



SUPPLEMENTARY MATERIAL TO  
**Energetic networks of lone pair– $\pi$  interactions in phycobiliprotein interfaces: structural organization, geometry, and cooperative stabilization**

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**Table S1. Cartesian coordinates of representative dimers**

The tables below present the Cartesian coordinates (xyz format) of the representative dimers selected for the Supplementary Material. R denotes the distance between the lone pair donor atom (O) and the centroid of the aromatic  $\pi$  system.  $\theta$  represents the angle between the donor–centroid vector and the normal to the aromatic ring plane, describing the approach of the lone pair toward the  $\pi$  system. All optimized structures correspond to true minima on the potential energy surface, with no imaginary frequencies.

Because the full dataset contains a large number of interacting pairs, only representative dimers illustrating the principal classes of lone pair– $\pi$  interactions were selected for detailed presentation in the Supplementary Material. The selected examples cover the main types of donor residues and aromatic  $\pi$  systems observed in the structural dataset and reproduce the characteristic geometrical parameters identified in the statistical analysis.

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**1. 4FOU - A:THR96:OG1 - B:TYR18**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
THR A96	OG1	TYR B18	5.11	57.17

**XYZ coordinates**

Atom	X	Y	Z
C	-47.9740	25.3270	80.8670
O	-49.1390	26.1040	80.5650
C	-47.2110	25.9910	82.0180
H	-48.2390	24.4320	81.1310
H	-48.9120	26.8930	80.3890
H	-47.7870	26.0510	82.7960
H	-46.4280	25.4610	82.2360
H	-46.9340	26.8820	81.7520
H	-47.3330	25.2730	79.9870
C	-53.1440	26.7670	83.9440
C	-52.1970	27.9510	84.0300
C	-50.8230	27.7790	83.8620
C	-52.6670	29.2380	84.3090
C	-49.9470	28.8510	83.9710
C	-51.7970	30.3120	84.4220
C	-50.4400	30.1110	84.2510
O	-49.5740	31.1680	84.3570
H	-53.6280	26.7020	84.7820
H	-52.6150	25.9580	83.8580
H	-50.4880	26.9320	83.6740
H	-53.5800	29.3760	84.4210
H	-49.0330	28.7210	83.8560
H	-52.1240	31.1620	84.6120
H	-49.9800	31.8320	84.6730
H	-53.8300	26.8760	83.1040

**2. 1CPC - L:THR96:OG1 - K:PHE18**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
THR L96	OG1	PHE K18	5.08	59.80

**XYZ coordinates**

Atom	X	Y	Z
C	11.0670	-28.2090	-6.4320
C	11.8900	-27.7530	-7.6390
C	12.6700	-26.6110	-7.5420
C	11.7760	-28.4370	-8.8380
C	13.3320	-26.0900	-8.6530
C	12.4610	-27.9130	-9.9520
C	13.2210	-26.7290	-9.8620
H	11.5890	-28.1100	-5.6210
H	10.8510	-29.1510	-6.5170
H	12.7530	-26.1840	-6.7200
H	11.2670	-29.2120	-8.9050
H	13.8440	-25.3170	-8.5750
H	12.4110	-28.3590	-10.7670
H	13.6430	-26.3840	-10.6150
H	10.1520	-27.6210	-6.3610
C	8.6210	-30.4880	-11.9670
O	8.5540	-29.3560	-11.0670
C	10.0640	-30.7940	-12.3830
H	8.3200	-31.2620	-11.4660
H	8.3900	-28.6580	-11.5050
H	10.6290	-30.8230	-11.5950
H	10.0960	-31.6520	-12.8350
H	10.3820	-30.1010	-12.9830
H	7.9920	-30.3250	-12.8420

**3. 2BV8 - P:TYR74:OH - K:TYR90**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
TYR K90	OH	TYR P74	4.90	74.72

**XYZ coordinates**

Atom	X	Y	Z
C	2.2490	46.8700	86.8180
C	2.3420	47.4430	88.2260
C	1.2890	47.3000	89.1630
C	3.4330	48.2530	88.5610
C	1.3240	47.9710	90.3810
C	3.4840	48.9290	89.7500
C	2.4210	48.7920	90.6520
O	2.4740	49.5430	91.7750
H	3.1250	46.5330	86.5720
H	2.0430	47.5970	86.2100
H	0.5660	46.7510	88.9610
H	4.1400	48.3340	87.9620
H	0.6350	47.8750	90.9990
H	4.2120	49.4700	89.9560
H	3.1810	49.9970	91.7760
H	1.4950	46.0850	86.7620
C	1.4710	55.4340	91.0980
C	0.7760	54.3180	90.3650
C	1.3080	53.0090	90.3600
C	-0.3900	54.5740	89.6510
C	0.6760	51.9690	89.6350
C	-1.0360	53.5650	88.9300
C	-0.5050	52.2720	88.9180
O	-1.1330	51.3230	88.1480
H	1.6180	55.1650	92.0180
H	0.8890	56.2100	91.1190
H	2.0840	52.8280	90.8390
H	-0.7470	55.4330	89.6530

Atom	X	Y	Z
H	1.0290	51.1090	89.6310
H	-1.8160	53.7530	88.4600
H	-1.7550	51.6820	87.7120
H	2.4170	55.6780	90.6150

**4. 1F99 - N:MET79:SD - K:PHE122**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
MET N79	SD	PHE K122	5.69	65.81

**XYZ coordinates**

Atom	X	Y	Z
C	-27.9410	38.8900	59.3320
C	-26.7160	38.9550	60.2390
C	-26.6930	39.8310	61.3110
C	-25.6500	38.0970	60.0320
C	-25.6100	39.8400	62.1720
C	-24.5740	38.1120	60.8960
C	-24.5540	38.9800	61.9680
H	-27.6700	38.6210	58.4400
H	-28.3340	39.7740	59.2540
H	-27.4050	40.4130	61.4520
H	-25.6590	37.5100	59.3110
H	-25.5950	40.4290	62.8910
H	-23.8590	37.5340	60.7550
H	-23.8300	38.9840	62.5510
H	-28.6710	38.1870	59.7330
C	-18.7680	37.7120	58.5160
C	-20.0970	37.8890	59.2390
S	-19.9610	38.5510	60.9210
C	-19.7100	40.2510	60.4960
H	-18.3890	38.5870	58.3390
H	-18.9330	37.2950	57.6560
H	-20.6600	38.4810	58.7160
H	-20.5470	37.0310	59.2780
H	-19.6130	40.7760	61.3060
H	-18.9070	40.3350	59.9580
H	-20.4720	40.5740	59.9910
H	-18.0830	37.1090	59.1120

**5. 1F99 - N:SER94:OG - M:PHE18**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
SER N94	OG	PHE M18	5.12	61.56

**XYZ coordinates**

Atom	X	Y	Z
C	-26.5750	21.9370	70.3080
C	-26.0230	23.3590	70.3590
C	-25.7200	24.0440	69.1940
C	-25.8180	23.9620	71.5850
C	-25.2110	25.3250	69.2730
C	-25.3090	25.2440	71.6530
C	-25.0040	25.9260	70.4980
H	-27.1790	21.8670	69.5520
H	-27.1010	21.7810	71.1080
H	-25.8580	23.6450	68.3660
H	-26.0240	23.5030	72.3670
H	-25.0060	25.7880	68.4930
H	-25.1720	25.6460	72.4800
H	-24.6600	26.7890	70.5420
H	-25.7670	21.2100	70.2270
C	-24.2480	23.3660	75.9470
O	-23.8090	22.6280	74.8140
H	-25.0830	22.9830	76.2580
H	-24.4400	24.2740	75.6660
H	-22.9890	22.7630	74.6920
H	-23.4960	23.3530	76.7360

**6. 1B33 - A:SER31:OG - J:TYR72**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
SER A31	OG	TYR J72	4.72	70.20

**XYZ coordinates**

Atom	X	Y	Z
C	84.5680	55.1380	62.0110
O	83.5100	54.3010	61.5580
H	85.0480	55.4890	61.2450
H	85.1990	54.6080	62.5230
H	83.2340	53.8280	62.1950
H	84.1750	55.9530	62.6190
C	85.7980	51.6340	57.5020
C	85.5740	53.1320	57.3700
C	85.5920	53.7530	56.1200
C	85.3930	53.9330	58.4950
C	85.4400	55.1300	55.9950
C	85.2440	55.3160	58.3790
C	85.2690	55.9040	57.1270
O	85.1320	57.2670	57.0050
H	85.1480	51.1680	56.9540
H	85.6360	51.3700	58.4210
H	85.7080	53.2360	55.3560
H	85.3710	53.5400	59.3380
H	85.4530	55.5280	55.1540
H	85.1290	55.8390	59.1390
H	85.2410	57.4890	56.2020
H	86.8120	51.3700	57.2010

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**7. 2BV8 - O:TYR74:OH - E:PHE63**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
TYR O74	OH	PHE E63	5.39	78.09

**XYZ coordinates**

Atom	X	Y	Z
C	31.8940	120.3860	59.0470
C	30.5110	120.0440	59.5600
C	30.3250	119.6500	60.8950
C	29.3960	120.1410	58.7190
C	29.0390	119.3630	61.3860
C	28.1050	119.8590	59.1830
C	27.9040	119.4700	60.5180
H	31.9000	120.2970	58.0810
H	32.5260	119.7380	59.3960
H	31.0600	119.5780	61.4600
H	29.5150	120.3980	57.8330
H	28.9250	119.1040	62.2720
H	27.3790	119.9290	58.6060
H	27.0490	119.2850	60.8330
H	32.1760	121.3970	59.3430
C	29.4980	121.1460	70.6350
C	29.2330	120.6950	69.2200
C	29.9220	119.6050	68.6740
C	28.2570	121.3270	68.4370
C	29.6440	119.1500	67.3780
C	27.9690	120.8840	67.1460
C	28.6630	119.7930	66.6200
O	28.3580	119.3370	65.3490
H	29.0260	121.9770	70.8010
H	30.4440	121.3310	70.7410
H	30.5740	119.1760	69.1790
H	27.7930	122.0540	68.7840
H	30.1090	118.4260	67.0260

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
H	27.3180	121.3130	66.6390
H	27.7540	119.8170	65.0170
H	29.1790	120.3810	71.3430

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**8. 4L1E - A:GLN33:OE1 - C:PHE28**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
GLN A33	OE1	PHE C28	5.04	57.50

**XYZ coordinates**

Atom	X	Y	Z
C	-64.2980	-4.9460	-31.8280
C	-65.3780	-4.0120	-31.3100
C	-66.0540	-4.5310	-30.0540
O	-65.4560	-5.2710	-29.2710
N	-67.3090	-4.1440	-29.8560
H	-63.7040	-5.1750	-31.0960
H	-63.7660	-4.4750	-32.4880
H	-64.9870	-3.1430	-31.1260
H	-66.0460	-3.8820	-32.0010
H	-67.6940	-3.6270	-30.4250
H	-67.7360	-4.4110	-29.1590
H	-64.7400	-5.8440	-32.2600
C	-61.3090	-6.8840	-25.7900
C	-62.6050	-6.4500	-25.1580
C	-63.0480	-7.0200	-23.9760
C	-63.3830	-5.4690	-25.7500
C	-64.2360	-6.6220	-23.3990
C	-64.5750	-5.0690	-25.1740
C	-64.9970	-5.6440	-23.9980
H	-61.0430	-6.2220	-26.4470
H	-61.4550	-7.7150	-26.2680
H	-62.5370	-7.6800	-23.5660
H	-63.1010	-5.0750	-26.5440
H	-64.5230	-7.0140	-22.6060
H	-65.0910	-4.4110	-25.5820
H	-65.7960	-5.3720	-23.6080
H	-60.5340	-7.0070	-25.0330

**9. 1B33 - O:GLN41:OE1 - K:TYR87**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
GLN O41	OE1	TYR K87	5.38	68.67

**XYZ coordinates**

Atom	X	Y	Z
C	111.3190	1.4800	72.0210
C	110.0370	0.7600	71.6620
C	109.9240	-0.6200	71.8120
C	108.9720	1.4430	71.0790
C	108.7770	-1.3140	71.3770
C	107.8180	0.7660	70.6420
C	107.7240	-0.6170	70.7890
O	106.6010	-1.2950	70.3280
H	111.6630	1.1320	72.8580
H	111.1340	2.4220	72.1600
H	110.6200	-1.0930	72.2070
H	109.0250	2.3660	70.9760
H	108.7230	-2.2360	71.4820
H	107.1180	1.2410	70.2550
H	106.0560	-0.7450	70.0020
H	112.0570	1.3540	71.2290
C	102.2830	4.4460	72.6030
C	103.6160	3.8410	72.9740
C	104.3110	3.2470	71.7820
O	105.1110	3.9130	71.1260
N	103.9810	2.0050	71.4610
H	101.5870	3.7830	72.7310
H	102.2890	4.6720	71.6600
H	104.1810	4.5220	73.3710
H	103.4840	3.1550	73.6460
H	103.4180	1.5710	71.9450
H	104.3300	1.6320	70.7690
H	102.0840	5.3310	73.2070

**10. 1ALL - A:GLY34:O - B:PHE31**

Donor residue	Donor atom	Aromatic residue	R (Å)	$\theta$ (°)
GLY A34	O	PHE B31	4.70	35.17

**XYZ coordinates**

Atom	X	Y	Z
N	5.3890	16.0670	10.0080
C	6.0910	16.4900	11.1890
C	7.0790	15.4710	11.7110
O	8.2350	15.8040	11.9580
H	4.5320	16.1310	10.0510
H	6.5620	17.3160	10.9960
H	5.4450	16.6880	11.8850
H	5.6360	15.0420	9.8250
H	6.7650	14.4390	11.8680
C	2.9170	16.5310	14.9570
C	4.0070	17.5050	14.5450
C	3.7150	18.6100	13.7450
C	5.3260	17.3170	14.9740
C	4.7120	19.5150	13.3790
C	6.3360	18.2120	14.6170
C	6.0240	19.3200	13.8130
H	3.2510	15.9730	15.6770
H	2.7230	15.9440	14.2100
H	2.8430	18.7450	13.4510
H	5.5330	16.5830	15.5060
H	4.5020	20.2480	12.8460
H	7.2080	18.0760	14.9090
H	6.6900	19.9220	13.5700
H	2.0200	17.0660	15.2690