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| **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

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| **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

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| --- |
| **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 |
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| 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 |

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| 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 |
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| 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 |

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| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **e) Table of helices** |
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| 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 |  **Unitrise**  | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |  **Residuesper 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 |  **Deviationfrom 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 |

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| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |
|  |
| **f) Helix-helix interactions** |
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|   | 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  |

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

 |
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|  |
| **h) Gamma turns** |
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|

|  |
| --- |
| 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 |

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**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** |
| **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**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  **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. ofstrands**  | 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 |  |  2  |  |  Antiparallel  |  |  No  |  |  1  |
| http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif |

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| 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 |
|

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| 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 |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  **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 |

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|  |
| 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 |
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| 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 | **Unitrise** | http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/templates/gif/1x1.gif | **Residuesper 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 | **Deviationfrom 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**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
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|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|   | 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  |

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| **g) Beta turns** |
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| 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  |
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| **h) gamma turns** |
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| 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 |

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