**Files:**

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| **S.No.** | **File Name** | **File Description** |
| 1. | Pdz.pdb | The WT PDZ pdb file |
| 2. | Coupling\_310K\_Pdz.mat | The input variables of PDZ for the MATLAB code. |
| 3. | BlockDetPdz.dat | Column 1: Residue Number starting from 1  Column 2: Block Number of the residue |
| 4. | CheY.pdb | The WT CheY pdb file |
| 5. | Coupling\_310K\_CheY.mat | The input variables of CheY for the MATLAB code. |
| 6. | BlockDetCheY.dat | Column 1: Residue Number starting from 1  Column 2: Block Number of the residue |
| 7. | CypA.pdb | The WT CypA pdb file |
| 8. | Coupling\_310K\_CypA.mat | The input variables of CypA for the MATLAB code. |
| 9. | BlockDetCypA.dat | Column 1: Residue Number starting from 1  Column 2: Block Number of the residue |
| 10 | Protein\_Mutantcol.pdb | The DCI of every residue is stored as b factor in this output pdb file |
| 11. | Fit Parameters.txt | Output file containing values of parameters of the single exponential model |

**Variables:**

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| --- | --- | --- |
| **S.No.** | **Variable Name** | **Variable Description** |
| 1. | nres | Total number of blocks |
| 2. | chiPwt | Positive coupling FE matrix of wild type |
| 3. | chiP\_mut | Positive coupling FE matrix of mutant |
| 4. | x2 | Binned and averaged distance from mutated site |
| 5. | y2 | Binned and averaged DCIs |
| 6. | param | Parameters after fitting: Amplitude, Error in amplitude, coupling distance (dc), Error in dc, Shift term, error in shift term, R2 |
| 7. | Edges1 | The changes in FE of all microstates |
| 8. | N1 | Number of microstates associated with the FE change in Edges1 variable |
| 9. | Edges2 | The changes in FE of folded well microstates |
| 10. | N2 | Number of microstates associated with the FE change in Edges2 variable |
| 11 | Fe\_wt | Free energy of structured blocks of wild type |
| 12 | Fe\_mut | Free energy of structured blocks of mutant |
| 13 | DCM | DCM of mutant |
| 13 | DCI | Averaged DCI of every residue |