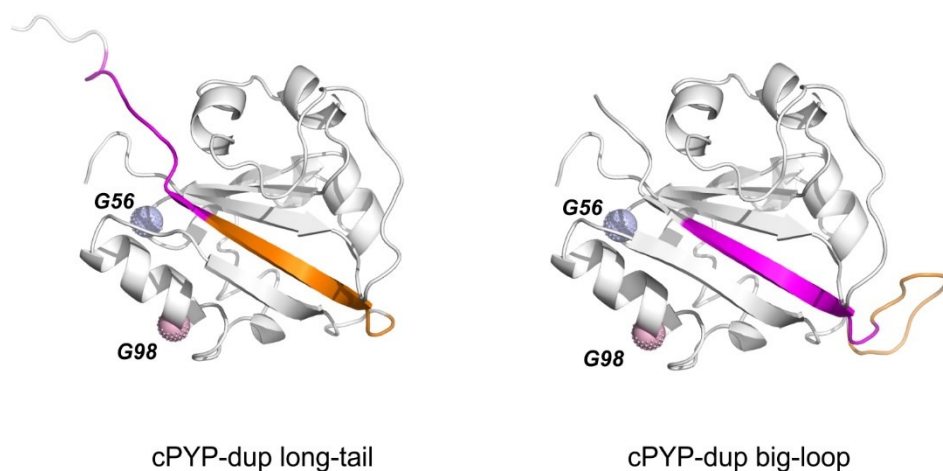


Figure S3. Locations of G56 and G98 in models of cPYP-dup in long-tail and big-loop conformations.

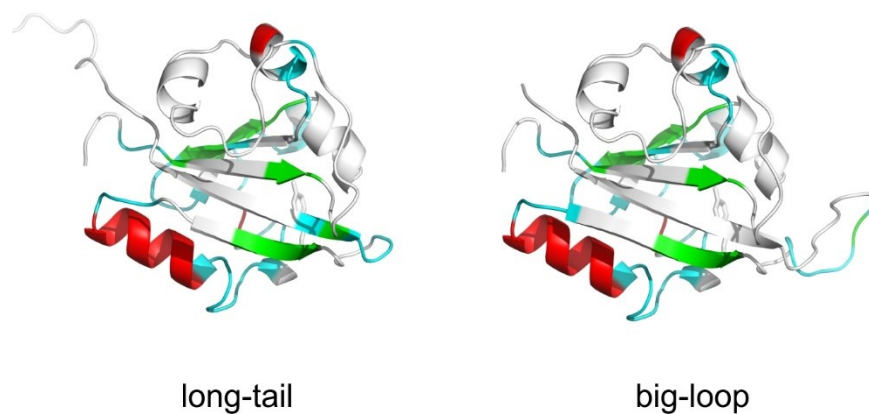


Figure S4. TALOS predictions for transient-state secondary structure mapped onto the models for long-tail (left), and big-loop (right) cPYP-dup (helix-red, sheet-green, loop-cyan). Approximately 66 of 150 residues are assigned, unassigned regions are colored white. This analysis did not permit a clear distinction to be made between the long-tail and big-loop structures.

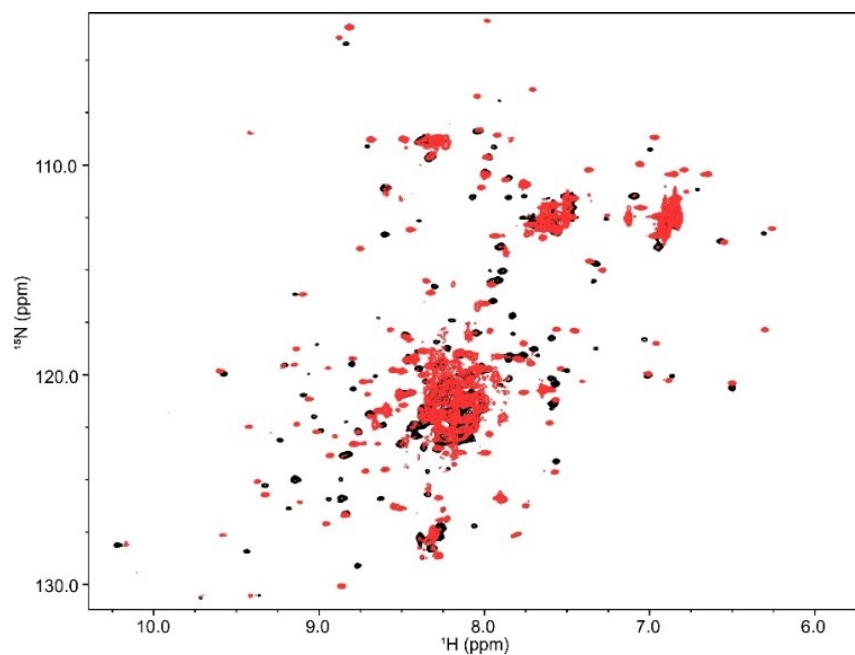


Figure S5. NH-HSQC spectra of dark-adapted cPYP-dup-E-helix (black peaks) and cPYP-dup-E-helix after blue-light irradiation (red peaks).

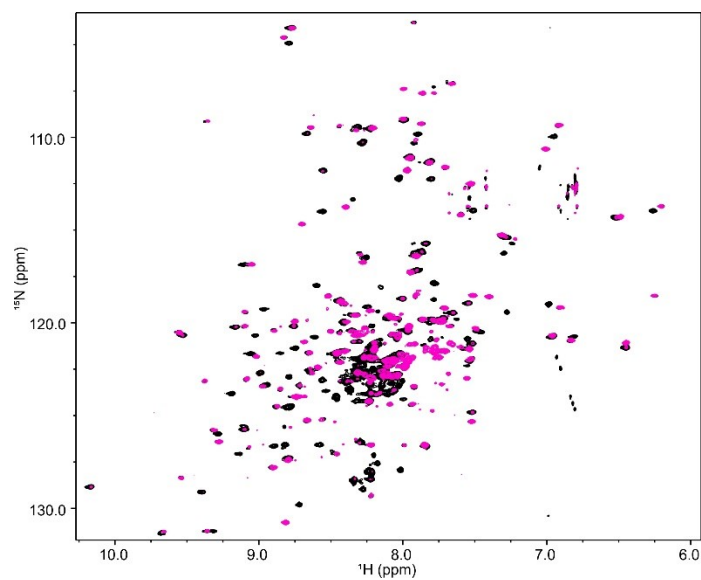


Figure S6. NH-HSQC spectra of dark-adapted cPYP-dup-E-helix (black peaks) and cPYP-dup-E-helix after addition of K-peptide (pink peaks).

TALOS files (chemical shifts) for the cPYP-dup – dark state (big loop):

153	8.120	0.000	H	4
154	120.833	0.000	N	4
605	54.549	0.000	CA	4
655	41.657	0.000	CB	4
921	175.172	0.000	C	4
57	8.198	0.000	H	5
58	114.278	0.000	N	5
516	57.425	0.000	CA	5
662	65.405	0.000	CB	5
851	171.983	0.000	C	5
69	8.889	0.000	H	6
70	115.727	0.000	N	6
524	57.978	0.000	CA	6
692	42.678	0.000	CB	6
855	172.987	0.000	C	6
187	9.241	0.000	H	7
188	122.710	0.000	N	7
561	55.796	0.000	CA	7
652	33.230	0.000	CB	7
875	175.673	0.000	C	7
147	9.147	0.000	H	8
148	120.609	0.000	N	8
562	62.147	0.000	CA	8
892	173.634	0.000	C	8
956	33.588	0.000	CB	8
237	9.417	0.000	H	9
238	125.377	0.000	N	9
544	54.884	0.000	CA	9
642	41.231	0.000	CB	9
867	175.981	0.000	C	9
185	8.972	0.000	H	10
186	122.607	0.000	N	10
587	61.348	0.000	CA	10
650	35.784	0.000	CB	10
877	174.087	0.000	C	10
235	8.877	0.000	H	11
236	126.034	0.000	N	11
547	53.907	0.000	CA	11
864	175.479	0.000	C	11
227	8.898	0.000	H	12
228	125.069	0.000	N	12
866	176.693	0.000	C	12
33	8.588	0.000	H	20
34	110.683	0.000	N	20
507	45.407	0.000	CA	20
945	174.516	0.000	C	20
21	8.431	0.000	H	21
22	108.838	0.000	N	21
610	45.296	0.000	CA	21
841	174.314	0.000	C	21
113	8.275	0.000	H	22
114	119.384	0.000	N	22
617	55.033	0.000	CA	22
696	32.038	0.000	CB	22
914	176.741	0.000	C	22
169	8.716	0.000	H	23
170	121.901	0.000	N	23
565	57.226	0.000	CA	23

683	29.485	0.000	CB	23
912	176.110	0.000	C	23
159	7.412	0.000	H	25
160	121.229	0.000	N	25
590	61.806	0.000	CA	25
653	31.783	0.000	CB	25
903	173.925	0.000	C	25
255	8.288	0.000	H	26
256	128.774	0.000	N	26
540	51.009	0.000	CA	26
633	19.696	0.000	CB	26
805	177.162	0.000	C	26
221	8.558	0.000	H	27
222	124.528	0.000	N	27
572	59.234	0.000	CA	27
870	176.822	0.000	C	27
137	7.310	0.000	H	37
138	120.299	0.000	N	37
591	54.443	0.000	CA	37
675	19.271	0.000	CB	37
901	178.360	0.000	C	37
55	7.146	0.000	H	38
56	114.052	0.000	N	38
515	55.698	0.000	CA	38
666	32.805	0.000	CB	38
846	176.337	0.000	C	38
105	7.361	0.000	H	39
106	119.348	0.000	N	39
592	56.416	0.000	CA	39
674	33.911	0.000	CB	39
902	175.867	0.000	C	39
171	8.397	0.000	H	40
172	121.677	0.000	N	40
584	52.788	0.000	CA	40
703	41.742	0.000	CB	40
927	176.402	0.000	C	40
111	8.568	0.000	H	41
112	119.420	0.000	N	41
534	56.903	0.000	CA	41
698	40.040	0.000	CB	41
918	177.923	0.000	C	41
19	8.467	0.000	H	42
20	108.932	0.000	N	42
505	46.150	0.000	CA	42
837	176.822	0.000	C	42
1005	8.136	0.000	H	43
1006	120.903	0.000	N	43
1007	58.276	0.000	CA	43
1009	28.938	0.000	CB	43
1010	179.032	0.000	C	43
173	8.358	0.000	H	44
174	121.763	0.000	N	44
585	57.473	0.000	CA	44
704	41.742	0.000	CB	44
911	179.833	0.000	C	44
75	7.853	0.000	H	45
76	117.252	0.000	N	45
526	56.578	0.000	CA	45
693	40.040	0.000	CB	45
859	177.033	0.000	C	45
11	7.985	0.000	H	46
12	108.368	0.000	N	46
502	44.821	0.000	CA	46

839	174.217	0.000	C	46
107	6.946	0.000	H	47
108	119.492	0.000	N	47
595	54.655	0.000	CA	47
676	42.934	0.000	CB	47
861	176.887	0.000	C	47
165	8.677	0.000	H	48
166	121.694	0.000	N	48
582	52.189	0.000	CA	48
985	19.112	0.000	CB	48
987	175.944	0.000	C	48
45	6.547	0.000	H	49
46	113.431	0.000	N	49
513	53.484	0.000	CA	49
667	39.614	0.000	CB	49
843	173.488	0.000	C	49
9	9.327	0.000	H	50
10	108.161	0.000	N	50
501	45.570	0.000	CA	50
835	173.278	0.000	C	50
199	8.153	0.000	H	51
200	123.602	0.000	N	51
626	51.743	0.000	CA	51
946	174.079	0.000	C	51
189	8.906	0.000	H	52
190	122.796	0.000	N	52
588	59.164	0.000	CA	52
649	42.338	0.000	CB	52
878	174.346	0.000	C	52
243	8.558	0.000	H	53
244	127.076	0.000	N	53
567	53.351	0.000	CA	53
639	31.443	0.000	CB	53
810	174.184	0.000	C	53
253	9.663	0.000	H	54
254	127.925	0.000	N	54
542	52.898	0.000	CA	54
634	46.424	0.000	CB	54
806	177.664	0.000	C	54
89	8.370	0.000	H	55
90	118.735	0.000	N	55
578	52.435	0.000	CA	55
694	41.146	0.000	CB	55
1	8.913	0.000	H	56
2	103.361	0.000	N	56
495	47.394	0.000	CA	56
833	173.763	0.000	C	56
73	7.957	0.000	H	57
74	116.461	0.000	N	57
519	53.972	0.000	CA	57
691	42.338	0.000	CB	57
857	177.243	0.000	C	57
13	8.660	0.000	H	58
14	108.575	0.000	N	58
503	45.668	0.000	CA	58
836	172.987	0.000	C	58
183	9.070	0.000	H	59
184	122.193	0.000	N	59
876	175.673	0.000	C	59
936	38.252	0.000	CB	59
937	53.310	0.000	CA	59
133	8.714	0.000	H	60
134	120.212	0.000	N	60

577	63.109	0.000	CA	60
896	176.321	0.000	C	60
934	38.142	0.000	CB	60
261	9.745	0.000	H	61
262	130.511	0.000	N	61
536	55.503	0.000	CA	61
632	42.934	0.000	CB	61
802	177.292	0.000	C	61
61	7.636	0.000	H	62
62	113.318	0.000	N	62
523	55.015	0.000	CA	62
664	34.166	0.000	CB	62
847	173.618	0.000	C	62
245	9.000	0.000	H	63
246	126.999	0.000	N	63
546	58.792	0.000	CA	63
637	41.316	0.000	CB	63
948	173.741	0.000	C	63
231	8.288	0.000	H	64
232	125.609	0.000	N	64
569	52.435	0.000	CA	64
710	40.380	0.000	CB	64
886	174.395	0.000	C	64
145	8.537	0.000	H	65
146	120.557	0.000	N	65
579	54.725	0.000	CA	65
688	18.079	0.000	CB	65
920	180.286	0.000	C	65
93	7.925	0.000	H	66
94	118.555	0.000	N	66
614	54.882	0.000	CA	66
905	179.865	0.000	C	66
103	7.588	0.000	H	67
104	118.843	0.000	N	67
602	58.142	0.000	CA	67
904	179.234	0.000	C	67
5	7.788	0.000	H	68
6	106.391	0.000	N	68
499	47.915	0.000	CA	68
51	8.411	0.000	H	72
52	112.490	0.000	N	72
522	45.830	0.000	CA	72
848	174.330	0.000	C	72
141	7.875	0.000	H	73
142	120.367	0.000	N	73
968	54.485	0.000	CA	73
969	30.317	0.000	CB	73
973	174.624	0.000	C	73
975	8.399	0.000	H	74
976	121.558	0.000	N	74
979	50.234	0.000	CA	74
981	41.600	0.000	CB	74
37	8.057	0.000	H	76
38	111.304	0.000	N	76
511	57.946	0.000	CA	76
929	31.666	0.000	CB	76
932	179.072	0.000	C	76
65	7.913	0.000	H	77
66	115.426	0.000	N	77
518	56.317	0.000	CA	77
689	29.400	0.000	CB	77
853	177.033	0.000	C	77
25	7.005	0.000	H	78

26	109.139	0.000	N	78
506	61.463	0.000	CA	78
668	31.953	0.000	CB	78
842	175.172	0.000	C	78
131	6.886	0.000	H	79
132	120.195	0.000	N	79
596	62.827	0.000	CA	79
679	36.294	0.000	CB	79
862	177.389	0.000	C	79
71	9.102	0.000	H	80
72	115.990	0.000	N	80
525	44.756	0.000	CA	80
856	174.379	0.000	C	80
99	7.794	0.000	H	81
100	119.023	0.000	N	81
616	54.542	0.000	CA	81
707	33.315	0.000	CB	81
908	174.832	0.000	C	81
117	9.593	0.000	H	82
118	119.744	0.000	N	82
531	54.787	0.000	CA	82
658	41.316	0.000	CB	82
887	176.661	0.000	C	82
259	9.385	0.000	H	83
260	130.318	0.000	N	83
537	62.342	0.000	CA	83
803	173.165	0.000	C	83
47	6.322	0.000	H	84
48	113.111	0.000	N	84
514	59.346	0.000	CA	84
844	175.172	0.000	C	84
31	7.861	0.000	H	85
32	110.683	0.000	N	85
508	55.373	0.000	CA	85
996	33.342	0.000	CB	85
59	7.346	0.000	H	86
60	114.504	0.000	N	86
665	43.104	0.000	CB	86
850	175.803	0.000	C	86
83	7.007	0.000	H	87
84	118.194	0.000	N	87
594	64.941	0.000	CA	87
677	33.230	0.000	CB	87
860	174.087	0.000	C	87
119	8.012	0.000	H	88
120	119.672	0.000	N	88
619	48.301	0.000	CA	88
700	18.760	0.000	CB	88
917	174.087	0.000	C	88
67	8.266	0.000	H	91
68	115.482	0.000	N	91
520	63.189	0.000	CA	91
631	68.044	0.000	CB	91
854	173.764	0.000	C	91
207	7.568	0.000	H	92
208	124.181	0.000	N	92
555	53.451	0.000	CA	92
670	37.997	0.000	CB	92
874	173.505	0.000	C	92
125	8.371	0.000	H	93
126	120.057	0.000	N	93
535	55.308	0.000	CA	93
686	64.894	0.000	CB	93

913	174.168	0.000	C	93
49	8.511	0.000	H	95
50	113.130	0.000	N	95
521	58.206	0.000	CA	95
663	29.825	0.000	CB	95
849	173.974	0.000	C	95
77	7.571	0.000	H	96
78	117.798	0.000	N	96
528	56.936	0.000	CA	96
681	39.359	0.000	CB	96
858	175.495	0.000	C	96
195	8.611	0.000	H	97
196	123.177	0.000	N	97
575	59.305	0.000	CA	97
648	38.167	0.000	CB	97
880	176.790	0.000	C	97
3	8.833	0.000	H	98
4	104.076	0.000	N	98
496	47.882	0.000	CA	98
834	176.369	0.000	C	98
211	6.491	0.000	H	99
212	120.359	0.000	N	99
629	58.286	0.000	CA	99
678	32.294	0.000	CB	99
863	179.234	0.000	C	99
81	8.523	0.000	H	101
82	117.906	0.000	N	101
529	59.216	0.000	CA	101
661	31.613	0.000	CB	101
899	179.752	0.000	C	101
101	7.720	0.000	H	102
102	118.843	0.000	N	102
708	29.570	0.000	CB	102
907	178.926	0.000	C	102
933	58.486	0.000	CA	102
15	7.812	0.000	H	103
16	108.575	0.000	N	103
504	46.808	0.000	CA	103
840	175.803	0.000	C	103
209	8.247	0.000	H	104
210	124.026	0.000	N	104
628	65.775	0.000	CA	104
646	31.443	0.000	CB	104
873	179.266	0.000	C	104
155	7.642	0.000	H	105
156	120.626	0.000	N	105
600	54.655	0.000	CA	105
654	17.994	0.000	CB	105
915	179.622	0.000	C	105
35	8.057	0.000	H	106
36	110.946	0.000	N	106
510	59.151	0.000	CA	106
930	63.785	0.000	CB	106
931	175.631	0.000	C	106
29	7.760	0.000	H	107
30	110.532	0.000	N	107
509	45.765	0.000	CA	107
982	173.324	0.000	C	107
85	8.098	0.000	H	108
86	118.158	0.000	N	108
612	51.951	0.000	CA	108
669	39.614	0.000	CB	108
949	173.192	0.000	C	108

161	7.867	0.000	H	109
162	121.763	0.000	N	109
560	55.145	0.000	CA	109
701	43.359	0.000	CB	109
884	174.994	0.000	C	109
229	8.926	0.000	H	110
230	125.648	0.000	N	110
865	173.764	0.000	C	110
938	53.228	0.000	CA	110
940	36.030	0.000	CB	110
115	9.140	0.000	H	111
116	119.528	0.000	N	111
532	60.746	0.000	CA	111
659	69.235	0.000	CB	111
893	170.834	0.000	C	111
251	8.378	0.000	H	112
252	127.732	0.000	N	112
541	54.298	0.000	CA	112
635	36.550	0.000	CB	112
807	175.091	0.000	C	112
149	8.865	0.000	H	113
150	120.746	0.000	N	113
580	56.310	0.000	CA	113
657	39.188	0.000	CB	113
898	172.631	0.000	C	113
109	8.815	0.000	H	114
110	119.312	0.000	N	114
533	55.308	0.000	CA	114
660	31.868	0.000	CB	114
895	175.350	0.000	C	114
225	9.160	0.000	H	115
226	124.837	0.000	N	115
549	58.369	0.000	CA	115
643	45.062	0.000	CB	115
868	172.614	0.000	C	115
95	7.312	0.000	H	116
96	118.699	0.000	N	116
593	61.242	0.000	CA	116
673	69.661	0.000	CB	116
900	173.650	0.000	C	116
97	7.847	0.000	H	126
98	119.023	0.000	N	126
615	61.766	0.000	CA	126
697	32.890	0.000	CB	126
906	175.657	0.000	C	126
217	8.349	0.000	H	127
218	124.490	0.000	N	127
553	56.773	0.000	CA	127
871	176.110	0.000	C	127
1004	32.554	0.000	CB	127
129	7.849	0.000	H	128
130	120.109	0.000	N	128
622	61.463	0.000	CA	128
923	175.026	0.000	C	128
967	33.469	0.000	CB	128
197	8.386	0.000	H	129
198	123.332	0.000	N	129
589	56.381	0.000	CA	129
647	30.847	0.000	CB	129
947	174.918	0.000	C	129
193	8.074	0.000	H	130
194	123.055	0.000	N	130
625	54.655	0.000	CA	130

711	33.741	0.000	CB	130
928	175.414	0.000	C	130
91	8.230	0.000	H	131
92	118.699	0.000	N	131
613	60.253	0.000	CA	131
695	69.065	0.000	CB	131
916	172.161	0.000	C	131
257	8.779	0.000	H	134
258	129.122	0.000	N	134
539	56.610	0.000	CA	134
709	32.209	0.000	CB	134
804	175.851	0.000	C	134
87	9.037	0.000	H	135
88	118.735	0.000	N	135
530	59.053	0.000	CA	135
685	35.273	0.000	CB	135
894	174.443	0.000	C	135
157	8.891	0.000	H	136
158	121.074	0.000	N	136
563	55.148	0.000	CA	136
897	173.666	0.000	C	136
970	34.480	0.000	CB	136
205	8.836	0.000	H	137
206	123.486	0.000	N	137
552	59.802	0.000	CA	137
671	33.571	0.000	CB	137
879	174.330	0.000	C	137
213	9.213	0.000	H	139
214	124.142	0.000	N	139
573	53.739	0.000	CA	139
983	36.741	0.000	CB	139
167	8.830	0.000	H	140
168	121.711	0.000	N	140
564	54.443	0.000	CA	140
684	37.827	0.000	CB	140
950	174.854	0.000	C	140
241	8.026	0.000	H	141
242	126.844	0.000	N	141
566	58.424	0.000	CA	141
640	33.060	0.000	CB	141
809	174.459	0.000	C	141
247	8.255	0.000	H	142
248	127.230	0.000	N	142
543	51.855	0.000	CA	142
636	19.441	0.000	CB	142
808	177.712	0.000	C	142
163	8.463	0.000	H	143
164	121.711	0.000	N	143
576	54.901	0.000	CA	143
702	42.338	0.000	CB	143
910	177.114	0.000	C	143
123	8.520	0.000	H	144
124	120.023	0.000	N	144
581	58.107	0.000	CA	144
699	63.532	0.000	CB	144
919	174.443	0.000	C	144
215	8.570	0.000	H	145
216	124.374	0.000	N	145
570	56.909	0.000	CA	145
645	32.805	0.000	CB	145
869	176.871	0.000	C	145
181	8.225	0.000	H	146
182	122.659	0.000	N	146

606	55.394	0.000	CA	146
881	177.275	0.000	C	146
942	42.037	0.000	CB	146
219	8.141	0.000	H	147
220	124.451	0.000	N	147
554	52.800	0.000	CA	147
644	18.845	0.000	CB	147
175	8.087	0.000	H	148
176	122.211	0.000	N	148
143	8.028	0.000	H	150
144	120.505	0.000	N	150
604	55.148	0.000	CA	150
687	42.082	0.000	CB	150
922	177.421	0.000	C	150
151	8.192	0.000	H	151
152	120.781	0.000	N	151
603	56.522	0.000	CA	151
656	30.081	0.000	CB	151
909	176.110	0.000	C	151
121	8.175	0.000	H	152
122	119.885	0.000	N	152

TALOS files (chemical shifts) for the cPYP-dup – transient state (long tail):

455	8.151	0.000	H	4
456	120.781	0.000	N	4
457	54.410	0.000	CA	4
459	41.637	0.000	CB	4
94	8.180	0.000	H	5
95	114.203	0.000	N	5
96	57.338	0.000	CA	5
98	65.587	0.000	CB	5
474	9.303	0.000	H	7
475	122.471	0.000	N	7
476	56.007	0.000	CA	7
477	33.032	0.000	CB	7
480	9.024	0.000	H	10
481	122.577	0.000	N	10
482	61.152	0.000	CA	10
483	36.226	0.000	CB	10
375	8.864	0.000	H	11
376	126.599	0.000	N	11
377	52.370	0.000	CA	11
379	37.645	0.000	CB	11
24	8.390	0.000	H	21
25	108.797	0.000	N	21
52	45.096	0.000	CA	21
269	8.716	0.000	H	23
270	121.892	0.000	N	23
271	57.160	0.000	CA	23
273	29.306	0.000	CB	23
399	8.273	0.000	H	26
400	128.603	0.000	N	26
401	51.217	0.000	CA	26
403	19.904	0.000	CB	26
26	8.483	0.000	H	42
27	108.797	0.000	N	42
28	45.895	0.000	CA	42
275	8.374	0.000	H	44
276	121.799	0.000	N	44
277	57.959	0.000	CA	44
279	41.459	0.000	CB	44

11	7.924	0.000	H	46
12	108.424	0.000	N	46
22	46.693	0.000	CA	46
491	6.999	0.000	H	47
492	119.770	0.000	N	47
493	54.440	0.000	CA	47
494	42.835	0.000	CB	47
76	6.549	0.000	H	49
77	113.504	0.000	N	49
78	53.435	0.000	CA	49
80	39.596	0.000	CB	49
312	8.910	0.000	H	52
313	122.731	0.000	N	52
314	51.394	0.000	CA	52
316	22.121	0.000	CB	52
380	8.522	0.000	H	53
381	126.319	0.000	N	53
382	53.080	0.000	CA	53
383	32.411	0.000	CB	53
390	9.602	0.000	H	54
391	127.531	0.000	N	54
392	52.725	0.000	CA	54
393	46.693	0.000	CB	54
430	8.376	0.000	H	55
431	118.816	0.000	N	55
432	52.370	0.000	CA	55
433	41.016	0.000	CB	55
1	8.825	0.000	H	56
2	103.280	0.000	N	56
37	47.225	0.000	CA	56
121	8.002	0.000	H	57
122	116.533	0.000	N	57
123	53.878	0.000	CA	57
124	42.435	0.000	CB	57
17	8.685	0.000	H	58
18	108.611	0.000	N	58
19	45.540	0.000	CA	58
293	9.151	0.000	H	59
294	122.218	0.000	N	59
295	53.523	0.000	CA	59
296	38.355	0.000	CB	59
212	8.739	0.000	H	60
213	120.308	0.000	N	60
214	63.015	0.000	CA	60
216	38.088	0.000	CB	60
465	9.716	0.000	H	61
466	130.294	0.000	N	61
467	55.386	0.000	CA	61
384	8.972	0.000	H	63
385	126.972	0.000	N	63
386	54.943	0.000	CA	63
388	41.371	0.000	CB	63
367	8.281	0.000	H	64
368	125.760	0.000	N	64
369	52.104	0.000	CA	64
370	40.395	0.000	CB	64
5	7.714	0.000	H	68
6	106.251	0.000	N	68
41	47.757	0.000	CA	68
66	8.025	0.000	H	76
67	110.941	0.000	N	76
68	57.781	0.000	CA	76
70	32.056	0.000	CB	76

105	7.963	0.000	H	77
106	115.601	0.000	N	77
107	56.184	0.000	CA	77
109	29.484	0.000	CB	77
15	6.969	0.000	H	78
16	108.518	0.000	N	78
48	61.418	0.000	CA	78
50	31.702	0.000	CB	78
201	6.891	0.000	H	79
202	120.261	0.000	N	79
203	62.660	0.000	CA	79
205	36.314	0.000	CB	79
116	9.112	0.000	H	80
117	116.160	0.000	N	80
118	44.653	0.000	CA	80
438	7.812	0.000	H	81
439	119.026	0.000	N	81
440	54.474	0.000	CA	81
442	33.420	0.000	CB	81
182	9.609	0.000	H	82
183	119.702	0.000	N	82
184	54.322	0.000	CA	82
186	41.282	0.000	CB	82
409	9.415	0.000	H	83
410	130.374	0.000	N	83
412	40.838	0.000	CB	83
495	62.148	0.000	CA	83
82	6.254	0.000	H	84
83	112.945	0.000	N	84
84	59.289	0.000	CA	84
86	38.975	0.000	CB	84
60	7.870	0.000	H	85
61	110.615	0.000	N	85
62	55.297	0.000	CA	85
64	33.210	0.000	CB	85
100	7.365	0.000	H	86
101	114.483	0.000	N	86
102	55.297	0.000	CA	86
103	43.145	0.000	CB	86
146	6.961	0.000	H	87
147	118.351	0.000	N	87
148	64.345	0.000	CA	87
150	43.056	0.000	CB	87
443	7.912	0.000	H	88
444	119.015	0.000	N	88
445	48.112	0.000	CA	88
507	18.681	0.000	CB	88
158	8.483	0.000	H	90
159	118.118	0.000	N	90
160	59.821	0.000	CA	90
162	31.879	0.000	CB	90
111	8.328	0.000	H	91
112	115.974	0.000	N	91
113	63.104	0.000	CA	91
115	68.071	0.000	CB	91
417	7.582	0.000	H	92
418	124.502	0.000	N	92
419	53.168	0.000	CA	92
421	37.734	0.000	CB	92
217	8.382	0.000	H	93
218	119.935	0.000	N	93
219	55.031	0.000	CA	93
220	64.878	0.000	CB	93

88	8.444	0.000	H	95
89	112.991	0.000	N	95
90	58.047	0.000	CA	95
92	29.839	0.000	CB	95
126	7.575	0.000	H	96
127	117.745	0.000	N	96
128	56.983	0.000	CA	96
130	39.242	0.000	CB	96
504	8.738	0.000	H	97
505	123.190	0.000	N	97
506	59.561	0.000	CA	97
3	8.885	0.000	H	98
4	103.802	0.000	N	98
39	47.846	0.000	CA	98
194	6.503	0.000	H	99
195	120.308	0.000	N	99
198	57.959	0.000	CA	99
200	32.234	0.000	CB	99
137	8.569	0.000	H	101
138	117.791	0.000	N	101
139	58.934	0.000	CA	101
140	31.702	0.000	CB	101
13	7.808	0.000	H	103
14	108.471	0.000	N	103
45	46.693	0.000	CA	103
340	8.281	0.000	H	104
341	123.430	0.000	N	104
342	65.587	0.000	CA	104
344	31.347	0.000	CB	104
500	7.590	0.000	H	105
501	120.671	0.000	N	105
502	54.401	0.000	CA	105
503	18.185	0.000	CB	105
497	7.759	0.000	H	107
498	110.821	0.000	N	107
499	45.769	0.000	CA	107
141	8.103	0.000	H	108
142	118.257	0.000	N	108
143	51.749	0.000	CA	108
145	39.330	0.000	CB	108
281	7.877	0.000	H	109
282	121.799	0.000	N	109
283	54.943	0.000	CA	109
285	39.330	0.000	CB	109
242	8.716	0.000	H	113
243	120.914	0.000	N	113
244	56.096	0.000	CA	113
245	39.064	0.000	CB	113
176	8.809	0.000	H	114
177	119.189	0.000	N	114
178	54.943	0.000	CA	114
180	32.145	0.000	CB	114
361	9.337	0.000	H	115
362	125.574	0.000	N	115
363	58.313	0.000	CA	115
365	45.362	0.000	CB	115
132	7.458	0.000	H	116
133	117.791	0.000	N	116
134	61.773	0.000	CA	116
136	69.224	0.000	CB	116
55	7.054	0.000	H	121
56	109.916	0.000	N	121
57	53.967	0.000	CA	121

58	35.072	0.000	CB	121
188	8.553	0.000	H	122
189	119.609	0.000	N	122
190	60.886	0.000	CA	122
192	69.579	0.000	CB	122
302	8.802	0.000	H	124
303	123.150	0.000	N	124
304	61.800	0.000	CA	124
306	71.885	0.000	CB	124
394	8.871	0.000	H	125
395	130.001	0.000	N	125
396	56.096	0.000	CA	125
398	32.056	0.000	CB	125
246	9.073	0.000	H	127
247	121.100	0.000	N	127
248	54.676	0.000	CA	127
250	34.718	0.000	CB	127
170	9.143	0.000	H	135
171	119.189	0.000	N	135
172	58.668	0.000	CA	135
174	63.636	0.000	CB	135
298	8.934	0.000	H	140
299	121.519	0.000	N	140
300	53.080	0.000	CA	140
301	38.000	0.000	CB	140
355	8.235	0.000	H	146
356	122.591	0.000	N	146
357	55.120	0.000	CA	146
359	41.991	0.000	CB	146
328	8.157	0.000	H	147
329	124.502	0.000	N	147
330	52.636	0.000	CA	147
332	18.839	0.000	CB	147
446	8.166	0.000	H	152
447	119.898	0.000	N	152
448	56.184	0.000	CA	152
449	30.637	0.000	CB	152

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1. Kumar, A., Burns, D. C., Al-Abdul-Wahid, M. S., and Woolley, G. A. (2013) A circularly permuted photoactive yellow protein as a scaffold for photoswitch design, *Biochemistry* 52, 3320-3331.