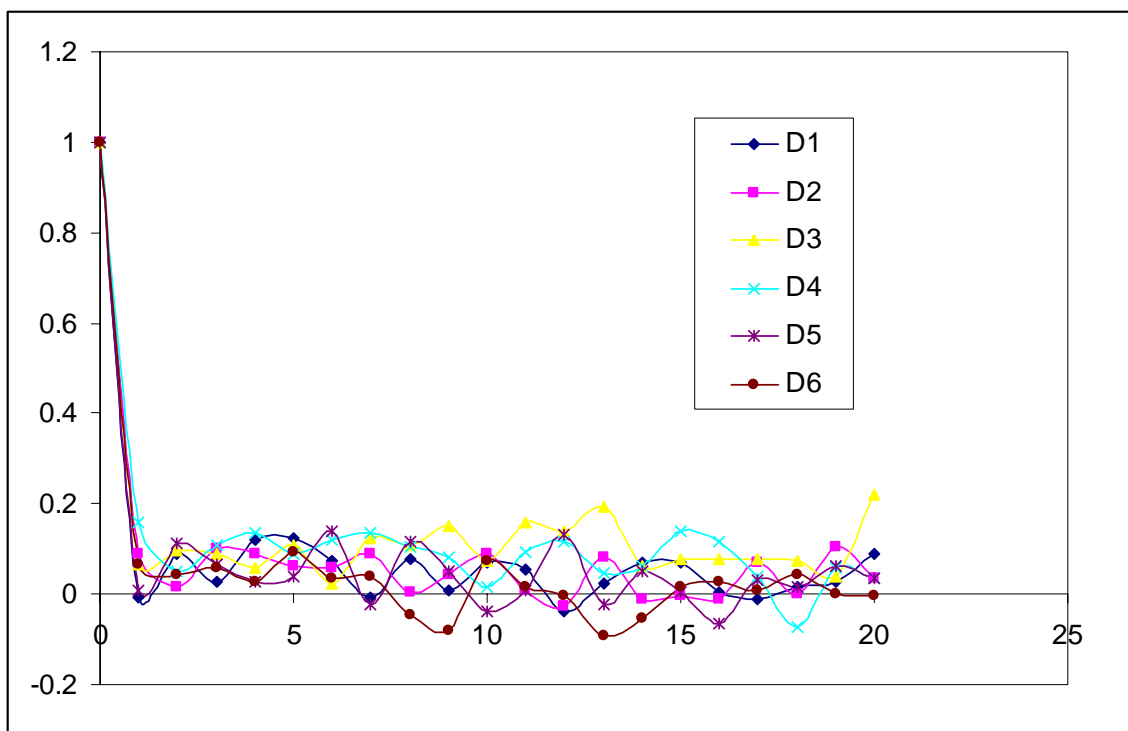


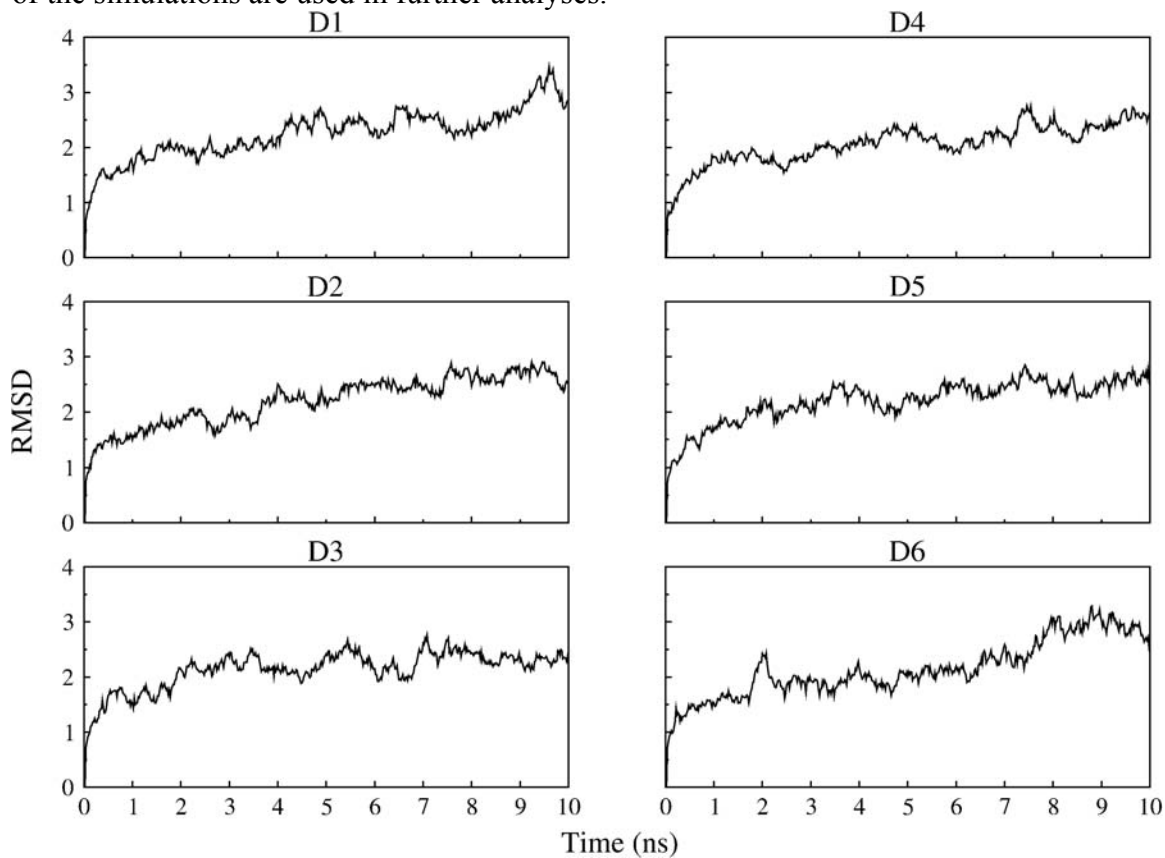
## SUPPLEMENTARY MATERIAL

For Tuncel et al. “Insights into Subunit Interactions in the Heterotetrameric Structure of Potato ADP-glucose Pyrophosphorylase”

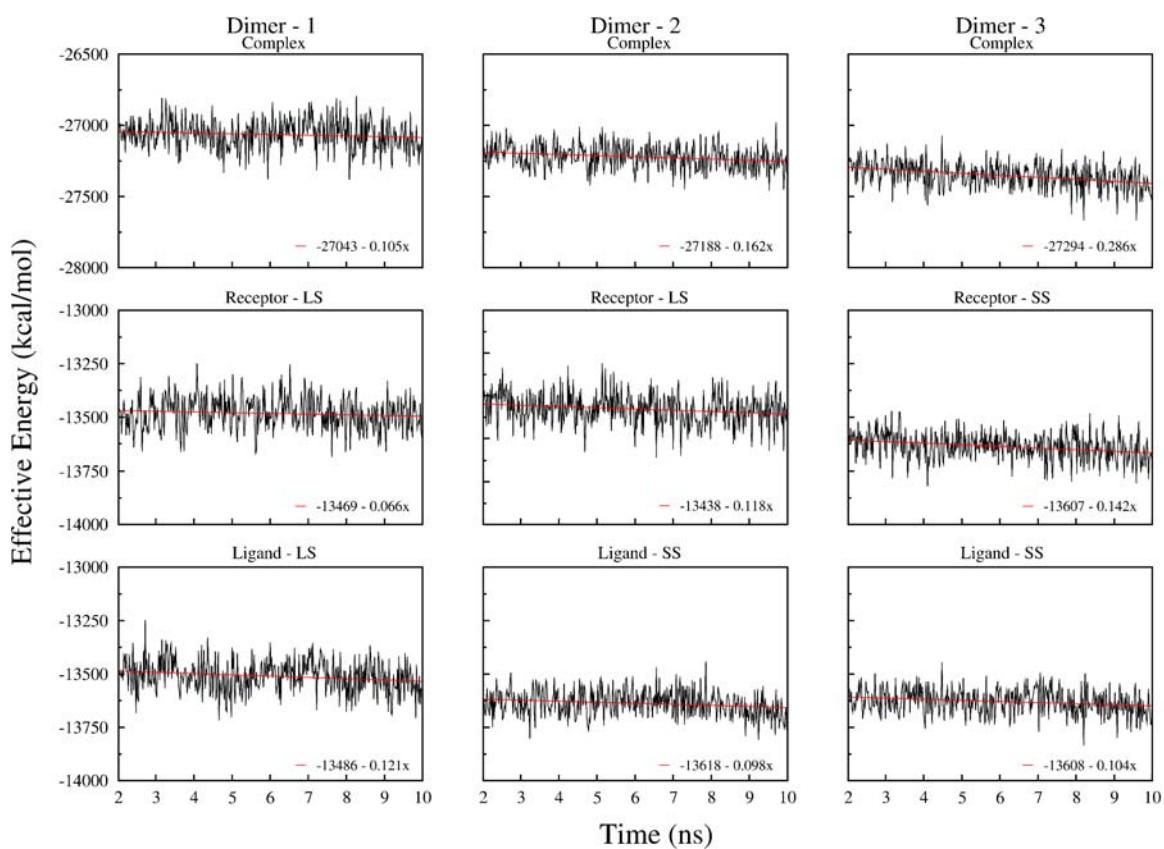
**Figure S1.** Autocorrelation functions for the effective free energies of the six dimers (D1-D6). Each lag in the x axis corresponds to 20 ps. The trajectory is obtained from the last 8 ns of the simulations.



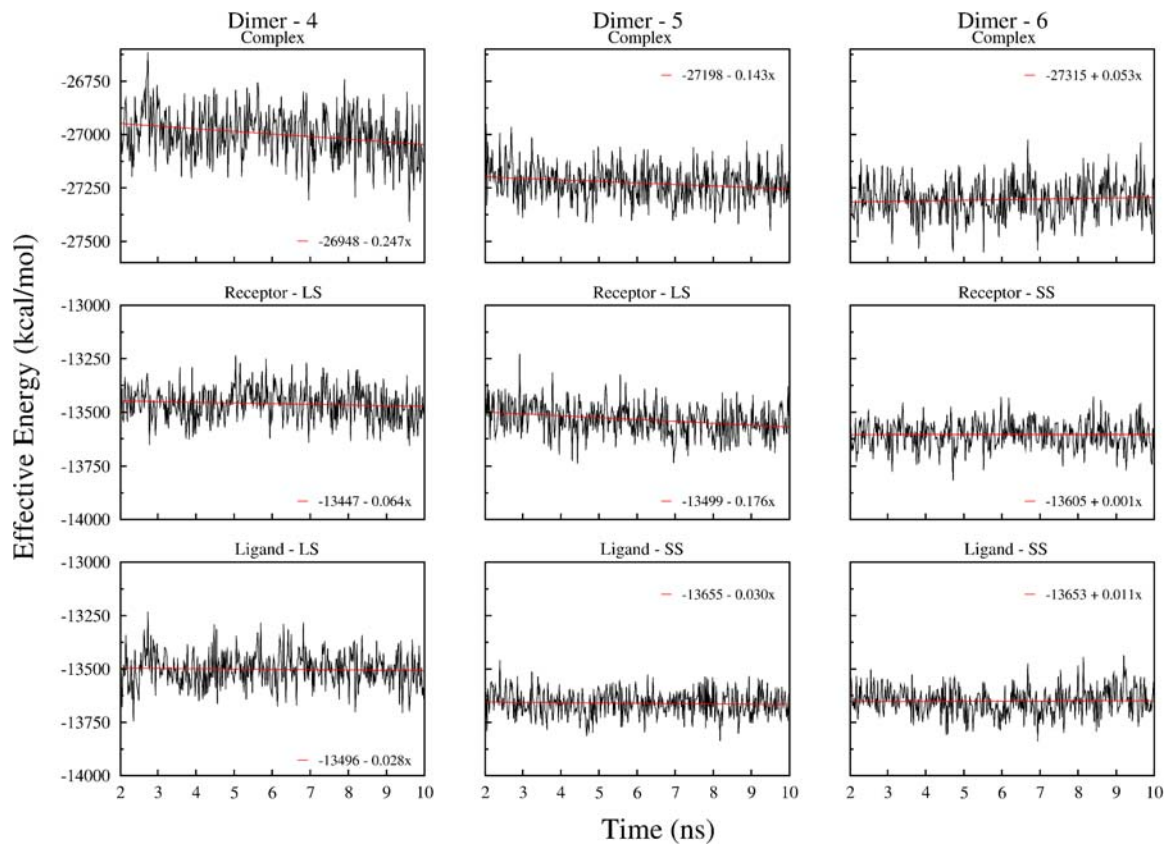
**Figure S2.** RMSD profiles of the six dimers during 10 ns simulations. The last 8 ns parts of the simulations are used in further analyses.



**Figure S3.** Graphs showing the  $E_{MM} + G_{sol}$  vs. Time for complex, receptor and ligand in each of the dimeric interactions. Regression lines are plotted in red. In each of the graphs complex means the corresponding dimer shown in **Figure 2b**. For homodimers both the receptor and ligand are the same structures.

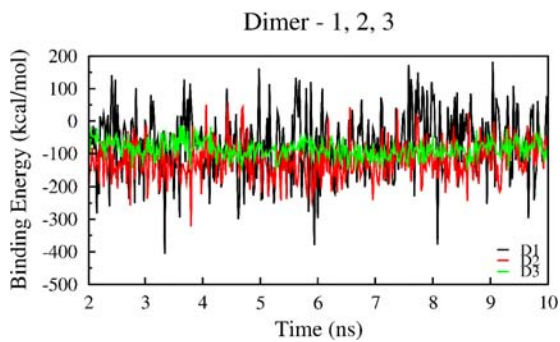


**a**

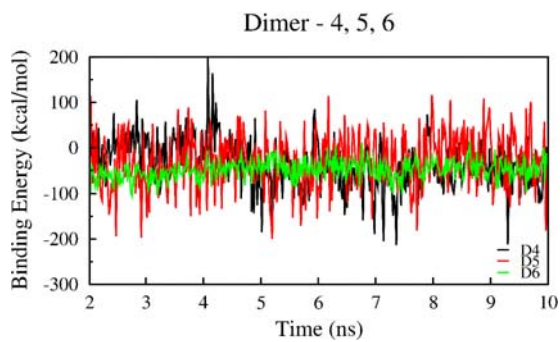


**b**

**Figure S4.**  $\Delta G$  values calculated as a sum of gas phase, polar and non-polar solvation free energies for each of the 400 snapshots. Time interval between the two consecutive frames is 20 ps constituting a total of 8 ns. (a) Binding free energies for the set1 dimers and (b) for the set2 dimers.



**a**



**b**

**Table S1.** List of interface residues of dimers (D1-D6) extracted from the MD trajectories.

| D1            |             | D2            |             | D3            |             |
|---------------|-------------|---------------|-------------|---------------|-------------|
| LS – Receptor | LS – Ligand | LS – Receptor | SS – Ligand | SS – Receptor | SS – Ligand |
| GLY37         | GLY38       | CYS39         | GLY40       | GLY40         | GLY40       |
| GLY38         | CYS39       | TYR40         | ALA41       | ALA41         | ASN42       |
| CYS39         | TYR40       | ALA74         | ASN42       | ASN42         | TYR43       |
| TYR40         | LEU275      | ARG75         | TYR43       | TYR43         | ARG78       |
| LEU285        | THR276      | THR76         | SER77       | ARG78         | SER82       |
| THR286        | GLN277      | GLY79         | ARG78       | SER82         | ASN83       |
| GLN287        | GLU278      | ASN80         | SER82       | ASN83         | ILE285      |
| GLU288        | PHE279      | GLY81         | ASN83       | ILE285        | THR287      |
| PHE289        | PRO280      | SER83         | MET84       | THR286        | LYS288      |
| PRO290        | GLN283      | PHE84         | ILE285      | LYS287        | PRO289      |
| GLN293        | TYR285      | LEU285        | THR286      | LYS288        | SER294      |
| TYR295        | PRO297      | THR286        | LYS287      | PRO289        | TYR296      |
| PRO297        | PHE301      | GLN287        | LYS288      | PRO291        | ARG298      |
| LYS298        | TYR302      | GLU288        | PRO289      | PHE295        | PRO301      |
| THR303        | THR303      | TYR295        | VAL290      | TYR296        | ILE302      |
| SER304        | SER304      | PRO297        | PRO291      | ARG298        | TYR303      |
| PRO305        | PRO305      | TYR302        | TYR296      | PRO301        | THR304      |
| ARG306        | ARG306      | THR303        | ARG298      | ILE302        | GLN305      |
| PHE307        | PHE307      | PRO305        | THR304      | TYR303        | PRO306      |
| LEU308        | LEU308      | PHE307        | GLN305      | THR304        | ARG307      |
| PRO309        | PRO309      | LEU308        | PRO306      | PRO306        | TYR308      |
| PRO310        | PRO310      | PRO309        | ARG307      | ARG307        | LEU309      |
| THR311        | THR311      | PRO310        | TYR308      | TYR308        | PRO310      |
| LYS312        | LYS312      | THR311        | LEU309      | LEU309        | PRO311      |
| ILE313        | ILE313      | LYS312        | PRO310      | PRO310        | SER312      |
| ASP314        | ASP314      | ILE313        | PRO311      | PRO311        | LYS313      |
| ASN315        | ASN315      | ASP314        | SER312      | SER312        | MET314      |
| CYS316        | CYS316      | ASN315        | LYS313      | LYS313        | LEU315      |
| LYS317        | LYS317      | CYS316        | MET314      | MET314        | ASP316      |
| ILE318        | ILE318      | LYS317        | LEU315      | LEU315        | ALA317      |
| LYS319        | LYS319      | ILE318        | ASP316      | ASP316        | ASP318      |
| ASP320        | ASP320      | LYS319        | ALA317      | ALA317        | VAL319      |
| ALA321        | ALA321      | ASP320        | ASP318      | ASP318        | THR320      |
| ILE322        | ILE322      | ALA321        | VAL319      | VAL319        | ASP321      |
| ILE323        | ILE323      | ILE322        | THR320      | THR320        | SER322      |
| SER324        | SER324      | ILE323        | ASP321      | ASP321        | VAL323      |
| HIS325        | HIS325      | SER324        | SER322      | SER322        | ILE324      |
| PHE328        | PHE328      | HIS325        | VAL323      | VAL323        | GLY325      |
| ARG330        | ARG330      | TYR362        | ILE324      | ILE324        | GLU326      |
| GLU341        | ARG342      | THR364        | GLY325      | GLY325        | ARG343      |
| ARG342        | TYR362      | GLU365        | GLU326      | GLU326        | TYR363      |
| TYR362        | GLN363      |               | LYS331      | ARG343        | THR365      |
| THR364        | THR364      |               | ARG343      | TYR363        | ALA366      |
| GLU365        | GLU365      |               | TYR363      | THR365        | ASP367      |
|               |             |               | THR365      |               |             |

| D4            |             | D5            |             | D6            |             |
|---------------|-------------|---------------|-------------|---------------|-------------|
| LS – Receptor | LS – Ligand | LS – Receptor | SS – Ligand | SS – Receptor | SS – Ligand |
| ASN65         | ASN65       | ARG28         | TYR62       | TYR62         | TYR62       |
| SER66         | ALA67       | ASN65         | ASN68       | ASN68         | ASN68       |
| ALA67         | PRO68       | SER66         | ALA70       | SER69         | ALA70       |
| PRO68         | ASN70       | ALA67         | ASN73       | ALA70         | ASN73       |
| ASN70         | ARG71       | PRO68         | ARG74       | ASN73         | ARG74       |
| ARG71         | ALA74       | ASN70         | SER77       | ARG74         | SER77       |
| ALA74         | ARG75       | ARG71         | ARG78       | SER77         | ARG78       |
| ARG75         | PHE78       | ILE73         | ALA81       | ARG78         | ALA81       |
| PHE78         | GLY79       | ALA74         | SER82       | ALA81         | SER82       |
| GLY79         | VAL82       | ARG75         | ASN83       | SER82         | MET84       |
| VAL82         | SER83       | PHE78         | MET84       | ASN83         | GLY85       |
| ASP86         | ASP86       | GLY79         | GLU90       | MET84         | GLY86       |
| GLY87         | GLY87       | ASN80         | PHE92       | ASN89         | ASN89       |
| PHE88         | PHE88       | VAL82         | VAL93       | GLU90         | GLU90       |
| VAL89         | GLU90       | SER83         | GLU94       | GLY91         | GLY91       |
| GLU90         | VAL91       | ASP86         | LEU96       | PHE92         | PHE92       |
| VAL91         | LEU92       | GLY87         | ALA98       | GLU94         | GLU94       |
| LEU92         | ALA93       | PHE88         | GLN100      | VAL95         | VAL95       |
| ALA93         | ALA94       | GLU90         | SER101      | LEU96         | LEU96       |
| ALA94         | GLN96       | VAL91         | PRO102      | ALA97         | ALA97       |
| THR95         | THR97       | LEU92         | GLN117      | ALA98         | ALA98       |
| GLN96         | PRO98       | ALA93         | TYR118      | GLN99         | GLN100      |
| THR97         | LYS115      | ALA94         | TRP120      | GLN100        | SER101      |
| PRO98         | TRP118      | GLN96         | LEU121      | SER101        | PRO102      |
| LYS115        | VAL119      | THR97         | GLU124      | PRO102        | GLN117      |
| PHE116        | GLU121      | PRO98         | HIS125      | GLN117        | TYR118      |
| TRP118        | ASP122      | PHE116        | THR126      | TYR118        | TRP120      |
| VAL119        | ALA123      | TRP118        |             | TRP120        | LEU121      |
| LYS124        | LYS124      | LYS124        |             | LEU121        | GLU124      |
| ASN125        | ASN125      | ASN125        |             | GLU124        | HIS125      |
| LYS126        | ASP360      | LYS126        |             | HIS125        |             |
| ASP360        | ASN395      | PHE307        |             | TYR308        |             |
| TYR361        |             |               |             |               |             |
| ASN395        |             |               |             |               |             |
| LYS432        |             |               |             |               |             |