|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table S4: Detailed secondary structure in ICP 7035 showing a) Secondary structure summary b) beta sheet c) beta hairpins, d) beta strands, e) helices, f) helix-helix interaction, g) beta turns, h) gamma turns**  **a) Secondary structure summary** http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif   |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | | | **Strand** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Alpha helix** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **3-10 helix** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Other** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Total residues** | | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | | | **4 (2.1%)** |  | **86 (44.6%)** |  | **12 (6.2%)** |  | **91 (47.2%)** |  | **193** |   [**b) Beta sheet**](http://www.ebi.ac.uk/thornton-srv/databases/cgi-bin/pdbsum/GetPage.pl?pdbcode=e493&pdb_type=UPLOAD&code=063658&template=protein.html&o=SHEETS&l=1&c=2&pdb_type=UPLOAD&code=063658&chain=NONE)http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif   |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | | | **Sheet** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **No.   strands** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Type** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Barrel** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Topology** | | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | | | **A** |  | **2** |  | **Antiparallel** |  | **N** |  | **1** | | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | |   **c) Beta hairpins** |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Strand 1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Strand 2** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Hairpin** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | **No.** |  | **Start** |  | **End** |  | **Length** |  | **Start** |  | **End** |  | **Length** |  | **class** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | 1. |  | Ala125 |  | Ala126 |  | 2 |  | Gly135 |  | Pro136 |  | 2 |  | 8:8 | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **d) Beta strands** |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
| |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | **No.** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Start** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **End** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Sheet** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. residue** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Edge** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gifSequence** |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | 1. |  | Ala125 |  | Ala126 |  | A |  | 2 |  | Yes | AA |  | | 2. |  | Gly135 |  | Pro136 |  | A |  | 2 |  | Yes | GP |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **e) Table of helices** |
|  |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | **No.** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Start** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **End** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Type** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. resid** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Length** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Unit rise** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residues per turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Pitch** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Deviation from ideal** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Sequence** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | \*1. |  | Ala2 |  | Thr4 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | AGT |  |  | | \*2. |  | Thr17 |  | Lys19 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | TIK |  |  | | \*3. |  | Pro21 |  | Ala25 |  | H |  | 5 |  | 8.07 |  | 1.48 |  | 3.59 |  | 5.30 |  | 21.4 |  | PAELA |  |  | | \*4. |  | Gly27 |  | Asn29 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | GAN |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 5. |  | Leu32 |  | Glu45 |  | H |  | 14 |  | 22.57 |  | 1.58 |  | 4.01 |  | 6.34 |  | 31.1 |  | LDIAVRLLEPIKAE |  |  | | 6. |  | Tyr51 |  | Ile65 |  | H |  | 15 |  | 22.31 |  | 1.45 |  | 3.67 |  | 5.32 |  | 11.3 |  | YADFYQLAGVVAVEI |  |  | | 7. |  | Ser96 |  | Phe103 |  | H |  | 8 |  | 11.71 |  | 1.41 |  | 3.82 |  | 5.41 |  | 13.4 |  | SDHLRDVF |  |  | | 8. |  | Asp111 |  | Ser118 |  | H |  | 8 |  | 12.87 |  | 1.56 |  | 3.59 |  | 5.58 |  | 13.2 |  | DQDIVALS |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 9. |  | Gly119 |  | Thr122 |  | G |  | 4 |  | 8.12 |  | 1.93 |  | 3.20 |  | 6.17 |  | 38.0 |  | GGHT |  |  | | 10. |  | Lys128 |  | Ser131 |  | H |  | 4 |  | 4.79 |  | 1.17 |  | 4.28 |  | 4.98 |  | 41.4 |  | KERS |  |  | | 11. |  | Ser147 |  | Ser154 |  | H |  | 8 |  | 12.55 |  | 1.48 |  | 3.74 |  | 5.54 |  | 12.9 |  | SHFKELLS |  |  | | 12. |  | Pro164 |  | Ser171 |  | H |  | 8 |  | 12.88 |  | 1.54 |  | 3.62 |  | 5.59 |  | 17.4 |  | PSDKALLS |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 13. |  | Phe175 |  | Ala184 |  | H |  | 10 |  | 15.76 |  | 1.53 |  | 3.59 |  | 5.50 |  | 2.6 |  | FRLLVEKYAA |  |  | | 14. |  | Glu186 |  | Ala191 |  | H |  | 6 |  | 9.67 |  | 1.53 |  | 3.50 |  | 5.33 |  | 4.7 |  | EDAFFA |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **f) Helix-helix interactions** |
|  |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Helix** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Interaction** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. interacting residues** | | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | |  |  | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | **No.** |  |  | **Helices** | |  | **types** | |  | **Distance (Å)** |  | **Angle (°)** |  | **type** | |  | **Total** |  | **Helix 1** |  | **Helix 2** | | 1. |  |  | 3 | 5 |  | H | H |  | 9.7 |  | 153.5 |  | c | n |  | 3 |  | 1 |  | 3 | | 2. |  |  | 5 | 6 |  | H | H |  | 10.9 |  | 108.8 |  | I | I |  | 10 |  | 6 |  | 4 | | 3. |  |  | 5 | 10 |  | H | H |  | 9.9 |  | -98.2 |  | N | C |  | 2 |  | 2 |  | 1 | | 4. |  |  | 7 | 8 |  | H | H |  | 9.9 |  | 107.9 |  | I | I |  | 6 |  | 3 |  | 4 | | 5. |  |  | 7 | 12 |  | H | H |  | 8.0 |  | -90.5 |  | N | I |  | 5 |  | 2 |  | 4 | | 6. |  |  | 7 | 13 |  | H | H |  | 12.0 |  | 86.2 |  | I | N |  | 3 |  | 3 |  | 1 | | 7. |  |  | 8 | 9 |  | H | G |  | 0.0 |  | -9.2 |  | C | I |  | 11 |  | 5 |  | 4 | | 8. |  |  | 8 | 11 |  | H | H |  | 8.4 |  | 93.5 |  | c | n |  | 5 |  | 3 |  | 3 | | 9. |  |  | 8 | 12 |  | H | H |  | 11.3 |  | -140.5 |  | I | I |  | 4 |  | 3 |  | 2 | | 10. |  |  | 8 | 13 |  | H | H |  | 9.5 |  | -49.3 |  | I | I |  | 12 |  | 5 |  | 4 | | 11. |  |  | 8 | 14 |  | H | H |  | 9.4 |  | -110.1 |  | I | C |  | 3 |  | 3 |  | 1 | | 12. |  |  | 9 | 11 |  | G | H |  | 6.9 |  | 95.5 |  | I | N |  | 5 |  | 3 |  | 3 | | 13. |  |  | 9 | 12 |  | G | H |  | 11.3 |  | -131.8 |  | N | I |  | 2 |  | 1 |  | 2 | | 14. |  |  | 9 | 14 |  | G | H |  | 10.4 |  | -117.2 |  | n | c |  | 3 |  | 3 |  | 1 | | 15. |  |  | 11 | 12 |  | H | H |  | 10.7 |  | -80.9 |  | I | I |  | 8 |  | 4 |  | 4 | | 16. |  |  | 11 | 13 |  | H | H |  | 7.6 |  | -118.8 |  | I | I |  | 10 |  | 4 |  | 6 | | 17. |  |  | 11 | 14 |  | H | H |  | 9.6 |  | 113.6 |  | N | I |  | 1 |  | 1 |  | 1 | | 18. |  |  | 12 | 13 |  | H | H |  | 4.3 |  | -99.5 |  | c | n |  | 7 |  | 4 |  | 3 | | 19. |  |  | 13 | 14 |  | H | H |  | 4.9 |  | -123.7 |  | c | n |  | 5 |  | 3 |  | 3 | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **g) Beta turns** |
|  |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+2** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **i to i+3** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | **No.** |  | **Turn** |  | **Sequence\*** |  | **type** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **CA-dist** |  | **H-bond** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | \*  1. |  | Asp6-Thr9 |  | DVST |  | IV |  | -50.2 |  | -51.4 |  | -171.0 |  | -49.6 |  | -57.4 |  | -47.0 |  | 6.0 |  | Yes | | \*  2. |  | Val7-Lys10 |  | VSTK |  | I |  | -49.6 |  | -57.4 |  | -47.0 |  | -80.7 |  | -20.8 |  | -179.6 |  | 4.7 |  | Yes | | \*  3. |  | Asn29-Leu32 |  | NNGL |  | II |  | -68.7 |  | 123.5 |  | -68.7 |  | 99.7 |  | -30.1 |  | - |  | 5.4 |  | No | | \*  4. |  | Phe46-Leu49 |  | FPIL |  | IV |  | -60.7 |  | -29.1 |  | -28.4 |  | -60.9 |  | -46.2 |  | -57.6 |  | 5.8 |  | No | | \*  5. |  | Asp91-Lys94 |  | DATK |  | I |  | -55.1 |  | -33.2 |  | - |  | -65.9 |  | -31.4 |  | 50.5 |  | 6.0 |  | No | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 6. |  | Thr138-Pro141 |  | TSDP |  | IV |  | -54.9 |  | -29.3 |  | -175.7 |  | -115.1 |  | 79.3 |  | -67.7 |  | 5.7 |  | Yes | | 7. |  | Asp140-Ile143 |  | DPLI |  | I |  | -62.2 |  | -21.8 |  | -21.3 |  | -83.4 |  | -18.7 |  | -70.3 |  | 5.4 |  | No | | 8. |  | Lys157-Leu160 |  | KEGL |  | II |  | -61.8 |  | 136.1 |  | -170.4 |  | 98.7 |  | -25.4 |  | - |  | 5.8 |  | No | | 9. |  | Asp172-Phe175 |  | DPVF |  | IV |  | -61.5 |  | 131.8 |  | -28.6 |  | 101.6 |  | -79.1 |  | 176.4 |  | 5.4 |  | Yes | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | |
|  |
|  |
| **h) Gamma turns** |
|  |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **i to i+2** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  |  | | **No.** |  | **Start** |  | **End** |  | **Sequence\*** |  | **type** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **CA-dist** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | 1. |  | Gly13 |  | Phe15 |  | G P F |  | INVERSE |  | -76.1 |  | 77.2 |  | 33.2 |  | 5.9 |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | |

**Detailed secondary structure in ICP 84023 showing a) Secondary structure summary b) beta sheet c) beta hairpins, d) beta strands, e) helices, f) helix-helix interaction, g) beta turns, h) gamma turns**

**a) Secondary structure summary**http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | |
| **Strand** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Alpha helix** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **3-10 helix** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Other** | **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | **Total residues** |
| **http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif** | | | | | | | | |
| **4 (2.0%)** |  | **96 (46.8%)** |  | **12 (5.9%)** |  | **93 (45.4%)** |  | **205** |

**b) Beta sheet**http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **Sheet** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **View** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. of strands** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Type** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Barrel** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Topology** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | A |  | [http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/rasmollogo3_5.gif](http://www.ebi.ac.uk/thornton-srv/databases/cgi-bin/pdbsum/RunRomLas.pl?pdb=e495NONE&origin=promotif&motif_type=7&script=YES&pdb_type=UPLOAD&code=071200&motif=1) |  | 2 |  | Antiparallel |  | No |  | 1 | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **c) Beta hairpins** |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Strand 1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Strand 2** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Hairpin** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | **No.** |  | **Start** |  | **End** |  | **Length** |  | **Start** |  | **End** |  | **Length** |  | **class** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | 1. |  | Ala125 |  | Ala126 |  | 2 |  | Gly135 |  | Pro136 |  | 2 |  | 8:8 | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | |
| **d) Beta strand** |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | **No.** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Start** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **End** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Sheet** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. resid** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Edge** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Sequence** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | 1. |  | Ala125 |  | Ala126 |  | A |  | 2 |  | Yes |  | AA | | 2. |  | Gly135 |  | Pro136 |  | A |  | 2 |  | Yes |  | GP | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | |
|  |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **e) Helices** |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | **No.** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Start** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **End** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Type** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. resid** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Length** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Unit rise** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residues per turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Pitch** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Deviation from ideal** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Sequence** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | \*1. |  | Ala2 |  | Thr4 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | AGT |  |  | | \*2. |  | Thr17 |  | Lys19 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | TIK |  |  | | \*3. |  | Pro21 |  | Ala25 |  | H |  | 5 |  | 8.15 |  | 1.50 |  | 3.60 |  | 5.40 |  | 21.2 |  | PAELA |  |  | | \*4. |  | Gly27 |  | Asn29 |  | G |  | 3 |  | - |  | - |  | - |  | - |  | - |  | GAN |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 5. |  | Leu32 |  | Glu45 |  | H |  | 14 |  | 22.64 |  | 1.59 |  | 3.95 |  | 6.27 |  | 30.2 |  | LDIAVRLLEPIKAE |  |  | | 6. |  | Tyr51 |  | Ile65 |  | H |  | 15 |  | 22.60 |  | 1.47 |  | 3.66 |  | 5.37 |  | 10.5 |  | YAYFYQLAGVVAVEI |  |  | | 7. |  | Ser96 |  | Phe103 |  | H |  | 8 |  | 11.94 |  | 1.45 |  | 3.76 |  | 5.45 |  | 14.1 |  | SDHLRDVF |  |  | | 8. |  | Asp111 |  | Ser118 |  | H |  | 8 |  | 12.86 |  | 1.55 |  | 3.62 |  | 5.61 |  | 12.7 |  | DQDIVALS |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 9. |  | Gly119 |  | Thr122 |  | G |  | 4 |  | 8.24 |  | 1.96 |  | 3.26 |  | 6.40 |  | 38.4 |  | GGHT |  |  | | 10. |  | Lys128 |  | Ser131 |  | H |  | 4 |  | 4.78 |  | 1.15 |  | 4.26 |  | 4.88 |  | 41.3 |  | KERS |  |  | | 11. |  | Ser147 |  | Ser154 |  | H |  | 8 |  | 12.75 |  | 1.51 |  | 3.80 |  | 5.73 |  | 17.3 |  | SHIKELLS |  |  | | 12. |  | Pro164 |  | Ser171 |  | H |  | 8 |  | 12.84 |  | 1.55 |  | 3.64 |  | 5.63 |  | 17.6 |  | PSDKALLS |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 13. |  | Phe175 |  | Ala184 |  | H |  | 10 |  | 15.62 |  | 1.50 |  | 3.59 |  | 5.40 |  | 3.1 |  | FRPLVEKYAA |  |  | | 14. |  | Glu186 |  | Ser201 |  | H |  | 16 |  | 24.17 |  | 1.47 |  | 3.71 |  | 5.45 |  | 12.3 |  | EDAIFADYAVAHHKLS |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
| **f) Helix- helix interactions**   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Helix** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Interaction** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **No. interacting residues** | | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | **No.** |  |  | **Helices** | |  | **types** | |  | **Distance (Å)** |  | **Angle (°)** |  | **type** | |  | **Total** |  | **Helix 1** |  | **Helix 2** | | 1. |  |  | 3 | 5 |  | H | H |  | 9.7 |  | 153.1 |  | c | n |  | 3 |  | 1 |  | 3 | | 2. |  |  | 5 | 6 |  | H | H |  | 11.0 |  | 110.4 |  | I | I |  | 10 |  | 5 |  | 5 | | 3. |  |  | 5 | 10 |  | H | H |  | 9.9 |  | -96.7 |  | N | I |  | 2 |  | 2 |  | 1 | | 4. |  |  | 6 | 14 |  | H | H |  | 10.8 |  | 171.1 |  | N | C |  | 8 |  | 4 |  | 4 | | 5. |  |  | 7 | 8 |  | H | H |  | 10.0 |  | 107.3 |  | I | I |  | 5 |  | 3 |  | 3 | | 6. |  |  | 7 | 12 |  | H | H |  | 7.9 |  | -91.7 |  | N | I |  | 5 |  | 2 |  | 4 | | 7. |  |  | 7 | 13 |  | H | H |  | 12.3 |  | 84.5 |  | N | N |  | 3 |  | 3 |  | 1 | | 8. |  |  | 7 | 14 |  | H | H |  | 13.8 |  | 50.4 |  | C | C |  | 1 |  | 1 |  | 1 | | 9. |  |  | 8 | 9 |  | H | G |  | 0.2 |  | 9.5 |  | C | I |  | 10 |  | 4 |  | 4 | | 10. |  |  | 8 | 11 |  | H | H |  | 8.3 |  | 92.5 |  | c | n |  | 2 |  | 2 |  | 2 | | 11. |  |  | 8 | 12 |  | H | H |  | 11.3 |  | -140.1 |  | I | I |  | 4 |  | 3 |  | 2 | | 12. |  |  | 8 | 13 |  | H | H |  | 9.8 |  | -48.4 |  | I | I |  | 12 |  | 5 |  | 5 | | 13. |  |  | 8 | 14 |  | H | H |  | 8.3 |  | -102.0 |  | I | I |  | 12 |  | 4 |  | 8 | | 14. |  |  | 9 | 11 |  | G | H |  | 6.9 |  | 97.4 |  | I | N |  | 6 |  | 3 |  | 3 | | 15. |  |  | 9 | 12 |  | G | H |  | 11.2 |  | -132.6 |  | N | I |  | 2 |  | 1 |  | 2 | | 16. |  |  | 9 | 14 |  | G | H |  | 9.5 |  | -107.5 |  | N | I |  | 3 |  | 2 |  | 2 | | 17. |  |  | 11 | 12 |  | H | H |  | 10.5 |  | -82.4 |  | I | I |  | 7 |  | 3 |  | 4 | | 18. |  |  | 11 | 13 |  | H | H |  | 7.6 |  | -120.9 |  | I | I |  | 10 |  | 4 |  | 5 | | 19. |  |  | 11 | 14 |  | H | H |  | 9.6 |  | 110.9 |  | N | I |  | 1 |  | 1 |  | 1 | | 20. |  |  | 12 | 13 |  | H | H |  | 4.4 |  | -101.4 |  | c | n |  | 7 |  | 4 |  | 3 | | 21. |  |  | 13 | 14 |  | H | H |  | 4.9 |  | -118.5 |  | c | n |  | 8 |  | 4 |  | 4 | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | |  | | --- | | **g) Beta turns** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+2** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **i to i+3** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | **No.** |  | **Turn** |  | **Sequence\*** |  | **type** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **CA-dist** |  | **H-bond** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | \*  1. |  | Asp6-Thr9 |  | DVST |  | IV |  | -58.6 |  | -40.0 |  | -176.9 |  | -42.4 |  | -69.8 |  | 178.6 |  | 6.4 |  | Yes | | \*  2. |  | Val7-Lys10 |  | VSTK |  | I |  | -42.4 |  | -69.8 |  | 178.6 |  | -93.7 |  | 2.7 |  | -175.5 |  | 4.7 |  | Yes | | \*  3. |  | Asn29-Leu32 |  | NNGL |  | II |  | -67.0 |  | 127.2 |  | -72.2 |  | 94.5 |  | -26.1 |  | - |  | 5.4 |  | No | | \*  4. |  | Phe46-Leu49 |  | FPIL |  | IV |  | -60.9 |  | -28.1 |  | -26.1 |  | -58.2 |  | -39.4 |  | -55.0 |  | 5.9 |  | No | | \*  5. |  | Asp91-Lys94 |  | DATK |  | I |  | -54.4 |  | -35.5 |  | - |  | -63.6 |  | -34.3 |  | -43.1 |  | 5.6 |  | No | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | 6. |  | Thr138-Pro141 |  | TSDP |  | VIII |  | -56.2 |  | -31.4 |  | -51.0 |  | -119.8 |  | 85.6 |  | -81.8 |  | 5.7 |  | Yes | | 7. |  | Asp140-Ile143 |  | DPLI |  | I |  | -64.8 |  | -7.6 |  | 31.2 |  | -117.6 |  | 21.9 |  | -61.4 |  | 5.7 |  | No | | 8. |  | Lys157-Leu160 |  | KEGL |  | II |  | -61.0 |  | 135.2 |  | 70.7 |  | 97.9 |  | -29.4 |  | - |  | 5.8 |  | No | | 9. |  | Asp172-Phe175 |  | DTVF |  | IV |  | -50.6 |  | -44.0 |  | -38.5 |  | -82.5 |  | -40.0 |  | -56.8 |  | 5.3 |  | Yes | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | | | | | | |  | |
| |  | | --- | | **h) gamma turns** | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Turn** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residue i+1** | | | | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **i to i+2** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | |  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  |  | | **No.** |  | **Start** |  | **End** |  | **Sequence\*** |  | **type** |  | **Phi** |  | **Psi** |  | **Chi1** |  | **CA-dist** |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | 1. |  | Gly13 |  | Phe15 |  | G P F |  | INVERSE |  | -75.2 |  | 72.0 |  | 33.0 |  | 6.0 |  |  | | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | | | | | | | | | | | | | | | | | | | | |