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Supplementary Information for

The crystal structures of *Arabidopsis* and *Chlamydomonas* phosphoribulokinase fill the last gap in the redox structural proteome of the Calvin-Benson cycle

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Supplementary Information

SI Materials and Methods

Activity Assay and Determination of pH and Temperature Dependence

Phosphoribulokinase activity was measured spectrophotometrically (Cary 60 UV-Vis; Agilent) at 25°C in 1 ml cuvette containing 50 mM Tris-HCl (pH 7.5), 10 mM $MgCl_2$, 20 mM KCl, 2 mM ATP, 2.5 mM phosphoenolpyruvate, 0.2 mM NADH, 5 U ml^{-1} pyruvate kinase, 6 U ml^{-1} lactate dehydrogenase and enzyme preparation. Following 1 min of blank acquisition, the reaction was started by the addition 0.5 mM ribulose-5-phosphate.

Temperature dependence was evaluated on aliquots of *At*PRK and *Cr*PRK desalted in PBS buffer and incubated for 20 min at temperatures ranging from 20°C to 60°C. Following incubation, the activity was assayed at 25°C as described above. Activities were measured on two independent protein purifications and are expressed as percentage of the highest measured activity.

The pH dependence of purified enzymes was determined in Britton-Robinson buffer for pH values ranging from 5.0 to 8.5. For pH values ranging from 9.0 to 10.0, 100 mM Glycine buffer was used. To ascertain that pH and buffer composition do not block pyruvate kinase and lactate dehydrogenase activity, their activity was controlled measuring the rate of NADH oxidation in a coupling assay performed at 25°C in 1 ml cuvette containing the above mentioned buffers and 10 mM $MgCl_2$, 20 mM KCl, 2 mM ADP, 0.2 mM NADH, 10 U ml^{-1} pyruvate kinase, 12 U ml^{-1} lactate dehydrogenase. Following 1 min of blank acquisition, the reaction was started by the addition 2.5 mM phosphoenolpyruvate and monitored spectrophotometrically at 340 nm.

Once the functionality of pyruvate kinase and lactate dehydrogenase was verified, to ascertain that their activity did not limit the measurements of PRK activity, the concentration of both enzymes was increased (i.e. from 5 to 15 U ml^{-1} for pyruvate kinase and 6 to 18 U ml^{-1} for lactate dehydrogenase) up to concentrations that did not increase PRK activity further.

Determined the experimental conditions, PRK activity was measured on a Cary 60 UV-Vis spectrophotometer (Agilent) at 25°C in 1 ml cuvette containing the above mentioned buffer at different pH values, 10 mM $MgCl_2$, 20 mM KCl, 2 mM ATP, 2.5 mM phosphoenolpyruvate, 0.2 mM NADH, 10 U ml^{-1} pyruvate kinase, 12 U ml^{-1} lactate dehydrogenase and enzyme preparation. Following 1 min of blank acquisition, the reaction was started by the addition 0.5 mM ribulose-5-phosphate. Activities were measured on two independent protein purifications and are expressed as percentage of the highest measured activity.

Crystallization and Data Collection.

Aliquots of 2 µl for both proteins were mixed to an equal volume of reservoir, and the prepared drop was equilibrated against 900 (*Cr*PRK) and 750 (*At*PRK) μl of reservoir.

*Cr*PRK crystals were obtained in different conditions of the Extension Kit from Hampton Research (solutions 22: 12% w/v PEG 20K, 0.1 M MES, pH 6.5; 26: 30% w/v PEG MME 5K, 0.1 M MES, pH 6.5, 0.2 M ammonium sulfate; 30: 10% w/v PEG 6K, 5% v/v MPD, 0.1 M HEPES, pH 7.5) and Structure screen 1 from Molecular Dimension (MD1-01-CF, solutions 35: 30% w/v PEG 4K, 0.1 M Tris-HCl, pH 8.5, 0.2 M lithium sulfate; and 50: 15% w/v PEG 8K, 0.5 M lithium sulfate). The conditions were optimized and the best diffracting crystal grew in about 10 days, from 22% w/v PEG MME 5K, 0.1 M MES, pH 6.5, 0.2 M ammonium sulfate. *Cr*PRK crystal appeared as needle-like, in the majority of the cases forming a cluster. Aggregates were manually separated and the thicker individuals fished.

*At*PRK crystals showed a bipiramidal morphology and grew in three to five weeks from a reservoir solution containing 1.4 – 1.7 M sodium malonate, pH 5.0. The best diffracting crystal of *At*PRK was obtained in 1.5 M sodium malonate, pH 5.0.

Crystals were mounted from the crystallization drop into cryo-loops, briefly soaked in a cryo-protectant solution containing 30% w/v PEG MME and 20% v/v PEG 200 for *Cr*PRK and 1.7 M sodium malonate, pH 5.0, and 30% v/v glycerol for *At*PRK, then frozen in liquid nitrogen. Diffraction images were recorded at 100 K at the Elettra synchrotron radiation source (Trieste, beam line XRD1) for *Cr*PRK and at the European Synchrotron Radiation Facility (Grenoble, beam line ID14-4) for *At*PRK. Data collection parameters are reported in Table S4.

The data at a resolution of 2.6 Å for *Cr*PRK and 2.5 Å for *At*PRK were processed using XDS (1) and scaled with SCALA (2). The correct space group was determined with POINTLESS (2) and confirmed in the structure solution stage. Data collection statistics are reported in Table S5.

Structure Solution and Refinement.

*Cr*PRK structure was solved by molecular replacement using the program PHASER (3) from PHENIX (4) starting from the coordinates of PRK from *Methanospirillum hungatei* (PDB code 5B3F) (5) deprived of sulfate ions and water molecules. The protein chain was traced by Autobuilt from PHENIX (4) and Buccaneer (6) from CCP4 package. The refinement was performed with REFMAC 5.8.0135 (7) selecting 5% of reflections for R_{free}. The manual rebuilding was performed with Coot (8). The residual electron density map showed the position of a sulfate ion for each monomer coming from the crystallization solution, which was added to the model. Water molecules were automatically added and, after a visual inspection, confirmed in the model if the relative electron density value in the ($2F_o - F_c$) maps exceeded 0.19 $e^-Å^{-3}$ (1.0 σ) and if they fell into an appropriate hydrogen bonding environment. The last refinement cycle was performed with PHENIX (4). The final model of *Cr*PRK lacks six residues at the C-terminal end of both chains.

The structure of *Cr*PRK without sulfate ions and waters, was used as initial model to solve the *At*PRK structure by molecular replacement using MOLREP (9). The refinement was performed as described for *Cr*PRK. The final model of AtPRK lacks three residues at the N-terminal domain and seven and ten residues at the C-terminal domain of chain A and B, respectively.

The refinement statistics of both structures are reported in Table S5. All structure figures were prepared using PyMOL (The PyMOL Molecular Graphics System, Schrödinger, LLC).

Small Angle X-ray Scattering Data Collection.

Data collection parameters are reported in Table S4. A Size Exclusion Chromatography SEC-SAXS experiment was performed using a HPLC system (Shimadzu) directly connected to the measurement capillary. A volume of 100 μl of reduced *Cr*PRK (6.1 mg ml^{-1}) was loaded onto a Superdex 200 10/300 GL column (GE Healthcare) pre-equilibrated in 50 mM Tris-HCl, 150 mM

KCl, pH 7.5. The sample was eluted at a flow rate of 0.5 ml min^{-1} and SAXS frames obtained by 1 s exposure were collected continuously. The automatic pipeline for SEC-SAXS data analysis implemented at BM29 was used to assess the quality of the collected data (10).

Small Angle X-ray Scattering Data Analysis.

Afterwards, a classification of the collected frames as buffer (0-14 ml) or protein frames (14-17.75 ml) was performed on the basis of the SAXS intensity trace (Fig. S13). Statistical test implemented in CorrMap (11) aided by visual inspection, was used to choose the superimposable buffer intensity profiles. The averaging of the buffer profiles, the subtraction of the averaged buffer intensity from the protein data and an automatic analysis of the subtracted protein profiles was performed with a Matlab script. The script used the tools of the ATSAS package (12) to automatically obtain from the subtracted intensity I(q): (i) the I(0) and the gyration radius (R_g) via the Guinier approximation (13) $I(q) = I(0)\cdot\exp[-(qR_g)^2/3]$; (ii) the pair-distance [p(r)] function, from which the maximum particle dimension (D_{max}) was estimated, in addition to an independent calculation of I(0) and R_g. Estimates of the MW were also determined both from the Porod invariant (14) as 0.6 times the Porod volume (V_p) for roughly globular particles (12) and by the invariant volume-of-correlation length (V_c), through a power-law relationship between V_c, R_g and MW that has been parametrized (15). The protein frames giving constant R_g values were scaled to the intensity of the elution maximum and averaged in order to obtain a single representative scattering profile with good signal to noise ratio, presented in the results and used for modelling.

Modeling from SAXS Data

The sequence and the homodimeric state of *Cr*PRK were given as inputs in GASBOR and a 2-fold symmetry was imposed in the calculations. A series of 10 models was generated. The similarity of the structures obtained by repeated calculations was checked by DAMAVER (16) in which the superposition is performed by the SUPCOMB code (17).

All programs used for SAXS data analysis and reconstruction, belong to the ATSAS package 2.7 (12). The graphical representations of the obtained three-dimensional models were built by using

PyMOL (The PyMOL Molecular Graphics System, Schrödinger, LLC).

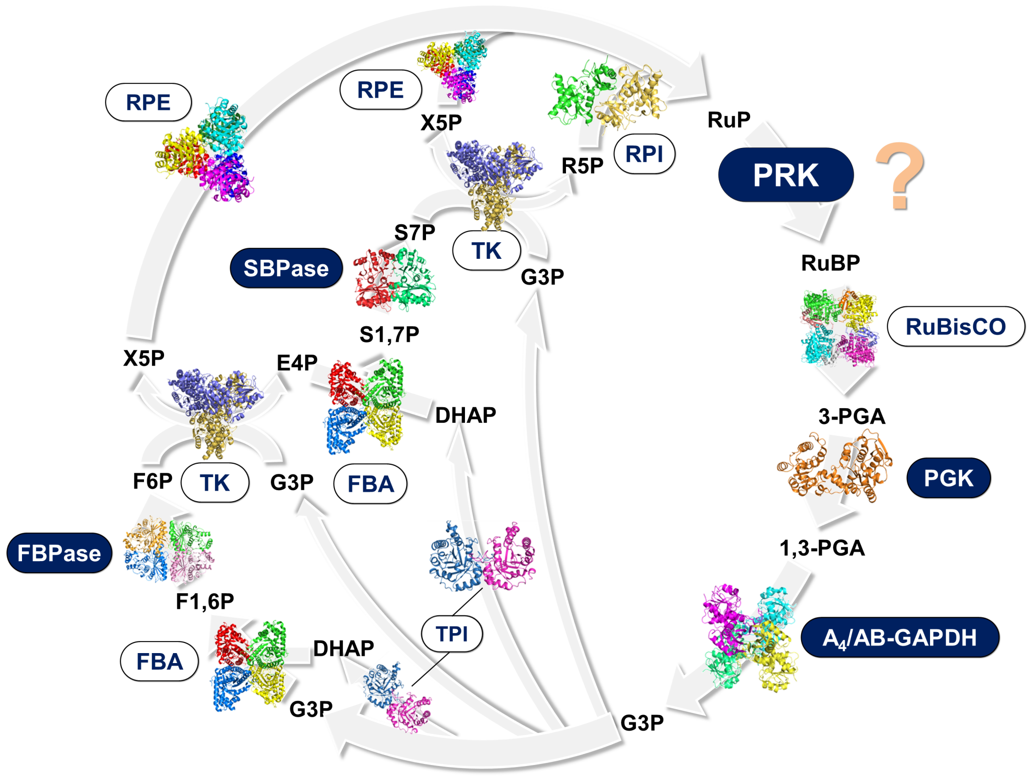

Fig. S1. Schematic representation of the CB cycle. The crystal structure of six chloroplast enzymes from different organisms: RuBisCO, ribulose-1,5-bisphosphate Carboxylase/Oxygenase from *Spinacia oleracia* (PDB ID code 1AUS) (18); GAPDH, glyceraldehyde-3-phosphatedehydrogenase from *Arabidopsis thaliana* (PDB ID code 3K2B) (19); TPI, triose phosphate isomerase from *Chlamydomonas reinhardtii* (PDB ID code 4MKN) (20); FBPase, fructose-1,6-bisphosphatase from *Pisum sativum* (PDB ID code 1DCU) (21); TK, transketolase from *Chlamydomonas reinhardtii* (PDB ID code 5ND5) (22); SBPase, sedoheptulose-1,7-bisphosphatase from *Physcomitrella patens* (PDB ID code 5IZ3) (23); RPE, ribulose-5-phosphate 3-epimerase from *Solanum tuberosa* (PDB ID code 1RPX) (24), is shown. For the remaining three enzymes, the crystal structure of the most homologous enzymes from non-photosynthetic organisms is reported: PGK, phosphoglycerate kinase from *Bacillus stearothermophilus* (PDB ID code 1PHP) (25) approximately 60% homologous to *Chlamydomonas reinhardtii* PGK1 (sequence accession number A8JC04); FBA, fructose-1,6-bisphosphatealdolase from *Toxoplasma gondii* (PDB ID code

5TJS) (26) approximately 55% homologous to *Arabidopsis thaliana* FBA1 (sequence accession number Q9SJU4); RPI, ribose-5-phosphateisomerase from *Toxoplasma gondii* (PDB ID code 4NML) approximately 50% homologous to *Spinacia oleracia* RPI (sequence accession number Q8RU73).

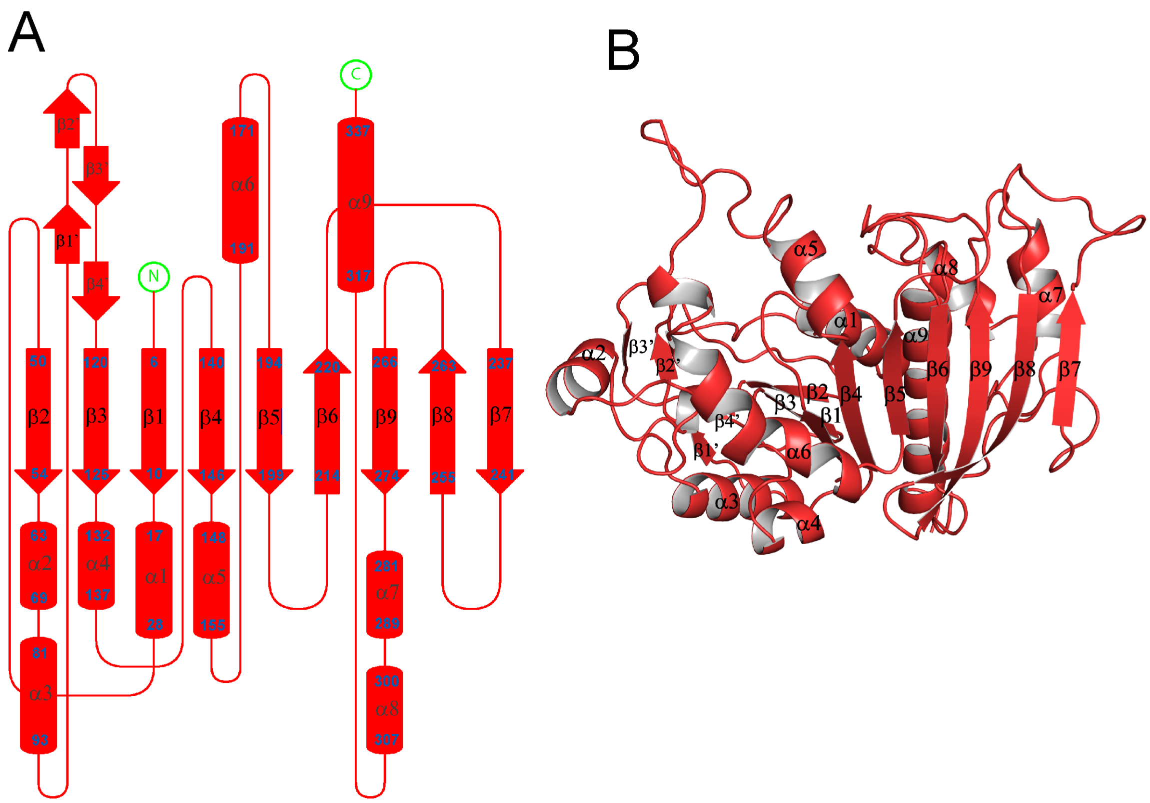

Fig. S2. Crystal structure of *At*PRK's monomer. (A) Topology diagram of *At*PRK. Similarly to *Cr*PRK (Fig. 2*A*), the monomer is composed by a mixed β-sheet of nine strands, by nine α-helices and four additional small β-strands indicated by β'. (B) Cartoon representation of the monomer structure of *At*PRK. Similarly to *Cr*PRK (Fig. 2*B*) the central β-sheet is sandwiched between helices α3, α4 and α6 and helices α1, α7, α8 and α9. The right end of the monomer consists of stand β7 involved in the dimer interface, while the four additional β-strands (β1' to β4') form the left external end of the dimer.

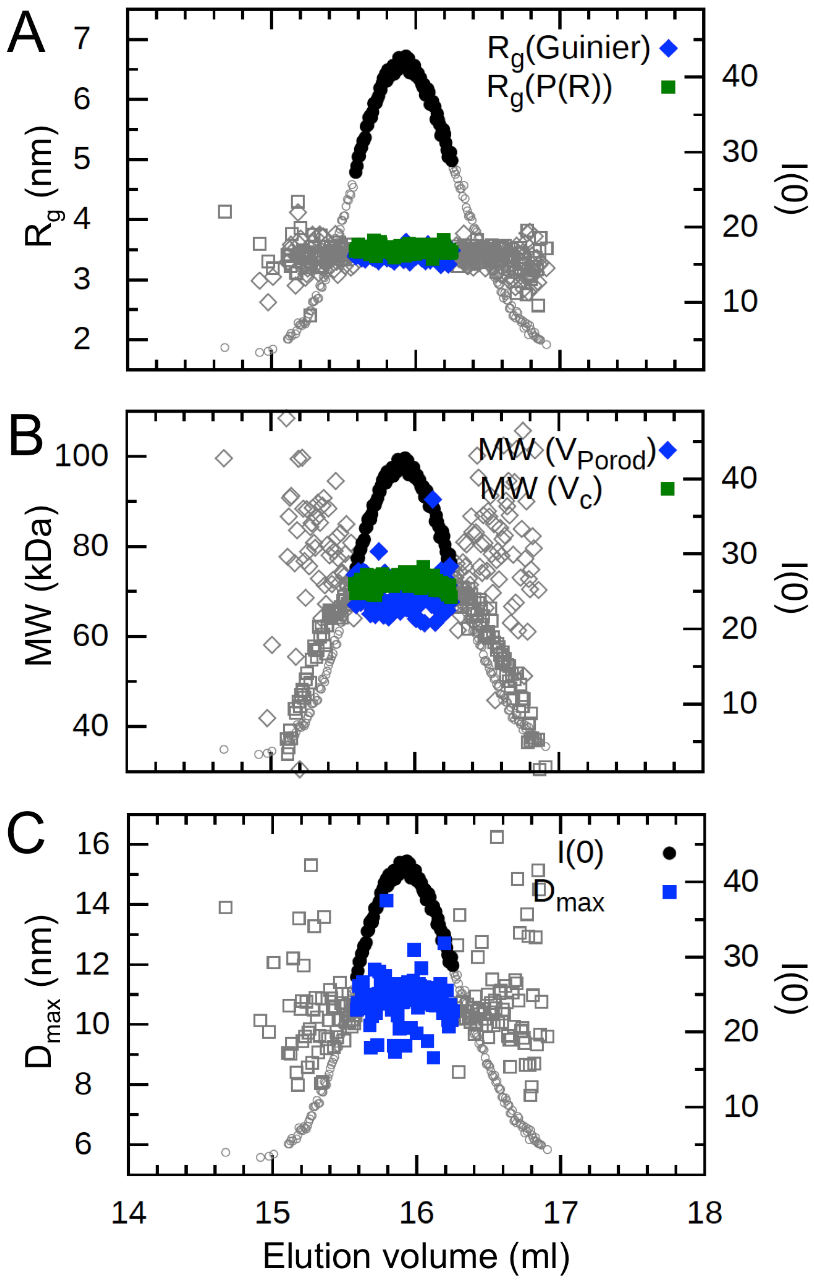

Fig. S3. Parameters determined by SEC-SAXS analysis of *Cr*PRK. (A) I(0) trace (dots) and R_g determined by the Guinier approximation (diamonds) and R_g calculated from the P(r) function (squares). (B) I(0) trace (dots) and MW estimated from the Porod volume (diamonds) and from the volume-of-correlation (squares). (C) I(0) trace (dots) and D_{max} estimated from the P(r) function (squares). The frames used in the average to obtain the representative scattering profile, are highlighted in black compared to the grey neglected frames.

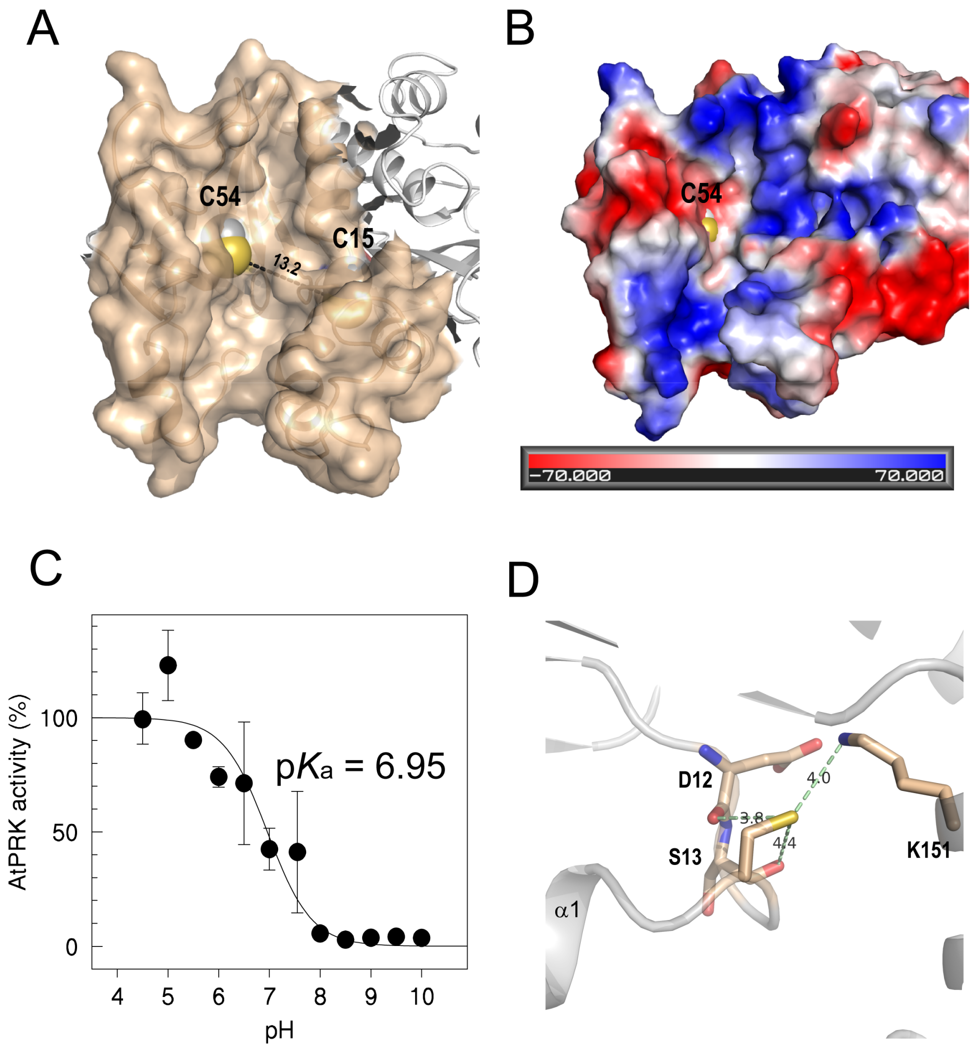

Fig. S4. Active site and TRX-dependent regulation of AtPRK. (A) The catalytic cavity is shown. The distance between the regulatory cysteines is higher than 13 Å. (B) Catalytic cavity electrostatic surface potential. The bottom of the catalytic cavity is marked by a positive potential. The negative potential region observed on the left side of the cavity, is suggested to be involved in the correct positioning of TRX close to regulatory cysteines. (C) The pK_a of Cys15 was determined by measuring the IAM-mediated inactivation as a function of pH. (D) Molecular environment of Cys15 considering a sphere of 5 Å centered on its thiol group. The hydrogen bonds between the thiol group and the neighboring residues and the corresponding distances, are shown.

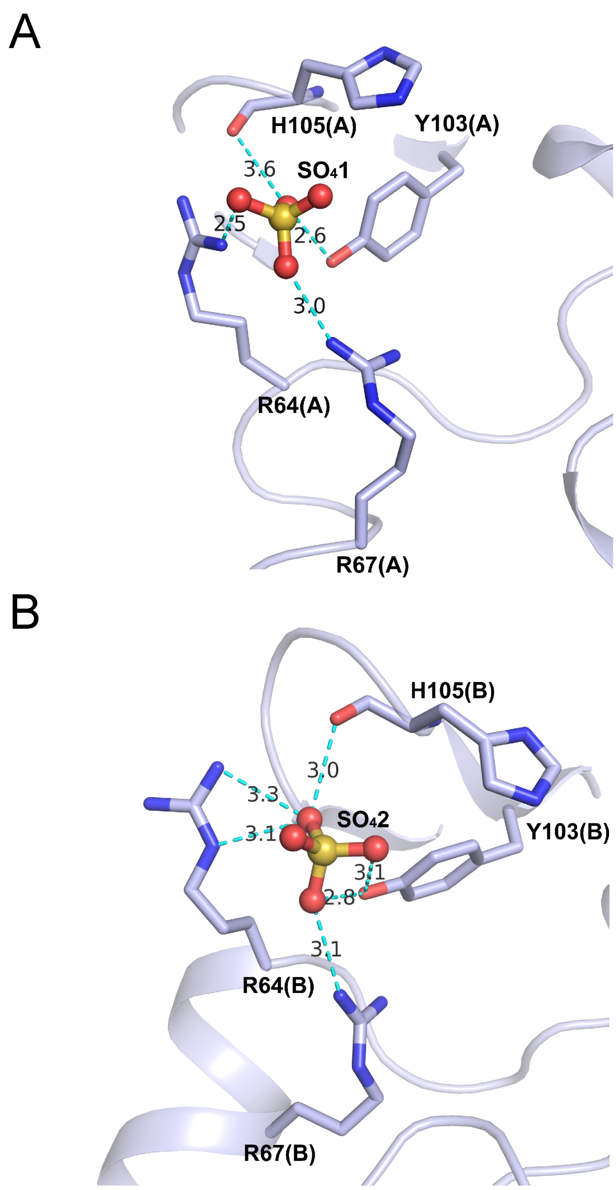

Fig. S5. Binding site of the sulfate ion in *Cr*PRK. The interactions between a sulfate ion coming from the crystallization solution, and protein residues in (A) subunit A and (B) subunit B, are represented. Salt-bridges are formed with Arg64 and Arg67, and hydrogen bonds with Tyr103 and His105.

A

```
                          10        20        30        40        50        60
                 =========+=========+=========+=========+=========+=========+
P. profundum     ------------------------------------------------------------
P. luminescens   ------------------------------------------------------------
E. amylovora     ------------------------------------------------------------
S. flexneri      ------------------------------------------------------------
S. medicae       ------------------------------------------------------------
R. meliloti      ------------------------------------------------------------
C. necator       ------------------------------------------------------------
R. rubrum        ------------------------------------------------------------
R. sphaeroides   ------------------------------------------------------------
A. cryptum       ------------------------------------------------------------
X. flavus        ------------------------------------------------------------
N. hamburgensis  ------------------------------------------------------------
N. vulgaris      ------------------------------------------------------------
R. palustris DX1 ------------------------------------------------------------
R. palustris Bis ------------------------------------------------------------
M. capsulatus    ------------------------------------------------------------
A. ferrooxidans  ------------------------------------------------------------
C. M. oxyfera    ------------------------------------------------------------
T. denitrificans ------------------------------------------------------------
A. vinosum       ------------------------------------------------------------
P. lunula        ---------------------------------MARSRSALFPALAALAALLLWAREAFL
L. polyedrum     ---------------------------MARSRSVVLPLAAAAVALVLLGHVAFVPPAPRP
B. natans        ------KTNVYAIASVVANVALVGVLLYTQTGEVGASVAASSRVHVAPRMVAPKFSMSGL
E. gracilis      -------------------------MMRYDQLIHEGPRQSSPSLLQLASVSATVFCAVFG
P. parvum        ------------------------------------------------MLSLSVGLSVAF
G. theta         -------------------------------------------MGTPLASRSSFASPVAL
T. pseudonana    ------------------------------------------------------------
O. sinensis      -------------------------------------MKLSLGIVALMAASASAFAPTAF
P. tricornutum   ---------------------------------------MKFAVFASLTATAAAFAPTAF
D. lutheri       ------------------------------------------------MRRSRVATPVQR
O. tauri         ------------------------------------------------------------
M. commoda       --------------------------------------------MASMTMSAACAQPLAA
P. sitchensis    ---------------------------------MACPAPTATSTPATVRSWNSQFCSNSP
P. patens        --------------------------------------MAAMACTSAASTALSTPRLAAV
S. oleracea      --------------------------------------MAVCTVYTIPTTTHLGSSFNQN
A. thaliana      --------------------------------------MAVSTIYSTQALNSTHFLTSSS
S. moellendorf.  --------------------------------------MAAACSSSGSSSRIGWFQASSS
T. aestivum      ------------------------------------------MAFCSPHTTTSLRSPCTT
P. trichocarpa   --------------------------------------MAVCTVYTTQSLNSTCSISTPT
M. crystallinum  --------------------------------------------------MAVSAYTVPT
P. sativum       ------------------------------------------------------------
C. variabilis    ---------------------------MQTAAAVQCKPVCRPMAARPHVARRPAQLAASA
C. reinhardtii   ------------------------------------------------------------
V. carteri       -----------------------------------------------MAFTMRAPAPRAT
G. sulphuraria   MELRDSLSTMGFVLPSTTSYVVYKSSSTIKSKKYNKRNYSSVSRVQVGGSKISSWSSNRL
G. kilaueensis   ------------------------------------------------------------
G. violaceus     ------------------------------------------------------------
T. elongatus     ------------------------------------------------------------
Synechocystis sp ------------------------------------------------------------
M. aeruginosa    ------------------------------------------------------------
Cyanothece sp    ------------------------------------------------------------
S. elongatus     ------------------------------------------------------------
A. variabilis    ------------------------------------------------------------
N. spumigena     ------------------------------------------------------------
A. boonei        ------------------------------------------------------------
F. placidus      ------------------------------------------------------------
A. profundus     ------------------------------------------------------------
A. veneficus     ------------------------------------------------------------
M. harundinacea  ------------------------------------------------------------
M. concilii      ------------------------------------------------------------
M. thermophila   ------------------------------------------------------------
M. hungatei      ------------------------------------------------------------
Methanolinea sp  ------------------------------------------------------------
M. boonei        ------------------------------------------------------------
M. limicola      ------------------------------------------------------------
M. petrolearia   ------------------------------------------------------------
M. palustris     ------------------------------------------------------------
M. marisnigri    ------------------------------------------------------------
M. liminatans    ------------------------------------------------------------
Gblocks
Annotation
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P. luminescens    ------------------------------------------------------------
E. amylovora      ------------------------------------------------------------
S. flexneri       ------------------------------------------------------------
S. medicae        ------------------------------------------------------------
R. meliloti       ------------------------------------------------------------
C. necator        ------------------------------------------------------------
R. rubrum         ------------------------------------------------------------
R. sphaeroides    ------------------------------------------------------------
A. cryptum        ------------------------------------------------------------
X. flavus         ------------------------------------------------------------
N. hamburgensis   ------------------------------------------------------------
N. vulgaris       ------------------------------------------------------------
R. palustris DX1  ------------------------------------------------------------
R. palustris Bis  ------------------------------------------------------------
M. capsulatus     ------------------------------------------------------------
A. ferrooxidans   ------------------------------------------------------------
C. M. oxyfera     ------------------------------------------------------------
T. denitrificans  ------------------------------------------------------------
A. vinosum        ------------------------------------------------------------
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L. polyedrum      RAARALTAMRGAANSVPTGLVWPSPEAEAKLREEDGIKMYPTHAWTDDMMPIVPATKE--
B. natans         RPAQREARVAAHGKGVVSTVALDAPVATSEDSMTWSSAKGNEVDAGMGQVHIEAAISNEV
E. gracilis       IGYTFSGGLVENYATTRPVQTQPAALILPKAVRYAGVSQGPQVESREARTALHAAATGTV
P. parvum         SPA--------------------------------------PSVVSQSRVAPRATVVE--
G. theta          -------------------------------------RVTNDKEMDVAIQQISMSLAS--
T. pseudonana     ------------------------MKFLVASLIASASAFSTINTPTLRGNSALAALKD--
O. sinensis       -----------------------------------MPANTLRAAAPASPSALNMALKE--
P. tricornutum    VPS-------------------------------------NLRGVAPSASSLNMALKE--
D. lutheri        VPQ--------------------------------------------TACTVLMATKT--
O. tauri          ---------------------MSASLGFSTSVRAAPVRATRDAVKPRATRARVVTTAK--
M. commoda        RKFQGS--------------------------------RVSGKSVVRAAKRNVTVKAE--
P. sitchensis     LAS-----------------------------------FSLAHTTRRPRRALVVCSVG--
P. patens         KPARSARPVH--------LTSAFHGQSVASVSQVAGFESSGVKYRSAGRRAVVVCKAA--
S. oleracea       NKQVFFNYKR----------------------------SSSSNNTLFTTRPSYVITCS--
A. thaliana       SSKQVF----------------------------------LYRRQPQTNRRFNTLITC--
S. moellendorf.   SSNIGILQHHPWRGSHASSLFSFPKLGARIGSSSGGSGSSGTSSSNRVRVLVCCAAGG--
T. aestivum       IPNSGFRQNQ----------------------VIFFTTRSSRRSNTRHGARTFQVSCA--
P. trichocarpa    KTHLGFNQRH-------------------------VVFYSTNKKTTKRASSAVITCSA--
M. crystallinum   TSHLGFNQKK---------------------QLFFCNKSAYKRVSFSSRPCVITCLAG--
P. sativum        --------------------------------------------------------AG--
C. variabilis     APIARPTFSS-------------------------TLNQRTLKAGRVASRVVVVKAEG--
C. reinhardtii    --------------------------MAFTMRAPAPRATAQSRVTANRARRSLVVRAD--
V. carteri        --------------------------------------AQSRVTASRASRRVLVVKAQ--
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T. elongatus      ------------------------------------------------------MSSK--
Synechocystis sp  ------------------------------------------------------MTTQ--
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S. elongatus      -------------------------------------------------------MSK--
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N. spumigena      ------------------------------------------------------MTTK--
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A. profundus      --------------------------------------------------MLKEKLIK--
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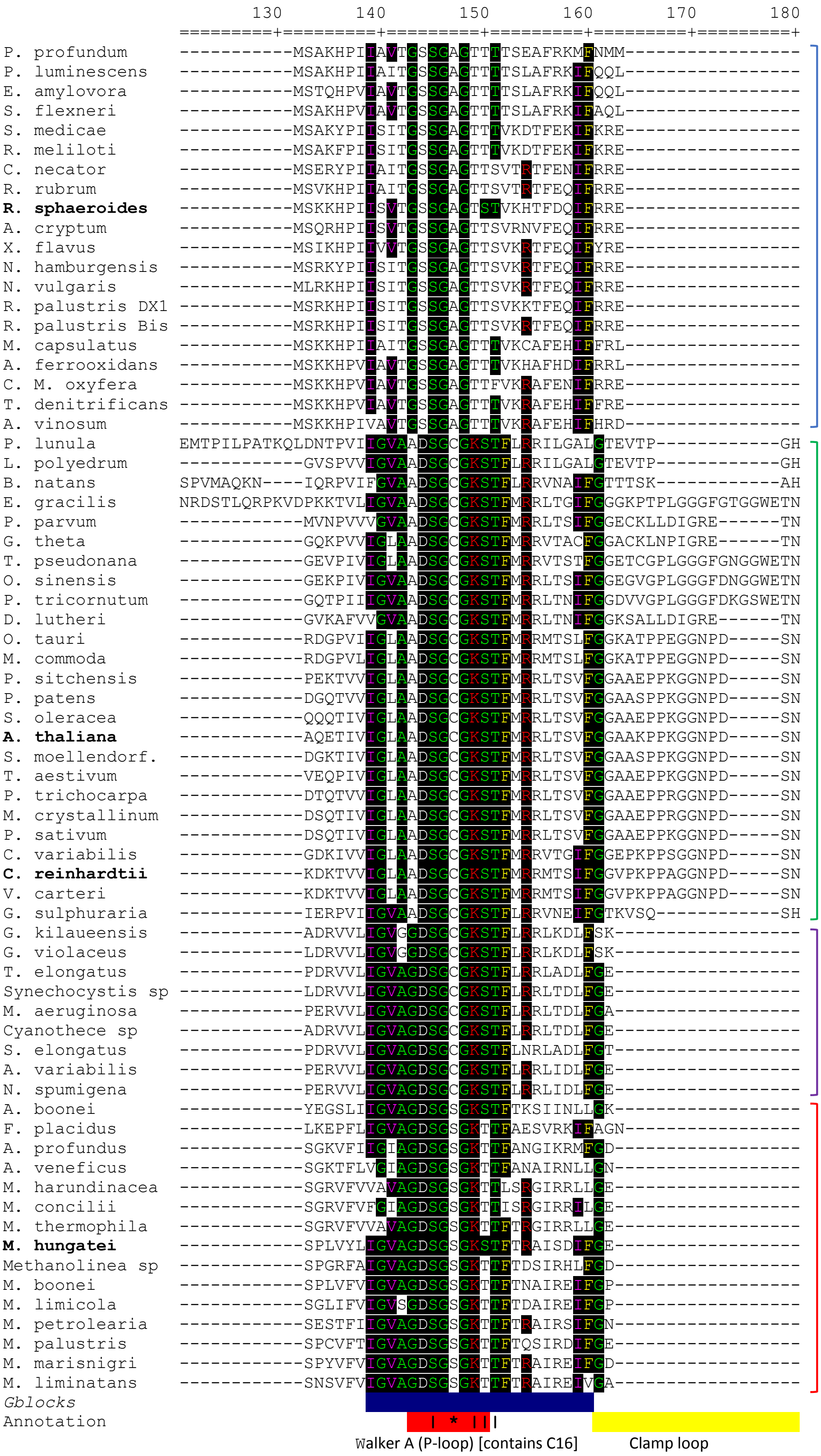

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A. cryptum -----------MSQRHPIISVTGSSGAGTTSVRNVFEQIFRRE-----------------
X. flavus -----------MSIKHPIIVVTGSSGAGTTSVKRTFEQIFYRE-----------------
N. hamburgensis -----------MSRKYPIISITGSSGAGTTSVKRTFEQIFRRE-----------------
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R. palustris DX1 -----------MSRKHPIISITGSSGAGTTSVKKTFEQIFRRE-----------------
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M. capsulatus -----------MSKKHPIIAITGSSGAGTTTVKCAFEHIFRL-----------------
A. ferrooxidans -----------MSKKHPVIAVTGSSGAGTTTVKHAFHDIFRRL-----------------
C. M. oxyfera -----------MSKKHPVIAVTGSSGAGTTFVKRAFENIFRRE-----------------
T. denitrificans -----------MSKKHPVIAVTGSSGAGTTTVKRAFEHIFFRE-----------------
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P. lunula EMTPILPATKQLDNTPVIIGVAADSGCGKSTFLRRILGALGTEVTP------------GH
L. polyedrum ------------GVSPVVIGVAADSGCGKSTFLRRILGALGTEVTP------------GH
B. natans SPVMAQKN----IQRPVIFGVAADSGCGKSTFLRRVNAIFGTTTSK------------AH
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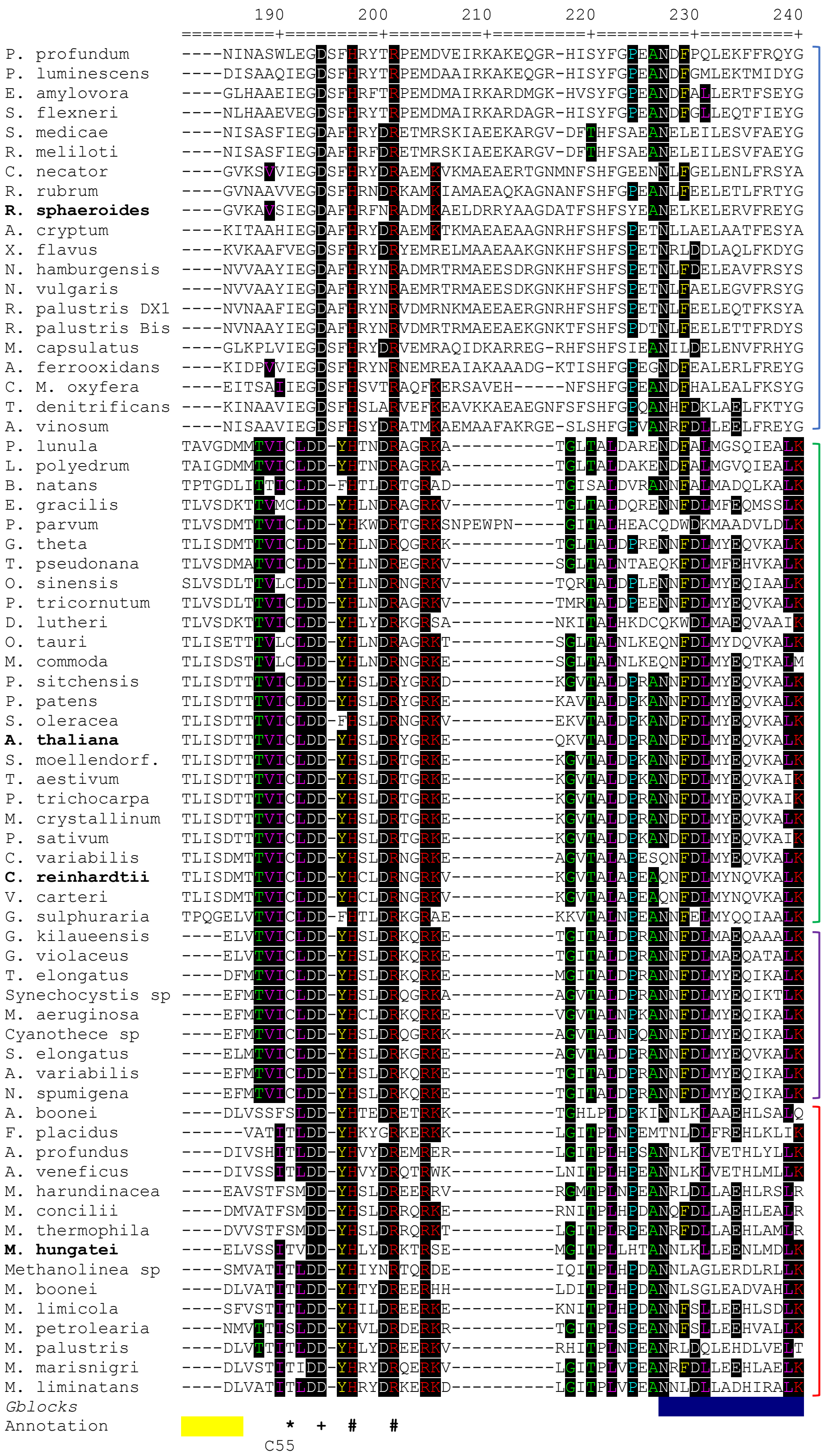
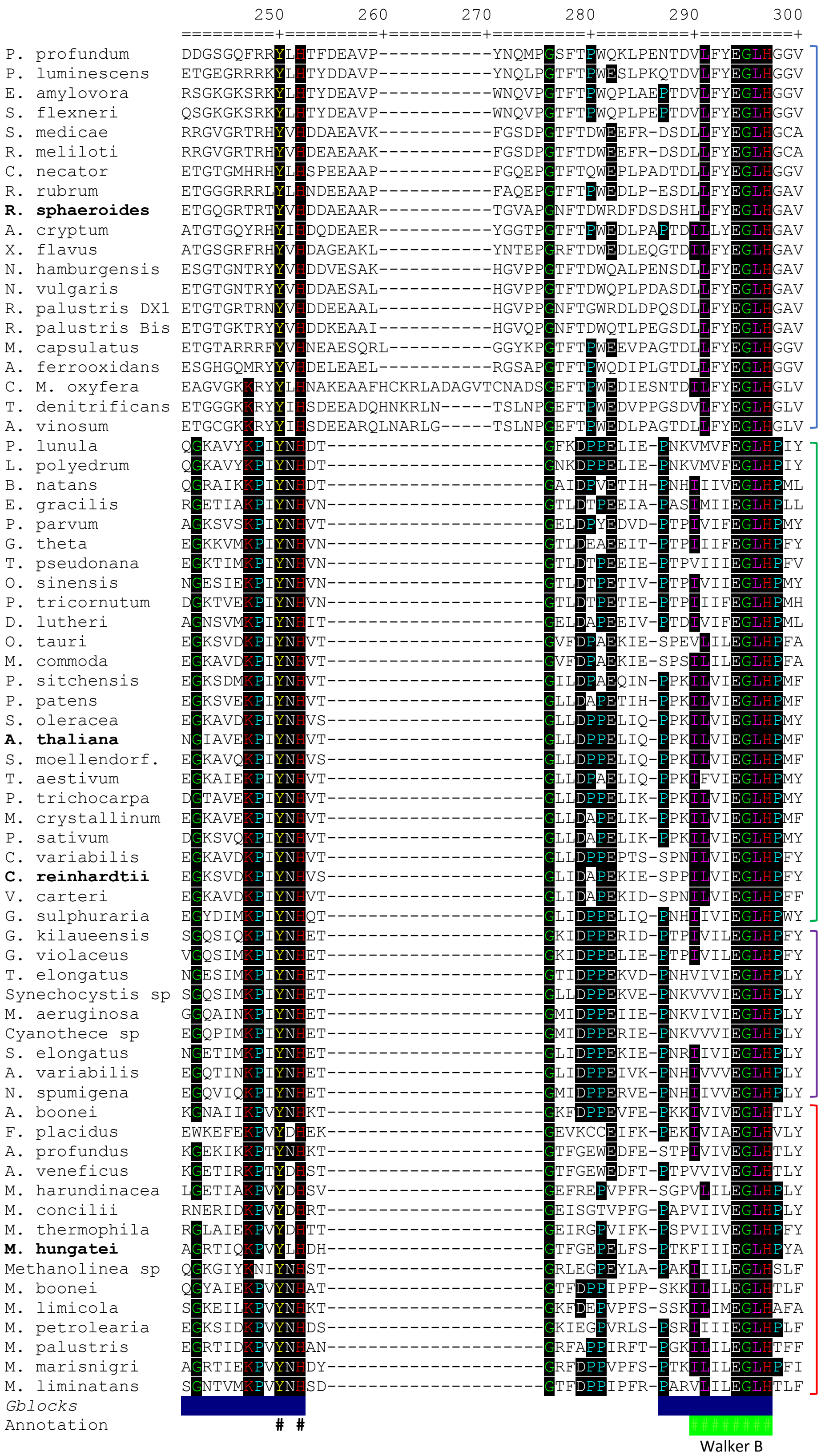
S. elongatus ------------PDRVVLIGVAGDSGCGKSTFLNRLADLFGT------------------
A. variabilis ------------PERVVLIGVAGDSGCGKSTFLRRLIDLFGE------------------
N. spumigena ------------PERVVLIGVAGDSGCGKSTFLRRLIDLFGE------------------
A. boonei ------------YEGSLIIGVAGDSGSGKSTFTKSIINLLGK------------------
F. placidus ------------LKEPFLIGVAGDSGSGKTTFAESVRKIFAGN-----------------
A. profundus ------------SGKVFIIGIAGDSGSGKTTFANGIKRMFGD------------------
A. veneficus ------------SGKTFLVGIAGDSGSGKTTFANAIRNLLGN------------------
M. harundinacea ------------SGRVFVVAVAGDSGSGKTTLSRGIRRLLGE------------------
M. concilii ------------SGRVFVFGIAGDSGSGKTTISRGIRRILGE------------------
M. thermophila ------------SGRVFVVAVAGDSGSGKTTFTRGIRRLLGE------------------
M. hungatei ------------SPLVYLIGVAGDSGSGKSTFTRAISDIFGE------------------
Methanolinea sp ------------SPGRFAIGVAGDSGSGKTTFTDSIRHLFGD------------------
M. boonei ------------SPLVFVIGVAGDSGSGKTTFTNAIREIFGP------------------
M. limicola ------------SGLIFVIGVSGDSGSGKTTFTDAIREIFGP------------------
M. petrolearia ------------SESTFIIGVAGDSGSGKTTFTRAIRSIFGN------------------
M. palustris ------------SPCVFTIGVAGDSGSGKTTFTQSIRDIFGE------------------
M. marisnigri ------------SPYVFVIGVAGDSGSGKTTFTRAIREIFGD------------------
M. liminatans ------------SNSVFVIGVAGDSGSGKTTFTRAIREIVGA------------------
Gblocks
Annotation
| * ||
Walker A (P-loop) [contains C16]
Clamp loop



190 200 210 220 230 240
P. profundum ----NINASWLEGDSFHRYTRPEMDVEIRKAKEQGR-HISYFGPEANDFPQLEKFFRQYG
P. luminescens ----DISAAQIEGDSFHRYTRPEMDAAIRKAKEQGR-HISYFGPEANDFGMLEKTMIDYG
E. amylovora ----GLHAAEIEGDSFHRFTRPEMDMAIRKARDMGK-HVSYFGPEANDFALLERTFSEYG
S. flexneri ----NLHAAEVEGDSFHRYTRPEMDMAIRKARDAGR-HISYFGPEANDFGLLEQTFIEYG
S. medicae ----NISASFIEGDAFHRYDRETMRSKIAEEKARGV-DFTHFSAEANELEILESVFAEYG
R. meliloti ----NISASFIEGDAFHRFDRETMRSKIAEEKARGV-DFTHFSAEANELEILESVFAEYG
C. necator ----GVKSVVIEGDSFHRYDRAEMKVKMAEAERTGNMNFSHFGEENNLFGELENLFRSYA
R. rubrum ----GVNAAVVEGDSFHRNDRKAMKIAMAEAQKAGNANFSHFGPEANLFEELETLFRTYG
R. sphaeroides ----GVKAVSIEGDAFHRFNRADMKAELDRRYAAGDATFSHFSYEANELKELERVFREYG
A. cryptum ----KITAAHIEGDAFHRYDRAEMKTKMAEAEAAGNRHFSHFSPETNLLAELAATFESYA
X. flavus ----KVKAAFVEGDSFHRYDRYEMRELMAAEAAKGNKHFSHFSPETNRLDDLAQLFKDYG
N. hamburgensis ----NVVAAYIEGDAFHRYNRADMRTRMAEESDRGNKHFSHFSPETNLFDELEAVFRSYS
N. vulgaris ----NVVAAYIEGDAFHRYNRAEMRTRMAEESDKGNKHFSHFSPETNLFAELEGVFRSYG
R. palustris DX1 ----NVNAAFIEGDAFHRYNRVDMRNKMAEEAERGNRHFSHFSPETNLFEELEQTFKSYA
R. palustris Bis ----NVNAAYIEGDAFHRYNRVDMRTRMAEEAEKGNKTFSHFSPDTNLFEELETTFRDYS
M. capsulatus ----GLKPLVIEGDSFHRYDRVEMRAQIDKARREG-RHFSHFSIEANILDELENVFRHYG
A. ferrooxidans ----KIDPVVIEGDSFHRYNRNEMREAIAKAAADG-KTISHFGPEGNDFEALERLFREYG
C. M. oxyfera ----EITSAIIEGDSFHSVTRAQFKERSAVEH-----NFSHFGPEANDFHALEALFKSYG
T. denitrificans ----KINAAVIEGDSFHSLARVEFKEAVKKAEAEGNFSFSHFGPQANHFDKLAELFKTYG
A. vinosum ----NISAAVIEGDSFHSYDRATMKAEMAAFAKRGE-SLSHFGPVANRFDLLEELFREYG
P. lunula TAVGDMMTVICLDD-YHTNDRAGRKA----------TGLTALDARENDFALMGSQIEALK
L. polyedrum TAIGDMMTVICLDD-YHTNDRAGRKA----------TGLTALDAKENDFALMGVQIEALK
B. natans TPTGDLITTICLDD-FHTLDRTGRAD----------TGISALDVRANNFALMADQLKALK
E. gracilis TLVSDKTTVMCLDD-YHLNDRAGRKV----------TGLTALDQRENNFDLMFEQMSSLK
P. parvum TLVSDMTTVICLDD-YHKWDRTGRKSNPEWPN-----GITALHEACQDWDKMAADVLDLK
G. theta TLISDMTTVICLDD-YHLNDRQGRKK----------TGLTALDPRENNFDLMYEQVKALK
T. pseudonana TLVSDMATVICLDD-YHLNDREGRKV----------SGLTALNTAEQKFDLMFEHVKALK
O. sinensis SLVSDLTTVLCLDD-YHLNDRNGRKV----------TQRTALDPLENNFDLMYEQIAALK
P. tricornutum TLVSDLTTVICLDD-YHLNDRAGRKV----------TMRTALDPEENNFDLMYEQVKALK
D. lutheri TLVSDKTTVICLDD-YHLYDRKGRSA----------NKITALHKDCQKWDLMAEQVAAIK
O. tauri TLISETTTVLCLDD-YHLNDRAGRKT----------SGLTALNLKEQNFDLMYDQVKALK
M. commoda TLISDSTTVLCLDD-YHLNDRNGRKE----------SGLTALNLKEQNFDLMYEQTKALM
P. sitchensis TLISDTTTVICLDD-YHSLDRYGRKD----------KGVTALDPRANNFDLMYEQVKALK
P. patens TLISDTTTVICLDD-YHSLDRYGRKE----------KAVTALDPKANNFDLMYEQVKALK
S. oleracea TLISDTTTVICLDD-FHSLDRNGRKV----------EKVTALDPKANDFDLMYEQVKALK
A. thaliana TLISDTTTVICLDD-YHSLDRYGRKE----------QKVTALDPRANDFDLMYEQVKALK
S. moellendorf. TLISDTTTVICLDD-YHSLDRTGRKE----------KGVTALDPKANNFDLMYEQVKALK
T. aestivum TLISDTTTVICLDD-YHSLDRTGRKE----------KGVTALDPKANDFDLMYEQVKAIK
P. trichocarpa TLISDTTTVICLDD-YHSLDRTGRKE----------KGVTALDPRANNFDLMYEQVKAIK
M. crystallinum TLISDTTTVICLDD-YHSLDRTGRKE----------KGVTALDPRANDFDLMYEQVKALK
P. sativum TLISDTTTVICLDD-YHSLDRTGRKE----------KGVTALDPKANDFDLMYEQVKAIK
C. variabilis TLISDMTTVICLDD-YHSLDRNGRKE----------AGVTALAPESQNFDLMYEQVKALK
C. reinhardtii TLISDMTTVICLDD-YHCLDRNGRKV----------KGVTALAPEAQNFDLMYNQVKALK
V. carteri TLISDMTTVICLDD-YHCLDRNGRKV----------KGVTALAPEAQNFDLMYNQVKALK
G. sulphuraria TPQGELVTVICLDD-FHTLDRKGRAE----------KKVTALNPEANNFELMYQQIAALK
G. kilaueensis ----ELVTVICLDD-YHSLDRKQRKE----------TGITALDPRANNFDLMAEQAAALK
G. violaceus ----ELVTVICLDD-YHSLDRKQRKE----------TGITALDPRANNFDLMAEQATALK
T. elongatus ----DFMTVICLDD-YHSLDRKQRKE----------MGITALDPRANNFDLMYEQIKALK
Synechocystis sp ----EFMTVICLDD-YHSLDRQGRKA----------AGVTALDPRANNFDLMYEQIKTLK
M. aeruginosa ----EFMTVICLDD-YHCLDRKQRKE----------VGVTALNPKANNFDLMYEQIKALK
Cyanothece sp ----EFMTVICLDD-YHSLDRQGRKK----------AGVTALNPQANNFDLMYEQIKALK
S. elongatus ----ELMTVICLDD-YHSLDRKGRKE----------AGVTALDPRANNFDLMYEQVKALK
A. variabilis ----EFMTVICLDD-YHSLDRKQRKE----------TGITALDPRANNFDLMYEQIKALK
N. spumigena ----EFMTVICLDD-YHSLDRKQRKE----------TGITALDPRANNFDLMYEQIKALK
A. boonei ----DLVSSFSLDD-YHTEDRETRKK----------TGHLPLDPKINNLKLAAEHLSALQ
F. placidus ------VATITLDD-YHKYGRKERKK----------LGITPLNPEMTNLDLFREHLKLIK
A. profundus ----DIVSHITLDD-YHVYDREMRER----------LGITPLHPSANNLKLVETHLYLLK
A. veneficus ----DIVSSITLDD-YHVYDRQTRWK----------LNITPLHPEANNLKLVETHLMLLK
M. harundinacea ----EAVSTFSMDD-YHSLDREERRV----------RGMTPLNPEANRLDLLAEHLRSLR
M. concilii ----DMVATFSMDD-YHSLDRRQRKE----------RNITPLHPDANQFDLLAEHLEALR
M. thermophila ----DVVSTFSMDD-YHSLDRRQRKT----------LGITPLRPEANRFDLLAEHLAMLR
M. hungatei ----ELVSSITVDD-YHLYDRKTRSE----------MGITPLLHTANNLKLLEENLMDLK
Methanolinea sp ----SMVATITLDD-YHIYNRTQRDE----------IQITPLHPDANNLAGLERDLRLLK
M. boonei ----DLVATITLDD-YHTYDREERHH----------LDITPLHPDANNLSGLEADVAHLK
M. limicola ----SFVSTITLDD-YHILDREERKE----------KNITPLHPDANNFSLLEEHLSDLK
M. petrolearia ----NMVTTISLDD-YHVLDRDERKR----------TGITPLSPEANNFSLLEEHVALLK
M. palustris ----DLVTTITLDD-YHLYDREERKV----------RHITPLNPEANRLDQLEHDLVELT
M. marisnigri ----DLVSTITIDD-YHRYDRQERKV----------LGITPLVPEANRFDLLEEHLAELK
M. liminatans ----DLVATITLDD-YHRYDRKERKD----------LGITPLVPEANNLDLLADHIRALK
Gblocks
Annotation * + # #
C55


250 260 270 280 290 300
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P. profundum DDGSGQFRRYLHTFDEAVP-----------YNQMPGSFTPWQKLPENTDVLFYEGLHGGV
P. luminescens ETGEGRRRKYLHTYDDAVP-----------YNQLPGTFTPWESLPKQTDVLFYEGLHGGV
E. amylovora RSGKGKSRKYLHTYDEAVP-----------WNQVPGTFTPWQPLAEPTDVLFYEGLHGGV
S. flexneri QSGKGKSRKYLHTYDEAVP-----------WNQVPGTFTPWQPLPEPTDVLFYEGLHGGV
S. medicae RRGVGRTRHYVHDDAEAVK-----------FGSDPGTFTDWEEFR-DSDLLFYEGLHGCA
R. meliloti RRGVGRTRHYVHDEAEAAK-----------FGSDPGTFTDWEEFR-DSDLLFYEGLHGCA
C. necator ETGTGMHRHYLHSPEEAAP-----------FGQEPGTFTQWEPLPADTDLLFYEGLHGGV
R. rubrum ETGGGRRRLYLHNDEEAAP-----------FAQEPGTFTPWEDLP-ESDLLFYEGLHGAV
R. sphaeroides ETGQGRTRTYVHDDAEAAR-----------TGVAPGNFTDWRDFDSDSHLLFYEGLHGAV
A. cryptum ATGTGQYRHYIHDQDEAER-----------YGGTPGTFTPWEDLPAPTDILLYEGLHGAV
X. flavus ATGSGRFRHYVHDAGEAKL-----------YNTEPGRFTDWEDLEQGTDILFYEGLHGAV
N. hamburgensis ESGTGNTRYYVHDDVESAK-----------HGVPPGTFTDWQALPENSDLLFYEGLHGAV
N. vulgaris ETGTGNTRYYVHDDAESAL-----------HGVPPGTFTDWQPLPDASDLLFYEGLHGAV
R. palustris DX1 ETGTGRTRNYVHDDEEAAL-----------HGVPPGNFTGWRDLDPQSDLLFYEGLHGAV
R. palustris Bis ETGTGKTRYYVHDDKEAAI-----------HGVQPGNFTDWQTLPEGSDLLFYEGLHGAV
M. capsulatus ETGTARRRFYVHNEAESQRL----------GGYKPGTFTPWEEVPAGTDLLFYEGLHGGV
A. ferrooxidans ESGHGQMRYYVHDELEAEL-----------RGSAPGTFTPWQDIPLGTDLLFYEGLHGGV
C. M. oxyfera EAGVGKKRYYLHNAKEAAFHCKRLADAGVTCNADSGEFTPWEDIESNTDILFYEGLHGLV
T. denitrificans ETGGGKKRYYIHSDEEADQHNKRLN-----TSLNPGEFTPWEDVPPGSDVLFYEGLHGLV
A. vinosum ETGCGKKRYYIHSDEEARQLNARLG-----TSLNPGEFTPWEDLPAGTDLLFYEGLHGLV
P. lunula QGKAVYKPIYNHDT---------------------GFKDPPELIE-PNKVMVFEGLHPIY
L. polyedrum QGKAVYKPIYNHDT---------------------GNKDPPELIE-PNKVMVFEGLHPIY
B. natans QGRAIKKPIYNHDT---------------------GAIDPVETIH-PNHIIIVEGLHPML
E. gracilis RGETIAKPIYNHVN---------------------GTLDTPEEIA-PASIMIIEGLHPLL
P. parvum AGKSVSKPIYNHVT---------------------GELDPYEDVD-PTPIVIFEGLHPMY
G. theta EGKKVMKPIYNHVN---------------------GTLDEAEEIT-PTPIIIFEGLHPFY
T. pseudonana EGKTIMKPIYNHVN---------------------GTLDTPEEIE-PTPVIIIEGLHPFV
O. sinensis NGESIEKPIYNHVN---------------------GTLDTPETIV-PTPIVIIEGLHPMY
P. tricornutum DGKTVEKPIYNHVN---------------------GTLDTPETIE-PTPIIIFEGLHPMH
D. lutheri AGNSVMKPIYNHIT---------------------GELDAPEEIV-PTDIVIFEGLHPML
O. tauri EGKSVDKPIYNHVT---------------------GVFDPAEKIE-SPEVLILEGLHPFA
M. commoda EGKAVDKPIYNHVT---------------------GVFDPAEKIE-SPSILILEGLHPFA
P. sitchensis EGKSDMKPIYNHVT---------------------GILDPAEQIN-PPKILVIEGLHPMF
P. patens EGKSVEKPIYNHVT---------------------GLLDAPETIH-PPKILVIEGLHPMF
S. oleracea EGKAVDKPIYNHVS---------------------GLLDPPELIQ-PPKILVIEGLHPMY
A. thaliana NGIAVEKPIYNHVT---------------------GLLDPPELIQ-PPKILVIEGLHPMF
S. moellendorf. EGKAVQKPIYNHVS---------------------GLLDPPELIQ-PPKILVIEGLHPMF
T. aestivum EGKAIEKPIYNHVT---------------------GLLDPAELIQ-PPKIFVIEGLHPMY
P. trichocarpa DGTAVEKPIYNHVT---------------------GLLDPPELIK-PPKILVIEGLHPMY
M. crystallinum EGKAVEKPIYNHVT---------------------GLLDAPELIK-PPKILVIEGLHPMF
P. sativum DGKSVQKPIYNHVT---------------------GLLDAPELIK-PPKILVIEGLHPMY
C. variabilis EGKAVDKPIYNHVT---------------------GLLDPPEPTS-SPNILVIEGLHPFY
C. reinhardtii EGKSVDKPIYNHVS---------------------GLIDAPEKIE-SPPILVIEGLHPFY
V. carteri EGKAVDKPIYNHVT---------------------GLIDAPEKID-SPNILVIEGLHPFF
G. sulphuraria EGYDIMKPIYNHQT---------------------GLIDPPELIQ-PNHIIVIEGLHPWY
G. kilaueensis SGQSIQKPIYNHET---------------------GKIDPPERID-PTPIVILEGLHPFY
G. violaceus VGQSIMKPIYNHET---------------------GKIDPPELIE-PTPIVILEGLHPFY
T. elongatus NGESIMKPIYNHET---------------------GTIDPPEKVD-PNHVIVIEGLHPLY
Synechocystis sp SGQSIMKPIYNHET---------------------GLLDPPEKVE-PNKVVVIEGLHPLY
M. aeruginosa GGQAINKPIYNHET---------------------GMIDPPEIIE-PNKVIVIEGLHPLY
Cyanothece sp EGQPIMKPIYNHET---------------------GMIDPPERIE-PNKVVVIEGLHPLY
S. elongatus NGETIMKPIYNHET---------------------GLIDPPEKIE-PNRIIVIEGLHPLY
A. variabilis EGQTINKPIYNHET---------------------GLIDPPEIVK-PNHIVVVEGLHPLY
N. spumigena EGQVIQKPIYNHET---------------------GMIDPPERVE-PNHIIVVEGLHPLY
A. boonei KGNAIIKPVYNHKT---------------------GKFDPPEVFE-PKKIVIVEGLHTLY
F. placidus EWKEFEKPVYDHEK---------------------GEVKCCEIFK-PEKIVIAEGLHVLY
A. profundus KGEKIKKPTYNHKT---------------------GTFGEWEDFE-STPIVIVEGLHTLY
A. veneficus KGETIRKPTYDHST---------------------GTFGEWEDFT-PTPVVIVEGLHTLY
M. harundinacea LGETIAKPVYDHSV---------------------GEFREPVPFR-SGPVLILEGLHPLY
M. concilii RNERIDKPVYDHRT---------------------GEISGTVPFG-PAPVIIVEGLHPLY
M. thermophila RGLAIEKPVYDHTT---------------------GEIRGPVIFK-PSPVIIVEGLHPFY
M. hungatei AGRTIQKPVYLHDH---------------------GTFGEPELFS-PTKFIIIEGLHPYA
Methanolinea sp QGKGIYKNIYNHST---------------------GRLEGPEYLA-PAKIIILEGLHSLF
M. boonei QGYAIEKPVYNHAT---------------------GTFDPPIPFP-SKKILILEGLHTLF
M. limicola SGKEILKPVYNHKT---------------------GKFDEPVPFS-SSKILIMEGLHAFA
M. petrolearia EGKSIDKPVYNHDS---------------------GKIEGPVRLS-PSRIIIIEGLHPLF
M. palustris EGRTIDKPVYNHAN---------------------GRFAPPIRFT-PGKILILEGLHTFF
M. marisnigri AGRTIEKPVYNHDY---------------------GRFDPPVPFS-PTKILILEGLHPFI
M. liminatans SGNTVMKPVYNHSD---------------------GTFDPPIPFR-PARVLILEGLHTLF
Gblocks
Annotation
# #
Walker B

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                          310       320       330       340       350       360
                 =========+=========+=========+=========+=========+=========+
P. profundum     VD-------GEVNAAEHVDLLIGMVPIVNLEWIQKIVRDTRDRGHSREAVMESIVRSMDD
P. luminescens   VT-------PQHNVASHVDLLVGVVPIVNLEWIQKLIRDTGERGHSQEAVMDSVVRSMDD
E. amylovora     VT-------PLHNVAENVDLLVGVVPIVNLEWIQKLVRDTSERGHSREAVMDSVVRSMED
S. flexneri      VT-------PQHNVAQHVDLLVGVVPIVNLEWIQKLIRDTSERGHSREAVMDSVVRSMED
S. medicae       VT-------DTINLAQHCDLKIGVVPVINLEWIQKIHRDKATRGYSTEAVTDTILRRMPD
R. meliloti      VT-------DTVNLAQHCDLKIGVVPVINLEWIQKIHRDKATRGYSTEAVTDTILRRMPD
C. necator       VT-------DSVNVAQYPNLLIGVVPVINLEWIQKLWRDKKQRGYSTEAVTDTILRRMPD
R. rubrum        VT-------DTVDVAQHADLKIGVVPVINVEWIQKLHRDRAARGYSTEAVTDTILRRMPD
R. sphaeroides   VN-------SEVNIAGLADLKIGVVPVINLEWIQKIHRDRATRGYTTEAVTDVILRRMHA
A. cryptum       RH-------GDIDTGRHADVKIGVVPVINLEWIQKIHRDRAARRYSTEAVMDTILRRMPD
X. flavus        VT-------DELNLAQHADLKIGVVPVINLEWIQKIHRDKATRGYTTEDVTDTIMRRMPD
N. hamburgensis  VT-------DKVNVAQYADLKIGVVPVINLEWIQKLHRDRSARGYSTEAVTDTILRRMPD
N. vulgaris      VT-------DKVNVAQYADLKIGVVPVINLEWIQKLHRDRNARGYSTEAVTDTILRRMPD
R. palustris DX1 IT-------EKVNVAQHADLKIGVVPVINLEWIQKLHRDRAARGYSTEAVTDTILRRMPD
R. palustris Bis MT-------ETVNVAQHADLKIGVVPVINLEWIQKLHRDRSDRGYSTEAVTDTILRRMPD
M. capsulatus    IT-------DRINVRKYVDLLVGVVPIVNLEWIQKIHRDTAERGYKPEDVTETILRRMDD
A. ferrooxidans  KT-------GAVDVTNYVDLLVGVVPVVNLEWIQKIHRDNAQRGYSAEAIVDTILRRMPD
C. M. oxyfera    KDISPDQKYGGYDVAQYVDLGIGVVPSVNLEWIQKIHRDHAERGYSPEATVDTIMRRMPD
T. denitrificans KT-------DTVDVAQHVDLGIGVVPIVNLEWIQKIHRDGAERGYSADVIVDTILRRMPD
A. vinosum       VT-------EDSNVAQHVDLGVGVVPIVNLEWIQKIHRDNLERGYSAEAIVDTIMRRMPD
P. lunula        DE----------KARAQLDLGIYIDIVNDVKFAWKVQRDVAERGWTEEQVRADIDKRLPD
L. polyedrum     DK----------KARDQLDLGIYIDIVNDVKFAWKVQRDVAERGWTEEQVREDIEKRLPD
B. natans        DK----------DVIESLDFTFYIDVSDPVKKAWKIERDMVERGHKKEDIIASIESRKPD
E. gracilis      DD----------RVAGLLDFSIYLDISDRVKFAWKIQRDMAERGWALEDIKKDIEKRKPD
P. parvum        DE----------RVNKALDLTVYLDITDEVKFAWKAQRDIAERGATMEEVQKAIDGRKPD
G. theta         DK----------RVEELMDFKIYVDITPEVKFNWKVQRDHEERGHSIESIKQQIEARKPD
T. pseudonana    DE----------RVRELIDFSLYLDISPDVKLNWKIQRDMEERGHSLESIMASIEARKPD
O. sinensis      DE----------RVRDLLDFSLYLDISDEVKLNWKIQRDMEERGHSLESILASIEARKPD
P. tricornutum   DK----------RVLDLLDFSLYLDISDDVKLNWKVQRDMEERGHSMESILASIEARKPD
D. lutheri       DD----------KVRSMLDLSIYLDISGXVKFAWKIQRDMQERGHSLESIKASIEGRKPD
O. tauri         DT----------RVRDMFDFKIYLDISDDVKFAWKIQRDMAERGHSLESIKASIEARKPD
M. commoda       DE----------RVRDMFDFKIYLDISDDVKFAWKIQRDMAERGHSLESIKASIEARKPD
P. sitchensis    DA----------RVRELLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIQARKPD
P. patens        DE----------RVRELLDFSIYLDISDDVKFAWKIQRDMAERGHSLESIKASIAARKPD
S. oleracea      DA----------RVRELLDFSIYLDISNEVKFAWKIQRDMKERGHSLESIKASIESRKPD
A. thaliana      DE----------RVRDLLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIEARKPD
S. moellendorf.  DS----------RVRELLDFSIYLDISDAVKFAWKIQRDMAERGHSLESIKASIAARKPD
T. aestivum      DE----------RVRELLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIEARKPD
P. trichocarpa   DQ----------RVRDLLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIEARKPD
M. crystallinum  DS----------RVRDLLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIEARKPD
P. sativum       DS----------RVRELLDFSIYLDISNEVKFAWKIQRDMAERGHSLESIKASIEARKPD
C. variabilis    DE----------RVNELVDFRIYLDISDEIKFAWKIQRDMAERGHSLESIKASIEARKPD
C. reinhardtii   DK----------RVAELLDFKIYLDISDDIKFAWKIQRDMAERGHSLESIKSSIAARKPD
V. carteri       DK----------RVADLLDFKIYLDISDDIKFAWKIQRDMAERGHSLQAIKSSIEARKPD
G. sulphuraria   DA----------RMKQLLDFTVYLDISDEVKVAWKIQRDMAERGHKLENILASIESRKPD
G. kilaueensis   DK----------RVRDLLDFKVYFDLSDPIKIQWKIQRDMAERGHSYDDVIRAIESRRPD
G. violaceus     DA----------RVRNLFDFKIYFDLSDPIKIQWKIQRDMAERGHTYEDVLKQIESRRPD
T. elongatus     DE----------RVRSLIDFSVYLDISDDVKIAWKIKRDMAERGHSYEDVIASINARRPD
Synechocystis sp DE----------RVRELVDFGVYLDISEEVKINWKIQRDMAERGHTYEDILASINARKPD
M. aeruginosa    DE----------RVRSLLDFSVYLDISDEVKVNWKIQRDMAERGHTYDDVMAAINSRKPD
Cyanothece sp    DE----------RVRSLVDFSVYLDISDEVKINWKIQRDMAERGHTYDDVIASINARKPD
S. elongatus     DE----------RVRELLDFSVYLDIDDEVKIAWKIQRDMAERGHSYEDVLASIEARRPD
A. variabilis    DE----------RVRSLLDFSVYFDISDEVKIAWKIQRDMAERGHRYEDVLAAINSRKPD
N. spumigena     DE----------RVRSLLDFSVYFDISDQVKIAWKIQRDMAERGHRYEDVLAQINSRKPD
A. boonei        DE-----------LRNYLDLKIYVDPSKDIKWLWKIKRDVEERGYKKEDVIKEIRAREPF
F. placidus      DG-----------IREILDYKIFVDPARIIKRKWKIKRDMEKRGYRKEEVIEEIIQRESD
A. profundus     DG-----------IRDYIDFKIFVDPARYIKRLWKIKRDVEERGYDRDKVIREIIRREPD
A. veneficus     DG-----------LRNYLDFRIFVDPARYIKRRWKIKRDVEERGYNRQKVVEEIIRRESD
M. harundinacea  TQ----------KLRREVDFGIFVDPSRAVKRRWKIRRDCGDRGYQRDLVMAEILAREPD
M. concilii      TE----------RLRSQIDFKIFVDPSRSVKRLWKIRRDVGERGYETGQVMAEILQREPD
M. thermophila   TE----------ELRKLSDFKIFVDPSRAVKRRWKLRRDVGERGYAPEDVMREILEREPD
M. hungatei      TK----------SLRALYDYTIFVDPERDVKYDWKIRRDMKKRNYDKNEVLREILQREPD
Methanolinea sp  TP----------GLRDLLDFSLYLDPASAVKREWKIKRDMEKRGYSEREVRDAIARREND
M. boonei        TP----------ALRDLVDFSVFVDPDREVKYAWKRQRDTGQRGYSPDEVNGEIARREAD
M. limicola      TP----------KLKSLTDFSIYVNPETNVKYEWKIKRDVNARGYDKEDVLSELEARRKD
M. petrolearia   TE----------KLRELIDFSIYVSPDTDVKYYWKIKRDVNLRGYREEEVLAELESRRAD
M. palustris     TP----------ALREHLDFTLFVEPDPEVKIEWKMRRDINNRGYTREQVMAELEPRERD
M. marisnigri    TG----------TLRDRIDFKLYVDPDPDVKRAWKIKRDVERRGYAPEAVLREMEERKPD
M. liminatans    TP----------ELRSLLDFSLFVDPDPAVKTLWKIRRDMQRRGYSRAEVLAEMEERKPD
Gblocks
Annotation                                         #  |+   #
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                            370       380       390       400       410       420
                   =========+=========+=========+=========+=========+=========+
P. profundum       YLNYITPQFSRTHINFQRVPT-----------VDTS----NPFSAKGIPSLD--ESFVVI
P. luminescens     YINYITPQFSRTHINFQRVPT-----------VDTS----NPFSAKAIPSLD--ESFIVI
E. amylovora       YINFITPQFSRTHINFQRVPT-----------VDTS----NPFAARGIPSLD--ESFVVV
S. flexneri        YINYITPQFSRTHLNFQRVPT-----------VDTS----NPFAAKGIPSLD--ESFVVI
S. medicae         YVHYICPQFSLTDINFQRVPI-----------VDTS----NPFIARWIPTPA--ESILVI
R. meliloti        YVNYICPQFSLTDINFQRVPI-----------VDTS----NPFIARWIPTPA--ESILVI
C. necator         YVNYICPQFSRTHVNFQRVPC-----------VDTS----NPFISREIPAPD--ESMVVI
R. rubrum          YVHYICPQFTRTDVNFQRVPL-----------VDTS----NPFVARHVPSAD--ESFVVI
R. sphaeroides     YVHCIVPQFSQTDINFQRVPV-----------VDTS----NPFIARWIPTAD--ESVVVI
A. cryptum         YVHYICPQFTETDINFQRVPT-----------VDTS----NPFIARWIPTAD--ESIVVI
X. flavus          YVRYICPQFTETDINFQRVPT-----------VDTS----NPFVARWIPTPD--ESMVVI
N. hamburgensis    YVNYICPQFAETDINFQRVPT-----------VDTS----NPFIARWIPTPD--ESMVVI
N. vulgaris        YVNYICPQFAETDINFQRVPT-----------VDTS----NPFISRWIPTPD--ESMVVI
R. palustris DX1   YVHYIVPQFAETDINFQRVPT-----------VDTS----NPFIARWIPTAD--ESMVVI
R. palustris Bis   YVHYIVPQFGETDINFQRVPT-----------VDTS----NPFIARWIPTPD--ESMVVI
M. capsulatus      YVKVITPQFSQTDINFQRVPT-----------VDTS----NPFIARDIPTPD--ESFVII
A. ferrooxidans    YIHYITPQFSRAHINFQRVPL-----------VDTS----NPFIARDIPTPD--ESMVVI
C. M. oxyfera      YINHLTPQFSRTHVNFQRVPT-----------VDTS----NPFIARDIPSAD--ESFVVI
T. denitrificans   YVNYITPQFSRTDINFQRVST-----------VDTS----NPFISRDIPTPD--ESFIVI
A. vinosum         YIRYITPQFSLTDINFQRVPT-----------VDTS----NPFIARDIPTPD--ESFVII
P. lunula          FSAYVDPQKANADVILRYEPS-----------DQGL----PYLKVKLIQKKG--GKFPPI
L. polyedrum       FSAYVDPQKADADVILRYEPS-----------DQGL----PYLKVKLIQKKG--GAFPPI
B. natans          FEKFVEPQKANADVIISIEPTKLDVA------PGEET---KYLNTRLIQKENQ-HGIRPV
E. gracilis        FDKYVAPQRAKADMVIEVLPSRLAPP------KDETAPL-EYLRVRLIQKTTT-KHFDPV
P. parvum          FAAYVEPQKAKADIIVQVLFSDL-I-------DDPTG---KFLKVRLITKNNL-KHISPA
G. theta           FDAYIDPQKNKADCVIQVLPTNL-VA------NDK-----THLNVKLIQCKGV-DHYAPT
T. pseudonana      FDAFIEPQKKFADYVIEVLPTDL---------DKEDK---KTLKVRAIQKKGV-ADFTPT
O. sinensis        FDAYIAPQKEFADLTIEVLPTQL---------DEEDK---KTLRVRCIQKEGV-SDFSPC
P. tricornutum     FDAYIDPQKQLADLIIEVLPTRL---------DQDDK---KTLRVRCIQKEGV-ENFDPC
D. lutheri         FDAFVAPQRANADIVIEVLPTQL-V-------NDAEG---KFLRVRFIQKAGL-DLIKAP
O. tauri           FDAFVDPQKEHADVVIEVLPTQL-IP------DDNEG---KILRVRMIMKENV-ENFDAP
M. commoda         FDEFVDPQKQYADIVIQVLPTQL-IP------DDNEG---KILRVRMIMKEGV-ENFDAP
P. sitchensis      FDAFIDPQKQYADVVIQVLPTEL-IP------EENEG---KVLRVRMVMKEGV-NFFNPV
P. patens          FDAYIDPQKQYADVVIQVLPTQL-IP------DDNEG---KVLRVRMVMKEGV-PFFEPV
S. oleracea        FDAYIDPQKQHADVVIEVLPTEL-IP------DDDEG---KVLRVRMIQKEGV-KFFNPV
A. thaliana        FDAFIDPQKQYADAVIEVLPTTL-IP------DDNEG---KVLRVRLIMKEGV-KYFSPV
S. moellendorf.    FDAYIDTQKQYADVVIQVLPTQL-IP------DDNEG---KVLRVRMIMKEGV-DNFEPV
T. aestivum        FDAFIDPQKQYADAVIEVLPTQL-IP------DDNEG---KVLRVKLIMKEGI-KFFNPV
P. trichocarpa     FDAYIDPQKQYADAVIEVLPTQL-IP------DDNEG---KVLRVKLIMKEGV-EFFSPV
M. crystallinum    FDAYIDPQKQYADAVIEVLPTQL-IP------GDNEG---KVLRVRLIQKEGV-QYFSPV
P. sativum         FEAYIDPQKQYADAVIEVLPTQL-IP------DDNEG---KILRVRLIQKAGV-KYFSPV
C. variabilis      FDAYIDPQKKKADMIIQVLPTQL-VP------DEKEG---KILRVRLIMKDGK-KLFDPV
C. reinhardtii     FDAYIDPQKKDADMIIQVLPTQL-VP------DDK-G---QYLRVRLIMKEGS-KMFDPV
V. carteri         FDAYIDPQKKDADMIIQVLPTQL-VP------DDK-G---QYLRVRLIQKEGS-KMFDPV
G. sulphuraria     FQQYIDPQKKDAVAVIQVLPTRL-IP------DDTEK---KVLRVRLIQREGI-QGFQSV
G. kilaueensis     FSAYIDPQKQHADVVLQILPSELPEK------KDGT----KKIKAAMVQVEGI-PNYDPP
G. violaceus       FSAYIDPQKQYADVVLQILPSEL---------PEKAGGI-KRVKACMVQVDGI-PNYDAP
T. elongatus       FMAYIDPQKQYADVVLQILPSQL-AK------EEKVG---NILRVRMLQREGI-PGFEPV
Synechocystis sp   FTAYIEPQKQYADVVIQVLPTRLI--------EDKES---KLLRVRLVQKEGV-KFFEPA
M. aeruginosa      FSAYIDPQRQYADVVIQVLPTKLL--------EDHES---KLLRVRLIQKEGV-ENFEPA
Cyanothece sp      FSAYIEPQREYADVVIQVLPTNL-IE------NDKES---KILRVRLIQKEGI-ENFQPV
S. elongatus       FKAYIEPQRGHADIVIRVMPTQL-IP------NDTER---KVLRVQLIQREGR-DGFEPA
A. variabilis      FQKYIEPQREFADVVLQVLPTNL-IK------DDTDR---KVLRVRMLQREGK-EGFEPA
N. spumigena       FEKFIEPQREFADVVLQVLPTNL-IK------NDTER---KVLRVRMLQREDK-EGFEPT
A. boonei          YKRYIDFQKIYADIVIKIDISKFS--------EEDSYSVETILKVLDFPLSGIEMPLSLS
F. placidus        YKRYVDFQKIYADVVIKIYPSSLESTERISTLLGME----EMYRVRLIFTNLS-FELDHV
A. profundus       YKRYIDFQKIYADVVIKILPSSIQSTERIKYLVDSRE---EVYKVRLILKKTD-IPLESV
A. veneficus       YKRYIDFQKIYADVVIKIFPTALQSVERITYLTEAPP---ELYKVRLILKSGDFVPTEPI
M. harundinacea    YKLYVDVQKVYAEAVVKIDDTRLGAPSF----LEDPG---ERYSVRLIQEVLE-AGPSAV
M. concilii        YKLYVDIQKIYAQIVIKIQDSRF-HPSL--LDSQSTL---DWYSVRLIMEIME-HPVSEV
M. thermophila     YKLYVDVQKVYAEMVIKIQDSRI-PPEWTEIARGSAR---EKYSVRIIQQILD-HPLDEV
M. hungatei        YFQYVFPQREVADAVIQISYSSYGKE------EGEKR---NVYRVMLSMPAQE-YCFEDI
Methanolinea sp    YRAYIAPQRDHADAVIEIGFSRFGRD------LGWKK---NIYRVSILQTATS-CSMDHI
M. boonei          YATYIEPQRCNADAIIRIGYSKYGKD------LGPAK---NVYSISLLQNPMD-QAVRNT
M. limicola        YENFVLPQSESADALIEISDSSFDSP------SLKDR---GVYKITLYQKRLD-KTVKNI
M. petrolearia     YENYVHPQIRFADAVIGISKSRY-AD------IMNER---GVYRVVLYQKKQD-RTIRNI
M. palustris       YQRFIAPQQKYADVVVRVRFSKYGRE------RGIRE---KIYQVSLSQNRIT-KSIEDV
M. marisnigri      YERYVAPQCLFADAVIRIAFSKYGRD------VSEKR---NVYRVTLCQSRLD-KSIGDV
M. liminatans      YERYIAPQRAYADAVIRIACSGY---------GEEASEERNVYRVTILQKKLL-QQMVEI
Gblocks
Annotation
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                        430       440       450       460       470       480
                 =========+=========+=========+=========+=========+=========+
P. profundum     RFRG-------------IEN---VDFP---YLLSMIQGSFMSRHNTLVVPGGKMS-----
P. luminescens   RFRD-------------LTQ---IDFP---YLLAMLQGSFVSSINTIVVPGGKMG-----
E. amylovora     HFQG-------------LED---IDFP---YLLSMLQGSFISHIKTLVVPGGKMG-----
S. flexneri      HFRN-------------LEG---IDFP---WLLAMLQGSFISHINTLVVPGGKMG-----
S. medicae       RFAK-------------PQS---IDFP---YLLSMLHNSYMSRANSIVVPGDKLD-----
R. meliloti      RFAK-------------PQS---IDFP---YLLSMLHNSYMSRANSIVVPGDKLD-----
C. necator       RFAN-------------PKG---IDFQ---YLLSMIHDSFMSRANTIVVPGGKME-----
R. rubrum        RFRD-------------PKG---IDFP---YLLNMLNDSFMSRPNTIVVPGGKME-----
R. sphaeroides   RFRN-------------PRG---IDFP---YLTSMIHGSWMSRANSIVVPGNKLD-----
A. cryptum       RFRD-------------PHG---IDFP---YLLAMLHGSFMSRANSIAVPGNKFD-----
X. flavus        RFRD-------------PHG---IDFP---YLLSMIHNSFMSRANSIVIPGNKQD-----
N. hamburgensis  RLKN-------------PRG---IDFP---YLLSMIPNSFMSRANSIVIHGSKMD-----
N. vulgaris      RLKN-------------PRG---IDFP---YLLSMIPSSFMSRANSIVIHGSKLD-----
R. palustris DX1 RFKN-------------PRG---IDFA---YLLSMIQGSFMSRANSIVIHGAKLD-----
R. palustris Bis RFKS-------------PRG---IDFA---YLLSMIQGSFMSRANSIVIHGSKMD-----
M. capsulatus    RFKE-------------PGKFN-VDFP---YLLAMLQNSFMSRHNSIVIPGGKMG-----
A. ferrooxidans  RFRD-------------PKE---ENFP---TLLQMLPGSFMSRSNTLVIPGTKMG-----
C. M. oxyfera    RFVD-------------PKRFG-VDFP---TLLVMINGSFISRRNTIVVPGGKMV-----
T. denitrificans RFRN-------------PQG---VDFP---YLLNMICNSFMSRRNTIVVPGGKMG-----
A. vinosum       RFKD-------------PKKLQ-IDFP---YLLSMIHDSFMSRRNSMVVPGGKMG-----
P. lunula        SLKK-------------DLSLT-GSKP--GATMKMYDDDWFGNPVTVVEMDGEIDMDNMA
L. polyedrum     SLKK-------------DLTLT-GSKP--GATLKMYDDDWFGNAVTVVEMDGEIDMDNME
B. natans        YMFEEEGSTVDWDPCAGPGAMA-CPYP--GTRVRYYNEMSGEKHAHVLEVDGVFG---ET
E. gracilis      YLIEKG-SSVTWKPC--GDNLQ-CEYP--GLQLAYYTEEYMGHPAEVLEMDGVIH---NL
P. parvum        YLMDEG-ASITWKPN--PNKLT-TSAP--GVLFKSYQDEWFGQSVSVLEMDGKID---SL
G. theta         YLWDEG-SDIEWVPP--RNKLA-SSAPGAGLKIYQKTEKWAGKDAAVIGMDGKYD---KI
T. pseudonana    YLFDEG-SEIEWAPS--ADKLS-SPAP--GIKLSYKQEQYFGADVAVVEMDGTFD---NI
O. sinensis      YLFDEG-STIAWTPA--PSKLS-SSGP--GLTMAYGTEDYYGKPAQVVEMDGTFD---NI
P. tricornutum   FLFDEG-SSIEWTPA--PTKLS-SPAP--GIKLAYYPEEFFGKDAQVLEMDGNFD---NI
D. lutheri       FLFDEG-STIEWTPC--GKKLT-CAYP--GIKFRYGTEMYMGSEVTVLEMDGRFD---KL
O. tauri         YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPDTYYGKEVTVLEMDGQFD---KL
M. commoda       YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPDTFFGEEVSVLEMDGQFD---KL
P. sitchensis    YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPDIYYDNEVSVLEMDGQFD---RL
P. patens        YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPDTYYGNEVSVLEMDGQFD---KL
S. oleracea      YLFDEG-STISWIPC--GRKLT-CSYP--GIKFSYGPDTFYGNEVTVVEMDGMFD---RL
A. thaliana      YLFDEG-STISWIPC--GRKLT-CSYP--GIKFNYEPDSYFDHEVSVLEMDGQFD---RL
S. moellendorf.  YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPDTYYDNEVSVLEMDGQFD---KL
T. aestivum      YLFDEG-STINWIPC--GRKLT-CSYP--GIKFSYGPDTYFGQEVSVLEMDGQFD---RL
P. trichocarpa   YLFDEG-SSISWIPC--GRKLT-CSYP--GIKFSYGPDAYYGHEVSVLEMDGQFD---RL
M. crystallinum  YLFDEG-SSITWIPC--GRKLT-CSYP--GIKFFYGPDTYFGNEVTVLEMDGQFD---RL
P. sativum       YLFDEG-STISWIPC--GRKLT-CSYP--GIKFFYGPETYKGNEVSVVEMDGQFD---RL
C. variabilis    YLFDQG-STVSWIPC--GRKLT-CSFP--GIKMFYGPDTYYGEEVSVLEMDGQFD---KL
C. reinhardtii   YLFDEG-STISWIPC--GRKLT-CSFP--GIKMFYGPDTWYGQEVSVLEMDGQFD---KL
V. carteri       YLFDEG-STISWIPC--GRKLT-CSFP--GIKMFYGPDTWYGQEVSVLEMDGQFD---KL
G. sulphuraria   YLYDEG-STIDWIPC--GRKLT-CSYP--GIKFHYGPDNWYNHDVSVLEVDGNFE---KL
G. kilaueensis   YLFDRAISDVCW-----KPNFP-NSDP--ELTFCYGTTDYFGRPASYLSIDGEFA----P
G. violaceus     YLFDRAISDVCWK----PNFPN-SDEE---LTFCYGTQDYFGRPASYLSIDGEFA----P
T. elongatus     YLFDEG-STITWIPC--GRKLT-CSYP--GIRLSYGPDEYYGHPVSVLEVDGRFE---KL
Synechocystis sp YLFDEG-STIDWRPC--GRKLT-CTYP--GIKMYYGPDNFMGNEVSLLEVDGRFE---NL
M. aeruginosa    YLFDEG-STIDWRPC--GRKLT-CTYP--GIKLYYGPDGFLGNEVSILELDGQFD---NL
Cyanothece sp    YLFDEG-STIDWRPC--GRKLT-CAYP--GLKMYYGPDNIFGNEVSILEIDGQFD---NL
S. elongatus     YLFDEG-STIQWTPC--GRKLT-CSYP--GIRLAYGPDTYYGHEVSVLEVDGQFE---NL
A. variabilis    YLFDEG-STINWTPC--GRKLT-CSYP--GMQLYYGSDVYYGRYVSVLEVDGQFD---NL
N. spumigena     YLFDEG-STINWTPC--GRKLT-CSYP--GMQVYYGSDVYYGRYVSVLEVDGQFD---NL
A. boonei        SLINT------------------SQKP---MMISYRDDFYYMKRVSRITFDGLIP-----
F. placidus      TLNVDL-----------SRLIK-ASER--DFAISFFSDYYYGKRASFIDIDGFLN-----
A. profundus     SLNIDI-----------SDLVK-ASER--DFSIGFFSDYYYAEKASFIDIDGFLN-----
A. veneficus     KLDIDL-----------SAFVR-ASEK--DFALGFFSDYYYEKPASFIDIDGLMN-----
M. harundinacea  DLKIDL-----------SAL---FSLPDGEFSISFQRDDYYGKRVSVLTVDGELH----R
M. concilii      SMNIDL-----------SKILR-RSEH--EFSIEFQRDDYYGKRVGIMTMDGEIH-----
M. thermophila   DLTIDL-----------SRIMR-LTER--EFSIEFQRDDYYGKRVGVMTLDGEFP----L
M. hungatei      ELNIDL-----------CDLFK-KSSH--DFSLSCISHTPDSRNMRALVVDGELM-----
Methanolinea sp  CLGMDL-----------VSLMS-SFDH--NFMVEYRVVTEAGRRMGRLAFDGGIP-----
M. boonei        SLSIDL-----------TSLLA-FHES--EFSIEFSTQRIECSFLRSLTFDGEMN-----
M. limicola      CLNFDL-----------FAINS-LADR--NFRFDFRVTERGGEKIGALSLDGEFQ----Y
M. petrolearia   NLNFDL-----------FAINS-LAER--GFSFDFSIIEKYEKKMGALSLDGEFR-----
M. palustris     DLSIDL-----------FSLLS-LSDR--NFLIEFSHEQRNDERTGELILDGELS-----
M. marisnigri    DLSIDL-----------FGLLS-LSER--DFMVEFTIEDVGGEAMGALTFDGELN-----
M. liminatans    GLSIDL-----------GEIFRLCERP---FLLEFGLSSLDGRELSALVLDGELA-----
Gblocks
Annotation                     *        *
                            C243     C249
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                         490       500       510       520       530       540
                   =========+=========+=========+=========+=========+=========+
P. profundum       -----------------------------------FAMELIVRPLIQQLIDTGKVG----
P. luminescens     -----------------------------------LAMELIMTPLVQRLLEGGKIS----
E. amylovora       -----------------------------------LAMELIMGPLVKRLIEGKKIG----
S. flexneri        -----------------------------------LAMELIMLPLVQRLMEGKKIE----
S. medicae         -----------------------------------LAMQLIFTPLIHKLLERKHRMS---
R. meliloti        -----------------------------------LAMQLIFTPLIHKLLERKHRMS---
C. necator         -----------------------------------LAMQLIFTPFVLRMMERRKRAAQ--
R. rubrum          -----------------------------------LSMQLIFTPFIWRFMDKRARALGR-
R. sphaeroides     -----------------------------------LAMQLILTPLIDRVVRESKVA----
A. cryptum         -----------------------------------LAMQLILTPIIMQLMDRKRRAQ---
X. flavus          -----------------------------------LAMQLLLTPLIMKLMDRKRRAG---
N. hamburgensis    -----------------------------------LAMQLILTPLILQLIDRKRRA----
N. vulgaris        -----------------------------------LAMQLILTPLILQLIERKKRA----
R. palustris DX1   -----------------------------------LAMQLILTPLIMQLIDRKRSVK---
R. palustris Bis   -----------------------------------LAMQLILTPLIMQLIERKRGAK---
M. capsulatus      -----------------------------------LAMEIIFRPILERMMADREKG----
A. ferrooxidans    -----------------------------------YAMELILGPRIERMLEDMHLTI---
C. M. oxyfera      -----------------------------------LAMELILAPIVHIMIENKLKA----
T. denitrificans   -----------------------------------FAMELILAPLIQDMIANKKK-----
A. vinosum         -----------------------------------FAMEIILQPIIERMMDARRV-----
P. lunula          DQLKEIEENLEGLAGS-PGELTEAMTKLRSSPGSQNGTGLLQTVIAMKVREVYERLTAKV
L. polyedrum       AQLKEIEDNLEGLPSKTPGELTEAMVKLKSSPGSQNGTGMLQTVIAMKFREVYEKLTGGK
B. natans          EELFFIEERLSNTNTKYFGELTKQMLKNKAAPGSGDGSGLIQALVALKMRESYERFTGRT
E. gracilis        KEGLYVEKFLHNTGAKEFGELTQELLKGQNSPGGDNGTGFMQTLAALKIREIYERATGE-
P. parvum          EELIYVESQLCNTGTKYYGELTEQMVNNKASPGSENGSGLFQTICAFKIREAFEAITA--
G. theta           DEMMYVEKQFASTGSKFVGEITKKMLEYEGQPGSNDGTGFLQTITALKVREVYEGIAKVK
T. pseudonana      QELVYVESNLGNTNSKFYGEVTQAMLSLADSPGSNNGTGLMQTLAAFAIRELYNKKSAAA
O. sinensis        QELVYVESQLSNTSTKFYGELTQAMLKLADAPGSNNGTGLMQTLAAFAIRELYEKKAAAA
P. tricornutum     QELVYVESALSNTKTKFYGEMTQAMLALATAPGSNNGTGLMQTLAAFAIRDIYEKKTAAA
D. lutheri         DELIYVESALTNTGAKFYGELTQQILKNKDAVGSDNGTGFFQTLCSFKIREAYEKATGKT
O. tauri           EELIYVESHLSNTSSKFYGEITQQMLKYQNGPGSNNGTGFFQTIVGLKVREVYERISGKE
M. commoda         EELIYVESHLSNTSTKFYGEITQQMLKYQNGPGSNNGTGLFQTLCGLKVRELYERISEKE
P. sitchensis      EELIYVESHLSNISTKFYGEVTQQMLKHADFPGSNNGTGLFQTIVGLKIRDVYEQLISQT
P. patens          DELIYVESHLSNISTKFYGEITQQMLKHADFPGSNNGTGLFQTICGLKIRSVYERILANQ
S. oleracea        DELIYVESHLSNLSTKFYGEVTQQMLKHQNFPGSNNGTGFFQTIIGLKIRDLFEQLVASR
A. thaliana        DELIYVESHLSNLSTKFYGEVTQQMLKHADFPGSNNGTGLFQTIVGLKIRDLYEQLIANK
S. moellendorf.    DELIYVESHLSNISTRFYGEITQQMLKHADFPGSNNGTGLFQTIVGLKIRDVFERITSKQ
T. aestivum        DELIYVESHLSNLSTKFYGEVTQQMLKHADFPGSNNGTGLFQTIVGLKIRDLYEQIIAER
P. trichocarpa     DELIYVESHLSNISTKFYGEVTQQMLKHADFPGSNNGTGLFQTIVGLKIRDLFEQIVASR
M. crystallinum    DELIYVESHLSNLSTKFYGEVTQQMLKHQDFPGSNNGTGLFQTIVGLKIRDLFEQLIASK
P. sativum         DELIYVESHLSNLSSKFYGEVTQQMLKHADFPGSNNGTGLFQTIVGLKIRDLFEQIVAS-
C. variabilis      EELIYMESHLSNTSAKFYGEITQQMLKNSSFPGSNNGTGLFQTIVGLKCREVYERITQK-
C. reinhardtii     EELIYVESHLSNTSAKFYGEITQQMLKNSGFPGSNNGTGLFQTIVGLKVREVYERIVKKD
V. carteri         EELIYVESHLSNTSAKFYGEITQQMLKNSGFPGSNNGTGLFQTIVGLKVREVYERIVKKD
G. sulphuraria     EELIYIESHLNNTSTKFYGEITQQLLRNSSAPGSNNGTGLFQVLTALKMRQLYEELTGKS
G. kilaueensis     DDSPELEQKLRNTSETRFGELASLILKHTDYPGSRDGTGFFQVLIGLKFRSIYEALIAQS
G. violaceus       EDSPELEEKLRNTSETRYGELASLILKHTDYPGSRDGTGFFQVLMSLKFRAIYEALTAQL
T. elongatus       DELIYIESHLSNTSTKHYGEVTELLLKHRDYPGSDNGSGLFQVLTGLKMRATYERLTSRD
Synechocystis sp   EEMVYVENHLSKTGTKYYGEMTELLLKHKDYPGTDNGTGLFQVLVGLKMRKVYEQLTAEA
M. aeruginosa      EEMIYIESHLSKTGTKYYGEMTELLLKHKDYPGSTNGTGLFQVLVGLKMRETYEKLMAAE
Cyanothece sp      EEMIYIEQHLSRTGTKYYGEMTHLLQQHKDYPGSNNGTGLFQVLVGLKMRETYEILTSV-
S. elongatus       EEMIYVEGHLSKTDTQYYGELTHLLLQHKDYPGSNNGTGLFQVLTGLKMRAAYERLTSQ-
A. variabilis      EEVIYIETHLSNTSTKYQGELTQLLLQHREYPGSNNGTGFFQVLTGLKMRAAYERLTAKE
N. spumigena       DEVIYVETHLSKTSTKYEGEMTHLLLQHREYPGSNNGTGLFQVLTGLKMRAAYERLTTK-
A. boonei          -------HEAIDSLERRIMEYTGFENYILERSKYVNGTQIAQLLVAWYFVEMMNNIFREI
F. placidus        ---VEIFESLLDALRDETGYKVRW-----EAREYVNSIEVAKLLLCWNLVEIIKMKG---
A. profundus       ---VDIFKSLFDSLRKEIGDG-----EIKVESEYVNAIEFSKLLVCWKLVEVLKHSLR--
A. veneficus       ---VELFSTLLDILKKEVGADVEWKMNT-----YVNAIEVAKLLVCWRFLELIKFRLEAE
M. harundinacea    SMVEGVEAKLKSLAG------STAPICDRAGGDRVTSTGMAQLLLSWRLLEKLQLHLDKA
M. concilii        ------QSMISDLEKKLGESLGTDGMISDRREEYVNAIGLAQLILTWNCVEKLDYLLQEE
M. thermophila     TMIKDLERKLCDFLGRDVPSVTEG--CQEDHGSYVNATEMTQLILIWRFLEKIANLAW--
M. hungatei        ------PDTIHKIERQIEFQTGISPINIFRGQEHITGTDLVRLILSWQIINGRIALSNHL
Methanolinea sp    ------REMAGDLRRKIEEQTGTQPADMFRGNAMVTATDMVRLIVSWRIINHLANLA---
M. boonei          ------YDTVRNLELSIEHQTGIHPIEMFAGRKVVTPTNIVQLLLSWRIINRRIFLQDHR
M. limicola        DVIRCLELNIEEQTG-------VSPVSLFEGRDYVTATEMIQLLLSWRIINRRIQMES--
M. petrolearia     ------HEVVSLLEKGIEMQTGIGPVSVYSDRSYVTATEMVELILSWRIINRRMDMKYGS
M. palustris       ------TRMVKRLETSIEEQTQVRPISDFHDHDYMTATEVVQLILAWRIIHQRVFLERCL
M. marisnigri      ------DAVARKLERNIEIQTQVEPIDLSQDSDYLTAGDMAQLILAWRIINRRIFIESAP
M. liminatans      ------ASAIRRLARTIGRETRSEAVNLFADRQYVTAGEIAELILAWRILNRWHVLEAAR
Gblocks
Annotation
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                          550        560
                   =========+=========+
P. profundum       --------------------
P. luminescens     --------------------
E. amylovora       --------------------
S. flexneri        --------------------
S. medicae         --------------------
R. meliloti        --------------------
C. necator         --------------------
R. rubrum          --------------------
R. sphaeroides     --------------------
A. cryptum         --------------------
X. flavus          --------------------
N. hamburgensis    --------------------
N. vulgaris        --------------------
R. palustris DX1   --------------------
R. palustris Bis   --------------------
M. capsulatus      --------------------
A. ferrooxidans    --------------------
C. M. oxyfera      --------------------
T. denitrificans   --------------------
A. vinosum         --------------------
P. lunula          GA------------------
L. polyedrum       --------------------
B. natans          IQIPKWGLFLDDY-------
E. gracilis        KA------------------
P. parvum          --------------------
G. theta           VPAQAN--------------
T. pseudonana      KLAATKETAASA--------
O. sinensis        KLAVIEA-------------
P. tricornutum     KAKAGVSAAAA---------
D. lutheri         VDASAAA-------------
O. tauri           VVAKA---------------
M. commoda         VVTAA---------------
P. sitchensis      TGASLEAAKA----------
P. patens          KNAATLQSAKA---------
S. oleracea        STATATAAKA----------
A. thaliana        ATARAEAKA-----------
S. moellendorf.    GSPVGAAAATSKV-------
T. aestivum        AGVPAEAAKV----------
P. trichocarpa     AKTPVEATKA----------
M. crystallinum    TAAPAAATKA----------
P. sativum         RAETPVGAAKA---------
C. variabilis      --------------------
C. reinhardtii     VVPV----------------
V. carteri         VVPA----------------
G. sulphuraria     IAPVLV--------------
G. kilaueensis     LAAAKV--------------
G. violaceus       LTASKAK-------------
T. elongatus       AATVTNR-------------
Synechocystis sp   KVPASV--------------
M. aeruginosa      AKVAASV-------------
Cyanothece sp      ESKVATQV------------
S. elongatus       AAPVAASV------------
A. variabilis      AKLAVQV-------------
N. spumigena       EAKLAVQV------------
A. boonei          ENAREKNIY-----------
F. placidus        --------------------
A. profundus       --------------------
A. veneficus       L-------------------
M. harundinacea    --------------------
M. concilii        GY------------------
M. thermophila     --------------------
M. hungatei        DQ------------------
Methanolinea sp    --------------------
M. boonei          --------------------
M. limicola        --------------------
M. petrolearia     GVSS----------------
M. palustris       HQDHNK--------------
M. marisnigri      GAGGTGRTVTGNNGHGCGRR
M. liminatans      SAHAKG--------------
Gblocks
Annotation
```

B

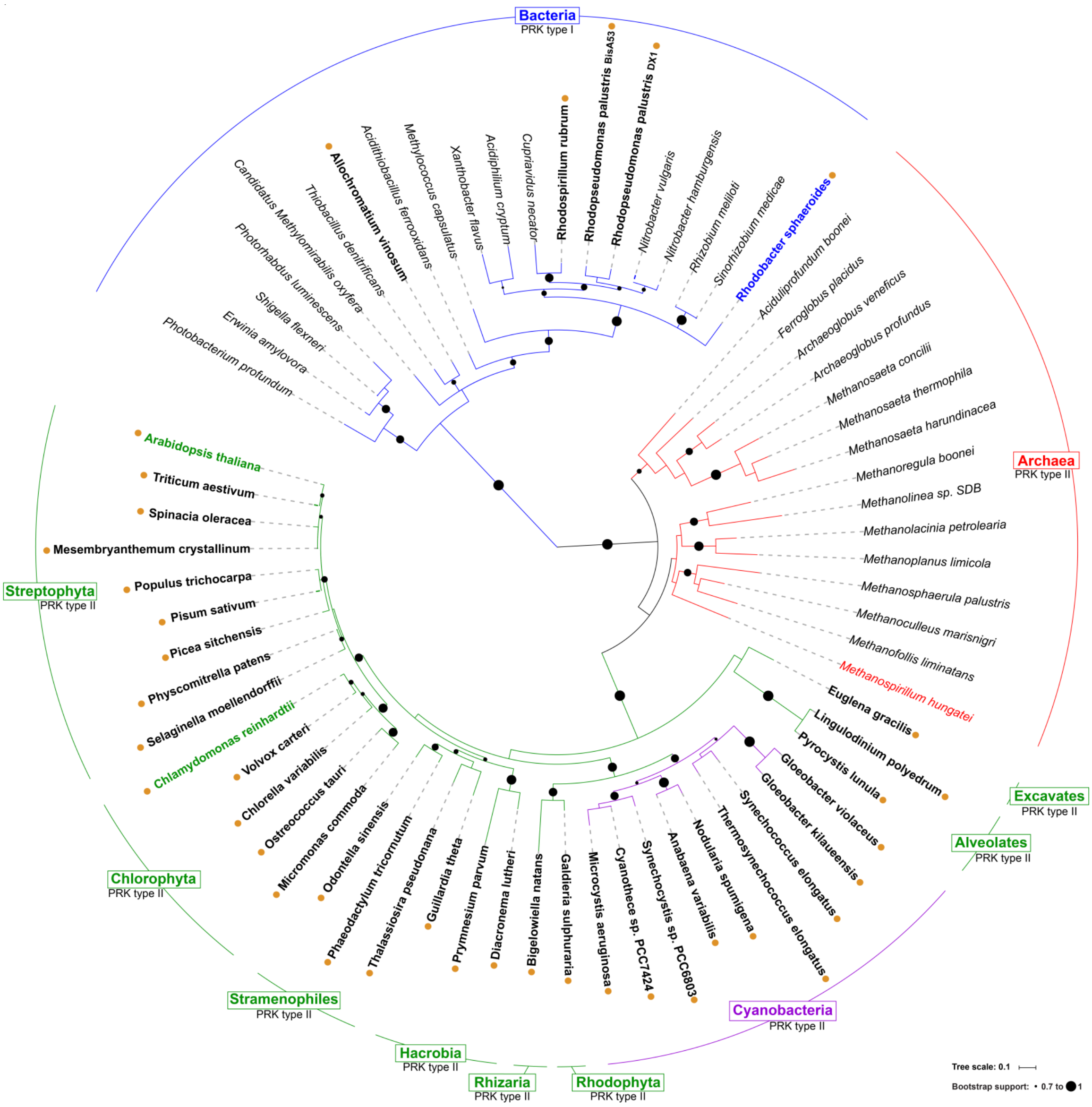
Bacteria
PRK type I
Rhodopseudomonas palustris BisA53
Rhodopseudomonas palustris DX1
Rhodospirillum rubrum
Cupriavidus necator
Acidiphilium cryptum
Xanthobacter flavus
Methylococcus capsulatus
Acidithiobacillus ferrooxidans
Allochromatium vinosum
Thiobacillus denitrificans
Candidatus Methylomirabilis oxyfera
Photorhabdus luminescens
Shigella flexneri
Erwinia amylovora
Photobacterium profundum
Nitrobacter vulgaris
Nitrobacter hamburgensis
Rhizobium meliloti
Sinorhizobium medicae
Rhodobacter sphaeroides
Aciduliprofundum boonei
Ferroglobus placidus
Archaeoglobus veneficus
Archaeoglobus profundus
Methanosaeta concilii
Methanosaeta thermophila
Methanosaeta harundinacea
Methanoregula boonei
Methanolinea sp. SDB
Methanolacinia petrolearia
Methanoplanus limicola
Methanosphaerula palustris
Methanoculleus marisnigri
Methanofollis liminatans
Methanospirillum hungatei
Archaea
PRK type II
Euglena gracilis
Lingulodinium polyedrum
Pyrocystis lunula
Gloeobacter violaceus
Gloeobacter kilauensis
Synechococcus elongatus
Thermosynechococcus elongatus
Nodularia spumigena
Anabaena variabilis
Synechocystis sp. PCC6803
Cyanothece sp. PCC7424
Microcystis aeruginosa
Galdieria sulphuraria
Bigelowiella natans
Diacronema lutheri
Prymnesium parvum
Guillardia theta
Thalassiosira pseudonana
Phaeodactylum tricornutum
Odontella sinensis
Micromonas commoda
Ostreococcus tauri
Chlorella variabilis
Volvox carteri
Chlamydomonas reinhardtii
Selaginella moellendorffii
Physcomitrella patens
Picea sitchensis
Pisum sativum
Populus trichocarpa
Mesembryanthemum crystallinum
Spinacia oleracea
Triticum aestivum
Arabidopsis thaliana
Streptophyta
PRK type II
Chlorophyta
PRK type II
Stramenophiles
PRK type II
Hacrobia
PRK type II
Rhizaria
PRK type II
Rhodophyta
PRK type II
Cyanobacteria
PRK type II
Alveolates
PRK type II
Excavates
PRK type II
Tree scale: 0.1
Bootstrap support: 0.7 to 1

Fig. S6. Sequence alignment and phylogenetic analysis of 69 PRKs. (A) The sequences annotated as PRKs were retrieved from Uniprot and aligned using the phylogeny webserver suite (www.phylogeny.fr) (27). Blue areas in the "Gblocks" line define the conserved areas, later used by the software to determine the phylogeny. The alignment was performed by MUSCLE and curation by Gblocks. Annotations used are as follow: black boxes within the sequences indicate conservation of the residue in more than 70% of the sequences. Walker A (P-loop) and Walker B motives are represented by a red or green area, respectively, and the clamp loop is highlighted by a yellow area. Bars (|) or Hashtags (#) denote residues implicated in Ru5P or ATP binding, respectively. Plus sign (+) indicates two Aspartate residues shown to be crucial for catalysis by mutagenesis in *R. sphaeroides* (28). Star signs (*) indicate Cys residues implicated in disulfide bridges (Cys16 with Cys55; Cys243 with Cys249) (29), numbers below are for *C. reinhardtii* PRK. Blue and red bars on the right side indicate clusters of bacterial and archeal PRK, respectively, while the green one indicates the cluster of eukaryotic and the purple one is for the cyanobacterial PRKs. Species names in bold are indicating the 4 species with known structure. Uniprot accessions numbers and other details, for all protein sequences are reported in Table S6. (B) The phylogeny was built with PhyML and the tree with TreeDyn. The visual was obtained with iTOL (http://itol.embl.de/) (30). Bootstrap values superior to 0.7 are represented by black circles with a radius proportional to the value. Branch lengths are represented by straight lines at indicated scale, while dashes are presented for the sake of clarity. The clades are colored in function of their kingdom (Bacteria in blue, Archaea in red and Eukaryotes in green) except Cyanobacteria clade which is in purple. Photosynthetic species are in bold indicated by a yellow circle while the others are italicized. Species for which the PRK has a known structure, *i.e. R. sphaeroides* (31), *M. hungatei* (5), *C. reinhardtii* and *A. thaliana*, are represented in the color of their kingdom.

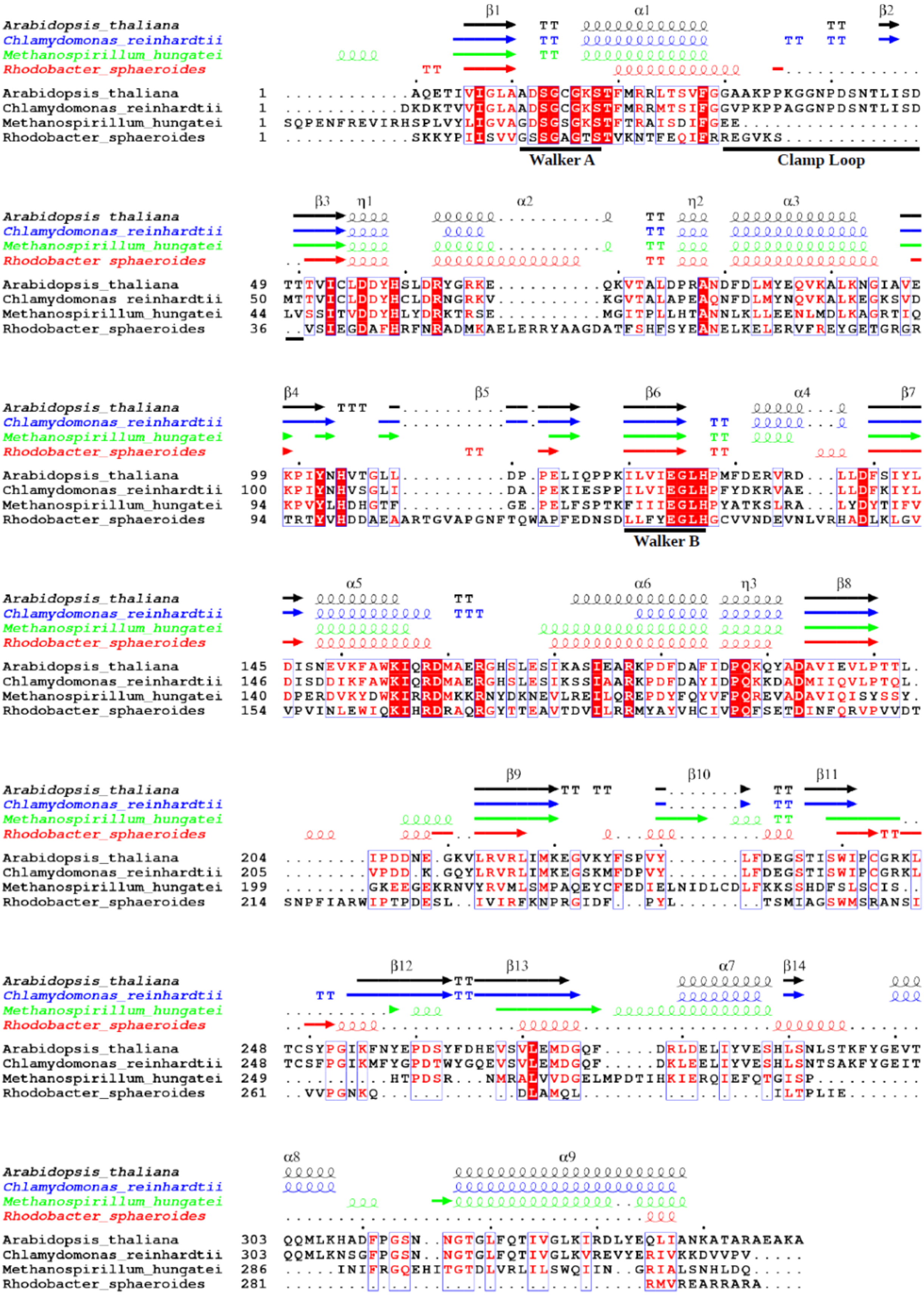
β1 α1 β2
Arabidopsis_thaliana 1 ............AQETIVIGLAADSGCGKSTFMRRLTSVFGGAAKPPKGGNPDSNTLISD
Chlamydomonas_reinhardtii 1 ...........DKDKTVVIGLAADSGCGKSTFMRRMTSIFGGVPKPPAGGNPDSNTLISD
Methanospirillum_hungatei 1 SQPENFREVIRHSPLVYLIGVAGDSGSGKSTFTRAISDIFGEE.................
Rhodobacter_sphaeroides 1 ............SKKYPIISVVGSSGAGTSTVKNTFEQIFRREGVKS.............
Walker A
Clamp Loop
β3 η1 α2 η2 α3
Arabidopsis_thaliana 49 TTVICLDDYHSLDRYGRKE..........QKVTALDPRANDFDLMYEQVKALKNGIAVE
Chlamydomonas_reinhardtii 50 MTTVICLDDYHCLDRNGRKV.........KGVTALAPEAQNFDLMYNQVKALKEGKSVD
Methanospirillum_hungatei 44 LVSSITVDDYHLYDRKTRSE..........MGITPLLHTANNLKLLEENLMDLKAGRTIQ
Rhodobacter_sphaeroides 36 ..VSIEGDAFHRFNRADMKAELERRYAAGDATFSHFSYEANELKELERVFREYGETGRGR
β4 β5 β6 α4 β7
Arabidopsis_thaliana 99 KPIYNHVTGLL..........DP.PELIQPPKILVIEGLHPMFDERVRD...LLDFSIYL
Chlamydomonas_reinhardtii 100 KPIYNHVSGLI..........DA.PEKIESPPILVIEGLHPFYDKRVAE...LLDFKIYL
Methanospirillum_hungatei 94 KPVYLHDHGTF..........GE.PELFSPTKFIIIEGLHPYATKSLRA...LYDYTIFV
Rhodobacter_sphaeroides 94 TRTYVHDDAEAARTGVAPGNFTQWAPFEDNSDLLFYEGLHGCVVNDEVNLVRHADLKLGV
Walker B
α5 α6 η3 β8
Arabidopsis_thaliana 145 DISNEVKFAWKIQRDMAERGHSLESIKASIEARKPDFDAFIDPQKQYADAVIEVLPTTL.
Chlamydomonas_reinhardtii 146 DISDDIKFAWKIQRDMAERGHSLESIKSSIAARKPDFDAYIDPQKKDADMIIQVLPTQL.
Methanospirillum_hungatei 140 DPERDVKYDWKIRRDMKKRNYDKNEVLREILQREPDYFQYVFPQREVADAVIQISYSSY.
Rhodobacter_sphaeroides 154 VPVINLEWIQKIHRDRAQRGYTTEAVTDVILRRMYAYVHCIVPQFSETDINFQRVPVVDT
β9 β10 β11
Arabidopsis_thaliana 204 ........IPDDNE.GKVLRVRLIMKEGVKYFSPVY.......LFDEGSTISWIPCGRKL
Chlamydomonas_reinhardtii 205 ........VPDD.K.GQYLRVRLIMKEGSKMFDPVY.......LFDEGSTISWIPCGRKL
Methanospirillum_hungatei 199 ........GKEEGEKRNVYRVMLSMPAQEYCFEDIELNIDLCDLFKKSSHDFSLSCIS..
Rhodobacter_sphaeroides 214 SNPFIARWIPTPDESL..IVIRFKNPRGIDF...PYL.......TSMIAGSWMSRANSI
β12 β13 α7 β14
Arabidopsis_thaliana 248 TCSYPGIKFNYEPDSYFDHEVSVLEMDGQF.....DRLDELIYVESHLSNLSTKFYGEVT
Chlamydomonas_reinhardtii 248 TCSFPGIKMFYGPDTWYGQEVSVLEMDGQF.....DKLEELIYVESHLSNTSAKFYGEIT
Methanospirillum_hungatei 249 ........HTPDSR...NMRALVVDGELMPDTIHKIERQIEFQTGISP..........
Rhodobacter_sphaeroides 261 ..VVPGNKQ..........DLAMQL..........ILTPLIE.......
α8 α9
Arabidopsis_thaliana 303 QQMLKHADFPGSN..NGTGLFQTIVGLKIRDLYEQLIANKATARAEAKA
Chlamydomonas_reinhardtii 303 QQMLKNSGFPGSN..NGTGLFQTIVGLKVREVYERIVKKDVVPV.....
Methanospirillum_hungatei 286 .....INIFRGQEHITGTDLVRLILSWQIIN..GRIALSNHLDQ.....
Rhodobacter_sphaeroides 281 ....RMVREARRARA....

Fig. S7. Sequence and structural alignment of the four structurally known PRKs. The alignment was performed with Espript (http://espript.ibcp.fr) (32) using the sequence and the structure of *At*PRK (Uniprot accession code P25697 and PDB ID code 6H7H); *Cr*PRK (Uniprot accession code P19824 and PDB ID code 6H7G); *Rs*PRK (Uniprot accession code P12033 and PDB ID code 1A7J) (31), *Mh*PRK (Uniprot accession code Q2FUB5 and PDB ID code 5B3F) (5). The sequence of both photosynthetic PRKs is much longer (349 and 344 residues for *At*PRK and *Cr*PRK, respectively) than bacterial (290 residues) and Archae (323 residues) PRKs. Sequence identities among considered PRKs are: 75% for *At*PRK *vs* *Cr*PRK; 35% for *At*PRK *vs* *Mh*PRK; 32% for *Cr*PRK *vs* *Mh*PRK; 22% for *At*PRK *vs* *Rs*PRK; 24% for *Cr*PRK *vs* *Rs*PRK. The sequence identities were calculated by Clustal Omega (33).

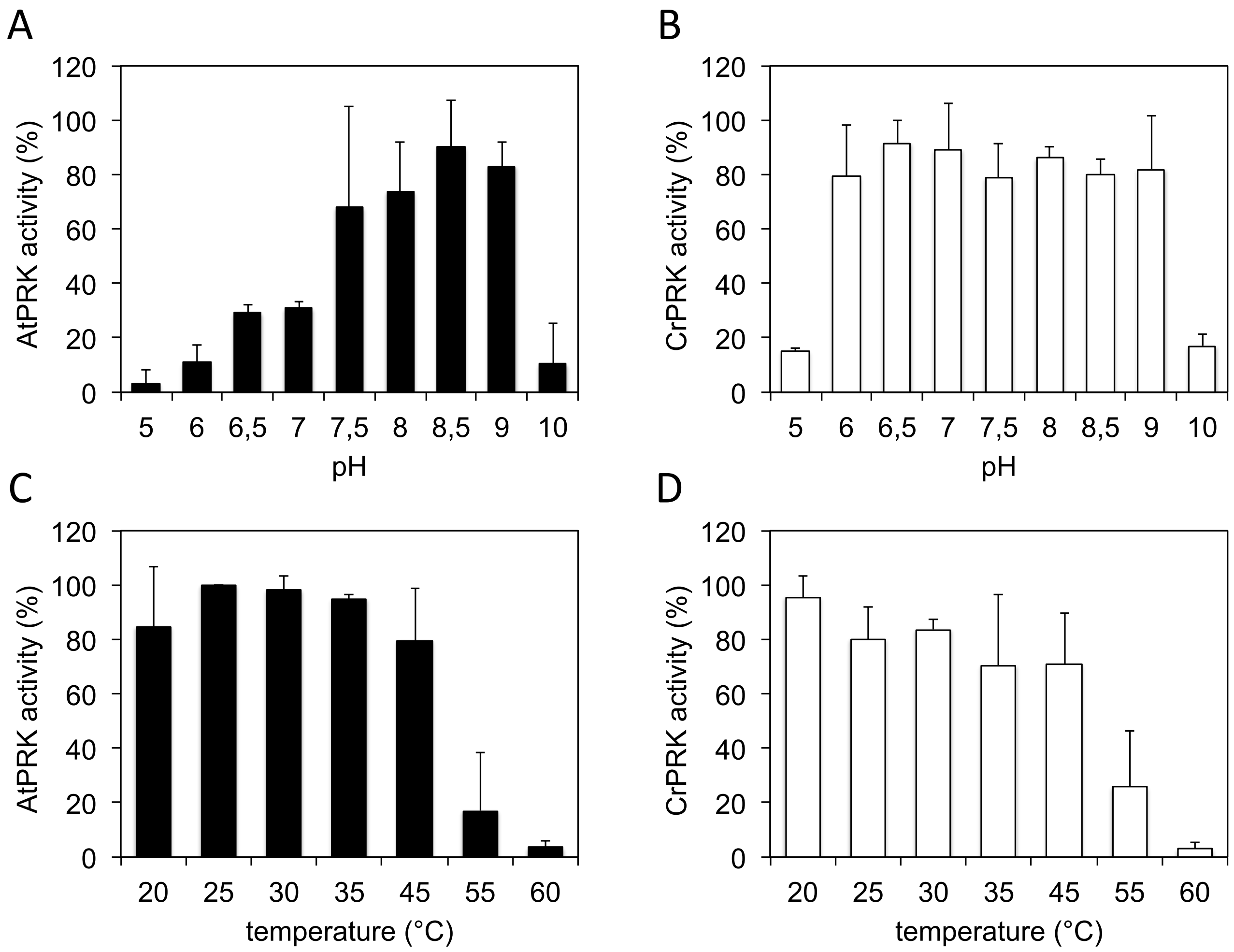

Fig. S8. pH and temperature dependence of photosynthetic PRKs. The enzyme activity of *At*PRK (A and C) and of *Cr*PRK (B and D) was evaluated at different pHs (upper panels) and temperatures (lower panels). Values are reported as means ± SD (n=3).

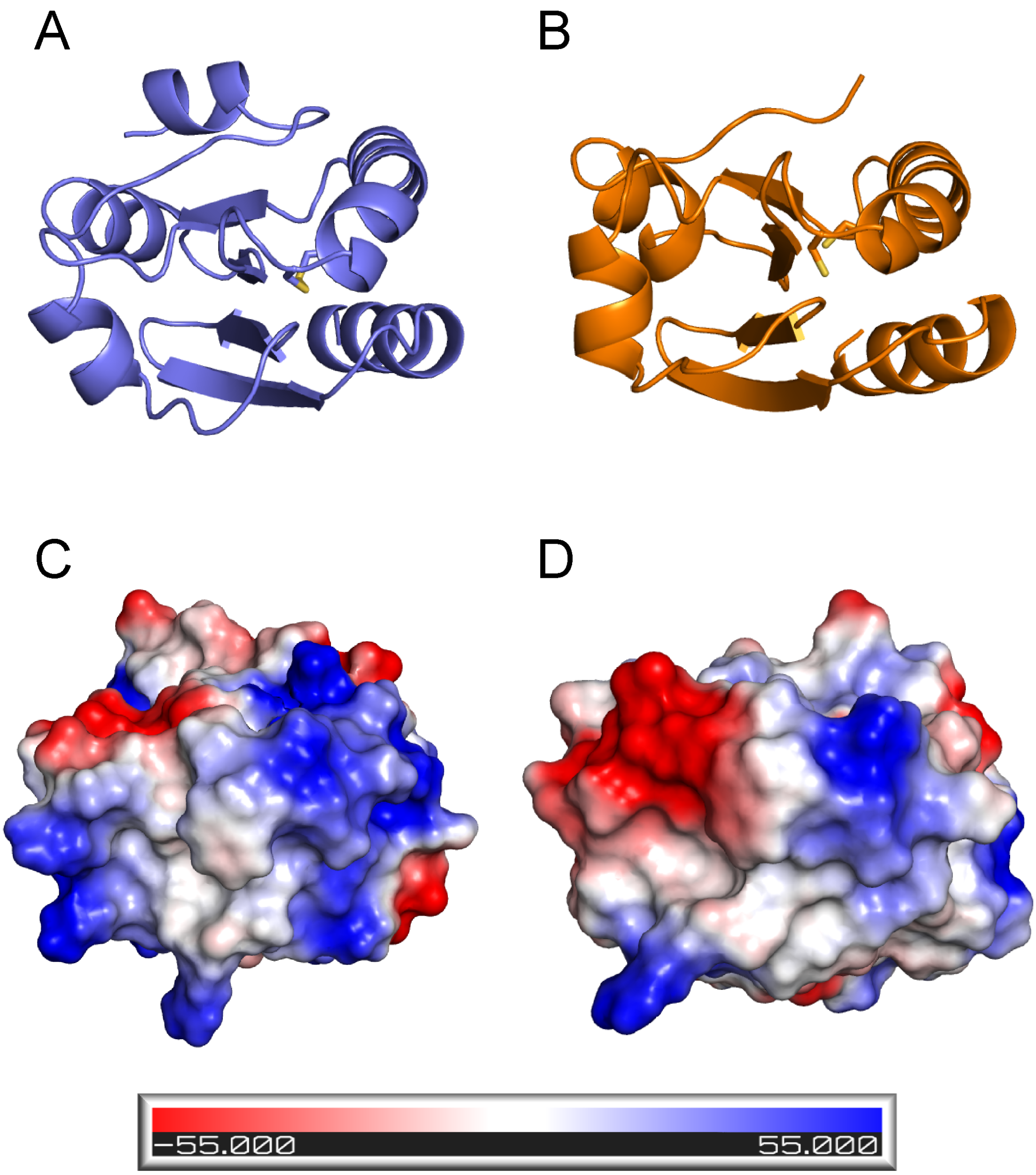

Fig. S9. Electrostatic surface potential of *A. thaliana* TRX-f1 and TRX-m2. Structure represented as ribbon (A, B) and electrostatic surface potential (C, D) of the homology model of *Arabidopsis thaliana* TRX-f1 (A, C) and TRX-m2 (B, D). The crystal structures of *Spinacia oleracea* TRX-f and TRX-m (PDB ID codes 1FAA and 1FB6) (34) were used as template to model *Arabidopsis thaliana* TRX-f1 and TRX-m2, respectively. The sequence identity of *Arabidopsis thaliana* TRXs with spinach enzymes is 59% and 75% for TRX-f1 and TRX-m2, respectively. The homology modelling was performed with Swiss-Model (35).

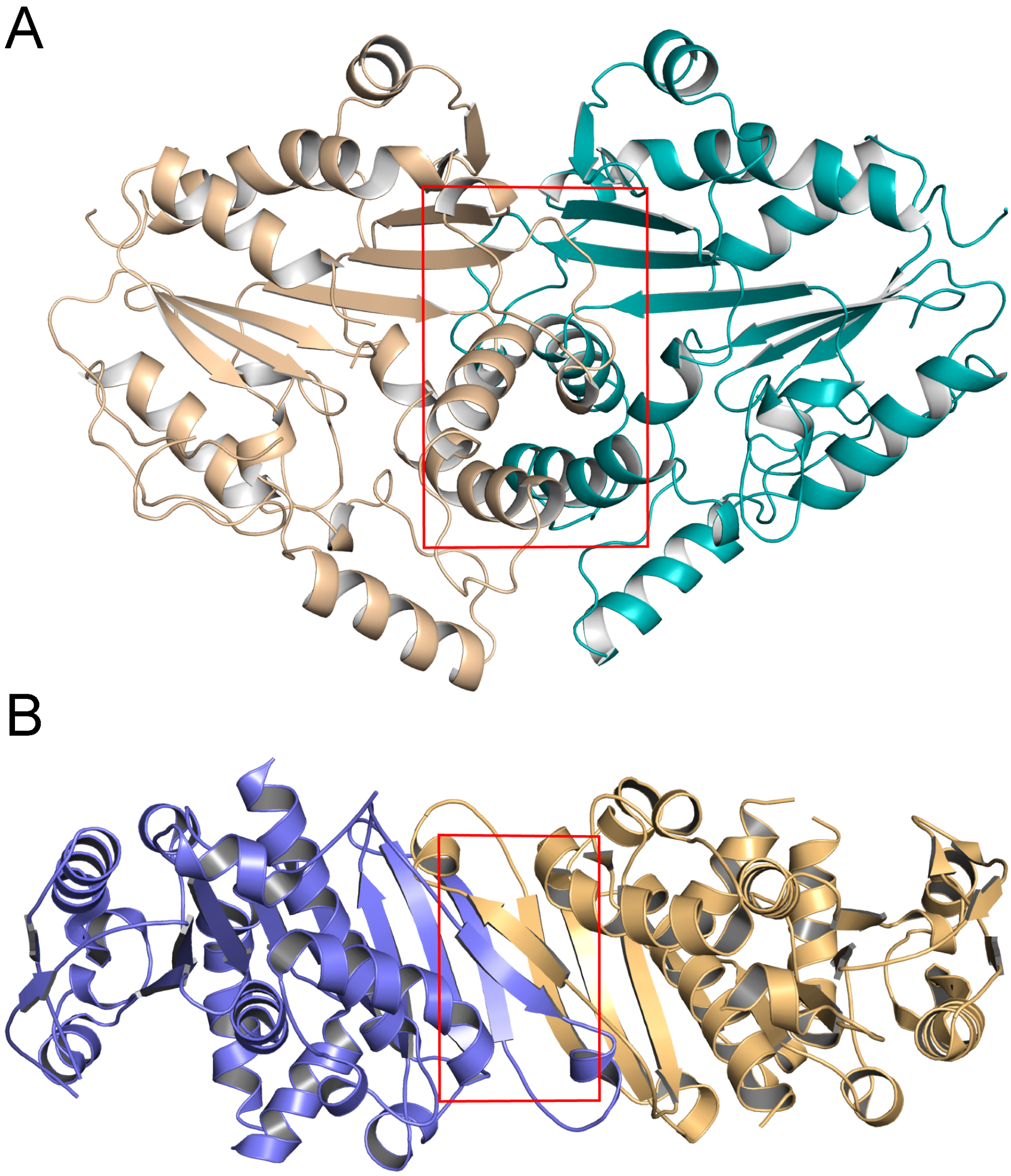

Fig. S10. Dimer interface of bacterial and Archaea PRKs. Dimer interface of (A), octameric *Rhodobacter sphaeroides* PRK (PDB ID code 1A7J) (31) and (B), dimeric *Methanospirillum hungatei* PRK (PDB ID code 5B3F) (5) is highlighted by a red box. The dimer interface of bacterial PRK is formed by three β-strands and one α-helix while in Archaea enzyme by two β-strands. The calculated dimer interface areas are 1667 and 1695 Å^2, respectively.

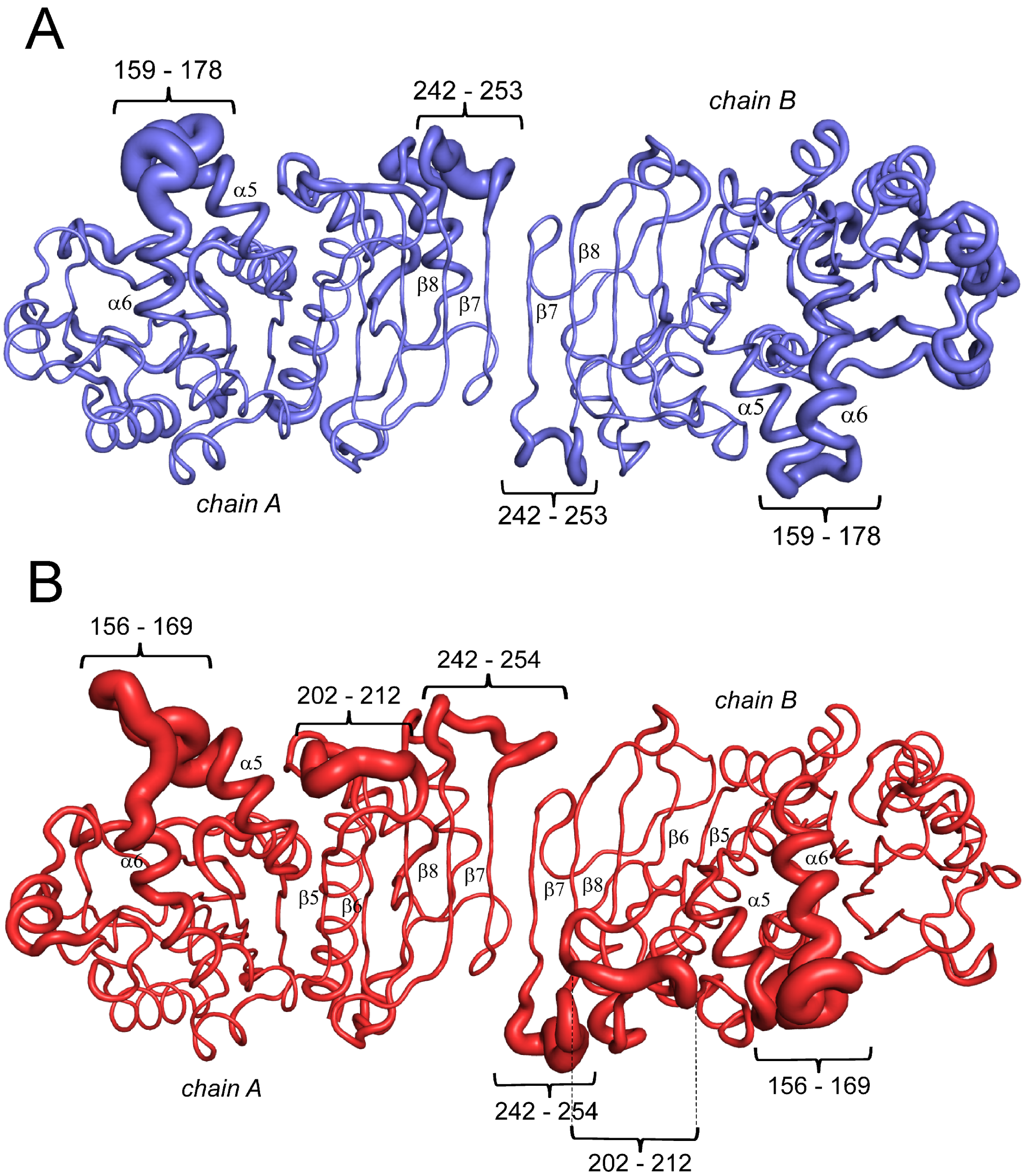

Fig. S11. Flexible and disordered regions in redox-sensitive PRKs. C_α trace of (A), *Cr*PRK and (B), *At*PRK. The trace thickness is proportional to the atomic B factor. *At*PRK shows a higher number of flexible regions compared to *Cr*PRK. The residues belonging to the flexible regions are reported.

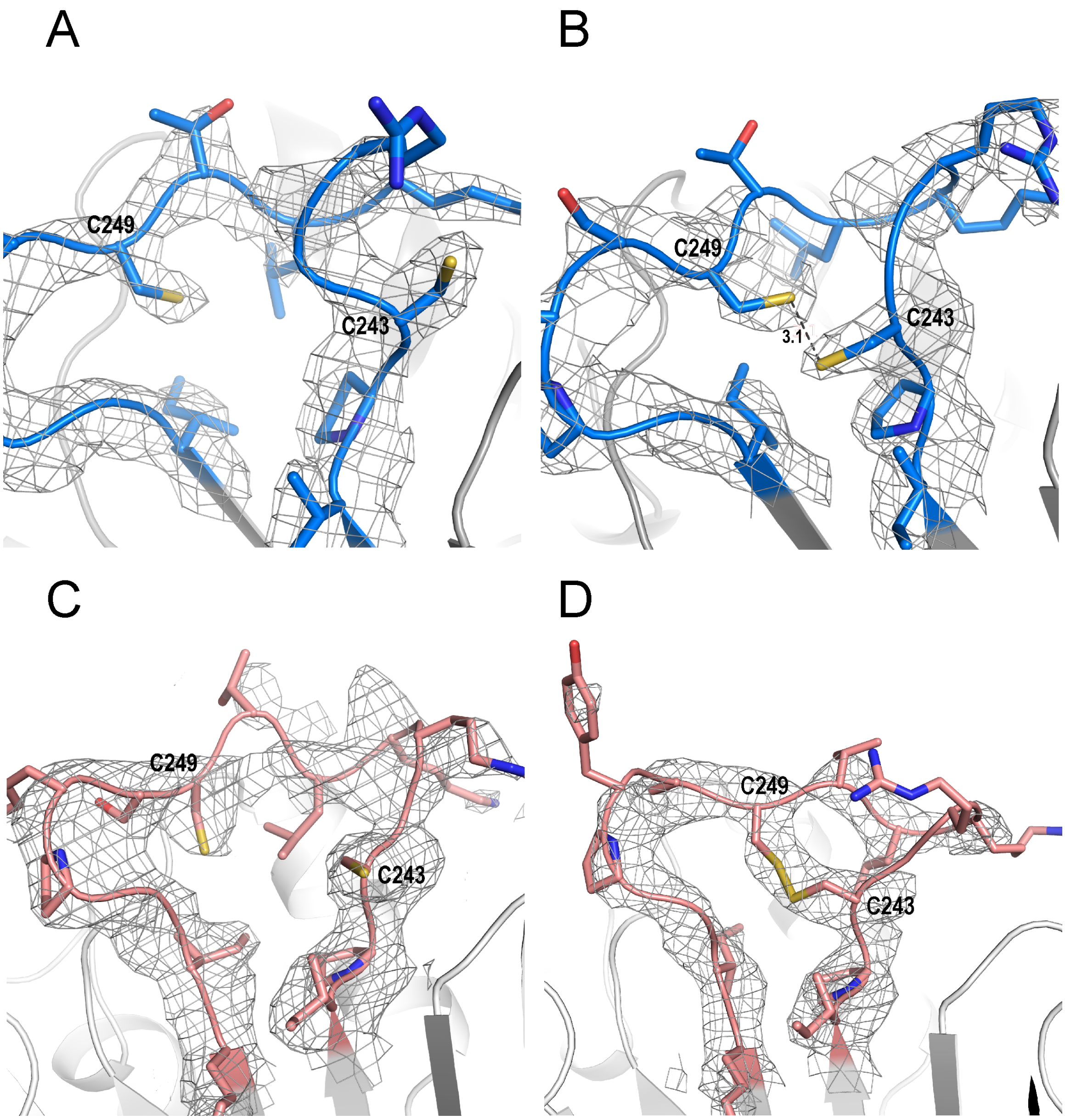

Fig. S12. Electron density of the C-terminal cysteine pair. $2F_o$-F_c electron density map contoured at 1.2σ and associated with Cys243 and Cys249 in (A), *Cr*PRK subunit A (B), *Cr*PRK subunit B (C), *At*PRK subunit A and (D), *At*PRK subunit B. In *Cr*PRK, both C-terminal cysteines are reduced even if in subunit B the thiol groups are only 3 Å apart. A disulfide bond is instead observed in subunits B of *At*PRK, while the thiol groups of the other cysteine pair (subunit A) lie very distantly.

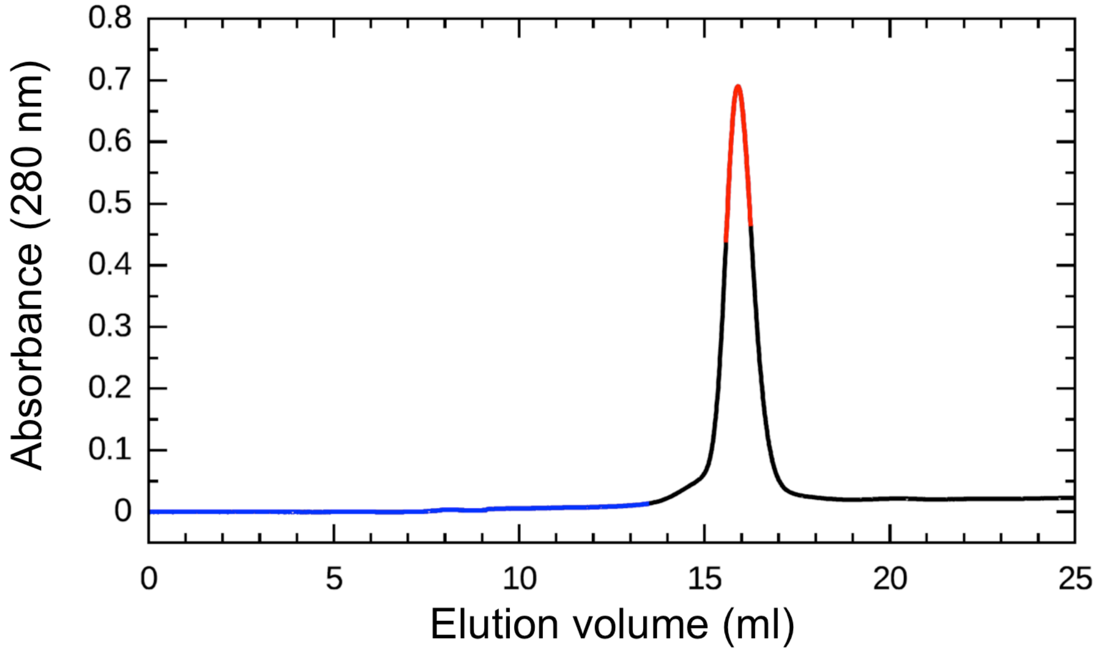

Fig. S13. UV trace of the chromatogram profile of *Cr*PRK analyzed in SEC-SAXS mode. Frames collected as buffer (from 0 to 14 ml) are highlighted in blue; frames collected as protein (from 14 to 17.5 ml) are highlighted in black; frames highlighted in red have been used for SAXS analysis.

Table S1. SEC-SAXS data analysis of reduced CrPRK.

Concentration (mg ml^{-1})	6.1 (injected)
Structural parameters	
q interval for Guinier linear fit (nm^{-1})	0.12-0.38
I(0) [from Guinier approximation]	42.0 ± 0.1
R_g (nm) [from Guinier approximation]	3.43 ± 0.01
q interval for Fourier inversion (nm^{-1})	0.12-3.5
I(0) [from P(R)]	42.4 ± 0.06
R_g (nm) [from P(R)]	3.55 ± 0.01
D_{max} (nm)	11.2±0.5
Porod volume estimate (nm^3)	115 ± 10
DAMMIN excluded volume (nm^3)	138 ± 1
Dry volume calculated from sequence (nm^3) (v=0.735 cm^3 g^{-1})	95
Molecular mass (kDa)	
From I(0)	70
From Vc	70
From Porod invariant	85
From Porod volume (x0.625)	72
From excluded volume (x0.5)	69
From sequence	77.8

Table S2. Accessibility values (ASA) for cysteine residues and a strictly conserved arginine.

Residue (*Cr*/*At*)	**ASA (Å^2)***			
	*Cr*PRK		*At*PRK	
	A	B	A	B
Cys16/15	14.5	8.5	7.6	10.6
Cys55/54	10.6	10.6	6.3	9.5
Cys61	55.9	58.7	/	/
Cys243	26.6	37.8	53.4	14.8
Cys249	42.4	31.1	14.8	50.6
Arg64/63	51.4	88.7	82.6	88.2

*Radius of the probe solvent molecule 1.4 Å

Table S3. Secondary structure element content in the structurally known PRKs.

PRK	Quaternary structure	Helix content (%)	Sheet content (%)	Other (%)
C. reinhardtii	Dimer	31.2	21.9	46.9
A. thaliana	Dimer	32.3	21.9	45.8
M. hungatei	Dimer	50.0	22.2	27.8
R. sphaeroides	Octamer	41.2	16.9	41.9

Table S4. X-ray (CrPRK and AtPRK) and SEC-SAXS (CrPRK) data collection parameters.

	*Cr*PRK	*At*PRK	*Cr*PRK SEC-mode
Detector	Pilatus 2M	ADSC Quantum Q315r	Pilatus 1M
Beam geometry (mm^2)	0.1 × 0.1	0.1 × 0.1	0.7 × 0.7
Wavelength (Å)	1.240	0.940	0.990
Capillary diameter (mm)	/	/	1.8
Sample-to-detector Distance (mm)	239.85	393.43	2872
Δϕ (°)	0.5	0.7	/
q* range (nm^{-1})	/	/	0.033-4.9
Exposure time (s)	5	5	1
Flow (ml/min)	/	/	0.5
Temperature (K)	100.0	100.0	277.15

*$q = 4\pi \sin(\theta)/\lambda$, where 2θ is the scattering angle and λ is the X-ray wavelength.

Table S5. X-ray data collection and refinement statistics.

	CrPRK	AtPRK
Data collection		
Unit cell (Å)	77.68, 83.55, 133.15, 90.00, 90.00, 90.00	116.30, 116.30, 106.81, 90.00, 90.00, 90.00
Space group	$P2_12_12_1$	$I4_1$
Resolution range* (Å)	44.38 – 2.60 (2.72 – 2.60)	82.23 – 2.47 (2.58 – 2.47)
Unique reflections	27230 (3280)	24824 (3107)
Completeness* (%)	99.6 (100.0)	97.6 (99.6)
R_{merge}*	0.076 (0.770)	0.091 (0.435)
$CC_{1/2}$	0.997 (0.743)	0.997 (0.947)
I/σ(I) *	13.6 (1.7)	11.2 (2.3)
Multiplicity*	5.1 (5.3)	6.9 (6.5)
Refinement		
Resolution range* (Å)	39.86 – 2.60 (2.69 - 2.60)	46.77 – 2.47 (2.57 – 2.47)
Reflection used	27162 (2666)	24672 (2786)
R/R_{free}*	0.227/0.262	0.226/0.281
rmsd from ideality (Å, °)	0.004, 0.915	0.011, 1.128
N° atoms		
Non-hydrogen atoms	5360	5385
Protein atoms	5319	5355
Solvent molecules	31	30
Hetero atoms	10	/
B value ($Å^2$)		
Mean	62.4	78.4
Wilson	59.0	52.5
Protein atoms	62.3	78.4
Solvent molecules	56.2	70.3
Hetero atoms	85.5	/
Ramachandran plot (%)[§]		
Most favoured	91.1	91.4
Allowed	7.4	6.0
Disallowed	1.5	2.7

*Values in parentheses refer to the last resolution shell
[§]As defined by MolProbity (35)

Table S6. Proteins used for phylogeny.

Organism	Organism - full description	Uniprot used	other Ref.	other Ref 2	Kingdom	Phylum	Photosynthetic	Reference and/or status of the uniprot entry
A. profundus	Archaeoglobus profundus	D2REP9		ADB58593	Archae	Euryarchaeota	no	Kono et al., 2017 (5)
M. concilii	Methanosaeta concilii	F4BW53		AEB68483	Archae	Euryarchaeota	no	Kono et al., 2017 (5)
M. hungatei	Methanospirillum hungatei	Q2FUB5		PDB: 5B3F	Archae	Euryarchaeota	no	Kono et al., 2017 (5)
M. marisnigri	Methanoculleus marisnigri	A3CWW0		ABN57860	Archae	Euryarchaeota	no	Kono et al., 2017 (5)
M. thermophila	Methanosaeta thermophila	A0B947		ABK15221	Archae	Euryarchaeota	no	Kono et al., 2017 (5)
A. boonei	Aciduliprofundum boonei (strain DSM 19572 / T469)	B5ICQ8			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
A. veneficus	Archaeoglobus veneficus (strain DSM 11195 / SNP6)	F2KMR8			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
F. placidus	Ferroglobus placidus (strain DSM 10642 / AEDII12DO)	D3RZ92			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. boonei	Methanoregula boonei (strain DSM 21154 / JCM 14090 / 6A8)	A7I4Y6			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. harundinacea	Methanosaeta harundinacea (strain 6Ac)	G7WL21			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. limicola	Methanoplanus limicola DSM 2279	H1YX11			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. liminatans	Methanofollis liminatans DSM 4140	J0SAT8			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. palustris	Methanosphaerula palustris (strain ATCC BAA-1556 / DSM 19958 / E1-9c)	B8GGS2			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
M. petrolearia	Methanolacinia petrolearia (strain DSM 11571 / OCM 486 / SEBR 4847) (Methanoplanus petrolearius)	E1RI35			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
Methanolinea sp	Methanolinea sp. SDB	A0A0Q0VL15			Archae	Euryarchaeota	no	Kono et al., 2017 (5) / protein predicted
A. ferrooxidans	Acidithiobacillus ferrooxidans (strain ATCC 23270 / DSM 14882 / CIP 104768 / NCIMB 8455) (Ferrobacillus ferrooxidans (strain ATCC 23270))	B7J555			Bacteria	Acidithiobacillia	no	Kono et al., 2017 (5) / protein inferred from homology
R. sphaeroides	Rhodobacter sphaeroides	AAA26113	P12033	PDB: 1A7J	Bacteria	α-Proteobacteria	yes (purple non-sulfur)	Hallenbeck and Kaplan, 1987 (36)
N. vulgaris	Nitrobacter vulgaris	P37100			Bacteria	α-Proteobacteria	no	*inferred by homology*
R. meliloti	Rhizobium meliloti (strain 1021) (Ensifer meliloti) (Sinorhizobium meliloti)	P58347			Bacteria	α-Proteobacteria	no	*inferred by homology*
S. medicae	Sinorhizobium medicae (strain WSM419) (Ensifer medicae)	P56887			Bacteria	α-Proteobacteria	no	*inferred by homology*
R. palustris DX	Rhodopseudomonas palustris (strain DX-1)	ADU46366		E6VEW3	Bacteria	α-Proteobacteria	yes (purple non-sulfur)	Kono et al., 2017 (5)
R. rubrum	Rhodospirillum rubrum	ABC23204		Q2RRP1	Bacteria	α-Proteobacteria	yes (purple non-sulfur)	Kono et al., 2017 (5)
A. cryptum	Acidiphilium cryptum (strain JF-5)	A5FWQ9			Bacteria	α-Proteobacteria	no	Kono et al., 2017 (5) / protein predicted
N. hamburgensis	Nitrobacter hamburgensis (strain DSM 10229 / NCIMB 13809 / X14)	Q1QGD6			Bacteria	α-Proteobacteria	no	Kono et al., 2017 (5) / protein inferred from homology
R. palustris Bi	Rhodopseudomonas palustris (strain BisA53)	Q07N64			Bacteria	α-Proteobacteria	yes (purple non-sulfur)	Kono et al., 2017 (5) / protein inferred from homology
X. flavus	Xanthobacter flavus	P23015			Bacteria	α-Proteobacteria	no	Meijer et al., 1991 (37)
Synechocystis sp	Synechocystis sp. (strain PCC 6803 / Kazusa)	P37101			Bacteria	Cyanobacteria	yes	Experimental evidence at transcript level
S. elongatus	Synechococcus elongatus PCC 7942	Q31PL2			Bacteria	Cyanobacteria	yes	Kobayashi et al., 2003 (38)
A. variabilis	Anabaena variabilis (strain ATCC 29413 / PCC 7937)	Q3MF31			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein inferred from homology
G. violaceus	Gloeobacter violaceus (strain PCC 7421)	Q7NI87			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein inferred from homology
T. elongatus	Thermosynechococcus elongatus (strain BP-1)	Q8DHN2			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein inferred from homology
Cyanothece sp	Cyanothece sp. (strain PCC 7424) (Synechococcus sp. (strain ATCC 29155))	B7KI62			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein predicted
G. kilaueensis	Gloeobacter kilaueensis JS1	U5QBM9			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein predicted
M. aeruginosa	Microcystis aeruginosa PCC 9701	I4INY9			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein predicted
N. spumigena	Nodularia spumigena CCY9414	A0ZEU1			Bacteria	Cyanobacteria	yes	Kono et al., 2017 (5) / protein predicted
E. amylovora	Erwinia amylovora	E5BA03			Bacteria	γ-Proteobacteria	no	*inferred by homology*
S. flexneri	Shigella flexneri	P0AEX6			Bacteria	γ-Proteobacteria	no	*inferred by homology*
M. capsulatus	Methylococcus capsulatus (strain ATCC 33009 / NCIMB 11132 / Bath)	Q602L2			Bacteria	γ-Proteobacteria	no	Kono et al., 2017 (5) / protein predicted
A. vinosum	Allochromatium vinosum (strain ATCC 17899 / DSM 180 / NBRC 103801 / NCIMB 10441 / D) (Chromatium vinosum)	D3RP02			Bacteria	γ-Proteobacteria	yes (purple sulfur)	Kono et al., 2017 (5) / protein inferred from homology
P. luminescens	Photorhabdus luminescens (Xenorhabdus luminescens)	A0A1B8YKC5			Bacteria	γ-Proteobacteria	no	Kono et al., 2017 (5) / protein inferred from homology
P. profundum	Photobacterium profundum (strain SS9)	Q6LVE1			Bacteria	γ-Proteobacteria	no	Kono et al., 2017 (5) / protein inferred from homology
C. M. oxyfera	Candidatus Methylomirabilis oxyfera	D5MHD4			Bacteria	unclassified	no	Kono et al., 2017 (5) / protein inferred from homology
T. denitrificans	Thiobacillus denitrificans (strain ATCC 25259)	Q3SG56			Bacteria	β-Proteobacteria	no	Kono et al., 2017 (5) / protein predicted
C. necator	Cupriavidus necator	P19923			Bacteria	β-Proteobacteria	no	Kossmann et al., 1989 (39)
E. gracilis	Euglena gracilis	Q24LT0			Excavates	Euglenozoa	yes	Experimental evidence at transcript level
G. theta	Guillardia theta	Q24LT4			Hacrobia#	Cryptophyta	yes	Experimental evidence at transcript level
D. lutheri	Diacronema lutheri (Monochrysis lutheri) **Pavlova lutheri**	Q24LT5			Hacrobia#	Haptophyceae	yes	Experimental evidence at transcript level
P. parvum	Prymnesium parvum	Q24LS8			Hacrobia#	Haptophyceae	yes	*Predicted protein*
C. variabilis	Chlorella variabilis	E1ZF27			Viridiplantae	Chlorophyte	yes	*inferred by homology*
M. commoda	Micromonas commoda	C1FFW3			Viridiplantae	Chlorophyte	yes	*inferred by homology*
O. tauri	Ostreococcus tauri	A0A090N369			Viridiplantae	Chlorophyte	yes	*inferred by homology*
V. carteri	Volvox carteri f. nagariensis	D8TRR7			Viridiplantae	Chlorophyte	yes	*Predicted protein*
C. reinhardtii	Chlamydomonas reinhardtii	P19824	A8IYP4	AAF36402	Viridiplantae	Chlorophyte	yes	Roesler and Ogren, 1990 (40)
G. sulphuraria	Galdieria sulphuraria	M2X324			Viridiplantae	Rhodophyta	yes	Kono et al., 2017 (5) / protein predicted
P. sativum	Pisum sativum	P93681			Viridiplantae	Streptophyta	yes	Experimental evidence at transcript level
P. sitchensis	Picea sitchensis (Sitka spruce) (Pinus sitchensis)	C0PS66			Viridiplantae	Streptophyta	yes	Experimental evidence at transcript level
P. patens	Physcomitrella patens	A9TRN4			Viridiplantae	Streptophyta	yes	*inferred by homology*
P. trichocarpa	Populus trichocarpa (Western balsam poplar) (Populus balsamifera subsp. trichocarpa)	B9GZT5			Viridiplantae	Streptophyta	yes	*inferred by homology*
S. moellendorf.	Selaginella moellendorffii	D8SU48			Viridiplantae	Streptophyta	yes	*inferred by homology*
M. crystallinum	Mesembryanthemum crystallinum	P27774			Viridiplantae	Streptophyta	yes	Michalowski et al., 1992 (41)
S. oleracea	Spinacia oleracea	P09559		CAA30499	Viridiplantae	Streptophyta	yes	Roesler and Ogren, 1990 (40)
T. aestivum	Triticum aestivum	P26302			Viridiplantae	Streptophyta	yes	Roesler and Ogren, 1990 (40)
A. thaliana	Arabidopsis thaliana	P25697			Viridiplantae	Streptophyta	yes	This Study and Roesler and Ogren, 1990 (40)
L. polyedrum	Lingulodinium polyedrum	Q24LT3			SAR-Alveolates*	Dinoflagellate	yes	Experimental evidence at transcript level
P. lunula	Pyrocystis lunula	Q24LT2			SAR-Alveolates*	Dinoflagellate	yes	Experimental evidence at transcript level
B. natans	Bigelowiella natans	Q24LS7			SAR-Rhizaria*	Cercozoa	yes	*Predicted protein*
O. sinensis	Odontella sinensis	Q95033			SAR-Stramenopiles*	Diatom	yes	Experimental evidence at transcript level
P. tricornutum	Phaeodactylum tricornutum	B5Y5F0			SAR-Stramenopiles*	Diatom	yes	*inferred by homology*
T. pseudonana	Thalassiosira pseudonana	B8BZ40			SAR-Stramenopiles*	Diatom	yes	*inferred by homology*

*Member of the SAR group (42) ; #Member of the Hacrobia Kingdom (43)

References

1. Kabsch W (2010) XDS. Acta Crystallogr D Biol Crystallogr 66(Pt 2):125–132.
2. Evans P (2006) Scaling and assessment of data quality. Acta Crystallogr D Biol Crystallogr 62(Pt 1):72–82.
3. McCoy AJ, et al. (2007) Phaser crystallographic software. J Appl Crystallogr 40(Pt 4):658–674.
4. Adams PD, et al. (2010) PHENIX: a comprehensive Python-based system for macromolecular structure solution. Acta Crystallogr D Biol Crystallogr 66(Pt 2):213–221.
5. Kono T, et al. (2017) A RuBisCO-mediated carbon metabolic pathway in methanogenic archaea. Nat Commun 8:14007.
6. Cowtan K (2006) The Buccaneer software for automated model building. 1. Tracing protein chains. Acta Crystallogr D Biol Crystallogr 62(Pt 9):1002–1011.
7. Murshudov GN, Vagin AA, Dodson EJ (1997) Refinement of macromolecular structures by the maximum-likelihood method. Acta Crystallogr D Biol Crystallogr 53(Pt 3):240–255.
8. Emsley P, Cowtan K (2004) Coot: model-building tools for molecular graphics. Acta Crystallogr D Biol Crystallogr 60(Pt 12 Pt 1):2126–2132.
9. Vagin A, Teplyakov A (2010) Molecular replacement with MOLREP. Acta Crystallogr D Biol Crystallogr 66(Pt 1):22–25.
10. Brennich ME, et al. (2016) Online data analysis at the ESRF bioSAXS beamline, BM29. J Appl Crystallogr 49:203–212.
11. Franke D, Jeffries CM, Svergun DI (2015) Correlation Map, a goodness-of-fit test for one-dimensional X-ray scattering spectra. Nat Methods 12(5):419–422.
12. Petoukhov MV, et al. (2012) New developments in the ATSAS program package for small-angle scattering data analysis. J Appl Crystallogr 45(Pt 2):342–350.
13. Guinier A (1939) La Diffraction des rayons x aux très petits angles: application à l'étude des

phénomènes ultramicroscopiques. Ann Phys 12:161–237.

14. Porod G (1982) General theory. *Small-Angle X-Ray Scattering*, eds Glatter O, Kratky O (Academic Press, London).
15. Rambo RP, Tainer JA (2013) Accurate assessment of mass, models and resolution by small-angle scattering. Nature 496(7446):477–481.
16. Svergun DI, Petoukhov MV, Kochet MH (2001) Determination of domain structure of proteins from X-ray solution scattering. Biophys J 80(6):2946–2953.
17. Volkov VV, Svergun DI (2003) Uniqueness of ab initio shape determination in small-angle scattering. J Appl Crystallogr 36:860–864.
18. Taylor TC, Andersson I (1997) Structure of a product complex of spinach Ribulose-1,5-Bisphosphate Carboxylase/Oxygenase. Biochemistry 36(13):4041-4046.
19. Fermani S, et al. (2010) The crystal structure of photosynthetic glyceraldehyde-3-phosphate dehydrogenase (isoform A4) from Arabidopsis thaliana in complex with NAD. Acta Crystallogr Sect F Struct Biol Cryst Commun 66(Pt6):621–626.
20. Zaffagnini M, et al. (2014) High resolution crystal structure and redox properties of chloroplastic triosephosphate isomerase from Chlamydomonas reinhardtii. Mol Plant 7(1):101-120.
21. Chiadmi M, Navaza A, Miginiac-Maslow M, Jacquot JP, Cherfils J (1999) Redox signalling in the chloroplast: Structure of oxidized pea fructose-1,6-bisphosphate phosphatase. EMBO J 18(23):6809–6815.
22. Pasquini M, et al. (2017) Structural basis for the magnesium-dependent activation of transketolase from Chlamydomonas reinhardtii. Biochim Biophys Acta 1861(8):2132-2145.
23. Gütle DD, et al. (2016) Chloroplast FBPase and SBPase are thioredoxin-linked enzymes with similar architecture but different evolutionary histories. Proc Natl Acad Sci USA 24(113):6779–6784.
24. Kopp J, Kopriva S, Süss KH, Schulz GE (1999) Structure and mechanism of the amphibolic

enzyme D-ribulose-5-phosphate 3-epimerase from potato chloroplasts. J Mol Biol 287(4):761-771.

25. Davies GJ, et al. (1994) Structure of the ADP complex of the 3-phosphoglycerate kinase from Bacillus stearothermophilus at 1.65 A. Acta Crystallogr D Biol Crystallogr 50(Pt 2):202-209.
26. Heron PW, Sygusch J (2017) Isomer activation controls stereospecificity of class I fructose-1,6-bisphosphate aldolases. J Biol Chem 292(48):19849-19860.
27. Dereeper A, et al. (2008) Phylogeny.fr: robust phylogenetic analysis for the non-specialist. Nucleic Acids Res 36 (Web Server issue):W465-W469.
28. Charlier HA, Runquist JA, Miziorko HM (1994) Evidence supporting catalytic roles for aspartate residues in phosphoribulokinase. Biochemistry 33(31):9343–9350.
29. Thieulin-Pardo G, Remy T, Lignon S, Lebrun R, Gontero B (2015) Phosphoribulokinase from Chlamydomonas reinhardtii: a Benson-Calvin cycle enzyme enslaved to its cysteine residues. Mol. Biosyst. 11(4):1134–1145.
30. Letunic I, Bork P (2016) Interactive tree of life (iTOL) v3: an online tool for the display and annotation of phylogenetic and other trees. Nucleic Acids Res 44(W1):242-245.
31. Harrison DH, Runquist JA, Holub A, Miziorko HM (1998) The crystal structure of phosphoribulokinase from Rhodobacter sphaeroides reveals a fold similar to that of adenylate kinase. Biochemistry 37(15):5074–5085.
32. Robert X, Gouet P (2014) Deciphering key features in protein structures with the new ENDscript server. Nucleic Acids Res 42:W320-W324.
33. Sievers F, et al. (2011) Fast, scalable generation of high-quality protein multiple sequence alignments using Clustal Omega. Mol Syst Biol 7:539-545.
34. Capitani G, et al. (2000) Crystal structures of two functionally different thioredoxins in spinach chloroplasts. J Mol Biol 302(1):135-154.
35. Bienert S, et al. (2017) The SWISS-MODEL Repository - new features and functionality.

Nucleic Acids Res 45(D1):D313-D319.

36. Hallenbeck PL, Kaplan S (1987) Cloning of the gene for phosphoribulokinase activity from Rhodobacter sphaeroides and its expression in Escherichia coli. J Bacteriol 169(8):3669-3678.
37. Meijer WG, et al. (1991) Identification and organization of carbon dioxide fixation genes in Xanthobacter flavus H4-14. Mol Gen Genet 225(2):320-330.
38. Kobayashi D, Tamoi M, Iwaki T, Shigeoka S, Wadano A (2003) Molecular characterization and redox regulation of phosphoribulokinase from the cyanobacterium Synechococcus sp. PCC 7942. Plant Cell Physiol 44(3):269–276.
39. Kossmann J, Klintworth R, Bowien B (1989) Sequence analysis of the chromosomal and plasmid genes encoding phosphoribulokinase from Alcaligenes eutrophus. Gene 85(1):247-252.
40. Roesler KR, Ogren WL (1990) Chlamydomonas reinhardtii phosphoribulokinase: sequence, purification and kinetics. Plant Physiol 93(1):188–193.
41. Michalowski CB, Derocher EJ, Bohnert HJ, Salvucci ME (1992) Phosphoribulokinase from ice plant: Transcription, transcripts and protein expression during environmental stress. Photosynth Res 31(2):27-38.
42. Burki F, et al. (2010) Evolution of Rhizaria: new insights from phylogenomic analysis of uncultivated protists. BMC Evol Biol 10:377-395.
43. Okamoto K, Kondo-Okamoto N, Ohsumi Y (2009) A landmark protein essential for mitophagy. Autophagy 5(8):1203-1205.