10 Appendix

Table 10.1: H-bonding and coordinating residues of cofactors

Cofactor	Residue/atom	Distance [Å]
P_{D1} (Mg^{2+})	D1-His198Nε2	2.2
P_{D2} (Mg^{2+})	D2-His197Nε2	2.2
Chl_{D2} (13^3 carbonyl)	D1-Gln199NεH	3.4
$Pheo_{D1}$ (13^1 carbonyl)	D1-Gln130NεH	3.5
$Pheo_{D1}$ (13^3 carbonyl)	D1-Tyr126OηH	2.7
$Pheo_{D1}$ (17^3 carbonyl)	D1-Tyr147OηH	2.9
$Chlz_{D1}$ (Mg^{2+})	D1-His118Nε2	2.8
$Chlz_{D2}$ (Mg^{2+})	D2-His117Nε2	2.5
Fe^{2+}	D1- His 215Nε2	2.0
	D1- His 272Nε2	2.1
	D2- His 214Nε2	2.1
	D2- His 268Nε2	2.3
Tyr_Z (OH)	D1-Gln165Nε	2.9
	D1-Glu189Oε1	3.2
	D1-His190Nε	3.9
Tyr_D (OH)	D2-Gln164Oε	2.6
	D2-His189Nε	2.6
Mn55	D1-Asp170Oε1	3.3
	D1-Asp170Oε2	2.6
	D1-Glu333Oε1	2.0
	D1-Glu333Oε2	2.2
Mn56	D1-His332Nε2	2.9
	D1-Glu189Oε2	3.1
Mn57	D1-Glu189Oε2	3.0
Cyt *b*-559 (Fe^{2+})	V-His41Nε2	2.1
	V-His42 Nε2	2.1
Cyt *c*-550 (Fe^{2+})	E-His23Nε2	2.2
	F-His24 Nε2	1.9

Table 10.2 Distances (Å) between cofactors of the PSIIcc reaction centre. Lower left closest edge-to-edge distances Upper right: centre-to-centre distances.

	P_{D1}*	P_{D2}*	Chl_{D1}*	Chl_{D2}*	$Pheo_{D1}$†	$Pheo_{D2}$†	$Chlz_{D1}$*	$Chlz_{D2}$*	Q_A‡	Fe^{2+}	Tyr_Z§	Try_D§	Mn¶	Cyt-*c*‖	Cyt-*b*‖
P_{D1}*	-	8.3	10.5	12.3	15.4	18.6	32.2	35.8	27.7	27.8	13.7	19.2	18.2	39.9	41.6
P_{D2}*	3.4	-	12.3	10.8	17.9	15.5	36.7	31.2	27.8	27.3	20.7	13.2	23.7	45.1	41.8
Chl_{D1}*	3.6	3.6	-	20.9	10.5	23.3	24.6	43.0	23.4	26.6	16.9	23.9	20.2	46.6	49.9
Chl_{D2}*	3.6	3.7		-	22.8	10.8	43.8	23.8	30.7	27.1	24.5	16.3	28.5	44.1	31.5
$Pheo_{D1}$†			3.8		-	21.3	24.6	44.0	13.9	17.9	23.0	31.0	27.9	52.6	46.5
$Pheo_{D2}$†				3.8		-	45.4	23.3	23.9	18.5	32.1	22.8	36.7	54.5	29.8
$Chlz_{D1}$*							-	66.8	32.9	40.1	27.6	47.6	29.3	54.5	68.7
$Chlz_{D2}$*								-	46.6	40.0	47.5	27.2	50.5	59.6	26.3
Q_A‡									-	9.0	36.7	40.0	41.8	65.8	47.2
Fe^{2+}										-	38.7	38.5	44.1	65.7	39.1
Tyr_Z§	7.7	15.6									-	28.0	6.3	30.5	51.0
Try_D§	14.2	7.9										-	28.7	44.6	44.6
Mn¶													-	28.0	55.8
Cyt-*c*‖	37.6	42.0												-	61.1
Cyt-*b*‖															-

* position of central Mg^{2+}

† centre of mass of N1 to N4 of the chlorin ring

‡ centre of mass

§ TyrOη

¶ Mn(57) was considered for all calculations

‖ position of central Fe^{2+} of haem

Table 10.3: Protein environment and coordination of cofactors within the ETC.

number	Coordination	Distance [Å][a]	Angle [°][b]	contacts	Hydrophobic contacts
P_{D1}	D1-His198	2.2	89		D1-Met183, D1-Ile192, D1-Thr286, D2-Leu279, D1-Phe186, D1-Val202, D1-Val205, D1-Phe206, D1-Ile290, sidechain of Chl_{D1} and Chl_{D2}
P_{D2}	D2-His197	2.5	87	π-stacking D2-Trp191 with D2-His197	D2-Leu279, D2-Leu182*, D2-Trp191, D2-Ser282, D1-Leu283*, D2-Phe185, D2-Val201, D1-Met183, D1-Val204, D2-Leu205, D2-Val286, sidechain $Chl_{D1}$and Chl_{D2}
Chl_{D1}	Indirect *via* D1-Thr179	5.1	35	D2-Met198 close to O1D	D1-Thr179, D1-Phe158, D1-Val157 D1-Phe119, D1-Thr179, D1-Phe180, D1-Met183, D1-Met172, D1-Ile176, D2-Met198, D2-Val201, D2-Leu205, phytolchain of P_{D1}, sidechain P_{D2} Z5, in van der Waals contact to P_{D1}, P_{D2} and $Pheo_{D1}$
Chl_{D2}	Indirect *via* backbone oxygen of D2-Va175	6.3	63	π-stacking D1-Phe206 possible H-bond to D1-Gln199	D2-Ile178, D2-Phe157, D2-Val156, D2-Gly118, D2-Ile178, D2-Phe179, D2-Leu182 D2-Pro171, D2-Val175, D1-Gln199, D1-Val202, D1-Phe206, in van der Waals contact to P_{D1}; P_{D2} and $Pheo_{D2}$
$Pheo_{D1}$	-	-	63	possible H-bond to D1-Tyr126 (2.4 Å), D1-130Gln and D1-Tyr147	D1-Tyr147, D1-Pro150, D1-Tyr126, D2-Ile213, D1-GlnA130, D1-Ile143, D2-Leu209, D2-Ala212, D2-Phe257, D1-Val283, D2-Leu205, phytolchain P_{D1} and Chl_{D1}
$Pheo_{D2}$	-	-	61	D1-Met214 is close by	D2-Phe146, D1-Pro149, D2-Phe125, D2-Met214, D2-Gln129, D2-Asn142, D1-Leu210, D1-Ala213, D1-Ile259, D2-Leu279, D1-Phe206 sidechain P_{D2}
$Chlz_{D1}$	D1-His118	3.0	85		D1-Thr40, D1-Pro39, D1-Ala43, D1-Leu114, D1-Leu121, D1-Ile136, unassigned TMH 8
$Chlz_{D2}$	D3-His117	2.5	88	possible H-bond to backbone D2-Leu91	D2-Cys40, D2-Pro39, D2-Leu43, D2-Phe113, D2Phe120, D2-Leu136, unassigned TMH 1

[a] distance of the coordinating residue to the central Mg^{2+}

[b] angle between the heterocycle plane normal and the pseudo-*C2*(Fe^{2+}) axis

Table 10.4: Protein environment of Chl*a* within the antenna proteins CP47 and CP43.

number	Coordination	Distance [Å][a]	Angle [°][b]	Orientation[c]	contacts	hydrophobic contacts
11	clostest CP47-Asp188		83	+		CP47-Asp188, CP47-Phe190, Chl*a*12
12	CP47-His201	2.6	86	+		CP47-Pro192, CP47-Ala205, CP47-Val208, CP47-Phe247, CP47-Val251, CP47-Thr25, Chla11, Chla13,
13	CP47-His202	2.2	68	+		CP47-Cys150, CP47-Phe153, CP47-His201, Chla12, Chla14, Chla16, phytolchain of Chl*a*12 and Chl*a*14
14	CP47-His455	2.4	43	+		CP47-Trp33, CP47-Val245, CP47-Ala249, CP47-Val252, CP47-Phe451, CP47-Phe458, CP47-Phe462, Chl*a*15 and Chl*a*26
15	CP47-His100	2.6	84	+		CP47-Val30, CP47-Trp33, CP47-Ala34, Chl*a*16, phytolchain of Chl*a*14
16	CP47-His157	2.0	51	+		CP47-Leu149, CP47-Phe153, CP47-Phe156, Chl*a*13 and Chl*a*15
17	closest CP47-Tyr40	5.2	70	+		CP47-Trp33, CP47-Met37, CP47-Tyr40, CP47-Thr44
21	CP47-His466	2.3	87	+	3 H-bonds from OBD and O1D to CP47-Ser239OH and CP47-Ser240OH	CP43-Leu42, CP43-Ala52, Chl*a*46, phytolchain of Chl*a*44, unassigned TMH 4
22	CP47-His216	2.5	78	-		CP47-Ala212, CP47-Phe139, Chla23, TMH 9
23	closest CP47-Ser241	4.1	84	-	π-stacking CP47-Phe39	CP47-Leu29, CP47-Val30, CP47-Trp33, CP47-Phe426, Chl*a*14, Chl*a*24, Chl*a*25 and Chl*a*27
24	CP47-His469	1.9	69	+		CP47-Thr10, CP47-Ile242, CP47-Phe464, CP47-Gly465, CP47-Trp468, CP47-Arg472, Chl*a*25 and Chl*a*26,
25	CP47-His23	2.5	68	+/short phytol		CP47-Ile13, CP47-His26, CP47-Ile234, CP47-Val237, CP47-Leu238, Chl*a*24, Chl*a*26 and Chl*a*27
26	CP47-His26	2.2	61	+		CP47-Leu29, CP47-Val30, CP47-Trp33, CP47-Phe426, Chl*a*14, Chl*a*24, Chl*a*25 and Chl*a*27
27	maybe CP47-His9	3.2	82	+		Chl*a*25

28	CP47-His142	3.8	75	+		CP47-Leu24, CP47-Ile20, CP47-Met138, CP47-Ile141, Chl*a*28, phytolchain of Chl*a*25
29	CP47-His114	2.2	77	-		CP47-Leu24, CP47-Ala110, Chl*a*28
33	CP43-His232	2.0	66	+/short phytol		CP43-Ala40, CP43-Val439, CP43-Gly440, CP43-Phe437, Chl*a*45 and Chl*a*46
34	CP43-His430	2.7	57	+		CP43-Phe70, CP43-Trp425, CP43-Ser429,
35	CP43-His117	2.4	88	-/no side chains		CP43-Ile89, CP43-Tyr297, CP43-Leu433, CP43-Phe437, CP43-Gly283, Chl*a*34 and Chl*a*46
37	CP43-Met67	3.8	83	+		CP43-Phe60, CP43-Trp425, Chl*a*34
41	CP43-His441	2.3	87	+	H-bond from CP43-Tyr274 to OBD	D1-Met127, D1-Gly128, D1-Trp131, CP43-Ile265, CP43-Leu442, CP43-Ala445, CP43-Gly277,
42	CP43-His251	2.1	63	+		CP43-Leu161, CP43-Gly247, CP43-Ala260, Chl*a*43, CP43-Trp259, CP43-Phe257, Chl*a*43
43	CP43-Ser275	3.4	79	+	maybe indirect	CP43-Met157, CP43-Leu161, CP43-Trp266, CP43-Tyr274, Chl*a*41, Chl*a*42 and Chl*a*45
44	CP43-His444	2.4	72	+	π-stacking CP43-Trp443	CP43-Ala172, CP43-Val233, CP43-Ile240, CP43-Phe289, CP43-Val296
45	CP43-His53	2.7	74	+		CP43-Leu272, CP43-His56, Chl*a*44 and Chl*a*46
46	CP43-His56	2.4	58	-		CP43-Ile60, CP43-Phe437, Chla34, Chl*a*44, Chl*a*45 and Chl*a*47, unassigned TMH 4
47	CP43-Asp39	6.0	78	-		CP43-Leu42, CP43-Ala52, Chl*a*46, phytolchain Chl*a*44, unassigned TMH 4
48	CP43-His164	2.7	77	-/few side chains		CP43-Leu50, CP43-His53 CP43-Phe163, CP43-Val167,
49	CP43-His132	3.3	73	-		CP43-Leu50, CP43-Phe127, CP43-Gly128, CP43-Pro137, Chl*a*48

[a] distance of the coordinating residue to the central Mg^{2+}

[b] angle between the heterocycle plane normal and the pseudo-*C2*(Fe^{2+}) axis

c "+" orientation unambiguously determined, whereas "-" indicates unsure orientation of the Chl*a*.

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Oct 2000 Diploma thesis on „Generation and crystallisation of surface mutants of "6-Hydroxy-D-Nicotine-Oxidase from *Arthrobacter nicotinovorans* and Characterisation and crystallisation of a Pyranose-Oxidase from *Peniophora gigantea*" in the group of Professor G. E. Schulz at the Albert-Ludwigs University of Freiburg, Germany.

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2002 The heart of photosynthesis: Crystallisation and X-ray studies of the Photosystem II. 9th International conference on the crystallization of biological macromolecules. Jena, Deutschland.

2003 Structural and functional analysis of photosystem II antenna proteins from spinach SfB429 Symposium in Potsdam, Germany.

2003 Structural investigations on PsbO, a regulatory subunit of the water oxidase. XIIth International Congress on "Genes, Gene Families and Isozymes" in Berlin, Germany.

2003 Cα–H•••O hydrogen bonds in protein structures: Photosystem I as an example of their importance. XVth International Conference on Horizons in Hydrogen Bond Research. Berlin, Germany.

2004 Biochemical characterization and crystal structure of water oxidizing Photosystem II from *Thermosynechococcus elongatus*. SfB448 Symposium in Caputh, Germany.

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2004 Crystal structure of photosystem II at 3.2 Å provides new details of protein-cofactor interactions. 22th European crystallographic meeting. Budapest, Hungaria.

Oral presentations

2002 The heart of photosynthesis: crystallization and X-ray studies of the photosystem II. 5th Heart of Europe Bio-Crystallography Meeting in Goslar.

2003 Crystallographic studies of Photosystem II from *Thermeosynechococcus elongatus*. ESRF (European Synchrotron Radiation Facility) in Grenoble, France.

2003 Crystallisation and X-ray studies of Photosystem II. Jahrestagung der Deutschen Gesellschaft für Kristallographie in Berlin an der Humboldt-Universität.

2003 Cα–H•••O hydrogen bonds in protein structures: Photosystem I as an example of their importance. 6th Heart of Europe Bio-Crystallography Meeting in Halle (Saale).

2004 Structural comparison of photosystem II structures at medium resolution. Seminar des SfB448 in Berlin.

2004 Crystal structure of the Photosystem II from *Thermosynechococcus elongatus* at 3.2 Å resolution. 7th Heart of Europe Bio-Crystallography Meeting in Krystowa, Poland.