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SUPPLEMENTARY MATERIAL TO

Energetic networks of lone pair–π interactions in phycobiliprotein interfaces: Structural organization, geometry and cooperative stabilization

LUKA M. BREBERINA[1], MARIO V. ZLATOVIĆ[2], SRĐAN Đ. STOJANOVIĆ[3] and MILAN R. NIKOLIĆ[1]*

[1]University of Belgrade – Faculty of Chemistry, Department of Biochemistry, Belgrade, Serbia, [2]University of Belgrade – Faculty of Chemistry, Department of Organic Chemistry, Belgrade, Serbia and [3]University of Belgrade, Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia, Department of Chemistry, Belgrade, Serbia

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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 π system. θ 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 π 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–π interactions were selected for detailed presentation in the Supplementary Material. The selected examples cover the main types of donor residues and aromatic π systems observed in the structural dataset and reproduce the characteristic geometrical parameters identified in the statistical analysis.

* Corresponding author. E-mail: mnikolic@chem.bg.ac.rs

Table S-I. Cartesian coordinates of representative dimers

1. 4F0U - A:THR96:OG1 - B:TYR18

Donor residue	Donor atom	Aromatic residue	R (Å)	θ (°)
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)	θ (°)
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)	θ (°)
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)	θ (°)
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)	θ (°)
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)	θ (°)
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

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

Donor residue	Donor atom	Aromatic residue	R (Å)	θ (°)
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

Atom	X	Y	Z
H	27.3180	121.3130	66.6390
H	27.7540	119.8170	65.0170
H	29.1790	120.3810	71.3430

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

Donor residue	Donor atom	Aromatic residue	R (Å)	θ (°)
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)	θ (°)
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)	θ (°)
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