Supplementary Data

Structural flexibility of the monomeric red fluorescent protein DsRed

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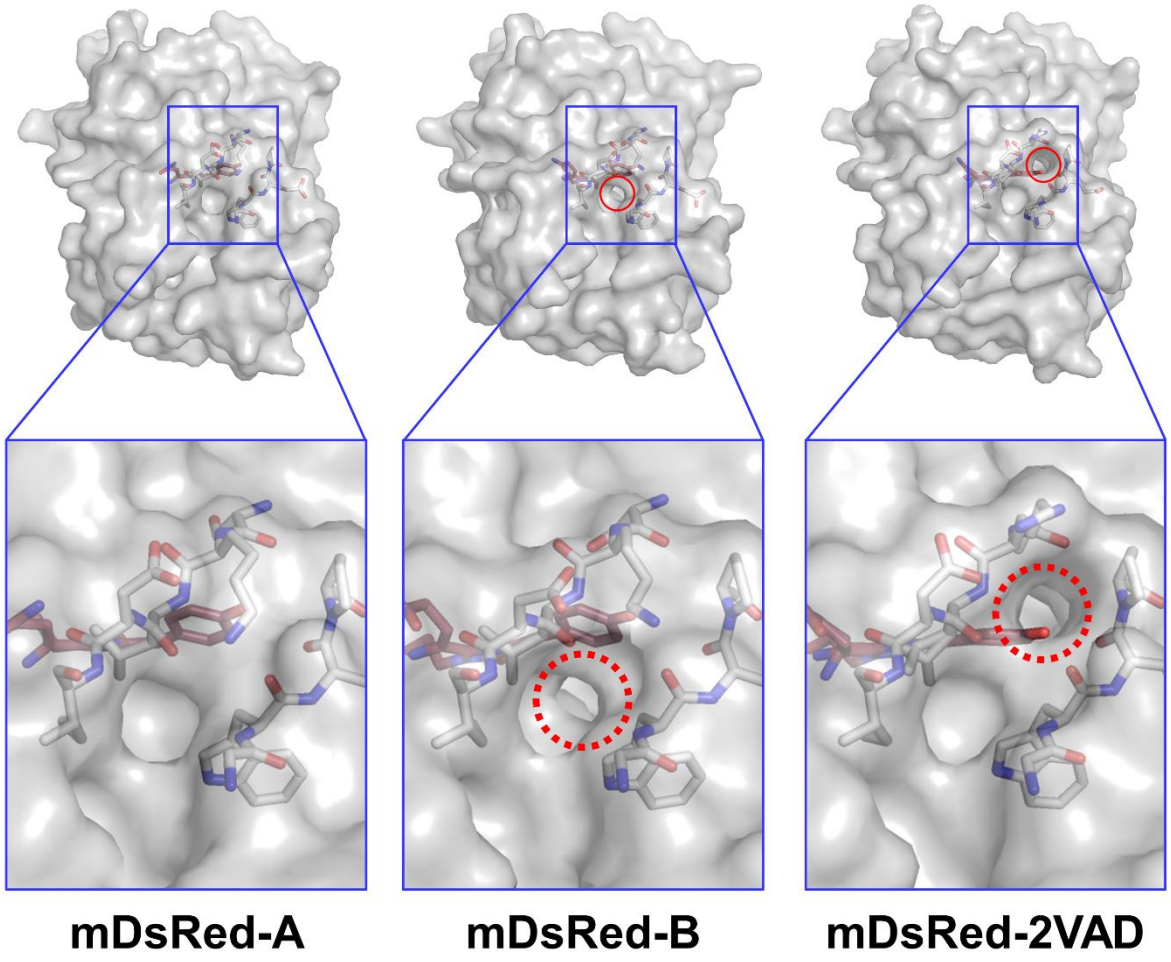
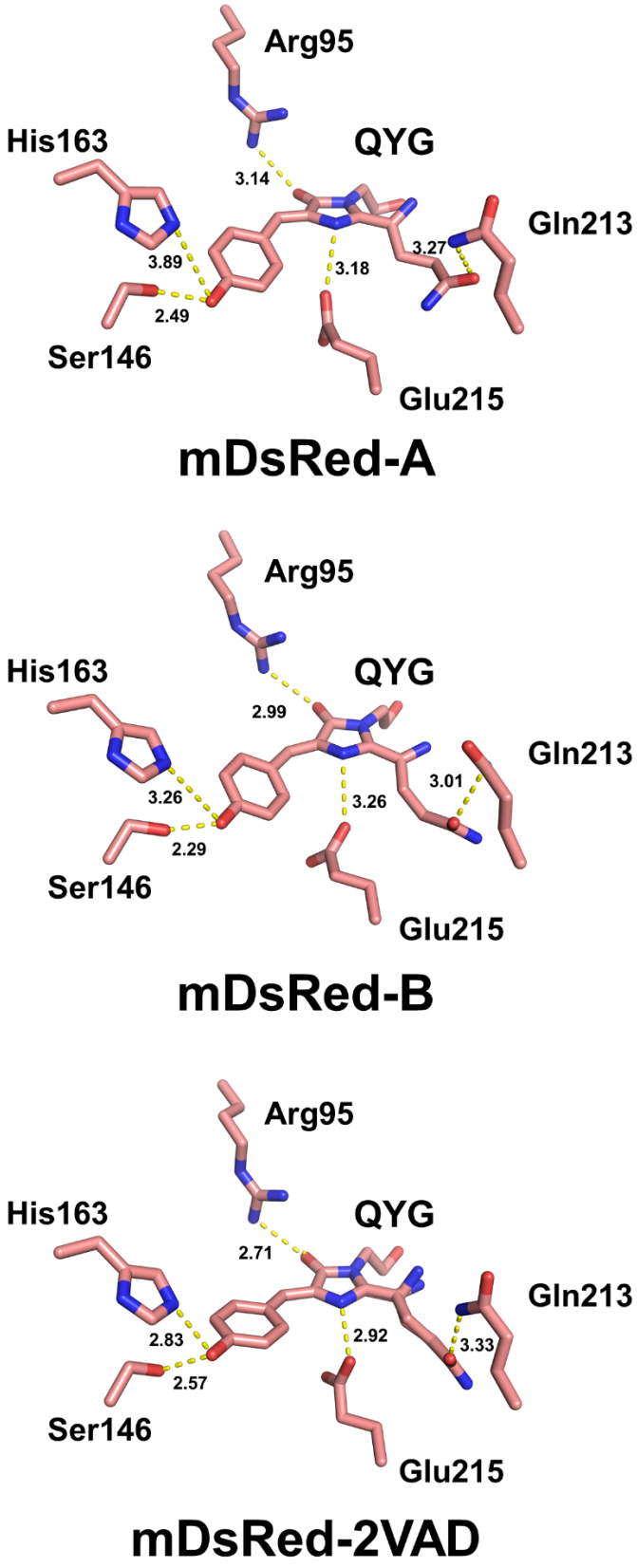


Supplementary Figure S1. Comparison of the surface structures of mDsRed-A, mDsRed-B, and mDsRed-2VAD. A hole connected with the chromophore was observed in mDsRed-B and mDsRed-2VAD.



Supplementary Figure S2. Hydrogen bond network in the vicinity of the mDsRed chromophores.

Table S1. Interface summary analyzed by PDBePISA.

	mDsRed-A		**mDsRed-B**	
Number of atoms				
interface	85	4.8%	79	4.5%
surface	962	54.8%	965	55.0%
total	1755	100.0%	1755	100.0%
Number of residues				
interface	24	11.0%	24	11.0%
surface	204	93.6%	208	95.4%
total	218	100.0%	218	100.0%
Solvent-accessible area, Å				
interface	695.1	7.0%	686.3	7.0%
total	9871.5	100.0%	9866.0	100.0%
Solvation energy, kcal/mol				
isolated structure	-207.8	100.0%	-203.3	100.0%
gain on complex formation	0.9	-0.4%	0.2	-0.1%
average gain	-0.8	0.4%	-1.2	0.6%
P-value	0.743		0.709	

Table S2. Interaction between mDsRed-A and mDsRed-B.

Hydrogen bonds		
mDsRed-A residue [atom]	Distance (Å)	mDsRed-B residue (atom)
Gly223 [O]	2.52	Lys36 [NZ]
Asp200 [OD1]	3.80	Lys166 [NZ]
Asp200 [OD1]	2.46	Lys198 [NZ]
Gly170 [O]	3.67	His204 [N]
Asp169 [O]	3.73	Glu206 [N]
Lys166 [NZ]	2.28	Asp200 [OD2]
Lys166 [NZ]	2.98	Ile201 [O]
His204 [N]	3.24	Gly170 [O]
Salt bridges		
mDsRed-A residue (atom)	Distance (Å)	mDsRed-B residue (atom)
Gly223 [O]	2.52	Lys36 [NZ]
Asp200 [OD1]	3.80	Lys166 [NZ]
Asp200 [OD1]	2.46	Lys198 [NZ]
Lys166 [NZ]	2.28	Asp200 [OD2]