Supporting Information:

Table S1. X-ray diffraction intensity measurements and data statistics of ΔPsbM-PSII.

Dataset	ΔPsbM_0.4MGy
Beamline	BL38B1, SPring-8
Wavelength (Å)	0.8
Averaged dose (MGy)	0.4
Space group	$P2_12_12_1$
Unit cell a, b, c (Å)	122.0, 227.0, 285.9
Resolution (Å)	48.8-2.2 (2.32-2.20)
Measured reflections	2,003,997 (272,075)
Unique reflections	385,629 (55,884)
R_{merge} (%)[i]	8.3(70.5)
$<I>/<\sigma(I)>$	13.6(2.2)
Completeness (%)	96.7(96.6)
Redundancy	5.2(4.9)
R_{pim} (%)[ii]	3.9(34.4)
CC(1/2)[iii]	99.8(82.2)

The dataset name is combined with the averaged X-ray dose. Numbers in parentheses are for the highest resolution shell.

(i) Linear merging R-value.

$$R_{merge} = \frac{\sum_{hkl}\sum_{i=1}^{N}\left|I_i(hkl) - \overline{I(hkl)}\right|}{\sum_{hkl}\sum_{i=1}^{N}I_i(hkl)}$$

$I_i(hkl)$ is an integrated intensity of one reflection. The suffix *i* is for equivalent reflections and *N* is their number. $I(\hbar kl)$ is an average for one unique reflection and the suffix *hkl* means unique reflections.

(ii) Precision-indicating merging R-value.

$$R_{pim} = \frac{\sum_{hkl} \left(\frac{1}{N-1} \right)^{1/2} \sum_{i=1}^{N} \left| I_i(hkl) - \overline{I(hkl)} \right|}{\sum_{hkl} \sum_{j=1}^{N} I_i(hkl)}$$

(iii) A correlation coefficient of integrated intensities between two half datasets randomly divided.

Table S2. Restrained least-squares refinement statistics of ΔPsbM-PSII.

Dataset	ΔPsbM_0.4MGy
Resolution (Å)	48.8 – 2.2
R / R_{free}	0.17 / 0.23
DPI (Å)	0.19
No. of chains	38
No. of residues	5147
No. of water molecules	2317
No. of ligand molecules	351
Averaged B-factor (Å^2)	42.0
R.M.S. deviations	
Bond lengths (Å)	0.016
Bond angles (deg)	2.34
Ramachandran plot (%)	
Favoured region	97.4
Allowed region	2.40
Outlier region	0.20

The dataset name is combined with the averaged X-ray dose.

Table S3. Transmembrane helices in the ΔPsbM-PSII structure and distances between two centers of transmembrane helix and dimer.

Subunit		Amino acid residue number in helix		Distance between helix and dimer centers (Å)		Averaged distance from dimer center (Å)	Difference of the distance (Å)	Averaged B-factor (Å²)
		start	last	A-monomer	B-monomer		B-A monomer	
PsbL		17	35	14.180	14.203	14.191	0.023	27.3
PsbT		4	22	17.245	17.242	17.243	-0.003	30.0
PsbB/C P47	I	19	39	23.537	23.670	23.604	0.132	30.6
	II	95	113	27.950	28.102	28.026	0.152	30.7
	III	138	158	44.132	44.263	44.197	0.131	34.8
	IV	197	217	48.592	48.731	48.661	0.139	36.5
	V	236	254	34.235	34.279	34.257	0.044	29.5
	VI	453	471	29.463	29.458	29.461	-0.005	28.4
PsbD/D2	A	31	54	53.490	53.394	53.442	-0.095	32.8
	B	110	129	46.245	46.141	46.193	-0.104	30.3
	C	142	160	35.626	35.586	35.606	-0.040	27.4
	D	194	213	29.725	29.732	29.729	0.007	24.4
	E	272	288	28.024	28.014	28.019	-0.011	25.6
PsbA/D1	A	31	54	34.028	34.040	34.034	0.012	27.4
	B	111	130	39.109	39.137	39.123	0.028	27.7
	C	143	161	41.703	41.729	41.716	0.026	26.9
	D	195	214	41.152	41.163	41.158	0.011	27.7
	E	276	292	44.882	44.890	44.886	0.009	27.8
PsbC/C P43	I	51	69	73.629	73.776	73.703	0.148	36.2
	II	112	130	80.560	80.682	80.621	0.122	39.5
	III	160	178	76.337	76.371	76.354	0.035	42.5
	IV	234	252	74.604	74.655	74.630	0.051	45.3
	V	271	289	58.035	58.141	58.088	0.106	33.3
	VI	425	445	54.094	54.169	54.131	0.076	31.1

Atomic coordinates (x, y, z) of the dimer center was (15.933, 19.660, 15.901) in Å unit.

Table S3. Transmembrane helices in the ΔPsbM-PSII structure and distances between two centers of transmembrane helix and dimer (continued).

Subunit		Amino acid residue number in helix		Distance between helix and dimer centers (Å)		Averaged distance from dimer center (Å)	Difference of the distances (Å)	Averaged B-factor (Å^2)
		start	last	A-monomer	B-monomer		B-A monomer	
PsbE		19	38	74.093	73.927	74.010	-0.166	48.8
PsbF		20	40	65.006	64.939	64.973	-0.066	39.0
PsbJ		11	30	67.928	67.928	67.928	0.000	44.6
PsbK		20	39	71.794	71.914	71.854	0.120	40.9
Psb30		20	37	78.354	78.446	78.400	0.092	53.1
PsbZ	1	3	25	89.240	89.456	89.348	0.216	53.8
	2	39	57	93.345	93.483	93.414	0.138	52.7
PsbI		3	22	48.608	48.629	48.618	0.021	39.2
PsbX		7	29	61.089	61.006	61.047	-0.083	47.5
PsbH		28	46	51.863	51.889	51.876	0.025	39.7

Atomic coordinates (x, y, z) of the dimer center was (15.933, 19.660, 15.901) in Å unit.

Table S4. Transmembrane helices in the 3WU2 structure superposed to ΔPsbM-PSII and distances between two centers of transmembrane helix and dimer.

Subunit		Amino acid residue number in helix		Distance between helix and dimer centers (Å)		Averaged distance from dimer center (Å)	Difference of the distance (Å)	Averaged B-factor (Å²)
		start	last	A-monomer	B-monomer		B-A monomer	
PsbL		17	35	14.636	14.648	14.642	0.012	31.6
PsbT		4	22	17.361	17.379	17.370	0.018	31.2
PsbB/C P47	I	19	39	23.332	23.380	23.356	0.048	30.3
	II	95	113	27.653	27.634	27.644	-0.019	31.6
	III	138	158	44.120	44.182	44.151	0.062	37.6
	IV	197	217	48.602	48.644	48.623	0.042	39.5
	V	236	254	34.406	34.414	34.410	0.008	30.1
	VI	453	471	29.648	29.659	29.654	0.011	31.1
PsbD/D2	A	31	54	53.757	53.699	53.728	-0.058	34.8
	B	110	129	46.506	46.468	46.487	-0.038	32.1
	C	142	160	35.922	35.886	35.904	-0.036	29.3
	D	194	213	30.004	30.016	30.010	0.012	26.8
	E	272	288	28.327	28.328	28.328	0.001	27.6
PsbA/D1	A	31	54	34.074	34.106	34.090	0.032	29.2
	B	111	130	39.202	39.239	39.221	0.037	29.5
	C	143	161	41.866	41.903	41.885	0.037	28.5
	D	195	214	41.449	41.458	41.454	0.009	29.0
	E	276	292	45.092	45.119	45.106	0.027	30.3
PsbC/CP43	I	51	69	73.803	73.908	73.856	0.105	40.41
	II	112	130	80.690	80.807	80.749	0.117	47.23
	III	160	178	76.407	76.486	76.447	0.079	46.04
	IV	234	252	74.612	74.683	74.648	0.071	48.59
	V	271	289	58.193	58.260	58.227	0.067	36.86
	VI	425	445	54.248	54.309	54.279	0.061	32.64

Atomic coordinates (x, y, z) of the dimer center was (15.933, 19.660, 15.901) in Å unit.

Table S4. Transmembrane helices in the 3WU2 structure superposed to ΔPsbM-PSII and distances between two centers of transmembrane helix and dimer (continued).

Subunit		Amino acid residue number in helix		Distance between helix and dimer centers (Å)		Averaged distance from dimer center (Å)	Difference of the distances (Å)	Averaged B-factor (Å^2)
		start	last	A-monomer	B-monomer		B-A monomer	
PsbE		19	38	74.250	74.070	74.160	-0.180	50.8
PsbF		20	40	65.175	65.067	65.121	-0.108	42.7
PsbJ		11	30	68.070	68.074	68.072	0.004	45.0
PsbK		20	39	71.981	72.091	72.036	0.110	46.0
Psb30		20	37	78.530	78.610	78.570	0.080	59.1
PsbZ	1	3	25	89.700	89.582	89.641	-0.118	67.6
	2	39	57	93.485	93.640	93.563	0.155	63.8
PsbI		3	22	48.613	48.619	48.616	0.006	40.1
PsbX		7	29	61.276	61.244	61.260	-0.032	51.0
PsbH		28	46	51.994	52.033	52.014	0.039	42.2

Atomic coordinates (x, y, z) of the dimer center was (15.933, 19.660, 15.901) in Å unit.

Table S5. Shift of ΔPsbM-PSII transmembrane helices from 3WU2.

Subunit		Amino acid residue number in helix		Shift of helix center from 3WU2 to ΔPsbM-PSII (Å)		Averaged shift (Å)	Averaged radial shift* (Å)	Averaged lateral shift** (Å)
		start	last	A-monomer	B-monomer			
PsbL		17	35	0.488	0.458	0.473	-0.451	-0.144
PsbT		4	22	0.355	0.316	0.335	-0.127	-0.310
PsbB/CP47	I	19	39	0.444	0.525	0.484	0.248	0.416
	II	95	113	0.415	0.588	0.502	0.382	0.324
	III	138	158	0.113	0.215	0.164	0.046	0.157
	IV	197	217	0.119	0.178	0.149	0.038	0.144
	V	236	254	0.231	0.233	0.232	-0.153	0.174
	VI	453	471	0.253	0.308	0.281	-0.193	0.204
PsbD/D2	A	31	54	0.307	0.366	0.336	-0.286	-0.176
	B	110	129	0.280	0.355	0.317	-0.294	-0.120
	C	142	160	0.298	0.301	0.299	-0.298	-0.097
	D	194	213	0.290	0.305	0.297	-0.281	-0.097
	E	272	288	0.307	0.315	0.311	-0.309	-0.038
PsbA/D1	A	31	54	0.202	0.166	0.184	-0.056	-0.175
	B	111	130	0.220	0.185	0.202	-0.097	-0.177
	C	143	161	0.221	0.242	0.231	-0.169	-0.158
	D	195	214	0.311	0.330	0.321	-0.296	-0.123
	E	276	292	0.244	0.267	0.276	-0.219	-0.167
PsbC/CP43	I	51	69	0.211	0.189	0.200	-0.153	-0.129
	II	112	130	0.207	0.184	0.196	-0.128	-0.148
	III	160	178	0.093	0.143	0.118	-0.093	-0.073
	IV	234	252	0.079	0.072	0.076	-0.018	-0.074
	V	271	289	0.182	0.198	0.190	-0.138	-0.131
	VI	425	445	0.222	0.210	0.216	-0.147	-0.158

* Negative values correspond to that the helix moves near the dimer center.

** The rotation axis passing through the dimer center from stromal to lumenal sides is defined, and the positive values indicate the right-handed rotation.

Table S5. Shift of ΔPsbM-PSII transmembrane helices from 3WU2 (continued).

Subunit		Amino acid residue numberin helix		Shift of helix center from 3WU2 to ΔPsbM-PSII (Å) (Å)		Averaged shift (Å)	Averaged radial shift* (Å)	Averaged lateral shift** (Å)
		start	last	A-monomer	B-monomer			
PsbE		19	38	0.296	0.247	0.271	-0.150	0.226
PsbF		20	40	0.296	0.212	0.254	-0.148	0.206
PsbJ		11	30	0.277	0.226	0.252	-0.144	0.207
PsbK		20	39	0.271	0.209	0.240	-0.182	0.156
Psb30		20	37	0.304	0.253	0.278	-0.170	0.220
PsbZ	1	3	25	0.558	0.177	0.367	-0.293	0.222
	2	39	57	0.343	0.213	0.278	-0.149	0.235
PsbI		3	22	0.224	0.178	0.201	0.002	-0.201
PsbX		7	29	0.291	0.298	0.294	-0.213	0.203
PsbH		28	46	0.196	0.197	0.197	-0.138	0.140

* Negative values correspond to that the helix moves near the dimer center.

** The rotation axis passing through the dimer center from stromal to lumenal sides is defined, and the positive values indicate the right-handed rotation.

Table S6. Atomic distances (Å) between two metal ions in the oxygen-evolving complex.

	ΔPsbM_0.4MGy	3WU2_0.43MGy[a]	4UB6_XFEL[b]	4UB8_XFEL[b]
Mn1-Mn2	2.77, 2.75	2.87, 2.76	2.61, 2.67	2.74, 2.68
Mn1-Mn3	3.41, 3.29	3.28, 3.29	3.18, 3.24	3.27, 3.10
Mn1-Mn4	4.98, 4.87	4.99, 4.92	4.97, 4.95	4.97, 4.89
Mn2-Mn3	2.87, 2.77	2.88, 2.92	2.67, 2.70	2.73, 2.71
Mn2-Mn4	5.31, 5.24	5.44, 5.38	5.18, 5.17	5.21, 5.27
Mn3-Mn4	2.84, 2.81	2.97, 2.89	2.83, 2.86	2.88, 2.91
Ca-Mn1	3.68, 3.51	3.55, 3.49	3.45, 3.51	3.49, 3.43
Ca-Mn2	3.40, 3.37	3.39, 3.30	3.29, 3.35	3.33, 3.32
Ca-Mn3	3.49, 3.42	3.42, 3.41	3.39, 3.47	3.41, 3.33
Ca-Mn4	3.83, 3.82	3.79, 3.80	3.86, 3.76	3.71, 3.76
Averaged difference*	—	0.016	-0.066	-0.065

The dataset name is combined with the averaged X-ray dose except the XFEL structures. Two values in each frame are corresponding to A- and B-monomers. *The averaged difference of atomic distances, calculated using the ΔPsbM-PSII structure as the standard. [a]Umena et al. 2011, and [b]Suga et al., 2015.