**New Facets of Larger Nest Motifs in Proteins**

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**Table SI** | Top twenty ranked dipeptides by occurrence frequency and their propensity (both given in parenthesis) in Nest

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| All | RL | LR | Simple | Larger |
| DG (3166/1.27) | DG (3127/1.13) | GL (1161/0.99) | LG (2401/1.11) | DG (920/**1.59**) |
| LG (2911/1.23) | LG (2891/0.96) | GK (1044/1.18) | DG (2246/1.18) | GL (779/**1.62**) |
| AG (2579/1.4) | AG (2551/1.2) | GA (771/0.97) | AG (2037/1.3) | SG (701/**1.76**) |
| TG (2523/1.37) | TG (2515/1.02) | GT (735/1) | TG (1974/1.23) | GK (683/1.45) |
| SG (2355/1.33) | SG (2342/1.08) | GS (683/0.95) | SG (1654/1.2) | TG (549/**1.79**) |
| NG (2001/0.89) | NG (1934/0.93) | GV (682/1.05) | NG (1497/0.87) | AG (542/**1.62**) |
| EG (1428/1.12) | EG (1408/0.99) | GE (670/1.09) | KG (1088/1.09) | LG (510/1.49) |
| KG (1419/1.06) | KG (1392/0.99) | GR (601/1.06) | EG (1059/1.05) | NG (504/0.96) |
| RG (1314/1.1) | RG (1289/1.01) | GI (517/0.99) | RG (1024/1.1) | GE (426/1.45) |
| GL (1190/**2.35**) | QG (1099/1.03) | GQ (460/0.96) | QG (899/1.17) | GT (425/**1.7**) |
| QG (1119/1.17) | FG (918/0.86) | GY (459/1.25) | FG (804/0.93) | GA (393/1.38) |
| GK (1106/**1.51**) | YG (887/0.87) | GD (447/1.06) | YG (787/0.97) | GS (387/1.38) |
| FG (934/0.99) | VG (717/1.04) | GF (433/1.07) | HG (611/0.89) | GV (387/**1.97**) |
| YG (914/1.04) | HG (715/0.84) | GG (351/0.92) | VG (579/1.24) | GR (383/1.22) |
| GG (870/**0.18**) | IG (671/1.05) | GN (338/0.94) | GG (566/**0.23**) | EG (369/1.31) |
| GA (798/**1.88**) | *LN* (524/1.16) | *NL* (253/1.24) | IG (537/1.28) | KG (331/1.02) |
| GT (744/**2.71**) | GG (519/0.89) | GH (240/0.99) | *LN* (443/1.31) | GD (314/1.06) |
| HG (738/0.91) | MG (516/1.03) | GM (191/1.03) | MG (428/1.16) | GG (304/**0.17**) |
| VG (721/1.36) | CG (412/0.8) | GW (191/1.09) | GK (423/1.41) | GI (298/**1.85**) |
| GS (712/**1.71**) | NN (410/1.31) | NA (155/1.12) | GL (411/**2.81**) | RG (290/1.09) |

Propensity values > 1.5 are in bold, and < 0.5 are in underlined bold. Non-gly peptides are italicized.

**Table SII** | Top twenty ranked secondary structures found in dipeptides by occurrence frequency and their propensity (both given in parenthesis) in Nest

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| All | RL | LR | Simple | Larger |
| Tt (13740/**2.72**) | hT (11254/**2.74**) | Tt (4457/**2.11**) | Tt (9236/**2.70**) | Tt (4504/**2.78**) |
| hT (11358/**2.53**) | Tt (9283/**3.08**) | hH (2794/**5.20**) | hT (8239/**2.50**) | hT (3119/**2.60**) |
| Hh (8518/**6.17**) | Hh (8483/**4.70**) | TT (1827/1.46) | Hh (7570/**5.33**) | SS (1457/**4.04**) |
| TT (4680/0.79) | TT (2853/0.64) | SS (1015/**4.69**) | TT (3858/0.84) | hH (1159/**3.87**) |
| hH (2802/**3.90**) | Gg (1727/**1.89**) | tT (981/**2.54**) | Gg (1663/**20.1**) | Hh (948/**9.09**) |
| CC (2200/**5.93**) | CC (1608/**6.50**) | gG (934/**15.2**) | hH (1643/**3.91**) | TT (822/0.59) |
| SS (2114/**6.41**) | CS (1183/**5.33**) | Te (813/1.39) | Te (1456/**1.80**) | CC (778/**3.99**) |
| Gg (1949/**20.9**) | SS (1099/**7.58**) | SC (604/**2.94**) | CC (1422/**7.54**) | tC (694/**2.62**) |
| Te (1895/**1.69**) | Te (1082/**1.86**) | CC (592/**4.96**) | CS (882/**7.59**) | CS (646/**2.32**) |
| CS (1528/**4.31**) | SC (691/**4.28**) | tS (503/**1.97**) | SC (793/**6.25**) | tT (622/1.10) |
| tT (1383/1.29) | tC (571/**5.31**) | tC (480/**1.99**) | tT (761/**1.95**) | tS (616/**1.62**) |
| SC (1295/**3.75**) | eS (406/**7.78**) | Th (415/**1.35**) | SS (657/**8.41**) | SC (502/**1.99**) |
| tC (1051/**3.34**) | tT (402/0.85) | CS (345/**2.74**) | gG (634/**49.8**) | Te (439/1.39) |
| gG (964/**41.7**) | he (315/0.59) | ht (339/0.34) | tC (357/**3.92**) | Th (420/0.60) |
| tS (705/**2.34**) | ht (293/0.11) | te (301/**1.67**) | he (314/0.54) | ht (413/0.30) |
| Th (666/0.19) | Th (251/0.09) | Gg (222/**27.1**) | eC (268/**4.78**) | gG (330/**31.2**) |
| ht (632/0.17) | hh (245/0.09) | Tg (178/0.77) | Th (246/0.09) | te (323/**2.54**) |
| eS (450/**4.90**) | Ct (219/0.31) | Se (134/0.88) | EE (228/**176**) | Gg (286/**22.3**) |
| he (370/0.44) | eC (210/3.61) | eT (118/**1.89**) | Ge (224/**2.16**) | hh (264/0.44) |
| te (350/**1.73**) | tS (202/**2.09**) | Sh (113/1.40) | ht (219/0.09) | eS (257/**4.47**) |

Propensity values > 1.5 are in bold, and < 0.5 are in underlined bold.



**Figure S1** | A color gradient tile showing the propensity values of the amino acids in position 1 and 2 in the Nest with respect to various datasets. All: All dipeptides in the data set including Nests; Nest\_All: Only Nest Dipeptides having either RL or LR enantiomeric conformational states; Nest\_RL: Dipeptides in Nest having only RL conformational state; Nest\_LR: Dipeptides in Nest having only LR conformational state; Simple Nest: Isolated dipeptides having either RL or LR conformational states; Larger Nest: Nests other than simple Nests. Here \_RL or \_LR data set means a subset screened to contain only RL or LR conformation dipeptides in them. Propensity values between 0.5 and 1.5 are uniformly colored by a deep blue color corresponding to 1 in the legend. Other values above 1.5 and below 0.5 are as per the legend.