

Supporting Information

Harrop et al. 10.1073/pnas.1402538111

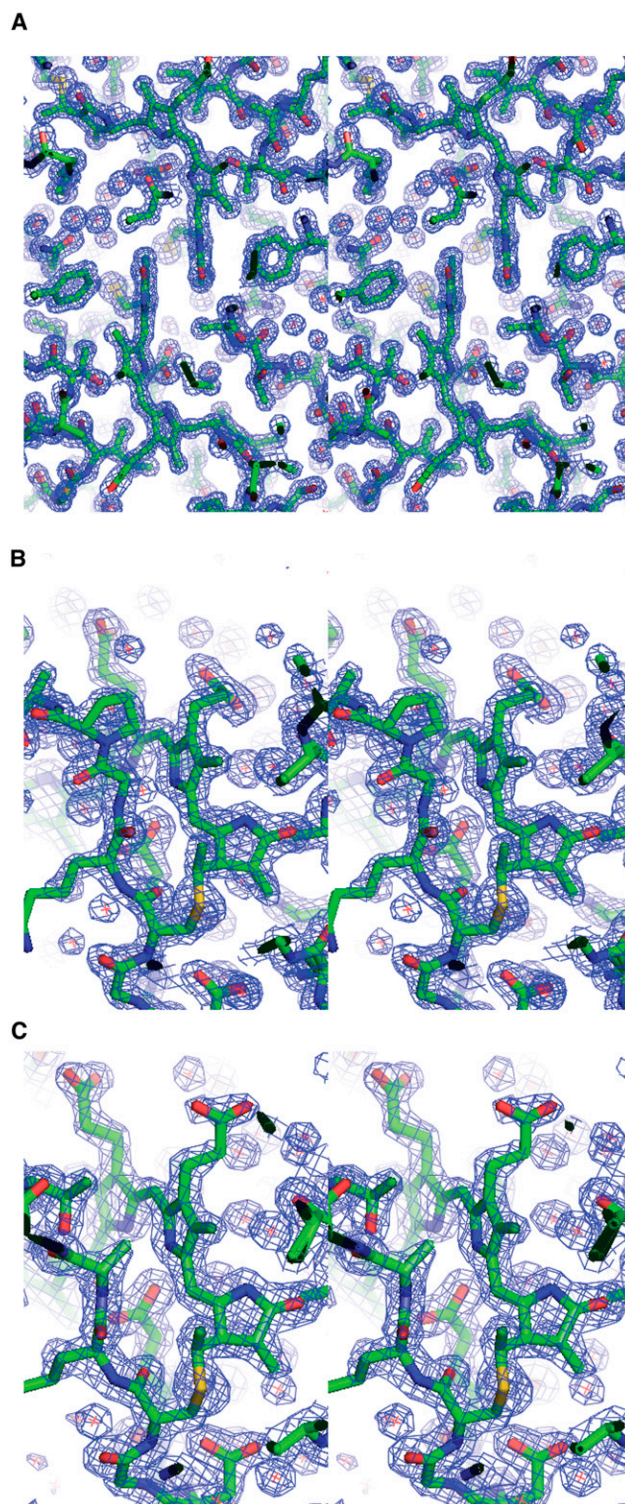


Fig. S1. Electron density. Stereograms showing sample electron density from the three crystal structures. (A) Electron density of PC645 centered on the offset-stacked $\beta 50/61$ chromophores (contoured at 2σ). (B) Electron density of PC612 centered on the chromophore in the α_1 subunit (contoured at 2σ). (C) Electron density of PE555 centered on the chromophore in the α_2 subunit (contoured at 1.5σ). The view is similar to that in B.

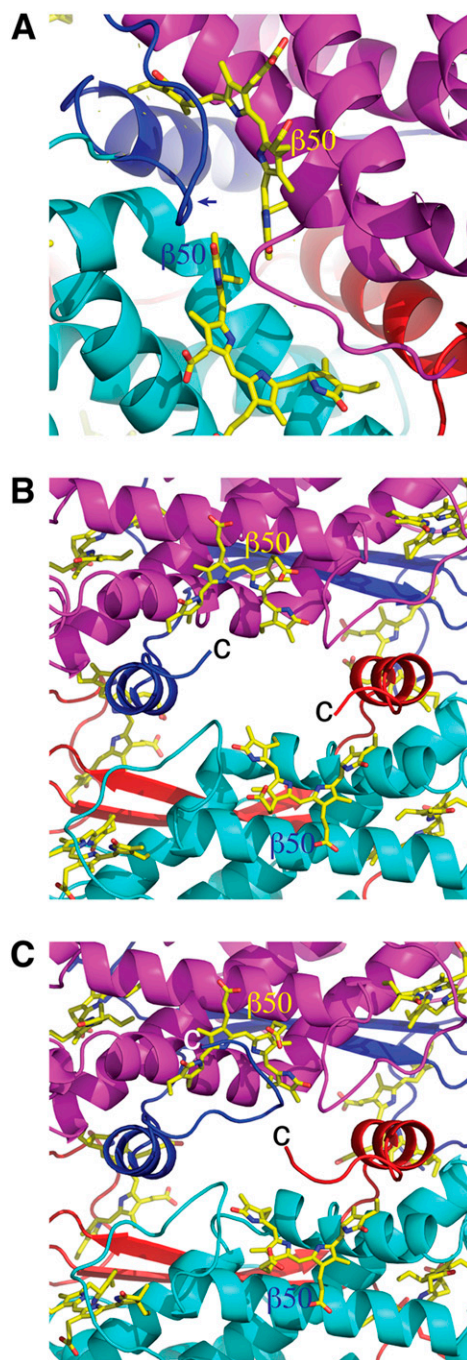


Fig. S2. Central $\beta 50/61$ chromophores viewed down the pseudo-twofold axis. (A) The two doubly linked $\beta 50/61$ DBV chromophores in the closed-form PC645. The blue arrow indicates the extended C-terminal loop of the α_1 subunit. (B and C) View down the pseudo-twofold axis showing the separation between the doubly linked $\beta 50/61$ chromophores in the open-form structures of PC612 (B) and PE555 (C).

Table S4. Matrix of Coulombic gas-phase couplings (cm^{-1}) calculated at the CIS/cc-pvtz level

Protein	Electronic coupling matrix							
PC645	MBV _{α18}	PCB _{β158}	PCB _{β82}	DBV _{β50/61}	MBV _{α18}	PCB _{β158}	PCB _{β82}	DBV _{β50/61}
	—	151	26	19	−7	5	69	−74
	PCB _{β158}	151	19	22	4	13	−19	37
	PCB _{β82}	26	19	−64	75	−19	−12	35
	DBV _{β50/61}	19	22	−64	−	45	32	647
	MBV _{α18}	−7	4	75	−76	−	24	14
	PCB _{β158}	5	13	−19	45	160	−	18
	PCB _{β82}	69	−19	−12	32	24	18	−
	DBV _{β50/61}	−74	37	35	647	14	32	−67
PC612	PCB _{α20}	PCB _{β158}	PCB _{β82}	DBV _{β50/61}	PCB _{α20}	PCB _{β158}	PCB _{β82}	DBV _{β50/61}
	—	146	20	29	−2	−2	40	−5
	PCB _{β158}	146	22	22	−2	8	3	−5
	PCB _{β82}	20	22	−	45	4	2	27
	DBV _{β50/61}	29	22	−67	−	−4	24	29
	PCB _{α20}	−2	−2	45	−5	−	130	19
	PCB _{β158}	−2	8	4	−4	130	−	19
	PCB _{β82}	40	3	2	24	19	19	−
PE555	PEB _{α20}	PEB _{β158}	PEB _{β82}	DBV _{β50/61}	PEB _{α20}	PEB _{β158}	PEB _{β82}	DBV _{β50/61}
	—	68	17	20	−13	5	26	−8
	PEB _{β158}	68	12	36	5	5	4	−2
	PEB _{β82}	17	12	−60	29	3	4	20
	DBV _{β50/61}	20	36	−60	0	1	24	4
	PEB _{α20}	−13	5	29	0	63	16	13
	PEB _{β158}	5	5	3	1	63	0	12
	PEB _{β82}	26	4	4	24	16	12	0
PE545	DBV _{β50/61}	−8	20	4	13	43	−56	0
	DBV _{α20}	PEB _{β158}	PEB _{β82}	PEB _{β50/61}	DBV _{α20}	PEB _{β158}	PEB _{β82}	PEB _{β50/61}
	—	51	17	4	−6	5	62	−64
	PEB _{β158}	51	11	29	5	9	−11	31
	PEB _{β82}	17	11	−56	62	−8	−4	29
	PEB _{β50/61}	4	29	−56	−61	25	27	166
	DBV _{α20}	−6	5	62	−61	49	18	4
	PEB _{β158}	5	9	−8	25	49	12	38
	PEB _{β82}	62	−11	−4	27	18	12	−58
	PEB _{β50/61}	−64	31	29	166	4	38	−58

