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ORIGINAL PAPER

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Three-dimensional model of zeaxanthin binding PsbS protein associated with nonphotochemical quenching of excess quanta of light energy absorbed by the photosynthetic apparatus

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Abstract A three-dimensional model of the PsbS protein was built with the help of homology-modeling methods. This protein is also known as CP22 and is associated with the protection of photosystem II of thylakoid from excess quanta of light energy absorbed by the photosynthetic apparatus. PsbS is reported to bind two molecules of zeaxanthin at low pH (<5.0) and is believed to be essential for rapid nonphotochemical quenching (qE) of chlorophyll a fluorescence in photosystem II. An attempt was made to explain the pH modulation of the conformation of protein through salt-bridges Glu^{-}(122)-Lys^{+}(113) and Glu^{-}(226)-Lys^{+}(217). Binding of two molecules of zeaxanthin in the three-dimensional model of PsbS is postulated. The molecular mechanism of photoprotection by PsbS is explained through the model.

Keywords PsbS protein · Homology modeling · Photoprotection · Nonphotochemical quenching · Zeaxanthin · Photosystem II

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Introduction

The photosythetic apparatus functions under light quanta in excess of what is required for photochemical reactions. The excess energy is deleterious to the system and also decreases the photosynthetic efficiency. Therefore, the system has a mechanism to dissipate the excess energy. The excess quanta of light energy are either fluoresced or dissipated as heat. Dissipation of energy as heat is reflected as nonphotochemical quenching of fluorescence. Nonphotochemical quenching consists of three components: (1) state transition (qT) (2) photoinhibition (qI); and (3) feedback deexcitation (qE). The feedback mechanism is rapid and protects the system from photodamage. The rapid feedback mechanism depends on a 22-kDa protein PsbS (also known as CP22), which belongs to the superfamily of the light-harvesting protein complexes (LHC) [1, 2]. The protein is the product of a nuclear gene *psbS*. It is a membrane protein with four membrane-spanning regions located at the junction of the distal antenna CP47/CP43 and chlorophyll a/b binding proteins of peripheral LHC II proteins [1–3]. Binding of chlorophylls to PsbS was not confirmed [1, 2]. PsbS is believed to bind two molecules of zeaxanthin at low pH (<5.0) [1]. PsbS with bound zeaxanthin is suggested to be functionally active in nonphotochemical quenching by a rapid feedback mechanism [1]. However, detailed structural information regarding the binding site of zeaxanthin in PsbS and its regulation by change in pH are not available.

A three-dimensional structure of PsbS could provide insight into the binding of zeaxanthin under low pH condition and the function of the protein in photoprotection. In the absence of an X-ray crystallographic structure of the

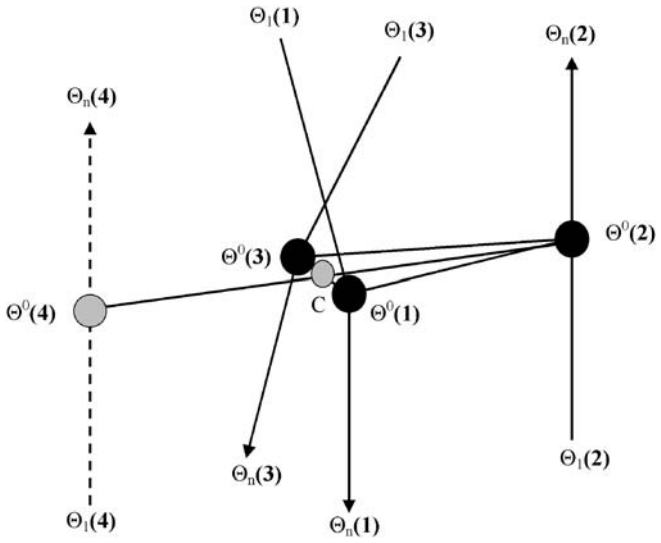

Fig. 1 Representation of axes of transmembrane helices of the Lhcb1 protein. The *arrowhead* represents the C-terminal end. The *broken line* represents the virtual fourth helix obtained by translation of the second helix of Lhcb1. $\Theta_1(i)$ and $\Theta_n(i)$ represent the projections of first and last Cα atoms on the axis of *i*th helix. $\Theta^0(i)$ represents the center of helix axis of *i*th helix. *C* represents the center of the transmembrane helix bundle

protein, we have made an attempt to build a three-dimensional model of PsbS applying principles of homology modeling using the X-ray crystallographic structure of LHC II [Protein Data Bank (PDB) ID 1rwt] as template [4]. However, the LHC II protein contains three membrane-spanning helices, whereas PsbS contains four. In the absence of a template homologous protein with four helices, it is not possible to straightforwardly apply homology modeling. Therefore, a chimera model is built with the structure of Lhcb1 and a fourth helix (reoriented second helix of Lhcb1). The role of PsbS in nonphotochemical quenching is explained with the help of the model.

Materials and methods

The protein sequence of PsbS was obtained from the SWISS-PROT database (Q9XF91, PSBS_ARATH, source *Arabidopsis thaliana*). The coordinates of the Lhcb1 protein were obtained from the PDB (ID 1rwt) [4].

Search for homology

Proteins homologous to PsbS were searched for in the PDB database using BLASTP 2.2.12 [5] and in the Conserved Domain Database (CDD V2.05) by reverse position-specific (RPS)-BLAST 2.2.11 [6]. The alignment of sequences of homologous chlorophyll a/b binding proteins (LHCs) with PsbS was performed using Clustal W 1.82 [7].

Homology modeling

Poor homology over the entire range of sequence and absence of a template protein containing four transmembrane helices in the homologous proteins LHCs poses problems for homology modeling. The problem was overcome by building a chimera model.

PsbS is assumed to have C2 symmetry with regard to orientation of the four membrane-spanning helices. The center of symmetry may lie at the center of the four membrane-spanning helices (H1–4). The orientation of the helical axes of the template protein (1rwt) were estimated and reported earlier [8]. The center of symmetry (C) is determined as the midpoint of the centers of the H1 and H3 helices. The fourth helix (H4) was generated theoretically by translating H2 along the vector $\mathbf{C\Theta^0(3)}$ such that $\Theta^0(3)$ and $\Theta^0(4)$ are equidistant from C (Fig. 1). A chimera model of PsbS was obtained from 1rwt truncated at Pro216 and the virtual helix as template using Modeller V6.2 [9] (Figs. 2 and 3). The salt-bridge between $Lys^+(217)$ and $Glu^-(226)$ in loop H3–H4 was predicted to be derived from the homology among LHC II and PsbS proteins. A stretch of sequence $Lys^+(113)$-$Glu^-(122)$ (KGILAQLNLE) in loop H1–H2 homologous to $Lys^+(217)$-$Glu^-(226)$ (KGA LAQLNIE) in the loop H3–H4 suggests a salt-bridge between $Lys^+(113)$ and $Glu^-(122)$. Distance restraints of 2.9±0.1 Å for salt-bridge formation at these two salt-bridges (OE1/OE2-NZ) were imposed during model building.

Fig. 2 Alignment of sequences of templates Lhcb1 and theoretically generated H4 helix along with sequence of PsbS for homology modeling of a chimera protein PsbS

```
>P1;1rwt.pdb
structureX:1rwt.pdb:14   :A:246  :A:LHCB1:Spinacia oleracea: 2.72: 1.00
SPWYGPDRVKYL---GPFS-GESPSYLTGEFPGDYGWDTAGLSADPETFAKNRELEVIHCRWAMLGALGCVFPEL
LARNG-VKFGEAVWFKAGSQIFSEGGLDYLGNPSLVHAQSILAIWACQVILMGAVE---GYRIAGGPLGEVVDPL
YPGG-SF-DPLGLADDPEAFAELKVKEIKNGRLAMFSMFGFFVQAIVTGKGPLENLA-DHLADPILAIWACQVIL
MGAVEGYRIAGGPLGEVVD-----*
>P1;H4
structureX:H4:  : :  : : H4: Theoretically generated helix
------------------------------------------------------------------------
------------------------------------------------------------------------
------------------------------------------------------------ILAIWACQVIL
MGAVEGYRIAGGPLGEVVD-----*
>P1;PsbS
sequence:PsbS:37  :A:265  :A:psbS:Arabidopsis:-1.00:-1.00
SPVALPSRRQSFVPLALFKPKTKAAPKKVEKPKSKVED--GIFGTSGGIGFTKANELFVGRVAMIGFAASLLGEA
LTGKGILAQLN----------------LETGIPIYEAEPLLLFFILFTLLGAIGALGDRGKFVDDPPTGLEKAV
IPPGKNVRSALGLKEQGPLFGFTKANELFVGRLAQLGIAFSLIGEIITGKGALAQLNIET-GIPIQDIEPLVLLN
VAFFFFAAINPGNGKFITDDGEES*
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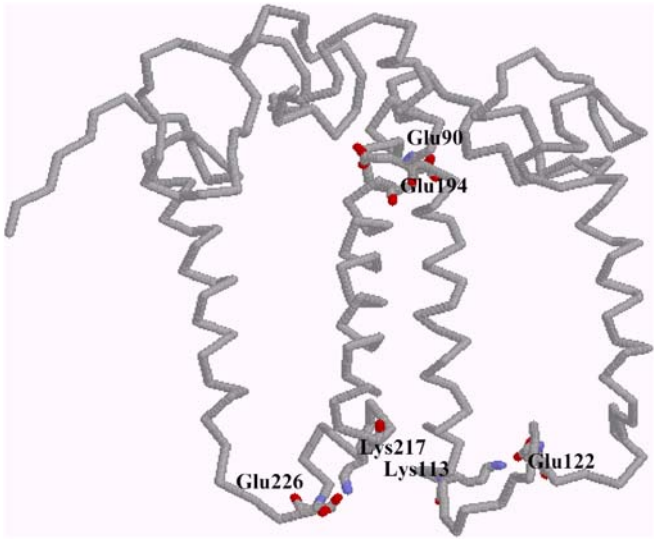

Fig. 3 Backbone structure of the PsbS protein. Residues Glu 90, 122, 194, 226 and Lys 113, 217 are shown. The figure is drawn with RASMOL (Molecular Visualization Program, RasMol V2.6, Roger Sayle, Glaxo Wellcome Research and Development, Stevenage, Hertfordshire, UK)

Binding of zeaxanthin to PsbS

PsbS is reported to interact with zeaxanthin in vitro in a similar manner during nonphotochemical quenching [10]. It is further postulated that two molecules of zeaxanthin may bind to PsbS under low pH (<5.0) conditions.

Low pH conditions on the lumenal side of PsbS were simulated by protonation and neutralization of the negative charge on the pH-sensitive and functionally important residues Glu122 and Glu226 using HyperChem 7.5 [11]. The model was optimized with the Bio+ force field (charmm22) [11] and the conjugate-gradient method followed by thorough refinement by "model" of Modeller V6.2 [9].

The pH-sensitive functionally important residues Glu122 and Glu226 are believed to interact with zeaxanthin [1, 3]. Further, Glu90 and Glu194 are conserved in PsbS and in all LHC except Lhcb4. These are chlorophyll-binding sites in LHCs. However, experiments could not ascertain binding of chlorophyll to PsbS [12, 13]. We postulate that these conserved Glu residues (90, 194) interact with zeaxanthin. The binding of zeaxanthin may be through weak interactions (H-bonds) between the carboxy group of Glu and hydroxy groups of zeaxanthins. A three-dimensional model of PsbS at low pH bound with two molecules of zeaxanthin (PsbS.2ZEX) suggests the feasibility of such interactions. H-bond pairs may be O23 (ZEX267)–OE2 Glu122, O3(ZEX267)–OE2 Glu194, O3 (ZEX266)–OE2 Glu90, and O23(ZEX266)–OE1 Glu226.

The all *trans* zeaxanthin molecule was built using the build module of HyperChem 7.5 [11]. In merge mode, the zeaxanthin molecules were oriented suitably with the PsbS model. The model of PsbS with two molecules of zeaxanthins was subjected to optimization using the optimization module of HyperChem [11] with the Bio+ force field by the conjugate-gradient method up to an root-mean-square deviation (RMSD) of 0.5 kcal mol^{-1} $Å^{-1}$ imposing restraints of 2.8±0.1 Å between atoms forming H-bond pairs. This model was again thoroughly refined using the model subroutine of Modeller V6.2 [9].

Comparison of models

The PsbS structures at high pH (>5.0) and low pH (<5.0) with bound zeaxanthin were compared by superimposition of Cα of the models using HyperChem 7.5 [11] and

Table 1 Helices in PsbS and PsbS.2ZEX proteins

Helix	Beginning		End		Length	Position
Apo PsbS protein						
1	Gly A	75	Thr A	79	5	Stromal
2	Gly A	81	Gly A	114	34	Membrane spanning
3	Pro A	132	Leu A	143	12	Membrane spanning
4	Gly A	179	Glu A	182	5	Stromal
5	Gln A	183	Gly A	216	34	Membrane spanning
6	Gly A	218	Leu A	223	6	Lumenal
7	Asp A	233	Asn A	251		Membrane spanning
					19	
Psbs.2ZEX						
1	GLY A	75	THR A	79	5	Stromal
2	GLY A	81	LYS A	113	33	Membrane spanning
3	PRO A	132	ILE A	146	15	Lumenal
4	GLN A	183	LEU A	203	21	Membrane spanning
5	ILE A	205	GLY A	216	12	Membrane spanning
6	GLY A	218	LEU A	223	6	Lumenal
7	PRO A	230	ASN A	251	22	Membrane spanning

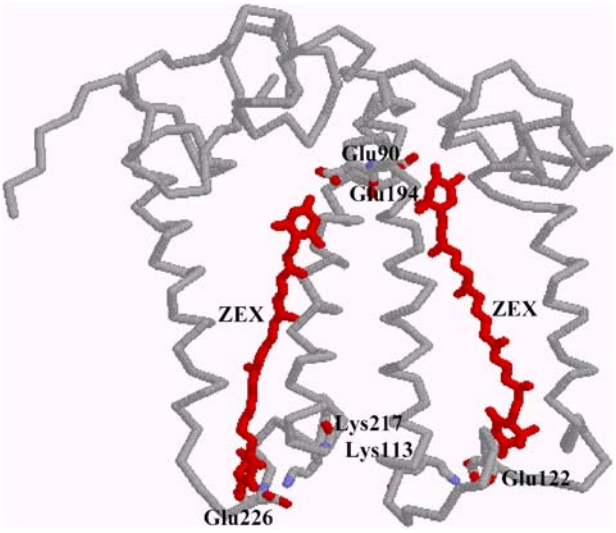

Fig. 4 Backbone structure of the PsbS protein with two molecules of all *trans* zeaxanthin (ZEX). Residues Glu 90, 122, 194, 226 and Lys 113, 217 are shown. The figure is drawn with RASMOL (Molecular Visualization Program, RasMol V2.6, Roger Sayle, Glaxo Wellcome Research and Development, Stevenage, Hertfordshire, UK)

measuring the RMSD. The conformational changes at individual residues in two states of the protein were determined by distances in the Ramachandran map using DIFFMAP [13] as follows:

Conformational distance

$$= \sqrt{\left[(\varphi_1 - \varphi_2)^2 + (\psi_1 - \psi_2)^2\right]} \qquad (1)$$

The coordinates of the theoretical models were deposited in the PDB. The ID codes for PsbS and PsbS.2ZEX are 2aui and 2avl, respectively.

Results

Sequence homology and alignment

RPS-BLAST search of CDD against 11,399 position-specific scoring matrices (PSSMs) suggests that chlorophyll a/b binding proteins (PSSM_Id: 25530) are structurally homologous to PsbS (conserved domain length 157 residues, 80.3% aligned, score=53.8 bits, and *E* value=$2e^{-08}$) [6]. The X-ray crystallographic structures of two chlorophyll a/b binding proteins, 1rwt (Lhcb1 of spinach, resolution 2.72 Å, score=31.2 bits, *E* value=0.22), and 1vcr (Lhcb1 of pea, resolution 9.5 Å, score=32.0 bits, *E* value=0.13) are suggested to be sequences producing significant alignments in the results of the BLASTP search of the PDB database (23,017 sequences) [5]. The structure of 1vcr is a low-resolution incomplete backbone structure. Therefore, the structure of 1rwt was chosen as the template for modeling.

Alignment of a set of sequences of LHC I and II proteins along with PsbS was obtained with Clutal W [7]. Alignment of sequences of templates Lhcb1 (PDB ID 1rwt) (14–216) and theoretically generated helix H4 (1–30) along with sequence of PsbS (*Arabidopsis*) (37–265) were used for homology modeling (Fig. 2).

Model of PsbS

The chimeric model of apo PsbS at pH >5.0 is shown in Fig. 3. The model has four membrane-spanning helices H1–H4 besides three other short helical segments, two on the stromal side and one on the lumenal side (Table 1). Distances OE1(Glu122)–NZ(Lys113) and OE2(Glu226)–NZ(Lys217) are 2.857 and 2.782 Å, respectively, forming salt-bridges for every restraint imposed. Protonation and charge neutralization of Glu122 and Glu 226 lead to the

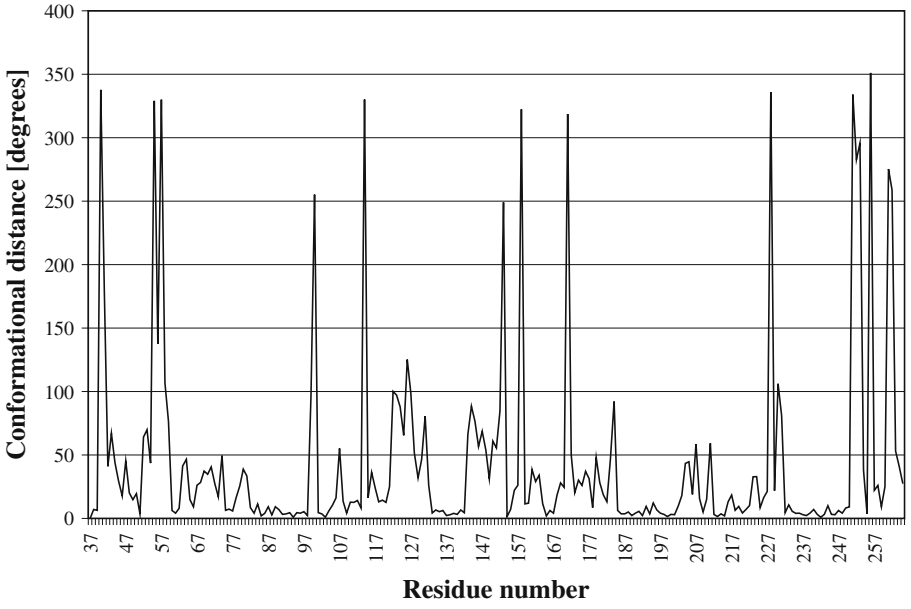

Fig. 5 Comparison of structures of PsbS and PsbS with two molecules of zeaxanthin bound to it. Conformational changes are depicted as residue-wise conformational distances between the two structures as expressed in Eq. 1 in the text using DIFFMAP [13]

Table 2 G-factors of PsbS and PsbS.2ZEX models

G-factor	PsbS	PsbS.2ZEX
Phi–Psi	2.96	−0.33
Chi1–Chi2	−0.50	−0.72
Chi1 only	0.28	−0.05
Chi3–Chi4	0.25	0.21
Omega	−0.27	−0.45
Dihedral	0.84	−0.38
Main chain bonds	−0.23	−0.09
Main chain angles	−0.67	−0.57
Main chain	−0.49	−0.37

breakdown of these salt-bridges. The simulation results in the separation of OE1(Glu122)–NZ(Lys113) and OE2 (Glu226)–NZ(Lys217) to 4.140 and 5.480 Å, respectively. PsbSH binds two zeaxanthin molecules through H-bonds between the hydroxy oxygens of xanthophylls and the carboxy oxygens of Glu yielding holoPsbS (PsbS.2ZEX). The distances OE2(Glu122)–O23(ZEX267), OE2(Glu194)–O3(ZEX267), OE1(Glu226)–O23(ZEX266), and OE2 (Glu90)–O3(ZEX266) are 3.385, 3.038, 3.055, and 2.985 Å, respectively (Fig. 4).

The structures of PsbS and PsbSH exhibit an RMS deviation of 1.205 Å, whereas that between PsbSH and PsbS.2ZEX is 0.447 Å. Residue-wise conformational distances in PsbS and PsbS.2ZEX calculated according to Eq. 1 by DIFFMAP [13] are shown in Fig. 5.

Quality of the model

The quality of structures was tested by PROCHECK online [14]. There are no short contacts and no bond-angle deviations except angle CA-CB-CG at LYS172 (17.2°) in PsbS.2ZEX.

Ramchandran maps of the models reveal that PsbS contains 79.1% of non-Gly-non-Pro residues in most favored, 14.8% in additionally allowed, 3.3% in generously allowed, and 2.7% in disallowed regions. PsbS.2ZEX contains 83.0, 12.6, 0.5, and 3.8% of non-Gly-non-Pro residues in most favored, additionally allowed, generously allowed, and disallowed regions, respectively. Ramchandran outliers are Leu41 (95.38, −179.34), Ser47 (41.08, 148.90), Lys154 (73.11, −45.27), Ser176 (82.93, 148.25), and Asn254 (58.86, −71.17) in PsbS and Ser47 (85.96, 144.49), Thr123 (111.02, 113.43), Arg152(75.88, −65.24), Lys154 (73.60, −45.80), Asp157 (119.37, 120.62), Ser176 (119.0, 157.48), and Asn254 (67.94, −34.48) in PsbS.2ZEX.

G-factors, which are statistical measures of how much the structural parameters of the model deviate from the standard ones, are depicted in Table 2. The overall G-factors of 0.32 and −0.36 for PsbS and PsbS.2ZEX, respectively, suggest that the models are good and acceptable.

Discussion

Three-dimensional model

It was established that PsbS is an essential component in nonphotochemical quenching of chlorophyll fluorescence due to deexcitation by a feedback mechanism (qE) [1, 2]. Although a sequence based schematic folding model for PsbS was proposed [1, 3], a three-dimensional structure of PsbS is not yet available. In the absence of an X-ray crystallographic structure of PsbS, the theoretical model serves as a starting point for investigating the molecular mechanism of nonphotochemical quenching by feedback

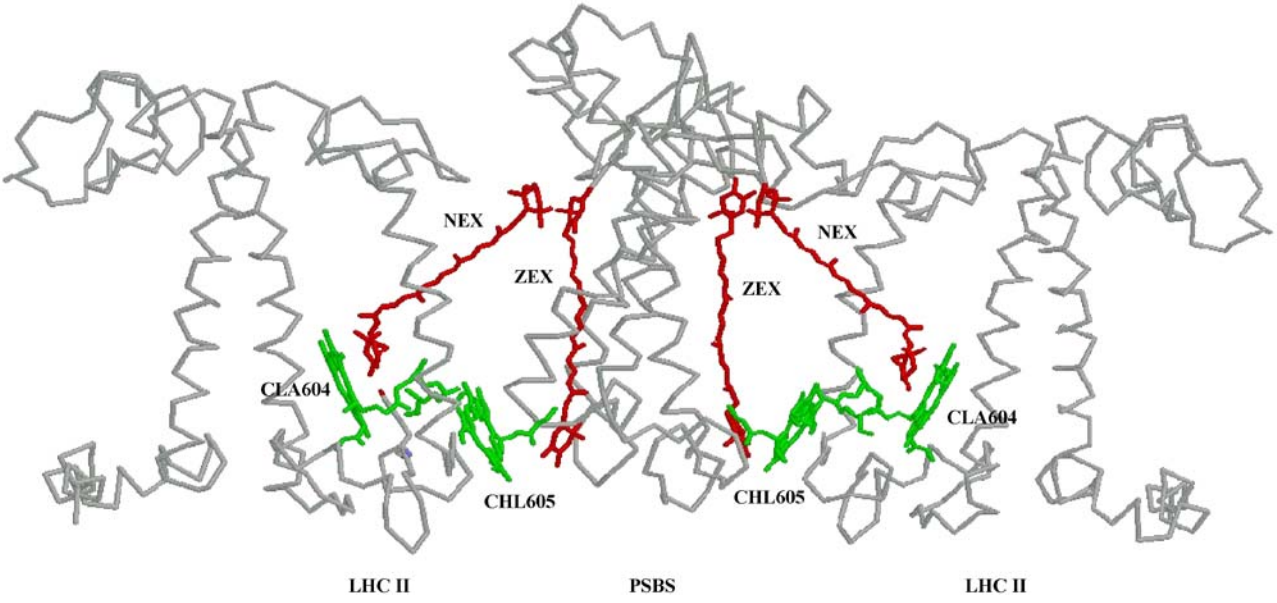

Fig. 6 A graphic overlap of structures of Lhcb1 on either side of PsbS to show a feasible interaction between chlorophyll a (CLA604) and zeaxanthin of PsbS (ZEX) through the molecular wire neoxanthin (NEX). There is possibility of interaction between chlorophyll b (CHL605) and zeaxanthin of PsbS

(qE). The model is similar to the schematic model with four transmembrane helices, one helix on the stromal side of the loop H2–H3 and two helices on the lumenal side of loop H1–H2 and loop H3–H4.

Functionally important residues

Site-directed mutagenesis studies suggest that Glu122 and Glu226 are functionally important residues [3, 15, 16]. These negatively charged residues might form salt-bridges with positively charged Lys113 and Lys 217, respectively. These salt-bridges imposed by restraint in the model are located in the H1–H2 and H3–H4 loop regions of PsbS on the lumenal side of the thylakoid. The salt-bridges may play an important role in the pH sensitivity of PsbS. The proposition of salt-bridges can be tested by site-directed mutation of these Lys residues. Besides, Glu90 and Glu194 are universally conserved in LHCs and PsbS, suggesting that they are functionally important. In LHCs, these residues ligate to chlorophylls. There is no experimental evidence of chlorophyll binding to PsbS [10]. We propose that if chlorophylls bind to PsbS, Glu90 and Glu194 may be the ligating sites. In the absence of chlorophyll, zeaxanthins may bind to these conserved Glu residues. Site-directed mutants could provide evidence for this proposition.

Sensitivity to pH

Decrease in pH (<5.0) in the lumen under high-light conditions may protonate the carboxylate group of Glu and make it charge neutral. Consequently, the salt-bridge may break, inducing a change in the conformation of PsbS. *In silico* simulation gives a result that corroborates this hypothesis. While there is a backbone conformational change with an RMSD 1.205, the change in the side-chain orientations at Lys113, Leu121, Glu122, Leu203, Gly204, Phe207, Lys 217, and Glu226 are significant.

The low pH conformation may be suitable for binding two molecules of zeaxanthin. A model suggests the feasibility of such binding (Fig. 4). The hydroxyl-group containing ends of zeaxanthin may form H-bonds with the Glu90–Glu122 and Glu194–Glu226 pairs. Besides H-bonds at both ends, the hydrophobic interaction of the nonpolar chain with hydrophobic residues of transmembrane helices H1 and H3 may further stabilize the binding. Changes in side-chain orientations of Leu203 and Phe207 with a break in helix H3 at Gly204 may be required to facilitate zeaxanthin binding.

Rapid-feedback mechanism (qE)

The model explains the rapid-feedback mechanism proposed by Niyogi et al. [1]. Lowering the pH in the lumen breaks down salt-bridges in PsbS, bringing about changes in the conformation of the protein, which in turn facilitates the binding of zeaxanthin. The inner ends of bound zeaxanthins are about 15 Å apart, which may facilitate the exchange of singlet excitons between zeaxanthins. Upon increasing pH again, salt-bridge formation may be energetically favored, leading to dissociation of zeaxanthin. PsbS with bound zeaxanthin may act as a site of nonphotochemical quenching by the rapid-feedback mechanism.

Ultrafast formation of the zeaxanthin cation

The mechanism requires a close contact ~3.5 Å between chlorophyll and zeaxanthin of PsbS [17]. Szabo et al. [2] suggest interaction of PsbS with LHC II, the site of quenching being shown at the interface. The crystallographic structure shows chlorophyll b (CHL605) on the periphery of LHC II (PDB ID 1rwt) [18]. However, interaction between chlorophyll a and zeaxanthin is expected. It is possible that neoxanthin of LHC II serves as a molecular wire to establish contact between chlorophyll a (CLA604) and zeaxanthin of PsbS (Fig. 6).

The first singlet excited state (S_1) of zeaxanthin has a short lifetime (10 ps), which facilitates rapid thermal dissipation of excitation energy. The lifetime of zeaxanthin S_1 in reconstituted LHC II was measured as 11 ps [19]. It was also measured by femtosecond transient absorption kinetics in intact thylakoids under maximal qE [20]. In the latter case, excitation of the S_1 state of zeaxanthin was observed after selective excitation of the first excited singlet state of chlorophyll a (Qy band).

Almost all the experimentally observed events could be explained with the help of the present three-dimensional model of zeaxanthin binding the PsbS protein. The model explains the molecular interaction between zeaxanthin and chlorophyll a in the protein matrix that leads to quenching of excess quanta absorbed by the pigments in the photosynthetic apparatus. The postulations made in the present model may be verified experimentally, which is likely to open new avenues for investigation of the molecular mechanism of nonphotochemical quenching.

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