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Scientific Reports

**Spectral and structural comparison between bright and dim green  
fluorescent proteins in *Amphioxus***

Erin K Bomati, Joy E Haley, Joseph P Noel and Dimitri D Deheyn

**Supplementary tables**

**Table S1.** Crystallographic statistics associated with characterization of bfloGFPa1 and bfloGFPc1 structures.

	<b>Statistic</b>	<b>Sub Category</b>	<b>bfloGFPa1</b>	<b>bfloGFPc1</b>
<b>DATA COLLECTION</b>	Space group		C 2 2 2(1)	C 2
	Cell Dimensions	a, b, c, $\alpha, \beta, \gamma$ (°)	59.25, 125.58, 106.47 90.0, 90.0, 90.0	158.76, 130.46, 106.33 90.0, 128.4, 90.0
	Resolution (Å)*		50.0 - 1.35(1.4 - 1.35)	50.0 - 1.95 (2.02 – 1.95)
	$R_{sym}$		4.7 (29.1)	5.5 (51.3)
	$I/\sigma$		37.9 (3.3)	34.3 (2.7)
	Completeness (%)		97.4 (83.9)	99.7 (98.2)
	Redundancy		6.7 (5.2)	5.3 (4.9)
<b>REFINEMENT</b>	Resolution (Å)		1.35	1.95
	No. Reflections		87211	123290
	$R_{work}/R_{free}$		.2939/.3214	.2944/.3216
	No. of atoms	Protein	3357	13224
		Ligand	38	152
		Water	501	581
	B-factor	Protein	13.2	41.7
		Ligand	9.0	42.0
		Water	25.2	38.4
R.m.s. deviations	Bond angles (°)			
	Bond lengths (Å)			

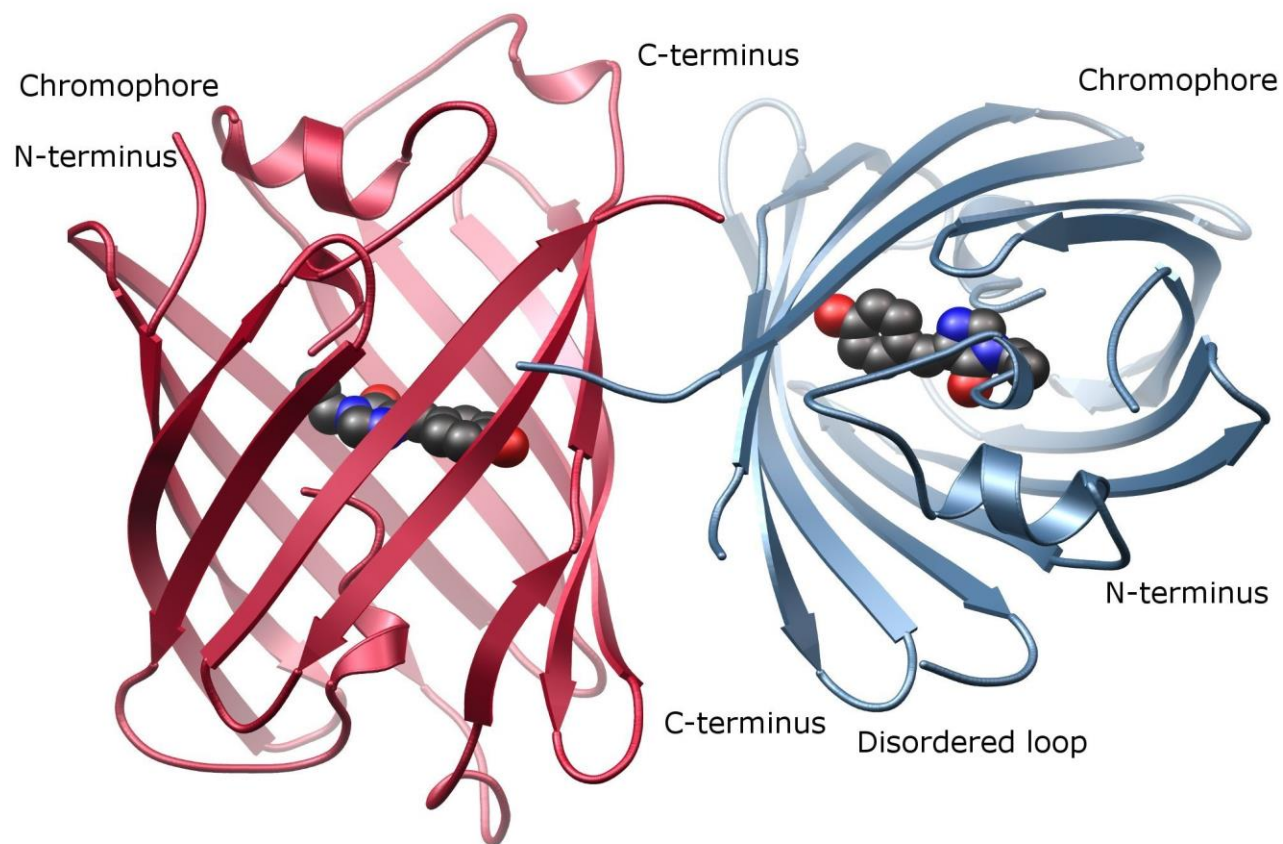
\* Number in parentheses refers to highest shell

**Table S2:** List of GFPs found with similar crystallographic resolution as bfpGFPa1, and their average B-factor values from the atoms comprising the chromophore (from PDB database and Lohman and Remington 2008).

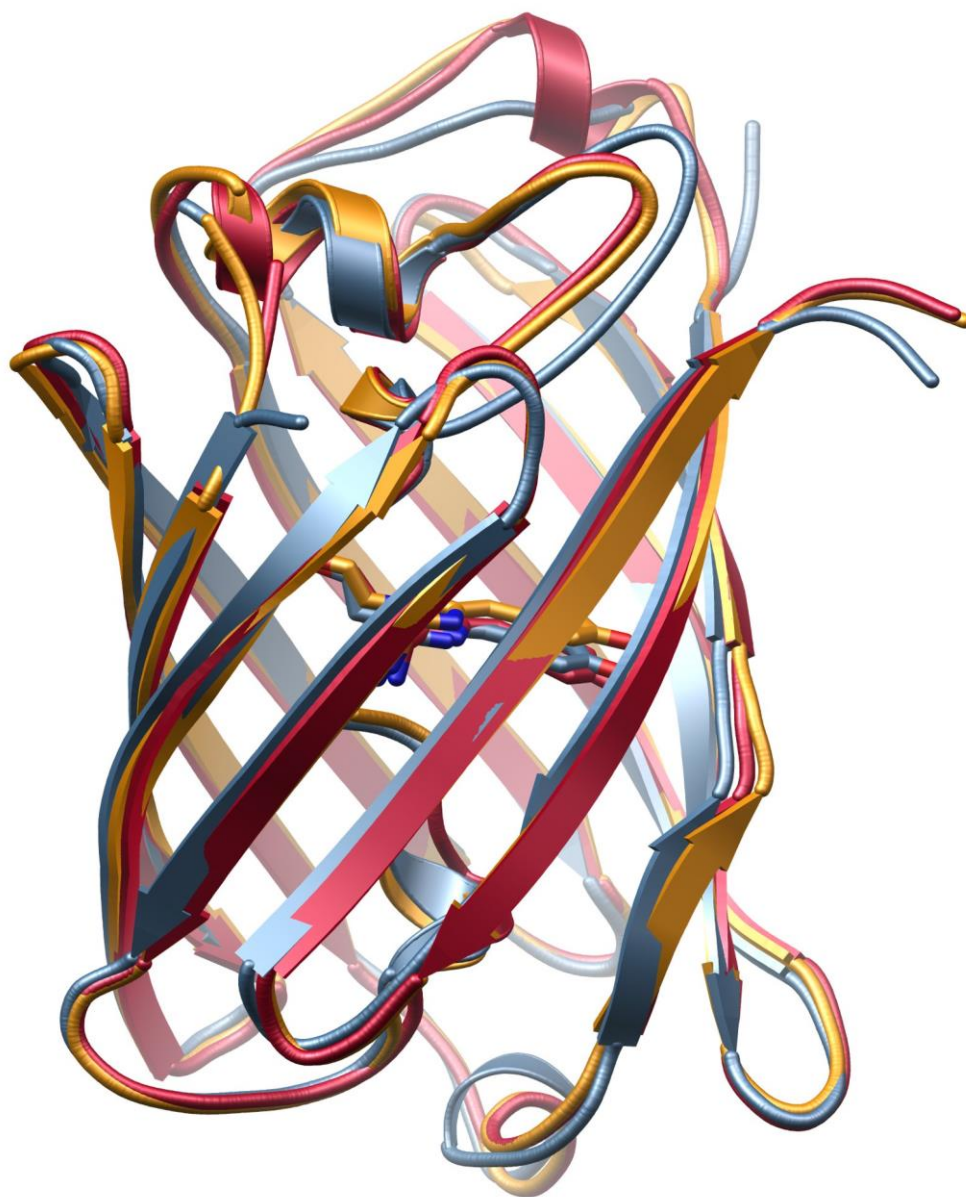
<b>PDB ID</b>	<b>B-factor</b>	<b>QE</b>
2DUG	21.1	<100%
2C9J	21.0	<100%
1XMZ	17.3	<100%
2QT2	15.9	<100%
2DUI	14.2	<100%
2DUE	13.6	<100%
2ZO6	12.6	<100%
1Q4A	11.7	<100%
1Q4E	11.0	<100%
2B3P	10.3	<100%
2GW3	10.2	<100%
2HRS	10.0	<100%
2O24	9.7	<100%
3CD1	9.5	<100%
3CB9	6.2	<100%
GFPa1	8.7	=100%

### Supplementary Figures

**Figure S1.** Ribbon representation of the bflGFPa1 dimer. Monomer A is colored blue, monomer B is colored rose. The GYG-derived chromophore is shown in space filling model with the carbon atoms colored black.



**Figure S2.** Overlay of structurally similar GFPs including bflGFPa1 in gold, bflGFPc1 in red, and copGFP (PDBid 2G3O) in blue. Chromophores are shown in ball-and-stick representation with carbon atoms color coordinated to match ribbon structure.



**Figure S3.** Overlay of bflGFPa1 and copGFP chromophore sites. Side chains and chromophores (CRO) are shown in ball-and-stick representation with carbon atoms colored gold (bflGFPa1) and blue (copGFP).

