**Files:**

| **Sl. No.** | **Filename** | **Structure** | **Protein** |
| --- | --- | --- | --- |
| 1 | gpcr1i | 1U19 | RHO |
| 2 | gpcr2i | 2LNL | CXCR1 |
| 3 | gpcr3i | 2RH1 | ADRB2 |
| 4 | gpcr4i | 3ODU | CXCR4 |
| 5 | gpcr5i | 3V2Y | S1PR1 |
| 6 | gpcr6i | 3VW7 | F2R |
| 7 | gpcr7i | 4BVN | ADRB1 |
| 8 | gpcr8i | 4DJH | OPRK1 |
| 9 | gpcr9i | 4DKL | OPRM1 |
| 10 | gpcr10i | 4N6H | OPRD1 |
| 11 | gpcr11i | 4OR2 | GRM1 |
| 12 | gpcr12i | 4PXZ | P2RY12 |
| 13 | gpcr13i | 4XES | NTSR1 |
| 14 | gpcr14i | 4XNV | P2RY1 |
| 15 | gpcr15i | 4XT1 | US28 |
| 16 | gpcr16i | 4YAY | AGTR1 |
| 17 | gpcr17i | 4Z35 | LPAR1 |
| 18 | gpcr18i | 4ZJ8 | HCRTR1 |
| 19 | gpcr19i | 5DHG | OPRL1 |
| 20 | gpcr20i | 5LWE | CCR9 |
| 21 | gpcr21i | 5NDD | F2RL1 |
| 22 | gpcr22i | 5TZR | FFAR1 |
| 23 | gpcr23i | 5UEN | ADORA1 |
| 24 | gpcr24i | 5UIW | CCR5 |
| 25 | gpcr25i | 5UNF | AGTR2 |
| 26 | gpcr26i | 5VBL | APLNR |
| 27 | gpcr27i | 5VEW | GLP1R |
| 28 | gpcr28i | 5ZBQ | NPY1R |
| 29 | gpcr29i | 5ZKP | PTAFR |
| 30 | gpcr30i | 5ZTY | CNR2 |
| 31 | gpcr31i | 6A94 | HTR2A |
| 32 | gpcr32i | 6BD4 | FZD4 |
| 33 | gpcr33i | 6C1R | C5AR1 |
| 34 | gpcr34i | 6D27 | PTGDR2 |
| 35 | gpcr35i | 6FFI | GRM5 |
| 36 | gpcr36i | 6GPX | CCR2 |
| 37 | gpcr37i | 6HLP | TACR1 |
| 38 | gpcr38i | 6IGK | EDNRB |
| 39 | gpcr39i | 6IIU | TBXA2R |
| 40 | gpcr40i | 6M9T | PTGER3 |
| 41 | gpcr41i | 6ME2 | MTNR1A |
| 42 | gpcr42i | 6ME6 | MTNR1B |
| 43 | gpcr43i | 6NIY | CALCR |
| 44 | gpcr44i | 6QZH | CCR7 |
| 45 | gpcr45i | 6RZ6 | CYSLTR2 |
| 46 | gpcr3a | 4LDE | ADRB2 |
| 47 | gpcr9a | 5C1M | OPRM1 |
| 48 | gpcr1a | 5W0P | RHO |
| 49 | gpcr8a | 6B73 | OPRK1 |
| 50 | gpcr23a | 6D9H | ADORA1 |
| 51 | gpcr16a | 6DO1 | AGTR1 |
| 52 | gpcr7a | 6H7N | ADRB1 |
| 53 | gpcr13a | 6OS9 | NTSR1 |

**Variables:**

| **Sl. No.** | **Variable** | **Description** |
| --- | --- | --- |
| 1 | PDBID\_gpcr | PDB ID of the structure |
| 2 | BlockDet\_gpcr | 1st column: residue indices 2nd column: corresponding block indices |
| 3 | TempDSC\_gpcr | Temperature vector for plotting DSC curves (only for structures used originally) |
| 4 | Cpd\_gpcr | Cp (only for structures used originally) |
| 5 | ene\_gpcr | vdW interaction energy |
| 6 | DS\_gpcr | Entropic cost |
| 7 | Tm\_gpcr | Melting temperature |
| 8 | fes\_298\_gpcr | 1D free energy landscape (FES) at 298 K |
| 9 | fes\_310\_gpcr | 1D FES at 310 K |
| 10 | fes\_Tm\_gpcr | 1D FES at Tm |
| 11 | Fpath\_298\_gpcr | Matrix of block folding probability against # of structured residues at 298 K |
| 12 | Fpath\_310\_gpcr | Matrix of block folding probability against # of structured residues at 310 K |
| 13 | Fpath\_Tm\_gpcr | Matrix of block folding probability against # of structured residues at Tm |
| 14 | fes2D\_298\_gpcr | 2D FES at 298 K |
| 15 | fes2D\_310\_gpcr | 2D FES at 310 K |
| 16 | fes2D\_Tm\_gpcr | 2D FES at Tm |
| 17 | fes2DResProb\_298\_gpcr | 3D matrix with block folding probabilities at each point on the 2D FES at 298 K |
| 18 | fes2DResProb\_310\_gpcr | 3D matrix with block folding probabilities at each point on the 2D FES at 310K |
| 19 | fes2DResProb\_Tm\_gpcr | 3D matrix with block folding probabilities at each point on the 2D FES at Tm |
| 20 | ResFoldProb\_298\_gpcr | Residue-wise folding probability at 298 K |
| 21 | ResFoldProb\_310\_gpcr | Residue-wise folding probability at 310 K |
| 22 | ResFoldProb\_Tm\_gpcr | Residue-wise folding probability at Tm |
| 23 | DeltaGc\_310\_gpcr | Mean thermodynamic coupling free energy of each residue at 310 K |
| 24 | CouplingMat\_310\_gpcr | Residue-residue thermodynamic coupling free energy matrix at 310 K |

Coupling free energies have not been calculated for GlpG and PagP.