**Supplementary Materials**

**for**

Dynamic Solvent Accessible Surface Areas of Proteogenic a - Amino Acids as a Function of Explored f,y Dihedral Angle Space Modelled using the Ac-Ala-Xaa-Ala-NH2 system and CHARMM36m Force Field.

William A. Burns 1, Sándor Lovas 2 and Charles R. Watts 3,\*

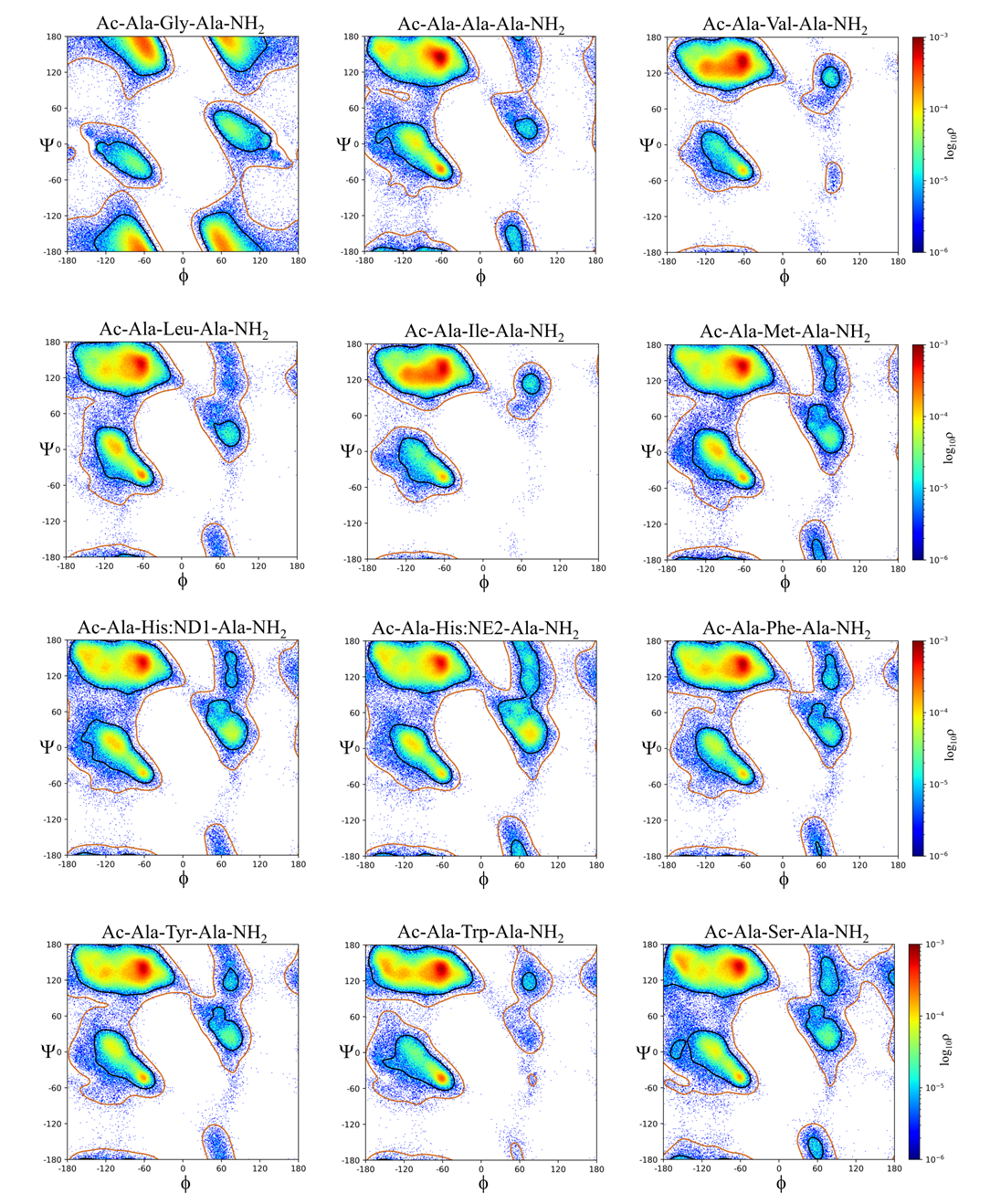
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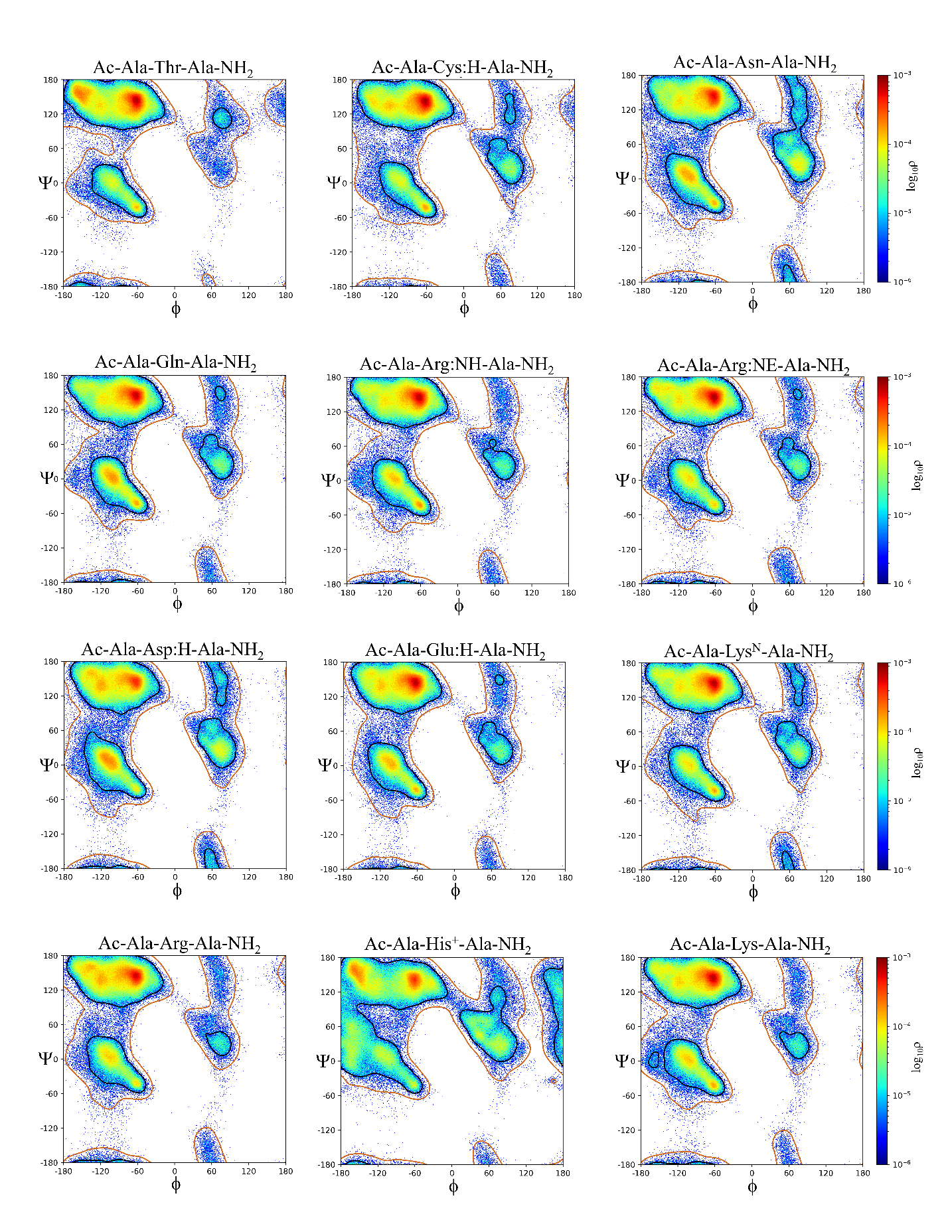
1 Health Partners Institute, Bloomington, Minnesota, USA, 55425; William.A.Burns@healthpartners.com

2 Department of Biomedical Sciences, Creighton University, Omaha, Nebraska, USA, 68178; SandorLovas@creighton.edu

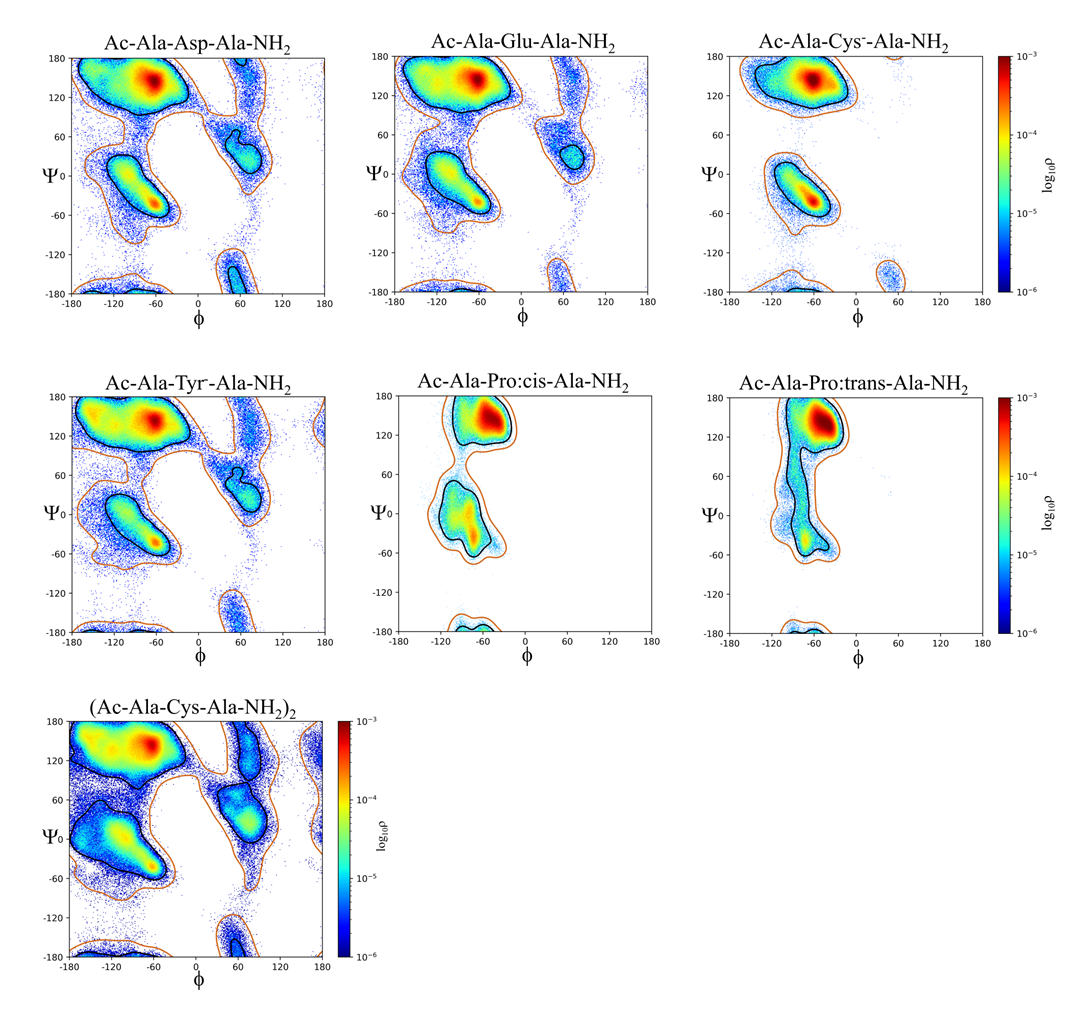
3 Department of Neurosurgery, Park Nicollet, Methodist Hospital, St. Louis Park, Minnesota, USA, 55426; charles.watts@parknicollet.com

**\*** Correspondence: charles.watts@parknicollet.com; Tel.: +1-952-933-3200, Fax: +1-952-993-7407

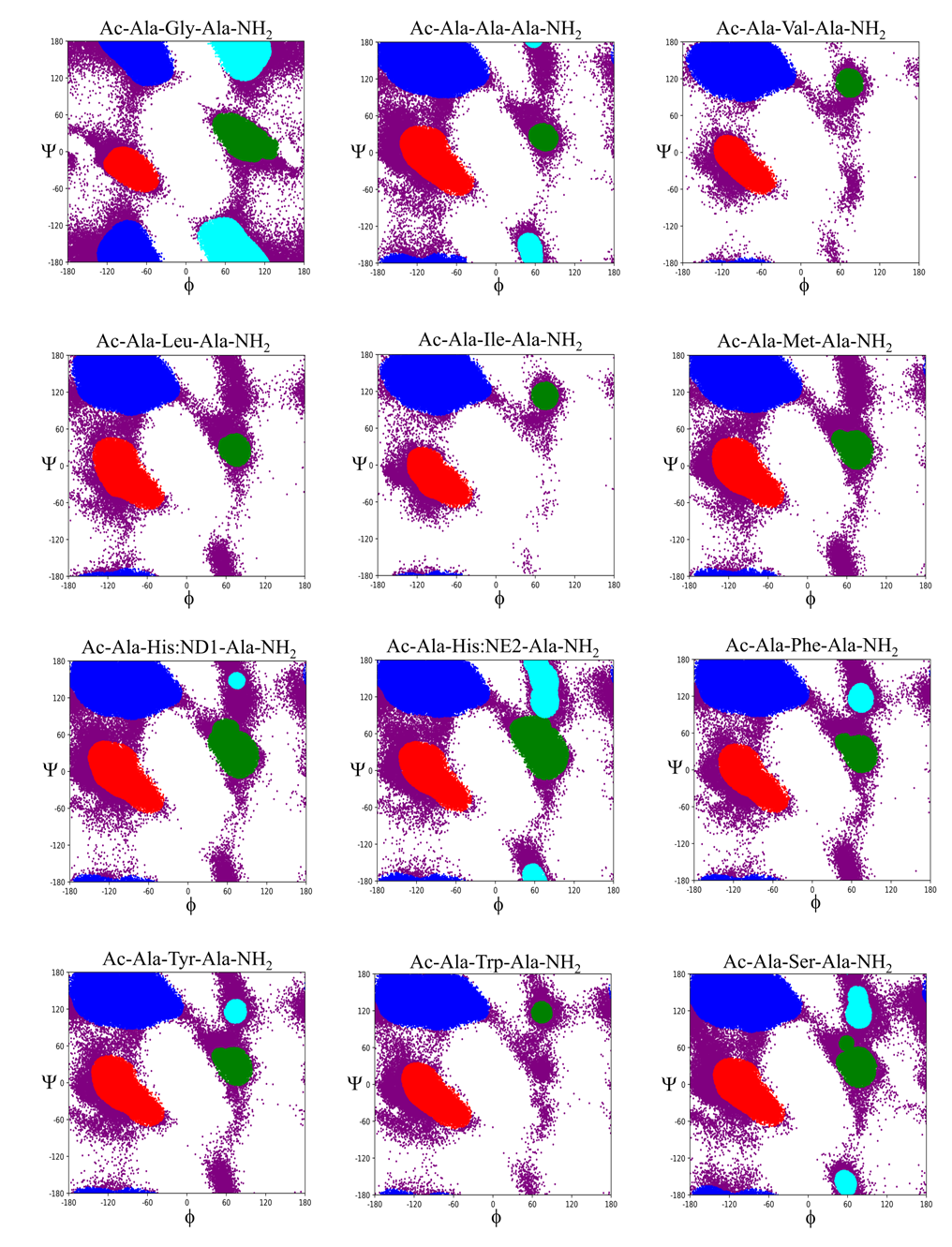
**Figure S1.** Two-dimensional histograms demonstrating the log10 scaled probabilities (r) of the sampled f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides. Black contour lines represent 98% of the sampled population, brown contour lines represent 99.8%.



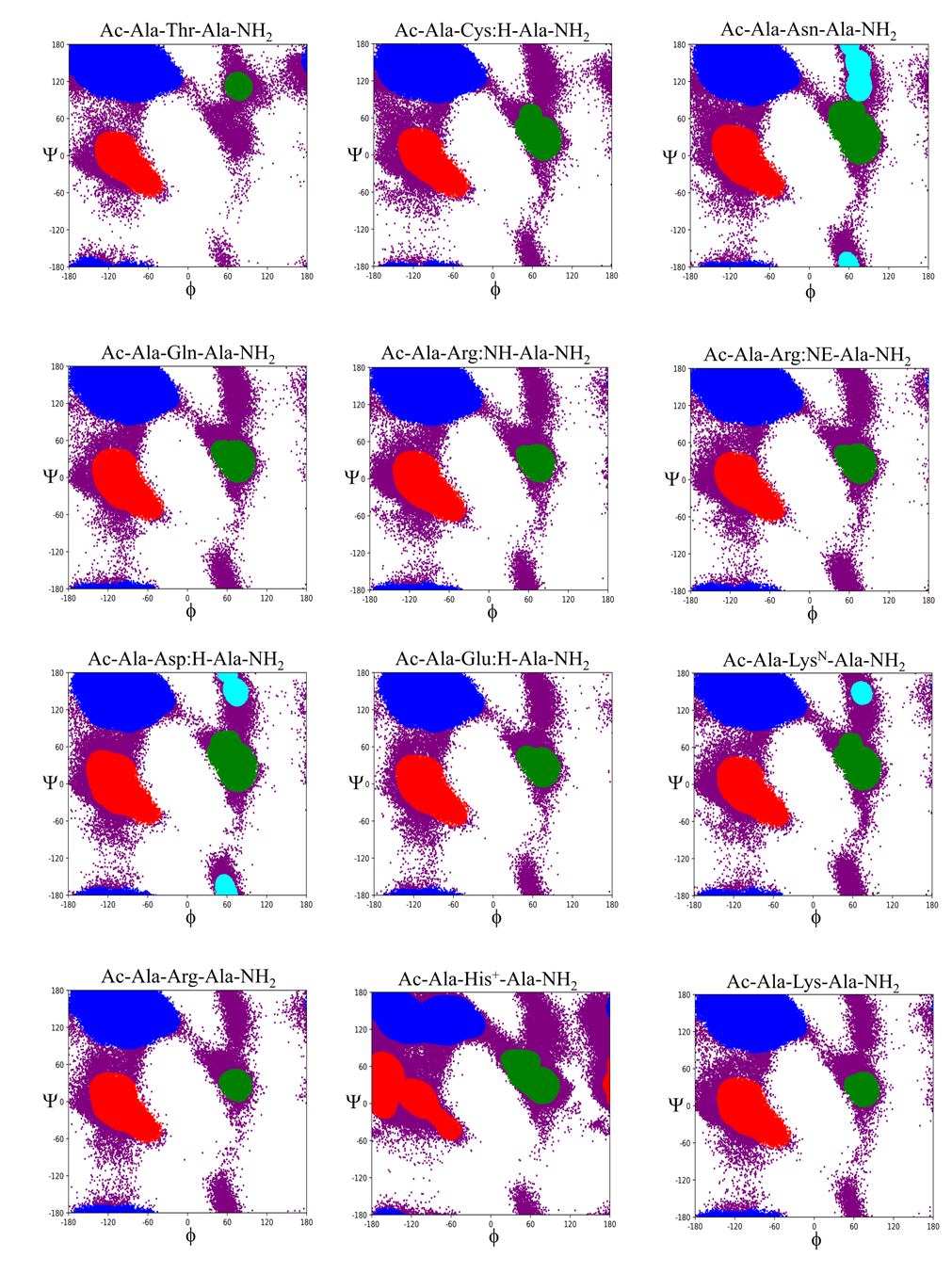
**Figure S1 (Cont.).** Two-dimensional histograms demonstrating the log10 scaled probabilities (r) of the sampled f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides. Black contour lines represent 98% of the sampled population, brown contour lines represent 99.8%.

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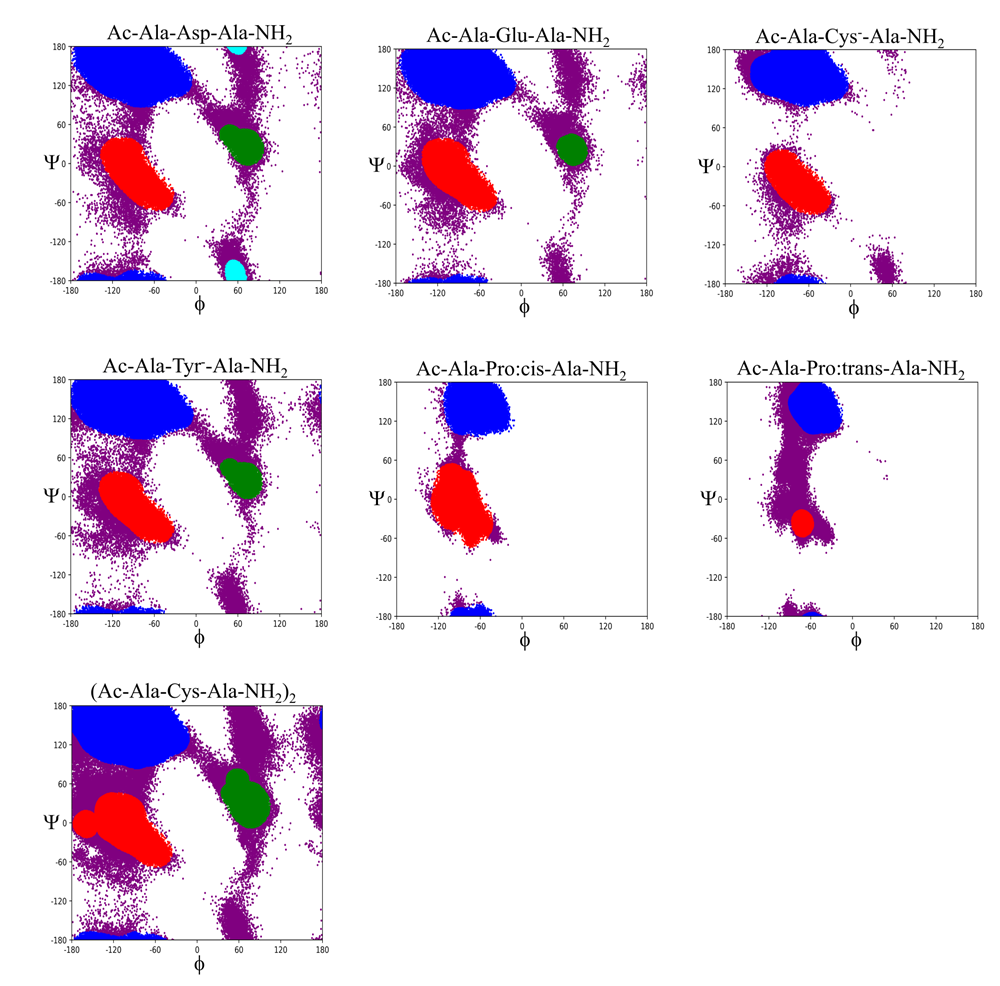
**Figure S1 (Cont.).** Two-dimensional histograms demonstrating the log10 scaled probabilities (r) of the sampled f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides. Black contour lines represent 98% of the sampled population, brown contour lines represent 99.8%.

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**Figure S2.** Sampled secondary structure classifications for the f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides as determined by density clustering. Blue, b, Red, a, Green, aL, Cyan, e, Purple, contiguous.

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**Figure S2 (Cont.).** Sampled secondary structure classifications for the f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides as determined by density clustering. Blue, b, Red, a, Green, aL, Cyan, e, Purple, contiguous.

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**Figure S2 (Cont.).** Sampled secondary structure classifications for the f,y space for the Xaa residues within the Ac-Ala-Xaa-Ala-NH2 peptides as determined by density clustering. Blue, b, Red, a, Green, aL, Cyan, e, Purple, contiguous.

**Table S1.** The probability () and number of conformations (n) of the f,y dihedral angles of the Xaa residue within the Ace-Ala-Xaa-Ala-NH2 peptides within the b, a, aL, e, or contiguous regions of f,y space as assigned by density clustering demonstrated in Figure S2. The results are compared using a c2-analysis.a,b,c Results are considered statistically significant for an a = 0.0001 using a right-tailed c2 distribution.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | b | a | aL | e | Cont. |
| r (n) | r (n) | r (n) | r(n) | r (n) |
| Gly | 0.4917 (196662) | 0.0430 (17215) | 0.0586 (23453) | 0.3596 (143841) | 0.0471 (18829) |
| Ala | 0.7636 (305439) | 0.1743 (69703) | 0.0104 (4180) | 0.0112 (4462) | 0.0405 (16216) |
| Val | 0.9086 (363456) | 0.0649 (25972) | 0.0103 (4104) | N/S | 0.0162 (6468) |
| Leu | 0.7395 (295814) | 0.2105 (84184) | 0.0148 (5931) | N/S | 0.0352 (14071) |
| Ile | 0.8868 (354725) | 0.0878 (35117) | 0.0094 (3762) | N/S | 0.0160 (6396) |
| Met | 0.7308 (292331) | 0.1987 (79486) | 0.0262 (10467) | N/S | 0.0443 (17716) |
| His:ND1 | 0.7088 (283537) | 0.1740 (69599) | 0.0672 (26869) | 0.0035 (1384) | 0.0465 (18611) |
| His:NE2 | 0.6600 (264018) | 0.1514 (60541) | 0.1219 (48753) | 0.0337 (13489) | 0.0330 (13199) |
| Phe | 0.8160 (326398) | 0.1096 (43854) | 0.0252 (10096) | 0.0094 (3755) | 0.0397 (15897) |
| Tyr | 0.7850 (313992) | 0.1441 (57656) | 0.0260 (10389) | 0.0067 (2666) | 0.0382 (15297) |
| Trp | 0.8425 (336997) | 0.1199 (47956) | 0.0057 (2262) | N/S | 0.0320 (12785) |
| Ser | 0.7517 (300689) | 0.1419 (56743) | 0.0320 (12795) | 0.0212 (8470) | 0.0533 (21303) |
| Thr | 0.8407 (336262) | 0.1198 (47939) | 0.0101 (4038) | N/S | 0.0294 (11761) |
| Cys:H | 0.7795 (311786) | 0.1359 (54394) | 0.0445 (17800) | N/S | 0.0402 (16065) |
| Asn | 0.6309 (252358) | 0.2149 (85950) | 0.1002 (40061) | 0.0248 (9929) | 0.0293 (11702) |
| Gln | 0.6964 (278560) | 0.2296 (91839) | 0.0338 (13506) | N/S | 0.0402 (16095) |
| Arg:NE | 0.7806 (312228) | 0.1493 (59737) | 0.0291 (11655) | N/S | 0.0410 (16380) |
| Arg:NH | 0.7415 (296611) | 0.1953 (78135) | 0.0242 (9693) | N/S | 0.0389 (15561) |

**Table S1 (Cont.).** The probability () and number of conformations (n) of the f,y dihedral angles of the Xaa residue within the Ace-Ala-Xaa-Ala-NH2 peptides within the b, a, aL, e, or contiguous regions of f,y space as assigned by density clustering demonstrated in Figure S2. The results are compared using a c2-analysis.a,b,c Results are considered statistically significant for an a = 0.0001 using a right-tailed c2 distribution.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | b | a | aL | e | Cont. |
| r (n) | r (n) | r (n) | r (n) | r (n) |
| Asp:H | 0.6281 (251242) | 0.2422 (96865) | 0.0806 (32255) | 0.0166 (6644) | 0.0325 (12994) |
| Glu:H | 0.7355 (294206) | 0.1981 (79260) | 0.0305 (12180) | N/S | 0.0359 (14354) |
| LysN | 0.7304 (292174) | 0.1751 (70037) | 0.0478 (19118) | 0.0056 (2257) | 0.0410 (16414) |
| Arg | 0.7781 (311234) | 0.1705 (68206) | 0.0147 (5880) | N/S | 0.0367 (14680) |
| His+ | 0.5942 (237698) | 0.2020 (80793) | 0.1073 (42938) | N/S | 0.0964 (38571) |
| Lys | 0.7530 (301189) | 0.1892 (75678) | 0.0180 (7189) | N/S | 0.0399 (15944) |
| Asp | 0.7675 (306995) | 0.1728 (69136) | 0.0209 (8362) | 0.0068 (2714) | 0.0320 (12793) |
| Glu | 0.8106 (324246) | 0.1506 (60238) | 0.0110 (4388) | N/S | 0.0278 (11128) |
| Cys- | 0.7757 (310270) | 0.2134 (85366) | N/S | N/S | 0.0109 (4364) |
| Tyr- | 0.8201 (328043) | 0.1228 (49108) | 0.0197 (7876) | N/S | 0.0374 (14973) |
| Cys-Cys | 0.7406 (592475) | 0.1690 (135173) | 0.0449 (35958) | N/S | 0.0455 (36394) |
| Pro:cis | 0.7859 (314375) | 0.2104 (84155) | N/S | N/S | 0.0037 (1470) |
| Pro:trans | 0.9204 (368141) | 0.0328 (13115) | N/S | N/S | 0.0469 (18744) |
| χ2-Statistic | 313922 | 144610 | 301107 | 25618 | 65608 |
| χ2-Critical | 61.6572 | 61.6572 | 60.1403 | 33.7199 | 61.6572 |
| p-value | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** |

a The Gly, Cys-Cys, Pro:cis, and Pro:trans peptides were excluded from the c2-analysis.

b N/S: not sampled region secondary to low population density (<1000 conformations within 10°).

c The standard deviation of r is

**Table S2.** Statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 0.1450 | 0.006373864 | Hydrophobic - Hydrophobic |
| Ala - Leu | 0.0241 | 0.007584145 | Hydrophobic - Hydrophobic |
| Ala - Ile | 0.1232 | 0.006580193 | Hydrophobic - Hydrophobic |
| Ala - Met | 0.0328 | 0.007625611 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 0.0548 | 0.007722739 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 0.1036 | 0.007900309 | Hydrophobic - Aromatic |
| Ala - Phe | 0.0524 | 0.007139246 | Hydrophobic - Aromatic |
| Ala - Tyr | 0.0214 | 0.007337620 | Hydrophobic - Aromatic |
| Ala - Trp | 0.0789 | 0.006948309 | Hydrophobic - Aromatic |
| Ala - Ser | 0.0119 | 0.007523000 | Hydrophobic - Polar |
| Ala - Thr | 0.0771 | 0.006961936 | Hydrophobic - Polar |
| Ala - Cys | 0.0159 | 0.007370159 | Hydrophobic - Polar |
| Ala - Asn | 0.1327 | 0.007982464 | Hydrophobic - Polar |
| Ala - Gln | 0.0672 | 0.007772721 | Hydrophobic - Polar |
| Ala - Arg:NE | 0.0170 | 0.007363713 | Hydrophobic - Polar |
| Ala - Arg:NH | 0.0221 | 0.007574363 | Hydrophobic - Polar |
| Ala - Asp:H | 0.1355 | 0.007989463 | Hydrophobic - Polar |
| Ala - Glu:H | 0.0281 | 0.007603429 | Hydrophobic - Polar |
| Ala - LysN | 0.0332 | 0.007627476 | Hydrophobic - Polar |
| Ala - Arg | 0.0145 | 0.007378318 | Hydrophobic - Positive Charge |
| Ala - His+ | 0.1694 | 0.008061832 | Hydrophobic - Positive Charge |
| Ala - Lys | 0.0106 | 0.007516276 | Hydrophobic - Positive Charge |
| Ala - Glu | 0.0470 | 0.007175681 | Hydrophobic - Negative Charge |
| Ala - Cys - | 0.0121 | 0.007392188 | Hydrophobic - Negative Charge |
| Ala - Tyr - | 0.0565 | 0.007111035 | Hydrophobic - Negative Charge |
| Val - Leu | 0.1691 | 0.006518825 | Hydrophobic - Hydrophobic |
| Val - Ile | 0.0218 | 0.005317401 | Hydrophobic - Hydrophobic |
| Val - Met | 0.1778 | 0.006567021 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 0.1998 | 0.006679560 | Hydrophobic - Aromatic |
| Val - His:NE2 | 0.2486 | 0.006884091 | Hydrophobic - Aromatic |
| Val - Phe | 0.0926 | 0.005995386 | Hydrophobic - Aromatic |
| Val - Tyr | 0.1236 | 0.006230288 | Hydrophobic - Aromatic |
| Val - Trp | 0.0661 | 0.005766699 | Hydrophobic - Aromatic |
| Val - Ser | 0.1569 | 0.006447585 | Hydrophobic - Polar |
| Val - Thr | 0.0679 | 0.005783111 | Hydrophobic - Polar |
| Val - Cys | 0.1291 | 0.006268578 | Hydrophobic - Polar |
| Val - Asn | 0.2777 | 0.006978220 | Hydrophobic - Polar |
| Val - Gln | 0.2122 | 0.006737285 | Hydrophobic - Polar |
| Val - Arg:NE | 0.1280 | 0.006260998 | Hydrophobic - Polar |
| Val - Arg:NH | 0.1671 | 0.006507441 | Hydrophobic - Polar |
| Val - Asp:H | 0.2805 | 0.006986225 | Hydrophobic - Polar |
| Val - Glu:H | 0.1731 | 0.006541250 | Hydrophobic - Polar |
| Val - LysN | 0.1782 | 0.006569186 | Hydrophobic - Polar |
| Val - Arg | 0.1305 | 0.006278168 | Hydrophobic - Positive Charge |
| Val - His+ | 0.3144 | 0.007068872 | Hydrophobic - Positive Charge |
| Val - Lys | 0.1556 | 0.006439737 | Hydrophobic - Positive Charge |
| Val - Asp | 0.1411 | 0.006348768 | Hydrophobic - Negative Charge |
| Val - Glu | 0.0980 | 0.006038726 | Hydrophobic - Negative Charge |
| Val - Cys - | 0.1329 | 0.006294464 | Hydrophobic - Negative Charge |
| Val - Tyr - | 0.0885 | 0.005961765 | Hydrophobic - Negative Charge |
| Leu - Ile | 0.1473 | 0.006720705 | Hydrophobic - Hydrophobic |
| Leu - Met | 0.0087 | 0.007747186 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 0.0307 | 0.007842808 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 0.0795 | 0.008017719 | Hydrophobic - Aromatic |
| Leu - Phe | 0.0765 | 0.007268959 | Hydrophobic - Aromatic |
| Leu - Tyr | 0.0455 | 0.007463887 | Hydrophobic - Aromatic |
| Leu - Trp | 0.1030 | 0.007081520 | Hydrophobic - Aromatic |
| Leu - Ser | 0.0122 | 0.007646206 | Hydrophobic - Polar |
| Leu - Thr | 0.1012 | 0.007094892 | Hydrophobic - Polar |
| Leu - Cys | 0.0400 | 0.007495878 | Hydrophobic - Polar |
| Leu - Asn | 0.1086 | 0.008098683 | Hydrophobic - Polar |
| Leu - Gln | 0.0431 | 0.007892030 | Hydrophobic - Polar |
| Leu - Arg:NE | 0.0411 | 0.007489540 | Hydrophobic - Polar |
| Leu - Asp:H | 0.1114 | 0.008105582 | Hydrophobic - Polar |
| Leu - LysN | 0.0091 | 0.007749021 | Hydrophobic - Polar |
| Leu - Arg | 0.0386 | 0.007503900 | Hydrophobic - Positive Charge |
| Leu - His+ | 0.1453 | 0.008176923 | Hydrophobic - Positive Charge |
| Leu - Lys | 0.0135 | 0.007639590 | Hydrophobic - Positive Charge |
| Leu - Asp | 0.0280 | 0.007563067 | Hydrophobic - Negative Charge |
| Leu - Glu | 0.0711 | 0.007304747 | Hydrophobic - Negative Charge |
| Leu - Cys - | 0.0362 | 0.007517539 | Hydrophobic - Negative Charge |
| Leu - Tyr - | 0.0806 | 0.007241254 | Hydrophobic - Negative Charge |
| Ile - Met | 0.1560 | 0.006767464 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 0.1780 | 0.006876723 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 0.2268 | 0.007075557 | Hydrophobic - Aromatic |
| Ile - Phe | 0.0708 | 0.006214294 | Hydrophobic - Aromatic |
| Ile - Tyr | 0.1018 | 0.006441218 | Hydrophobic - Aromatic |
| Ile - Trp | 0.0443 | 0.005993965 | Hydrophobic - Aromatic |
| Ile - Ser | 0.1351 | 0.006651628 | Hydrophobic - Polar |
| Ile - Thr | 0.0461 | 0.006009756 | Hydrophobic - Polar |
| Ile - Cys | 0.1073 | 0.006478261 | Hydrophobic - Polar |
| Ile - Asn | 0.2559 | 0.007167172 | Hydrophobic - Polar |
| Ile - Gln | 0.1904 | 0.006932807 | Hydrophobic - Polar |
| Ile - Arg:NE | 0.1062 | 0.006470927 | Hydrophobic - Polar |
| Ile - Arg:NH | 0.1453 | 0.006709664 | Hydrophobic - Polar |
| Ile - Asp:H | 0.2587 | 0.007174966 | Hydrophobic - Polar |
| Ile - Glu:H | 0.1513 | 0.006742459 | Hydrophobic - Polar |
| Ile - LysN | 0.1564 | 0.006769565 | Hydrophobic - Polar |
| Ile - Arg | 0.1087 | 0.006487542 | Hydrophobic - Positive Charge |
| Ile - His+ | 0.2926 | 0.007255464 | Hydrophobic - Positive Charge |
| Ile - Lys | 0.1338 | 0.006644021 | Hydrophobic - Positive Charge |
| Ile - Asp | 0.1193 | 0.006555887 | Hydrophobic - Negative Charge |
| Ile - Glu | 0.0762 | 0.006256118 | Hydrophobic - Negative Charge |
| Ile - Cys - | 0.1111 | 0.006503312 | Hydrophobic - Negative Charge |
| Ile - Tyr - | 0.0667 | 0.006181864 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 0.0220 | 0.007882914 | Hydrophobic - Aromatic |
| Met - His:NE2 | 0.0708 | 0.008056955 | Hydrophobic - Aromatic |
| Met - Phe | 0.0852 | 0.007312213 | Hydrophobic - Aromatic |
| Met - Tyr | 0.0542 | 0.007506018 | Hydrophobic - Aromatic |
| Met - Trp | 0.1117 | 0.007125912 | Hydrophobic - Aromatic |
| Met - Ser | 0.0209 | 0.007687338 | Hydrophobic - Polar |
| Met - Thr | 0.1099 | 0.007139201 | Hydrophobic - Polar |
| Met - Cys | 0.0487 | 0.007537830 | Hydrophobic - Polar |
| Met - Asn | 0.0999 | 0.008137528 | Hydrophobic - Polar |
| Met - Gln | 0.0344 | 0.007931887 | Hydrophobic - Polar |
| Met - Arg:NE | 0.0498 | 0.007531528 | Hydrophobic - Polar |
| Met - Arg:NH | 0.0107 | 0.007737610 | Hydrophobic - Polar |
| Met - Asp:H | 0.1027 | 0.008144394 | Hydrophobic - Polar |
| Met - Arg | 0.0473 | 0.007545807 | Hydrophobic - Positive Charge |
| Met - His+ | 0.1366 | 0.008215398 | Hydrophobic - Positive Charge |
| Met - Lys | 0.0222 | 0.007680757 | Hydrophobic - Positive Charge |
| Met - Asp | 0.0367 | 0.007604648 | Hydrophobic - Negative Charge |
| Met - Glu | 0.0798 | 0.007347791 | Hydrophobic - Negative Charge |
| Met - Cys - | 0.0449 | 0.007559371 | Hydrophobic - Negative Charge |
| Met - Tyr - | 0.0893 | 0.007284673 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 0.0488 | 0.008148943 | Aromatic - Aromatic |
| His:ND1 - Phe | 0.1072 | 0.007413448 | Aromatic - Aromatic |
| His:ND1 - Tyr | 0.0762 | 0.007604673 | Aromatic - Aromatic |
| His:ND1 - Trp | 0.1337 | 0.007229756 | Aromatic - Aromatic |
| His:ND1 - Ser | 0.0429 | 0.007783696 | Aromatic - Polar |
| His:ND1 - Thr | 0.1319 | 0.007242854 | Aromatic - Polar |
| His:ND1 - Cys | 0.0707 | 0.007636074 | Aromatic - Polar |
| His:ND1 - Asn | 0.0779 | 0.008228616 | Aromatic - Polar |
| His:ND1 - Gln | 0.0124 | 0.008025308 | Aromatic - Polar |
| His:ND1 - Arg:NE | 0.0718 | 0.007629853 | Aromatic - Polar |
| His:ND1 - Arg:NH | 0.0327 | 0.007833349 | Aromatic - Polar |
| His:ND1 - Asp:H | 0.0807 | 0.008235405 | Aromatic - Polar |
| His:ND1 - Glu:H | 0.0267 | 0.007861457 | Aromatic - Polar |
| His:ND1 - LysN | 0.0216 | 0.007884718 | Aromatic - Polar |
| His:ND1 - Arg | 0.0693 | 0.007643949 | Aromatic - Positive Charge |
| His:ND1 - His+ | 0.1146 | 0.008305632 | Aromatic - Positive Charge |
| His:ND1 - Lys | 0.0442 | 0.007777196 | Aromatic - Positive Charge |
| His:ND1 - Asp | 0.0587 | 0.007702040 | Aromatic - Negative Charge |
| His:ND1 - Glu | 0.1018 | 0.007448542 | Aromatic - Negative Charge |
| His:ND1 - Cys - | 0.0669 | 0.007657339 | Aromatic - Negative Charge |
| His:ND1 - Tyr - | 0.1113 | 0.007386285 | Aromatic - Negative Charge |
| His:NE2 - Phe | 0.1560 | 0.007598249 | Aromatic - Aromatic |
| His:NE2 - Tyr | 0.1250 | 0.007784936 | Aromatic - Aromatic |
| His:NE2 - Trp | 0.1825 | 0.007419135 | Aromatic - Aromatic |
| His:NE2 - Ser | 0.0917 | 0.007959906 | Aromatic - Polar |
| His:NE2 - Thr | 0.1807 | 0.007431899 | Aromatic - Polar |
| His:NE2 - Cys | 0.1195 | 0.007815613 | Aromatic - Polar |
| His:NE2 - Asn | 0.0291 | 0.008395493 | Aromatic - Polar |
| His:NE2 - Gln | 0.0364 | 0.008196326 | Aromatic - Polar |
| His:NE2 - Arg:NE | 0.1206 | 0.007809535 | Aromatic - Polar |
| His:NE2 - Arg:NH | 0.0815 | 0.008008467 | Aromatic - Polar |
| His:NE2 - Asp:H | 0.0319 | 0.008402148 | Aromatic - Polar |
| His:NE2 - Glu:H | 0.0755 | 0.008035963 | Aromatic - Polar |
| His:NE2 - LysN | 0.0704 | 0.008058719 | Aromatic - Polar |
| His:NE2 - Arg | 0.1181 | 0.007823308 | Aromatic - Positive Charge |
| His:NE2 - His+ | 0.0658 | 0.008470992 | Aromatic - Positive Charge |
| His:NE2 - Lys | 0.0930 | 0.007953550 | Aromatic - Positive Charge |
| His:NE2 - Asp | 0.1075 | 0.007880077 | Aromatic - Negative Charge |
| His:NE2 - Glu | 0.1506 | 0.007632494 | Aromatic - Negative Charge |
| His:NE2 - Cys - | 0.1157 | 0.007836390 | Aromatic - Negative Charge |
| His:NE2 - Tyr - | 0.1601 | 0.007571749 | Aromatic - Negative Charge |
| Phe - Tyr | 0.0310 | 0.007011361 | Aromatic - Aromatic |
| Phe - Trp | 0.0265 | 0.006602841 | Aromatic - Aromatic |
| Phe - Ser | 0.0643 | 0.007205140 | Aromatic - Polar |
| Phe - Thr | 0.0247 | 0.006617179 | Aromatic - Polar |
| Phe - Cys | 0.0365 | 0.007045407 | Aromatic - Polar |
| Phe - Asn | 0.1851 | 0.007683635 | Aromatic - Polar |
| Phe - Gln | 0.1196 | 0.007465501 | Aromatic - Polar |
| Phe - Arg:NE | 0.0354 | 0.007038664 | Aromatic - Polar |
| Phe - Arg:NH | 0.0745 | 0.007258752 | Aromatic - Polar |
| Phe - Asp:H | 0.1879 | 0.007690906 | Aromatic - Polar |
| Phe - Glu:H | 0.0805 | 0.007289077 | Aromatic - Polar |
| Phe - LysN | 0.0856 | 0.007314157 | Aromatic - Polar |
| Phe - Arg | 0.0379 | 0.007053941 | Aromatic - Positive Charge |
| Phe - His+ | 0.2218 | 0.007766057 | Aromatic - Positive Charge |
| Phe - Lys | 0.0630 | 0.007198118 | Aromatic - Positive Charge |
| Phe - Asp | 0.0485 | 0.007116850 | Aromatic - Negative Charge |
| Phe - Cys - | 0.0403 | 0.007068448 | Aromatic - Negative Charge |
| Tyr - Trp | 0.0575 | 0.006816843 | Aromatic - Aromatic |
| Tyr - Ser | 0.0333 | 0.007401749 | Aromatic - Polar |
| Tyr - Thr | 0.0557 | 0.006830732 | Aromatic - Polar |
| Tyr - Asn | 0.1541 | 0.007868296 | Aromatic - Polar |
| Tyr - Gln | 0.0886 | 0.007655426 | Aromatic - Polar |
| Tyr - Arg:NH | 0.0435 | 0.007453947 | Aromatic - Polar |
| Tyr - Asp:H | 0.1569 | 0.007875397 | Aromatic - Polar |
| Tyr - Glu:H | 0.0495 | 0.007483481 | Aromatic - Polar |
| Tyr - LysN | 0.0546 | 0.007507912 | Aromatic - Polar |
| Tyr - His+ | 0.1908 | 0.007948804 | Aromatic - Positive Charge |
| Tyr - Lys | 0.0320 | 0.007394914 | Aromatic - Positive Charge |
| Tyr - Asp | 0.0175 | 0.007315832 | Aromatic - Negative Charge |
| Tyr - Glu | 0.0256 | 0.007048457 | Aromatic - Negative Charge |
| Tyr - Cys - | 0.0093 | 0.007268755 | Aromatic - Negative Charge |
| Tyr - Tyr - | 0.0351 | 0.006982634 | Aromatic - Negative Charge |
| Trp - Ser | 0.0908 | 0.007015997 | Aromatic - Polar |
| Trp - Cys | 0.0630 | 0.006851855 | Aromatic - Polar |
| Trp - Asn | 0.2116 | 0.007506558 | Aromatic - Polar |
| Trp - Gln | 0.1461 | 0.007283122 | Aromatic - Polar |
| Trp - Arg:NE | 0.0619 | 0.006844922 | Aromatic - Polar |
| Trp - Arg:NH | 0.1010 | 0.007071043 | Aromatic - Polar |
| Trp - Asp:H | 0.2144 | 0.007514000 | Aromatic - Polar |
| Trp - Glu:H | 0.1070 | 0.007102169 | Aromatic - Polar |
| Trp - LysN | 0.1121 | 0.007127907 | Aromatic - Polar |
| Trp - Arg | 0.0644 | 0.006860630 | Aromatic - Positive Charge |
| Trp - His+ | 0.2483 | 0.007590903 | Aromatic - Positive Charge |
| Trp - Lys | 0.0895 | 0.007008785 | Aromatic - Positive Charge |
| Trp - Asp | 0.0750 | 0.006925295 | Aromatic - Negative Charge |
| Trp - Glu | 0.0319 | 0.006642219 | Aromatic - Negative Charge |
| Trp - Cys - | 0.0668 | 0.006875545 | Aromatic - Negative Charge |
| Trp - Tyr - | 0.0224 | 0.006572328 | Aromatic - Negative Charge |
| Ser - Thr | 0.0890 | 0.007029493 | Polar - Polar |
| Ser - Cys | 0.0278 | 0.007434007 | Polar - Polar |
| Ser - Asn | 0.1208 | 0.008041452 | Polar - Polar |
| Ser - Gln | 0.0553 | 0.007833288 | Polar - Polar |
| Ser - Arg:NE | 0.0289 | 0.007427617 | Polar - Polar |
| Ser - Arg:NH | 0.0102 | 0.007636504 | Polar - Polar |
| Ser - Asp:H | 0.1236 | 0.008048399 | Polar - Polar |
| Ser - Glu:H | 0.0162 | 0.007665334 | Polar - Polar |
| Ser - LysN | 0.0213 | 0.007689187 | Polar - Polar |
| Ser - Arg | 0.0264 | 0.007442096 | Polar - Positive Charge |
| Ser - His= | 0.1575 | 0.008120243 | Polar - Positive Charge |
| Ser - Asp | 0.0158 | 0.007501750 | Polar - Negative Charge |
| Ser - Glu | 0.0589 | 0.007241244 | Polar - Negative Charge |
| Ser - Cys - | 0.0240 | 0.007455848 | Polar - Negative Charge |
| Ser - Tyr - | 0.0684 | 0.007177189 | Polar - Negative Charge |
| Thr - Cys | 0.0612 | 0.006865674 | Polar - Polar |
| Thr - Asn | 0.2098 | 0.007519173 | Polar - Polar |
| Thr - Gln | 0.1443 | 0.007296124 | Polar - Polar |
| Thr - Arg:NE | 0.0601 | 0.006858754 | Polar - Polar |
| Thr - Arg:NH | 0.0992 | 0.007084434 | Polar - Polar |
| Thr - Asp:H | 0.2126 | 0.007526603 | Polar - Polar |
| Thr - Glu:H | 0.1052 | 0.007115502 | Polar - Polar |
| Thr - LysN | 0.1103 | 0.007141192 | Polar - Polar |
| Thr - Arg | 0.0626 | 0.006874432 | Polar - Positive Charge |
| Thr - His+ | 0.2465 | 0.007603379 | Polar - Positive Charge |
| Thr - Lys | 0.0877 | 0.007022295 | Polar - Positive Charge |
| Thr - Asp | 0.0732 | 0.006938968 | Polar - Negative Charge |
| Thr - Glu | 0.0301 | 0.006656473 | Polar - Negative Charge |
| Thr - Cys - | 0.0650 | 0.006889317 | Polar - Negative Charge |
| Thr - Tyr - | 0.0206 | 0.006586733 | Polar - Negative Charge |
| Cys - Asn | 0.1486 | 0.007898649 | Polar - Polar |
| Cys - Gln | 0.0831 | 0.007686619 | Polar - Polar |
| Cys - Arg:NH | 0.038 | 0.007485980 | Polar - Polar |
| Cys - Asp:H | 0.1514 | 0.007905722 | Polar - Polar |
| Cys - Glu:H | 0.0440 | 0.007515388 | Polar - Polar |
| Cys - LysN | 0.0491 | 0.007539716 | Polar - Polar |
| Cys - His+ | 0.1853 | 0.007978851 | Polar - Positive Charge |
| Cys - Lys | 0.0265 | 0.007427202 | Polar - Positive Charge |
| Cys - Asp | 0.0120 | 0.007348467 | Polar - Negative Charge |
| Cys - Glu | 0.0311 | 0.007082325 | Polar - Negative Charge |
| Cys - Tyr - | 0.0406 | 0.007016819 | Polar - Negative Charge |
| Asn - Gln | 0.0655 | 0.008275543 | Polar - Polar |
| Asn - Arg:NE | 0.1497 | 0.007892635 | Polar - Polar |
| Asn - Arg:NH | 0.1106 | 0.008089523 | Polar - Polar |
| Asn - Glu:H | 0.1046 | 0.008116745 | Polar - Polar |
| Asn - LysN | 0.0995 | 0.008139275 | Polar - Polar |
| Asn - Arg | 0.1472 | 0.007906263 | Polar - Positive Charge |
| Asn - His+ | 0.0367 | 0.008547664 | Polar - Positive Charge |
| Asn - Lys | 0.1221 | 0.008035161 | Polar - Positive Charge |
| Asn - Asp | 0.1366 | 0.007962440 | Polar - Negative Charge |
| Asn - Glu | 0.1797 | 0.007717500 | Polar - Negative Charge |
| Asn - Cys - | 0.1448 | 0.007919209 | Polar - Negative Charge |
| Asn - Tyr - | 0.1892 | 0.007657430 | Polar - Negative Charge |
| Gln - Arg:NE | 0.0842 | 0.007680439 | Polar - Polar |
| Gln - Arg:NH | 0.0451 | 0.007882629 | Polar - Polar |
| Gln - Asp:H | 0.0683 | 0.008282294 | Polar - Polar |
| Gln - Glu:H | 0.0391 | 0.007910563 | Polar - Polar |
| Gln - LysN | 0.0340 | 0.007933679 | Polar - Polar |
| Gln - Arg | 0.0817 | 0.007694443 | Polar - Positive Charge |
| Gln - His+ | 0.1022 | 0.008352126 | Polar - Positive Charge |
| Gln - Lys | 0.0566 | 0.007826830 | Polar - Positive Charge |
| Gln - Asp | 0.0711 | 0.007752155 | Polar - Negative Charge |
| Gln - Glu | 0.1142 | 0.007500351 | Polar - Negative Charge |
| Gln - Cys - | 0.0793 | 0.007707744 | Polar - Negative Charge |
| Gln - Tyr - | 0.1237 | 0.007438528 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 0.0391 | 0.007479634 | Polar - Polar |
| Arg:NE - Asp:H | 0.1525 | 0.007899714 | Polar - Polar |
| Arg:NE - Glu:H | 0.0451 | 0.007509067 | Polar - Polar |
| Arg:NE - LysN | 0.0502 | 0.007533415 | Polar - Polar |
| Arg:NE - His+ | 0.1864 | 0.007972898 | Polar - Positive Charge |
| Arg:NE - Lys | 0.0276 | 0.007420806 | Polar - Positive Charge |
| Arg:NE - Asp | 0.0131 | 0.007342002 | Polar - Negative Charge |
| Arg:NE - Glu | 0.0300 | 0.007075617 | Polar - Negative Charge |
| Arg:NE - Tyr - | 0.0395 | 0.007010049 | Polar - Negative Charge |
| Arg:NH - Asp:H | 0.1134 | 0.008096430 | Polar - Polar |
| Arg:NH - LysN | 0.0111 | 0.007739447 | Polar - Polar |
| Arg:NH - Arg | 0.0366 | 0.007494013 | Polar - Positive Charge |
| Arg:NH - His+ | 0.1473 | 0.008167851 | Polar - Positive Charge |
| Arg:NH - Lys | 0.0115 | 0.007629879 | Polar - Positive Charge |
| Arg:NH - Asp | 0.0260 | 0.007553257 | Polar - Negative Charge |
| Arg:NH - Glu | 0.0691 | 0.007294590 | Polar - Negative Charge |
| Arg:NH - Cys - | 0.0342 | 0.007507670 | Polar - Negative Charge |
| Arg:NH - Tyr - | 0.0786 | 0.007231008 | Polar - Negative Charge |
| Asp:H - Glu:H | 0.1074 | 0.008123628 | Polar - Polar |
| Asp:H - LysN | 0.1023 | 0.008146139 | Polar - Polar |
| Asp:H - Arg | 0.1500 | 0.007913329 | Polar - Positive Charge |
| Asp:H - His+ | 0.0339 | 0.008554200 | Polar - Positive Charge |
| Asp:H - Lys | 0.1249 | 0.008042114 | Polar - Positive Charge |
| Asp:H - Asp | 0.1394 | 0.007969457 | Polar - Negative Charge |
| Asp:H - Glu | 0.1825 | 0.007724739 | Polar - Negative Charge |
| Asp:H - Cys - | 0.1476 | 0.007926263 | Polar - Negative Charge |
| Asp:H - Tyr - | 0.1920 | 0.007664726 | Polar - Negative Charge |
| Glu:H - Arg | 0.0426 | 0.007523389 | Polar - Positive Charge |
| Glu:H - His+ | 0.1413 | 0.008194812 | Polar - Positive Charge |
| Glu:H - Lys | 0.0175 | 0.007658734 | Polar - Positive Charge |
| Glu:H - Asp | 0.0320 | 0.007582404 | Polar - Negative Charge |
| Glu:H - Glu | 0.0751 | 0.007324767 | Polar - Negative Charge |
| Glu:H - Cys - | 0.0402 | 0.007536993 | Polar - Negative Charge |
| Glu:H - Tyr- | 0.0846 | 0.007261448 | Polar - Negative Charge |
| LysN - Arg | 0.0477 | 0.007547691 | Polar - Positive Charge |
| LysN - His+ | 0.1362 | 0.008217129 | Polar - Positive Charge |
| LysN - Lys | 0.0226 | 0.007682608 | Polar - Positive Charge |
| LysN - Asp | 0.0371 | 0.007606518 | Polar - Negative Charge |
| LysN - Glu | 0.0802 | 0.007349725 | Polar - Negative Charge |
| LysN - Cys - | 0.0453 | 0.007561251 | Polar - Negative Charge |
| LysN - Tyr - | 0.0897 | 0.007286624 | Polar - Negative Charge |
| Arg - His+ | 0.1839 | 0.007986388 | Positive Charge - Positive Charge |
| Arg - Lys | 0.0251 | 0.007435298 | Positive Charge - Positive Charge |
| Arg - Asp | 0.0106 | 0.007356650 | Positive Charge - Negative Charge |
| Arg - Glu | 0.0325 | 0.007090815 | Positive Charge - Negative Charge |
| Arg - Tyr- | 0.0420 | 0.007025388 | Positive Charge - Negative Charge |
| His+ - Lys | 0.1588 | 0.008114014 | Positive Charge - Positive Charge |
| His+ - Asp | 0.1733 | 0.008042006 | Positive Charge - Negative Charge |
| His+ - Glu | 0.2164 | 0.007799565 | Positive Charge - Negative Charge |
| His+ - Cys - | 0.1815 | 0.007999204 | Positive Charge - Negative Charge |
| His+ - Tyr- | 0.2259 | 0.007740132 | Positive Charge - Negative Charge |
| Lys - Asp | 0.0145 | 0.007495006 | Positive Charge - Negative Charge |
| Lys - Glu | 0.0576 | 0.007234257 | Positive Charge - Negative Charge |
| Lys - Cys - | 0.0227 | 0.007449062 | Positive Charge - Negative Charge |
| Lys - Tyr- | 0.0671 | 0.007170140 | Positive Charge - Negative Charge |
| Asp - Glu | 0.0431 | 0.007153399 | Negative Charge - Negative Charge |
| Asp - Cys - | 0.0082 | 0.007370561 | Negative Charge - Negative Charge |
| Asp - Tyr- | 0.0526 | 0.007088550 | Negative Charge - Negative Charge |
| Glu - Cys - | 0.0349 | 0.007105246 | Negative Charge - Negative Charge |
| Glu - Tyr- | 0.0095 | 0.006812261 | Negative Charge - Negative Charge |
| Cys -  - Tyr- | 0.0444 | 0.007039954 | Negative Charge - Negative Charge |

**Table S3.** Non-statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Asp | 0.0039 | 0.007438484 | Hydrophobic - Negative Charge |
| Leu - Arg:NH | 0.0020 | 0.007696747 | Hydrophobic - Polar |
| Leu - Glu:H | 0.0040 | 0.007725352 | Hydrophobic - Polar |
| Met - Glu:H | 0.0047 | 0.007766065 | Hydrophobic - Polar |
| Met - LysN | 0.0004 | 0.007789610 | Hydrophobic - Polar |
| Phe - Glu | 0.0054 | 0.006841703 | Aromatic - Negative Charge |
| Phe - Tyr- | 0.0041 | 0.006773871 | Aromatic - Negative Charge |
| Tyr - Cys | 0.0055 | 0.007246351 | Aromatic - Polar |
| Tyr - Arg:NE | 0.0044 | 0.007239795 | Aromatic - Polar |
| Tyr - Arg | 0.0069 | 0.007254649 | Aromatic - Positive Charge |
| Trp - Thr | 0.0018 | 0.006410712 | Aromatic - Polar |
| Ser - Lys | 0.0013 | 0.007578893 | Polar - Positive Charge |
| Cys - Arg:NE | 0.0011 | 0.007272771 | Polar - Polar |
| Cys - Arg | 0.0014 | 0.007287558 | Polar - Positive Charge |
| Cys - Cys - | 0.0038 | 0.007301601 | Polar - Negative Charge |
| Asn - Asp:H | 0.0028 | 0.008479442 | Polar - Polar |
| Arg:NE - Arg | 0.0025 | 0.007281039 | Polar - Positive Charge |
| Arg:NE - Cys - | 0.0049 | 0.007295095 | Polar - Negative Charge |
| Arg:NH - Glu:H | 0.0060 | 0.007715749 | Polar - Polar |
| Glu:H - LysN | 0.0051 | 0.007767895 | Polar - Polar |
| Arg - Cys - | 0.0024 | 0.007309836 | Positive Charge - Negative Charge |

**Table S4.** Statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 0.1094 | 0.005615946 | Hydrophobic - Hydrophobic |
| Ala - Leu | 0.0362 | 0.006913843 | Hydrophobic - Hydrophobic |
| Ala - Ile | 0.0865 | 0.005876199 | Hydrophobic - Hydrophobic |
| Ala - Met | 0.0244 | 0.006835687 | Hydrophobic - Hydrophobic |
| Ala - His:NE2 | 0.0229 | 0.006479832 | Hydrophobic - Aromatic |
| Ala - Phe | 0.0647 | 0.006101369 | Hydrophobic - Aromatic |
| Ala - Tyr | 0.0302 | 0.006418371 | Hydrophobic - Aromatic |
| Ala - Trp | 0.0544 | 0.006200807 | Hydrophobic - Aromatic |
| Ala - Ser | 0.0324 | 0.006399481 | Hydrophobic - Polar |
| Ala - Thr | 0.0545 | 0.006199862 | Hydrophobic - Polar |
| Ala - Cys | 0.0384 | 0.006347080 | Hydrophobic - Polar |
| Ala - Asn | 0.0406 | 0.006941969 | Hydrophobic - Polar |
| Ala - Gln | 0.0553 | 0.007032044 | Hydrophobic - Polar |
| Ala - Arg:NE | 0.0250 | 0.006462341 | Hydrophobic - Polar |
| Ala - Arg:NH | 0.0210 | 0.006812417 | Hydrophobic - Polar |
| Ala - Asp:H | 0.0679 | 0.007104612 | Hydrophobic - Polar |
| Ala - Glu:H | 0.0238 | 0.006831605 | Hydrophobic - Polar |
| Ala - His+ | 0.0277 | 0.006857949 | Hydrophobic - Positive Charge |
| Ala - Lys | 0.0149 | 0.006769807 | Hydrophobic - Positive Charge |
| Ala - Glu | 0.0237 | 0.006473187 | Hydrophobic - Negative Charge |
| Ala - Cys - | 0.0391 | 0.006932442 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 0.0515 | 0.006228044 | Hydrophobic - Negative Charge |
| Val - Leu | 0.1456 | 0.005913683 | Hydrophobic - Hydrophobic |
| Val - Ile | 0.0229 | 0.004658341 | Hydrophobic - Hydrophobic |
| Val - Met | 0.1338 | 0.005822117 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 0.1091 | 0.005613262 | Hydrophobic - Aromatic |
| Val - His:NE2 | 0.0865 | 0.005399875 | Hydrophobic - Aromatic |
| Val - Phe | 0.0447 | 0.004939346 | Hydrophobic - Aromatic |
| Val - Tyr | 0.0792 | 0.005325966 | Hydrophobic - Aromatic |
| Val - Trp | 0.0550 | 0.005061664 | Hydrophobic - Aromatic |
| Val - Ser | 0.0770 | 0.005303186 | Hydrophobic - Polar |
| Val - Thr | 0.0549 | 0.005060506 | Hydrophobic - Polar |
| Val - Cys | 0.0710 | 0.005239833 | Hydrophobic - Polar |
| Val - Asn | 0.1500 | 0.005946542 | Hydrophobic - Polar |
| Val - Gln | 0.1647 | 0.006051452 | Hydrophobic - Polar |
| Val - Arg:NE | 0.0844 | 0.005378874 | Hydrophobic - Polar |
| Val - Arg:NH | 0.1304 | 0.005794778 | Hydrophobic - Polar |
| Val - Asp:H | 0.1773 | 0.006135629 | Hydrophobic - Polar |
| Val - Glu:H | 0.1332 | 0.005817324 | Hydrophobic - Polar |
| Val - LysN | 0.1102 | 0.005623084 | Hydrophobic - Polar |
| Val - Arg | 0.1056 | 0.005581672 | Hydrophobic - Positive Charge |
| Val - His+ | 0.1371 | 0.005848239 | Hydrophobic - Positive Charge |
| Val - Lys | 0.1243 | 0.005744625 | Hydrophobic - Positive Charge |
| Val - Asp | 0.1079 | 0.005602489 | Hydrophobic - Negative Charge |
| Val - Glu | 0.0857 | 0.005391899 | Hydrophobic - Negative Charge |
| Val - Cys - | 0.1485 | 0.005935417 | Hydrophobic - Negative Charge |
| Val - Tyr- | 0.0579 | 0.005094994 | Hydrophobic - Negative Charge |
| Leu - Ile | 0.1227 | 0.006161373 | Hydrophobic - Hydrophobic |
| Leu - Met | 0.0118 | 0.007082332 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 0.0365 | 0.006911663 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 0.0591 | 0.006739512 | Hydrophobic - Aromatic |
| Leu - Phe | 0.1009 | 0.006376481 | Hydrophobic - Aromatic |
| Leu - Tyr | 0.0664 | 0.006680441 | Hydrophobic - Aromatic |
| Leu - Trp | 0.0906 | 0.006471693 | Hydrophobic - Aromatic |
| Leu - Ser | 0.0686 | 0.006662294 | Hydrophobic - Polar |
| Leu - Thr | 0.0907 | 0.006470788 | Hydrophobic - Polar |
| Leu - Cys | 0.0746 | 0.006611976 | Hydrophobic - Polar |
| Leu - Gln | 0.0191 | 0.007272032 | Hydrophobic - Polar |
| Leu - Arg:NE | 0.0612 | 0.006722697 | Hydrophobic - Polar |
| Leu - Arg:NH | 0.0152 | 0.007059875 | Hydrophobic - Polar |
| Leu - Asp:H | 0.0317 | 0.007342228 | Hydrophobic - Polar |
| Leu - Glu:H | 0.0124 | 0.007078392 | Hydrophobic - Polar |
| Leu - LysN | 0.0354 | 0.006919642 | Hydrophobic - Polar |
| Leu - Arg | 0.0400 | 0.006886032 | Hydrophobic - Positive Charge |
| Leu - His+ | 0.0085 | 0.007103821 | Hydrophobic - Positive Charge |
| Leu - Lys | 0.0213 | 0.007018767 | Hydrophobic - Positive Charge |
| Leu - Asp | 0.0377 | 0.006902917 | Hydrophobic - Negative Charge |
| Leu - Glu | 0.0599 | 0.006733123 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 0.0877 | 0.006497795 | Hydrophobic - Negative Charge |
| Ile - Met | 0.1109 | 0.006073542 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 0.0862 | 0.005873634 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 0.0636 | 0.005670054 | Hydrophobic - Aromatic |
| Ile - Phe | 0.0218 | 0.005233355 | Hydrophobic - Aromatic |
| Ile - Tyr | 0.0563 | 0.005599712 | Hydrophobic - Aromatic |
| Ile - Trp | 0.0321 | 0.005348954 | Hydrophobic - Aromatic |
| Ile - Ser | 0.0541 | 0.005578051 | Hydrophobic - Polar |
| Ile - Thr | 0.0320 | 0.005347858 | Hydrophobic - Polar |
| Ile - Cys | 0.0481 | 0.005517855 | Hydrophobic - Polar |
| Ile - Asn | 0.1271 | 0.006192918 | Hydrophobic - Polar |
| Ile - Gln | 0.1418 | 0.006293722 | Hydrophobic - Polar |
| Ile - Arg:NE | 0.0615 | 0.005650058 | Hydrophobic - Polar |
| Ile - Arg:NH | 0.1075 | 0.006047340 | Hydrophobic - Polar |
| Ile - Asp:H | 0.1544 | 0.006374701 | Hydrophobic - Polar |
| Ile - Glu:H | 0.1103 | 0.006068948 | Hydrophobic - Polar |
| Ile - LysN | 0.0873 | 0.005883021 | Hydrophobic - Polar |
| Ile - Arg | 0.0827 | 0.005843452 | Hydrophobic - Positive Charge |
| Ile - His+ | 0.1142 | 0.006098587 | Hydrophobic - Positive Charge |
| Ile - Lys | 0.1014 | 0.005999298 | Hydrophobic - Positive Charge |
| Ile - Asp | 0.0850 | 0.005863340 | Hydrophobic - Negative Charge |
| Ile - Glu | 0.0628 | 0.005662459 | Hydrophobic - Negative Charge |
| Ile - Cys - | 0.1256 | 0.006182236 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 0.0350 | 0.005380505 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 0.0247 | 0.006833483 | Hydrophobic - Aromatic |
| Met - His:NE2 | 0.0473 | 0.006659311 | Hydrophobic - Aromatic |
| Met - Phe | 0.0891 | 0.006291654 | Hydrophobic - Aromatic |
| Met - Tyr | 0.0546 | 0.006599522 | Hydrophobic - Aromatic |
| Met - Trp | 0.0788 | 0.006388131 | Hydrophobic - Aromatic |
| Met - Ser | 0.0568 | 0.006581152 | Hydrophobic - Polar |
| Met - Thr | 0.0789 | 0.006387213 | Hydrophobic - Polar |
| Met - Cys | 0.0628 | 0.006530209 | Hydrophobic - Polar |
| Met - Asn | 0.0162 | 0.007109792 | Hydrophobic - Polar |
| Met - Gln | 0.0309 | 0.007197767 | Hydrophobic - Polar |
| Met - Arg:NE | 0.0494 | 0.006642293 | Hydrophobic - Polar |
| Met - Asp:H | 0.0435 | 0.007268681 | Hydrophobic - Polar |
| Met - LysN | 0.0236 | 0.006841553 | Hydrophobic - Polar |
| Met - Arg | 0.0282 | 0.006807558 | Hydrophobic - Positive Charge |
| Met - Lys | 0.0095 | 0.006941793 | Hydrophobic - Positive Charge |
| Met - Asp | 0.0259 | 0.006824636 | Hydrophobic - Negative Charge |
| Met - Glu | 0.0481 | 0.006652845 | Hydrophobic - Negative Charge |
| Met - Cys - | 0.0147 | 0.007100489 | Hydrophobic - Negative Charge |
| Met - Tyr- | 0.0759 | 0.006414572 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 0.0226 | 0.006477506 | Aromatic - Aromatic |
| His:ND1 - Phe | 0.0644 | 0.006098899 | Aromatic - Aromatic |
| His:ND1 - Tyr | 0.0299 | 0.006416023 | Aromatic - Aromatic |
| His:ND1 - Trp | 0.0541 | 0.006198377 | Aromatic - Aromatic |
| His:ND1 - Ser | 0.0321 | 0.006397126 | Aromatic - Polar |
| His:ND1 - Thr | 0.0542 | 0.006197431 | Aromatic - Polar |
| His:ND1 - Cys | 0.0381 | 0.006344705 | Aromatic - Polar |
| His:ND1 - Asn | 0.0409 | 0.006939798 | Aromatic - Polar |
| His:ND1 - Gln | 0.0556 | 0.007029901 | Aromatic - Polar |
| His:ND1 - Arg:NE | 0.0247 | 0.006460009 | Aromatic - Polar |
| His:ND1 - Arg:NH | 0.0213 | 0.006810205 | Aromatic - Polar |
| His:ND1 - Asp:H | 0.0682 | 0.007102491 | Aromatic - Polar |
| His:ND1 - Glu:H | 0.0241 | 0.006829399 | Aromatic - Polar |
| His:ND1 - His+ | 0.0280 | 0.006855752 | Aromatic - Positive Charge |
| His:ND1 - Lys | 0.0152 | 0.006767581 | Aromatic - Positive Charge |
| His:ND1 - Glu | 0.0234 | 0.006470858 | Aromatic - Negative Charge |
| His:ND1 - Cys - | 0.0394 | 0.006930268 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 0.0512 | 0.006225624 | Aromatic - Negative Charge |
| His:NE2 - Phe | 0.0418 | 0.005903093 | Aromatic - Aromatic |
| His:NE2 - Tyr | 0.0073 | 0.006230191 | Aromatic - Aromatic |
| His:NE2 - Trp | 0.0315 | 0.006005815 | Aromatic - Aromatic |
| His:NE2 - Ser | 0.0095 | 0.006210729 | Aromatic - Polar |
| His:NE2 - Thr | 0.0316 | 0.006004839 | Aromatic - Polar |
| His:NE2 - Cys | 0.0155 | 0.006156722 | Aromatic - Polar |
| His:NE2 - Asn | 0.0635 | 0.006768363 | Aromatic - Polar |
| His:NE2 - Gln | 0.0782 | 0.006860717 | Aromatic - Polar |
| His:NE2 - Arg:NH | 0.0439 | 0.006635422 | Aromatic - Polar |
| His:NE2 - Asp:H | 0.0908 | 0.006935079 | Aromatic - Polar |
| His:NE2 - Glu:H | 0.0467 | 0.006655121 | Aromatic - Polar |
| His:NE2 - LysN | 0.0237 | 0.006486019 | Aromatic - Polar |
| His:NE2 - Arg | 0.0191 | 0.006450150 | Aromatic - Positive Charge |
| His:NE2 - His+ | 0.0506 | 0.006682161 | Aromatic - Positive Charge |
| His:NE2 - Lys | 0.0378 | 0.006591668 | Aromatic - Positive Charge |
| His:NE2 - Asp | 0.0214 | 0.006468173 | Aromatic - Negative Charge |
| His:NE2 - Cys - | 0.0620 | 0.006758591 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 0.0286 | 0.006033932 | Aromatic - Negative Charge |
| Phe - Tyr | 0.0345 | 0.005835561 | Aromatic - Aromatic |
| Phe - Trp | 0.0103 | 0.005595382 | Aromatic - Aromatic |
| Phe - Ser | 0.0323 | 0.005814778 | Aromatic - Polar |
| Phe - Thr | 0.0102 | 0.005594335 | Aromatic - Polar |
| Phe - Cys | 0.0263 | 0.005757058 | Aromatic - Polar |
| Phe - Asn | 0.1053 | 0.006406967 | Aromatic - Polar |
| Phe - Gln | 0.1200 | 0.006504455 | Aromatic - Polar |
| Phe - Arg:NE | 0.0397 | 0.005883889 | Aromatic - Polar |
| Phe - Arg:NH | 0.0857 | 0.006266364 | Aromatic - Polar |
| Phe - Asp:H | 0.1326 | 0.006582842 | Aromatic - Polar |
| Phe - Glu:H | 0.0885 | 0.006287219 | Aromatic - Polar |
| Phe - LysN | 0.0655 | 0.006107940 | Aromatic - Polar |
| Phe - Arg | 0.0609 | 0.006069837 | Aromatic - Positive Charge |
| Phe - His+ | 0.0924 | 0.006315834 | Aromatic - Positive Charge |
| Phe - Lys | 0.0796 | 0.006220014 | Aromatic - Positive Charge |
| Phe - Asp | 0.0632 | 0.006088986 | Aromatic - Negative Charge |
| Phe - Glu | 0.0410 | 0.005895798 | Aromatic - Negative Charge |
| Phe - Cys - | 0.1038 | 0.006396643 | Aromatic - Negative Charge |
| Phe - Tyr- | 0.0132 | 0.005625551 | Aromatic - Negative Charge |
| Tyr - Trp | 0.0242 | 0.005939451 | Aromatic - Aromatic |
| Tyr - Thr | 0.0243 | 0.005938464 | Aromatic - Polar |
| Tyr - Cys | 0.0082 | 0.006092002 | Aromatic - Polar |
| Tyr - Asn | 0.0708 | 0.006709545 | Aromatic - Polar |
| Tyr - Gln | 0.0855 | 0.006802699 | Aromatic - Polar |
| Tyr - Arg:NH | 0.0512 | 0.006575416 | Aromatic - Polar |
| Tyr - Asp:H | 0.0981 | 0.006877687 | Aromatic - Polar |
| Tyr - Glu:H | 0.0540 | 0.006595294 | Aromatic - Polar |
| Tyr - LysN | 0.0310 | 0.006424618 | Aromatic - Polar |
| Tyr - Arg | 0.0264 | 0.006388404 | Aromatic - Positive Charge |
| Tyr - His+ | 0.0579 | 0.006622578 | Aromatic - Positive Charge |
| Tyr - Lys | 0.0451 | 0.006531260 | Aromatic - Positive Charge |
| Tyr - Asp | 0.0287 | 0.006406600 | Aromatic - Negative Charge |
| Tyr - Glu | 0.0065 | 0.006223280 | Aromatic - Negative Charge |
| Tyr - Cys - | 0.0693 | 0.006699688 | Aromatic - Negative Charge |
| Tyr - Tyr- | 0.0213 | 0.005967881 | Aromatic - Negative Charge |
| Trp - Ser | 0.0220 | 0.005919033 | Aromatic - Polar |
| Trp - Cys | 0.0160 | 0.005862339 | Aromatic - Polar |
| Trp - Asn | 0.0950 | 0.006501732 | Aromatic - Polar |
| Trp - Gln | 0.1097 | 0.006597820 | Aromatic - Polar |
| Trp - Arg:NE | 0.0294 | 0.005986940 | Aromatic - Polar |
| Trp - Arg:NH | 0.0754 | 0.006363224 | Aromatic - Polar |
| Trp - Asp:H | 0.1223 | 0.006675111 | Aromatic - Polar |
| Trp - Glu:H | 0.0782 | 0.006383763 | Aromatic - Polar |
| Trp - LysN | 0.0552 | 0.006207273 | Aromatic - Polar |
| Trp - Arg | 0.0506 | 0.006169784 | Aromatic - Positive Charge |
| Trp - His+ | 0.0821 | 0.006411947 | Aromatic - Positive Charge |
| Trp - Lys | 0.0693 | 0.006317585 | Aromatic - Positive Charge |
| Trp - Asp | 0.0529 | 0.006188622 | Aromatic - Negative Charge |
| Trp - Glu | 0.0307 | 0.005998645 | Aromatic - Negative Charge |
| Trp - Cys - | 0.0935 | 0.006491559 | Aromatic - Negative Charge |
| Ser - Thr | 0.0221 | 0.005918043 | Polar - Polar |
| Ser - Asn | 0.0730 | 0.006691477 | Polar - Polar |
| Ser - Gln | 0.0877 | 0.006784879 | Polar - Polar |
| Ser - Arg:NE | 0.0074 | 0.006192479 | Polar - Polar |
| Ser - Arg:NH | 0.0534 | 0.006556978 | Polar - Polar |
| Ser - Asp:H | 0.1003 | 0.006860062 | Polar - Polar |
| Ser - Glu:H | 0.0562 | 0.006576912 | Polar - Polar |
| Ser - LysN | 0.0332 | 0.006405746 | Polar - Polar |
| Ser - Arg | 0.0286 | 0.006369425 | Polar - Positive Charge |
| Ser - His+ | 0.0601 | 0.006604272 | Polar - Positive Charge |
| Ser - Lys | 0.0473 | 0.006512697 | Polar - Positive Charge |
| Ser - Asp | 0.0309 | 0.006387675 | Polar - Negative Charge |
| Ser - Glu | 0.0087 | 0.006203796 | Polar - Negative Charge |
| Ser - Cys - | 0.0715 | 0.006681593 | Polar - Negative Charge |
| Ser - Tyr- | 0.0191 | 0.005947560 | Polar - Negative Charge |
| Thr - Cys | 0.0161 | 0.005861339 | Polar - Polar |
| Thr - Asn | 0.0951 | 0.006500831 | Polar - Polar |
| Thr - Gln | 0.1098 | 0.006596932 | Polar - Polar |
| Thr - Arg:NE | 0.0295 | 0.005985961 | Polar - Polar |
| Thr - Arg:NH | 0.0755 | 0.006362303 | Polar - Polar |
| Thr - Asp:H | 0.1224 | 0.006674233 | Polar - Polar |
| Thr - Glu:H | 0.0783 | 0.006382845 | Polar - Polar |
| Thr - LysN | 0.0553 | 0.006206329 | Polar - Polar |
| Thr - Arg | 0.0507 | 0.006168834 | Polar - Positive Charge |
| Thr - His+ | 0.0822 | 0.006411033 | Polar - Positive Charge |
| Thr - Lys | 0.0694 | 0.006316657 | Polar - Positive Charge |
| Thr - Asp | 0.0530 | 0.006187676 | Polar - Negative Charge |
| Thr - Glu | 0.0308 | 0.005997668 | Polar - Negative Charge |
| Thr - Cys - | 0.0936 | 0.006490656 | Polar - Negative Charge |
| Cys - Asn | 0.0790 | 0.006641381 | Polar - Polar |
| Cys - Gln | 0.0937 | 0.006735477 | Polar - Polar |
| Cys - Arg:NE | 0.0134 | 0.006138311 | Polar - Polar |
| Cys - Arg:NH | 0.0594 | 0.006505846 | Polar - Polar |
| Cys - Asp:H | 0.1063 | 0.006811205 | Polar - Polar |
| Cys - Glu:H | 0.0622 | 0.006525936 | Polar - Polar |
| Cys - LysN | 0.0392 | 0.006353397 | Polar - Polar |
| Cys - Arg | 0.0346 | 0.006316775 | Polar - Positive Charge |
| Cys - His+ | 0.0661 | 0.006553509 | Polar - Positive Charge |
| Cys - Lys | 0.0533 | 0.006461214 | Polar - Positive Charge |
| Cys - Asp | 0.0369 | 0.006335177 | Polar - Negative Charge |
| Cys - Glu | 0.0147 | 0.006149728 | Polar - Negative Charge |
| Cys - Cys - | 0.0775 | 0.006631422 | Polar - Negative Charge |
| Cys - Tyr- | 0.0131 | 0.005891141 | Polar - Negative Charge |
| Asn - Gln | 0.0147 | 0.007298778 | Polar - Polar |
| Asn - Arg:NE | 0.0656 | 0.006751620 | Polar - Polar |
| Asn - Arg:NH | 0.0196 | 0.007087421 | Polar - Polar |
| Asn - Asp:H | 0.0273 | 0.007368720 | Polar - Polar |
| Asn - Glu:H | 0.0168 | 0.007105867 | Polar - Polar |
| Asn - LysN | 0.0398 | 0.006947745 | Polar - Polar |
| Asn - Arg | 0.0444 | 0.006914272 | Polar - Positive Charge |
| Asn - His+ | 0.0129 | 0.007131198 | Polar - Positive Charge |
| Asn - Lys | 0.0257 | 0.007046474 | Polar - Positive Charge |
| Asn - Asp | 0.0421 | 0.006931087 | Polar - Negative Charge |
| Asn - Glu | 0.0643 | 0.006762001 | Polar - Negative Charge |
| Asn - Tyr- | 0.0921 | 0.006527714 | Polar - Negative Charge |
| Gln - Arg:NE | 0.0803 | 0.006844200 | Polar - Polar |
| Gln - Arg:NH | 0.0343 | 0.007175671 | Polar - Polar |
| Gln - Asp:H | 0.0126 | 0.007453639 | Polar - Polar |
| Gln - Glu:H | 0.0315 | 0.007193890 | Polar - Polar |
| Gln - LysN | 0.0545 | 0.007037746 | Polar - Polar |
| Gln - Arg | 0.0591 | 0.007004703 | Polar - Positive Charge |
| Gln - His+ | 0.0276 | 0.007218912 | Polar - Positive Charge |
| Gln - Lys | 0.0404 | 0.007135230 | Polar - Positive Charge |
| Gln - Asp | 0.0568 | 0.007021302 | Polar - Negative Charge |
| Gln - Glu | 0.0790 | 0.006854442 | Polar - Negative Charge |
| Gln - Cys - | 0.0162 | 0.007289717 | Polar - Negative Charge |
| Gln - Tyr- | 0.1068 | 0.006623425 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 0.0460 | 0.006618343 | Polar - Polar |
| Arg:NE - Asp:H | 0.0929 | 0.006918739 | Polar - Polar |
| Arg:NE - Glu:H | 0.0488 | 0.006638092 | Polar - Polar |
| Arg:NE - LysN | 0.0258 | 0.006468546 | Polar - Polar |
| Arg:NE - Arg | 0.0212 | 0.006432579 | Polar - Positive Charge |
| Arg:NE - His+ | 0.0527 | 0.006665201 | Polar - Positive Charge |
| Arg:NE - Lys | 0.0399 | 0.006574475 | Polar - Positive Charge |
| Arg:NE - Asp | 0.0235 | 0.006450651 | Polar - Negative Charge |
| Arg:NE - Cys - | 0.0641 | 0.006741824 | Polar - Negative Charge |
| Arg:NE - Tyr- | 0.0265 | 0.006015145 | Polar - Negative Charge |
| Arg:NH - Asp:H | 0.0469 | 0.007246801 | Polar - Polar |
| Arg:NH - LysN | 0.0202 | 0.006818303 | Polar - Polar |
| Arg:NH - Arg | 0.0248 | 0.006784191 | Polar - Positive Charge |
| Arg:NH - Asp | 0.0225 | 0.006801328 | Polar - Negative Charge |
| Arg:NH - Glu | 0.0447 | 0.006628933 | Polar - Negative Charge |
| Arg:NH - Cys - | 0.0181 | 0.007078090 | Polar - Negative Charge |
| Arg:NH - Tyr- | 0.0725 | 0.006389769 | Polar - Negative Charge |
| Asp:H - Glu:H | 0.0441 | 0.007264842 | Polar - Polar |
| Asp:H - LysN | 0.0671 | 0.007110256 | Polar - Polar |
| Asp:H - Arg | 0.0717 | 0.007077551 | Polar - Positive Charge |
| Asp:H - His+ | 0.0402 | 0.007289620 | Polar - Positive Charge |
| Asp:H - Lys | 0.0530 | 0.007206760 | Polar - Positive Charge |
| Asp:H - Asp | 0.0694 | 0.007093980 | Polar - Negative Charge |
| Asp:H - Glu | 0.0916 | 0.006928870 | Polar - Negative Charge |
| Asp:H - Cys - | 0.0288 | 0.007359745 | Polar - Negative Charge |
| Asp:H - Tyr- | 0.1194 | 0.006700420 | Polar - Negative Charge |
| Glu:H - LysN | 0.0230 | 0.006837475 | Polar - Polar |
| Glu:H - Arg | 0.0276 | 0.006803459 | Polar - Positive Charge |
| Glu:H - Lys | 0.0089 | 0.006937774 | Polar - Positive Charge |
| Glu:H - Asp | 0.0253 | 0.006820548 | Polar - Negative Charge |
| Glu:H - Glu | 0.0475 | 0.006648651 | Polar - Negative Charge |
| Glu:H - Cys - | 0.0153 | 0.007096560 | Polar - Negative Charge |
| Glu:H - Tyr- | 0.0753 | 0.006410222 | Polar - Negative Charge |
| LysN - His+ | 0.0269 | 0.006863796 | Polar - Positive Charge |
| LysN - Lys | 0.0141 | 0.006775730 | Polar - Positive Charge |
| LysN - Glu | 0.0245 | 0.006479381 | Polar - Negative Charge |
| LysN - Cys - | 0.0383 | 0.006938226 | Polar - Negative Charge |
| LysN - Tyr- | 0.0523 | 0.006234482 | Polar - Negative Charge |
| Arg - His+ | 0.0315 | 0.006829911 | Positive Charge - Positive Charge |
| Arg - Lys | 0.0187 | 0.006741402 | Positive Charge - Positive Charge |
| Arg - Glu | 0.0199 | 0.006443475 | Positive Charge - Negative Charge |
| Arg - Cys - | 0.0429 | 0.006904706 | Positive Charge - Negative Charge |
| Arg - Tyr- | 0.0477 | 0.006197157 | Positive Charge - Negative Charge |
| His+ - Lys | 0.0128 | 0.006963716 | Positive Charge - Positive Charge |
| His+ - Asp | 0.0292 | 0.006846934 | Positive Charge - Negative Charge |
| His+ - Glu | 0.0514 | 0.006675717 | Positive Charge - Negative Charge |
| His+ - Cys - | 0.0114 | 0.007121924 | Positive Charge - Negative Charge |
| His+ - Tyr- | 0.0792 | 0.006438291 | Positive Charge - Negative Charge |
| Lys - Asp | 0.0164 | 0.006758648 | Positive Charge - Negative Charge |
| Lys - Glu | 0.0386 | 0.006585136 | Positive Charge - Negative Charge |
| Lys - Cys - | 0.0242 | 0.007037089 | Positive Charge - Negative Charge |
| Lys - Tyr- | 0.0664 | 0.006344321 | Positive Charge - Negative Charge |
| Asp - Glu | 0.0222 | 0.006461516 | Negative Charge - Negative Charge |
| Asp - Cys - | 0.0406 | 0.006921545 | Negative Charge - Negative Charge |
| Asp - Tyr- | 0.0500 | 0.006215913 | Negative Charge - Negative Charge |
| Glu - Cys - | 0.0628 | 0.006752220 | Negative Charge - Negative Charge |
| Glu - Tyr- | 0.0278 | 0.006026795 | Negative Charge - Negative Charge |
| Cys -  - Tyr- | 0.0906 | 0.006517581 | Negative Charge - Negative Charge |

**Table S5.** Non-statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - His:ND1 | 0.0003 | 0.006658699 | Hydrophobic - Aromatic |
| Ala - LysN | 0.0008 | 0.006666982 | Hydrophobic - Polar |
| Ala - Arg | 0.0038 | 0.006632091 | Hydrophobic - Positive Charge |
| Ala - Asp | 0.0015 | 0.006649621 | Hydrophobic - Negative Charge |
| Leu - Asn | 0.0044 | 0.007184966 | Hydrophobic - Polar |
| Leu - Cys - | 0.0029 | 0.007175761 | Hydrophobic - Negative Charge |
| Met - Arg:NH | 0.0034 | 0.006983354 | Hydrophobic - Polar |
| Met - Glu:H | 0.0006 | 0.007002074 | Hydrophobic - Polar |
| Met - His+ | 0.0033 | 0.007027779 | Hydrophobic - Positive Charge |
| His:ND1 - LysN | 0.0011 | 0.006664721 | Aromatic - Polar |
| His:ND1 - Arg | 0.0035 | 0.006629819 | Aromatic - Positive Charge |
| His:ND1 - Asp | 0.0012 | 0.006647354 | Aromatic - Negative Charge |
| His:NE2 - Arg:NE | 0.0021 | 0.006275481 | Aromatic - Polar |
| His:NE2 - Glu | 0.0008 | 0.006286648 | Aromatic - Negative Charge |
| Tyr - Ser | 0.0022 | 0.006146578 | Aromatic - Polar |
| Tyr - Arg:NE | 0.0052 | 0.006211998 | Aromatic - Polar |
| Trp - Thr | 0.0001 | 0.005702621 | Aromatic - Polar |
| Trp - Tyr- | 0.0029 | 0.005733247 | Aromatic - Negative Charge |
| Ser - Cys | 0.0060 | 0.006072097 | Polar - Polar |
| Thr - Tyr- | 0.0030 | 0.005732225 | Polar - Negative Charge |
| Asn - Cys - | 0.0015 | 0.007202865 | Polar - Negative Charge |
| Arg:NE - Glu | 0.0013 | 0.006268619 | Polar - Negative Charge |
| Arg:NH - Glu:H | 0.0028 | 0.006979358 | Polar - Polar |
| Arg:NH - His+ | 0.0067 | 0.007005146 | Polar - Positive Charge |
| Arg:NH - Lys | 0.0061 | 0.006918880 | Polar - Positive Charge |
| Glu:H - His+ | 0.0039 | 0.007023808 | Polar - Positive Charge |
| LysN - Arg | 0.0046 | 0.006638137 | Polar - Positive Charge |
| LysN - Asp | 0.0023 | 0.006655650 | Polar - Negative Charge |
| Arg - Asp | 0.0023 | 0.006620701 | Positive Charge - Negative Charge |

**Table S6.** Statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Leu | 0.0044 | 0.001933816 | Hydrophobic - Hydrophobic |
| Ala - Met | 0.0158 | 0.002320209 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 0.0568 | 0.003312400 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 0.1115 | 0.004200117 | Hydrophobic - Aromatic |
| Ala - Phe | 0.0148 | 0.002289267 | Hydrophobic - Aromatic |
| Ala - Tyr | 0.0156 | 0.002314059 | Hydrophobic - Aromatic |
| Ala - Trp | 0.0047 | 0.001549032 | Hydrophobic - Aromatic |
| Ala - Ser | 0.0216 | 0.002490914 | Hydrophobic - Polar |
| Ala - Cys | 0.0341 | 0.002817847 | Hydrophobic - Polar |
| Ala - Asn | 0.0898 | 0.003886258 | Hydrophobic - Polar |
| Ala - Gln | 0.0234 | 0.002541156 | Hydrophobic - Polar |
| Ala - Arg:NE | 0.0187 | 0.002407337 | Hydrophobic - Polar |
| Ala - Arg:NH | 0.0138 | 0.002257836 | Hydrophobic - Polar |
| Ala - Asp:H | 0.0702 | 0.003562151 | Hydrophobic - Polar |
| Ala - Glu:H | 0.0201 | 0.002448105 | Hydrophobic - Polar |
| Ala - LysN | 0.0374 | 0.002896657 | Hydrophobic - Polar |
| Ala - Arg | 0.0043 | 0.001930039 | Hydrophobic - Positive Charge |
| Ala - His+ | 0.0969 | 0.003993618 | Hydrophobic - Positive Charge |
| Ala - Lys | 0.0076 | 0.002050606 | Hydrophobic - Positive Charge |
| Ala - Asp | 0.0105 | 0.002150358 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 0.0093 | 0.002109726 | Hydrophobic - Negative Charge |
| Val - Leu | 0.0045 | 0.001930005 | Hydrophobic - Hydrophobic |
| Val - Met | 0.0159 | 0.002317034 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 0.0569 | 0.003310177 | Hydrophobic - Aromatic |
| Val - His:NE2 | 0.1116 | 0.004198364 | Hydrophobic - Aromatic |
| Val - Phe | 0.0149 | 0.002286049 | Hydrophobic - Aromatic |
| Val - Tyr | 0.0157 | 0.002310875 | Hydrophobic - Aromatic |
| Val - Trp | 0.0046 | 0.001544272 | Hydrophobic - Aromatic |
| Val - Ser | 0.0217 | 0.002487956 | Hydrophobic - Polar |
| Val - Cys | 0.0342 | 0.002815233 | Hydrophobic - Polar |
| Val - Asn | 0.0899 | 0.003884363 | Hydrophobic - Polar |
| Val - Gln | 0.0235 | 0.002538257 | Hydrophobic - Polar |
| Val - Arg:NE | 0.0188 | 0.002404277 | Hydrophobic - Polar |
| Val - Arg:NH | 0.0139 | 0.002254573 | Hydrophobic - Polar |
| Val - Asp:H | 0.0703 | 0.003560084 | Hydrophobic - Polar |
| Val - Glu:H | 0.0202 | 0.002445096 | Hydrophobic - Polar |
| Val - LysN | 0.0375 | 0.002894115 | Hydrophobic - Polar |
| Val - Arg | 0.0044 | 0.001926221 | Hydrophobic - Positive Charge |
| Val - His+ | 0.0970 | 0.003991775 | Hydrophobic - Positive Charge |
| Val - Lys | 0.0077 | 0.002047013 | Hydrophobic - Positive Charge |
| Val - Asp | 0.0106 | 0.002146932 | Hydrophobic - Negative Charge |
| Val - Tyr- | 0.0094 | 0.002106234 | Hydrophobic - Negative Charge |
| Leu - Ile | 0.0054 | 0.001895328 | Hydrophobic - Hydrophobic |
| Leu - Met | 0.0114 | 0.002455248 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 0.0524 | 0.003408353 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 0.1071 | 0.004276197 | Hydrophobic - Aromatic |
| Leu - Phe | 0.0104 | 0.002426029 | Hydrophobic - Aromatic |
| Leu - Tyr | 0.0112 | 0.002449437 | Hydrophobic - Aromatic |
| Leu - Trp | 0.0091 | 0.001744813 | Hydrophobic - Aromatic |
| Leu - Ser | 0.0172 | 0.002617159 | Hydrophobic - Polar |
| Leu - Thr | 0.0047 | 0.001922359 | Hydrophobic - Polar |
| Leu - Cys | 0.0297 | 0.002930040 | Hydrophobic - Polar |
| Leu - Asn | 0.0854 | 0.003968359 | Hydrophobic - Polar |
| Leu - Gln | 0.0190 | 0.002665023 | Hydrophobic - Polar |
| Leu - Arg:NE | 0.0143 | 0.002537744 | Hydrophobic - Polar |
| Leu - Arg:NH | 0.0094 | 0.002396392 | Hydrophobic - Polar |
| Leu - Asp:H | 0.0658 | 0.003651547 | Hydrophobic - Polar |
| Leu - Glu:H | 0.0157 | 0.002576449 | Hydrophobic - Polar |
| Leu - LysN | 0.0330 | 0.003005910 | Hydrophobic - Polar |
| Leu - His+ | 0.0925 | 0.004073556 | Hydrophobic - Positive Charge |
| Leu - Lys | 0.0032 | 0.002202239 | Hydrophobic - Positive Charge |
| Leu - Asp | 0.0061 | 0.002295411 | Hydrophobic - Negative Charge |
| Leu - Glu | 0.0038 | 0.001956508 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 0.0049 | 0.002257392 | Hydrophobic - Negative Charge |
| Ile - Met | 0.0168 | 0.002288230 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 0.0578 | 0.003290079 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 0.1125 | 0.004182537 | Hydrophobic - Aromatic |
| Ile - Phe | 0.0158 | 0.002256805 | Hydrophobic - Aromatic |
| Ile - Tyr | 0.0166 | 0.002281993 | Hydrophobic - Aromatic |
| Ile - Trp | 0.0037 | 0.001500709 | Hydrophobic - Aromatic |
| Ile - Ser | 0.0226 | 0.002461153 | Hydrophobic - Polar |
| Ile - Cys | 0.0351 | 0.002791574 | Hydrophobic - Polar |
| Ile - Asn | 0.0908 | 0.003867251 | Hydrophobic - Polar |
| Ile - Gln | 0.0244 | 0.002511991 | Hydrophobic - Polar |
| Ile - Arg:NE | 0.0197 | 0.002376531 | Hydrophobic - Polar |
| Ile - Arg:NH | 0.0148 | 0.002224960 | Hydrophobic - Polar |
| Ile - Asp:H | 0.0712 | 0.003541405 | Hydrophobic - Polar |
| Ile - Glu:H | 0.0211 | 0.002417818 | Hydrophobic - Polar |
| Ile - LysN | 0.0384 | 0.002871106 | Hydrophobic - Polar |
| Ile - Arg | 0.0053 | 0.001891475 | Hydrophobic - Positive Charge |
| Ile - His+ | 0.0979 | 0.003975124 | Hydrophobic - Positive Charge |
| Ile - Lys | 0.0086 | 0.002014351 | Hydrophobic - Positive Charge |
| Ile - Asp | 0.0115 | 0.002115814 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 0.0103 | 0.002074505 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 0.0410 | 0.003641510 | Hydrophobic - Aromatic |
| Met - His:NE2 | 0.0957 | 0.004464256 | Hydrophobic - Aromatic |
| Met - Trp | 0.0205 | 0.002165201 | Hydrophobic - Aromatic |
| Met - Ser | 0.0058 | 0.002914318 | Hydrophobic - Polar |
| Met - Thr | 0.0161 | 0.002310668 | Hydrophobic - Polar |
| Met - Cys | 0.0183 | 0.003198259 | Hydrophobic - Polar |
| Met - Asn | 0.0740 | 0.004170324 | Hydrophobic - Polar |
| Met - Gln | 0.0076 | 0.002957376 | Hydrophobic - Polar |
| Met - Arg:NE | 0.0029 | 0.002843215 | Hydrophobic - Polar |
| Met - Asp:H | 0.0544 | 0.003870080 | Hydrophobic - Polar |
| Met - Glu:H | 0.0043 | 0.002877814 | Hydrophobic - Polar |
| Met - LysN | 0.0216 | 0.003267908 | Hydrophobic - Polar |
| Met - Arg | 0.0115 | 0.002452274 | Hydrophobic - Positive Charge |
| Met - His+ | 0.0811 | 0.004270549 | Hydrophobic - Positive Charge |
| Met - Lys | 0.0082 | 0.002548251 | Hydrophobic - Positive Charge |
| Met - Asp | 0.0053 | 0.002629190 | Hydrophobic - Negative Charge |
| Met - Glu | 0.0152 | 0.002339155 | Hydrophobic - Negative Charge |
| Met - Tyr- | 0.0065 | 0.002596063 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 0.0547 | 0.005051555 | Aromatic - Aromatic |
| His:ND1 - Phe | 0.0420 | 0.003621874 | Aromatic - Aromatic |
| His:ND1 - Tyr | 0.0412 | 0.003637594 | Aromatic - Aromatic |
| His:ND1 - Trp | 0.0615 | 0.003205733 | Aromatic - Aromatic |
| His:ND1 - Ser | 0.0352 | 0.003752582 | Aromatic - Polar |
| His:ND1 - Thr | 0.0571 | 0.003305725 | Aromatic - Polar |
| His:ND1 - Cys | 0.0227 | 0.003977120 | Aromatic - Polar |
| His:ND1 - Asn | 0.0330 | 0.004793769 | Aromatic - Polar |
| His:ND1 - Gln | 0.0334 | 0.003786119 | Aromatic - Polar |
| His:ND1 - Arg:NE | 0.0381 | 0.003697634 | Aromatic - Polar |
| His:ND1 - Arg:NH | 0.0430 | 0.003602089 | Aromatic - Polar |
| His:ND1 - Asp:H | 0.0134 | 0.004534991 | Aromatic - Polar |
| His:ND1 - Glu:H | 0.0367 | 0.003724304 | Aromatic - Polar |
| His:ND1 - LysN | 0.0194 | 0.004033342 | Aromatic - Polar |
| His:ND1 - Arg | 0.0525 | 0.003406211 | Aromatic - Positive Charge |
| His:ND1 - His+ | 0.0401 | 0.004881210 | Aromatic - Positive Charge |
| His:ND1 - Lys | 0.0492 | 0.003475947 | Aromatic - Positive Charge |
| His:ND1 - Asp | 0.0463 | 0.003535713 | Aromatic - Negative Charge |
| His:ND1 - Glu | 0.0562 | 0.003325699 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 0.0475 | 0.003511149 | Aromatic - Negative Charge |
| His:NE2 - Phe | 0.0967 | 0.004448254 | Aromatic - Aromatic |
| His:NE2 - Tyr | 0.0959 | 0.004461063 | Aromatic - Aromatic |
| His:NE2 - Trp | 0.1162 | 0.004116517 | Aromatic - Aromatic |
| His:NE2 - Ser | 0.0899 | 0.004555312 | Aromatic - Polar |
| His:NE2 - Thr | 0.1118 | 0.004194855 | Aromatic - Polar |
| His:NE2 - Cys | 0.0774 | 0.004741991 | Aromatic - Polar |
| His:NE2 - Asn | 0.0217 | 0.005445109 | Aromatic - Polar |
| His:NE2 - Gln | 0.0881 | 0.004582978 | Aromatic - Polar |
| His:NE2 - Arg:NE | 0.0928 | 0.004510154 | Aromatic - Polar |
| His:NE2 - Arg:NH | 0.0977 | 0.004432159 | Aromatic - Polar |
| His:NE2 - Asp:H | 0.0413 | 0.005218730 | Aromatic - Polar |
| His:NE2 - Glu:H | 0.0914 | 0.004532045 | Aromatic - Polar |
| His:NE2 - LysN | 0.0741 | 0.004789242 | Aromatic - Polar |
| His:NE2 - Arg | 0.1072 | 0.004274490 | Aromatic - Positive Charge |
| His:NE2 - His+ | 0.0146 | 0.005522246 | Aromatic - Positive Charge |
| His:NE2 - Lys | 0.1039 | 0.004330266 | Aromatic - Positive Charge |
| His:NE2 - Asp | 0.1010 | 0.004378385 | Aromatic - Negative Charge |
| His:NE2 - Glu | 0.1109 | 0.004210614 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 0.1022 | 0.004358573 | Aromatic - Negative Charge |
| Phe - Trp | 0.0195 | 0.002132012 | Aromatic - Aromatic |
| Phe - Ser | 0.0068 | 0.002889745 | Aromatic - Polar |
| Phe - Thr | 0.0151 | 0.002279598 | Aromatic - Polar |
| Phe - Cys | 0.0193 | 0.003175883 | Aromatic - Polar |
| Phe - Asn | 0.0750 | 0.004153189 | Aromatic - Polar |
| Phe - Gln | 0.0086 | 0.002933163 | Aromatic - Polar |
| Phe - Arg:NE | 0.0039 | 0.002818022 | Aromatic - Polar |
| Phe - Asp:H | 0.0554 | 0.003851610 | Aromatic - Polar |
| Phe - Glu:H | 0.0053 | 0.002852927 | Aromatic - Polar |
| Phe - LysN | 0.0226 | 0.003246013 | Aromatic - Polar |
| Phe - Arg | 0.0105 | 0.002423020 | Aromatic - Positive Charge |
| Phe - His+ | 0.0821 | 0.004253817 | Aromatic - Positive Charge |
| Phe - Lys | 0.0072 | 0.002520111 | Aromatic - Positive Charge |
| Phe - Asp | 0.0043 | 0.002601925 | Aromatic - Negative Charge |
| Phe - Glu | 0.0142 | 0.002308468 | Aromatic - Negative Charge |
| Phe - Tyr- | 0.0055 | 0.002568447 | Aromatic - Negative Charge |
| Tyr - Trp | 0.0203 | 0.002158610 | Aromatic - Aromatic |
| Tyr - Ser | 0.0060 | 0.002909424 | Aromatic - Polar |
| Tyr - Thr | 0.0159 | 0.002304493 | Aromatic - Polar |
| Tyr - Cys | 0.0185 | 0.003193800 | Aromatic - Polar |
| Tyr - Asn | 0.0742 | 0.004166905 | Aromatic - Polar |
| Tyr - Gln | 0.0078 | 0.002952553 | Aromatic - Polar |
| Tyr - Arg:NE | 0.0031 | 0.002838198 | Aromatic - Polar |
| Tyr - Asp:H | 0.0546 | 0.003866396 | Aromatic - Polar |
| Tyr - Glu:H | 0.0045 | 0.002872858 | Aromatic - Polar |
| Tyr - LysN | 0.0218 | 0.003263544 | Aromatic - Polar |
| Tyr - Arg | 0.0113 | 0.002446456 | Aromatic - Positive Charge |
| Tyr - His+ | 0.0813 | 0.004267210 | Aromatic - Positive Charge |
| Tyr - Lys | 0.0080 | 0.002542652 | Aromatic - Positive Charge |
| Tyr - Asp | 0.0051 | 0.002623764 | Aromatic - Negative Charge |
| Tyr - Glu | 0.0150 | 0.002333055 | Aromatic - Negative Charge |
| Tyr - Tyr- | 0.0063 | 0.002590568 | Aromatic - Negative Charge |
| Trp - Ser | 0.0263 | 0.002347207 | Aromatic - Polar |
| Trp - Thr | 0.0044 | 0.001534705 | Aromatic - Polar |
| Trp - Cys | 0.0388 | 0.002691652 | Aromatic - Polar |
| Trp - Asn | 0.0945 | 0.003795752 | Aromatic - Polar |
| Trp - Gln | 0.0281 | 0.002400459 | Aromatic - Polar |
| Trp - Arg:NE | 0.0234 | 0.002258318 | Aromatic - Polar |
| Trp - Arg:NH | 0.0185 | 0.002098226 | Aromatic - Polar |
| Trp - Asp:H | 0.0749 | 0.003463185 | Aromatic - Polar |
| Trp - Glu:H | 0.0248 | 0.002301727 | Aromatic - Polar |
| Trp - LysN | 0.0421 | 0.002774050 | Aromatic - Polar |
| Trp - Arg | 0.0090 | 0.001740627 | Aromatic - Positive Charge |
| Trp - His+ | 0.1016 | 0.003905601 | Aromatic - Positive Charge |
| Trp - Lys | 0.0123 | 0.001873423 | Aromatic - Positive Charge |
| Trp - Asp | 0.0152 | 0.001982113 | Aromatic - Negative Charge |
| Trp - Glu | 0.0053 | 0.001577270 | Aromatic - Negative Charge |
| Trp - Tyr- | 0.0140 | 0.001937956 | Aromatic - Negative Charge |
| Ser - Thr | 0.0219 | 0.002482029 | Polar - Polar |
| Ser - Cys | 0.0125 | 0.003324175 | Polar - Polar |
| Ser - Asn | 0.0682 | 0.004267655 | Polar - Polar |
| Ser - Arg:NH | 0.0078 | 0.002864909 | Polar - Polar |
| Ser - Asp:H | 0.0486 | 0.003974771 | Polar - Polar |
| Ser - LysN | 0.0158 | 0.003391239 | Polar - Polar |
| Ser - Arg | 0.0173 | 0.002614370 | Polar - Positive Charge |
| Ser - His+ | 0.0753 | 0.004365646 | Polar - Positive Charge |
| Ser - Lys | 0.0140 | 0.002704601 | Polar - Positive Charge |
| Ser - Asp | 0.0111 | 0.002780993 | Polar - Negative Charge |
| Ser - Glu | 0.0210 | 0.002508571 | Polar - Negative Charge |
| Ser - Tyr- | 0.0123 | 0.002749695 | Polar - Negative Charge |
| Thr - Cys | 0.0344 | 0.002809997 | Polar - Polar |
| Thr - Asn | 0.0901 | 0.003880570 | Polar - Polar |
| Thr - Gln | 0.0237 | 0.002532448 | Polar - Polar |
| Thr - Arg:NE | 0.0190 | 0.002398144 | Polar - Polar |
| Thr - Arg:NH | 0.0141 | 0.002248031 | Polar - Polar |
| Thr - Asp:H | 0.0705 | 0.003555945 | Polar - Polar |
| Thr - Glu:H | 0.0204 | 0.002439065 | Polar - Polar |
| Thr - LysN | 0.0377 | 0.002889021 | Polar - Polar |
| Thr - Arg | 0.0046 | 0.001918560 | Polar - Positive Charge |
| Thr - His+ | 0.0972 | 0.003988083 | Polar - Positive Charge |
| Thr - Lys | 0.0079 | 0.002039805 | Polar - Positive Charge |
| Thr - Asp | 0.0108 | 0.002140061 | Polar - Negative Charge |
| Thr - Tyr- | 0.0096 | 0.002099230 | Polar - Negative Charge |
| Cys - Asn | 0.0557 | 0.004466373 | Polar - Polar |
| Cys - Gln | 0.0107 | 0.003361988 | Polar - Polar |
| Cys - Arg:NE | 0.0154 | 0.003262018 | Polar - Polar |
| Cys - Arg:NH | 0.0203 | 0.003153302 | Polar - Polar |
| Cys - Asp:H | 0.0361 | 0.004187411 | Polar - Polar |
| Cys - Glu:H | 0.0140 | 0.003292220 | Polar - Polar |
| Cys - Arg | 0.0298 | 0.002927549 | Polar - Positive Charge |
| Cys - His+ | 0.0628 | 0.004560096 | Polar - Positive Charge |
| Cys - Lys | 0.0265 | 0.003008401 | Polar - Positive Charge |
| Cys - Asp | 0.0236 | 0.003077260 | Polar - Negative Charge |
| Cys - Glu | 0.0335 | 0.002833468 | Polar - Negative Charge |
| Cys - Tyr- | 0.0248 | 0.003049006 | Polar - Negative Charge |
| Asn - Gln | 0.0664 | 0.004297174 | Polar - Polar |
| Asn - Arg:NE | 0.0711 | 0.004219420 | Polar - Polar |
| Asn - Arg:NH | 0.0760 | 0.004135946 | Polar - Polar |
| Asn - Asp:H | 0.0196 | 0.004969623 | Polar - Polar |
| Asn - Glu:H | 0.0697 | 0.004242812 | Polar - Polar |
| Asn - LysN | 0.0524 | 0.004516509 | Polar - Polar |
| Asn - Arg | 0.0855 | 0.003966520 | Polar - Positive Charge |
| Asn - His+ | 0.0071 | 0.005287459 | Polar - Positive Charge |
| Asn - Lys | 0.0822 | 0.004026564 | Polar - Positive Charge |
| Asn - Asp | 0.0793 | 0.004078268 | Polar - Negative Charge |
| Asn - Glu | 0.0892 | 0.003897599 | Polar - Negative Charge |
| Asn - Tyr- | 0.0805 | 0.004056991 | Polar - Negative Charge |
| Gln - Arg:NE | 0.0047 | 0.003026215 | Polar - Polar |
| Gln - Arg:NH | 0.0096 | 0.002908698 | Polar - Polar |
| Gln - Asp:H | 0.0468 | 0.004006448 | Polar - Polar |
| Gln - Glu:H | 0.0033 | 0.003058745 | Polar - Polar |
| Gln - LysN | 0.0140 | 0.003428312 | Polar - Polar |
| Gln - Arg | 0.0191 | 0.002662284 | Polar - Positive Charge |
| Gln - His+ | 0.0735 | 0.004394507 | Polar - Positive Charge |
| Gln - Lys | 0.0158 | 0.002750943 | Polar - Positive Charge |
| Gln - Asp | 0.0129 | 0.002826083 | Polar - Negative Charge |
| Gln - Glu | 0.0228 | 0.002558467 | Polar - Negative Charge |
| Gln - Tyr- | 0.0141 | 0.002795290 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 0.0049 | 0.002792548 | Polar - Polar |
| Arg:NE - Asp:H | 0.0515 | 0.003922936 | Polar - Polar |
| Arg:NE - LysN | 0.0187 | 0.003330334 | Polar - Polar |
| Arg:NE - Arg | 0.0144 | 0.002534868 | Polar - Positive Charge |
| Arg:NE - His+ | 0.0782 | 0.004318506 | Polar - Positive Charge |
| Arg:NE - Lys | 0.0111 | 0.002627829 | Polar - Positive Charge |
| Arg:NE - Asp | 0.0082 | 0.002706389 | Polar - Negative Charge |
| Arg:NE - Glu | 0.0181 | 0.002425604 | Polar - Negative Charge |
| Arg:NE - Tyr- | 0.0094 | 0.002674219 | Polar - Negative Charge |
| Arg:NH - Asp:H | 0.0564 | 0.003833011 | Polar - Polar |
| Arg:NH - Glu:H | 0.0063 | 0.002827768 | Polar - Polar |
| Arg:NH - LysN | 0.0236 | 0.003223922 | Polar - Polar |
| Arg:NH - Arg | 0.0095 | 0.002393346 | Polar - Positive Charge |
| Arg:NH - His+ | 0.0831 | 0.004236985 | Polar - Positive Charge |
| Arg:NH - Lys | 0.0062 | 0.002491593 | Polar - Positive Charge |
| Arg:NH - Asp | 0.0033 | 0.002574314 | Polar - Negative Charge |
| Arg:NH - Glu | 0.0132 | 0.002277301 | Polar - Negative Charge |
| Arg:NH - Tyr- | 0.0045 | 0.002540472 | Polar - Negative Charge |
| Asp:H - Glu:H | 0.0501 | 0.003948084 | Polar - Polar |
| Asp:H - LysN | 0.0328 | 0.004240846 | Polar - Polar |
| Asp:H - Arg | 0.0659 | 0.003649548 | Polar - Positive Charge |
| Asp:H - His+ | 0.0267 | 0.005054022 | Polar - Positive Charge |
| Asp:H - Lys | 0.0626 | 0.003714719 | Polar - Positive Charge |
| Asp:H - Asp | 0.0597 | 0.003770702 | Polar - Negative Charge |
| Asp:H - Glu | 0.0696 | 0.003574521 | Polar - Negative Charge |
| Asp:H - Tyr- | 0.0609 | 0.003747679 | Polar - Negative Charge |
| Glu:H - LysN | 0.0173 | 0.003359921 | Polar - Polar |
| Glu:H - Arg | 0.0158 | 0.002573616 | Polar - Positive Charge |
| Glu:H - His+ | 0.0768 | 0.004341363 | Polar - Positive Charge |
| Glu:H - Lys | 0.0125 | 0.002665227 | Polar - Positive Charge |
| Glu:H - Asp | 0.0096 | 0.002742716 | Polar - Negative Charge |
| Glu:H - Glu | 0.0195 | 0.002466070 | Polar - Negative Charge |
| Glu:H - Tyr- | 0.0108 | 0.002710976 | Polar - Negative Charge |
| LysN - Arg | 0.0331 | 0.003003482 | Polar - Positive Charge |
| LysN - His+ | 0.0595 | 0.004609212 | Polar - Positive Charge |
| LysN - Lys | 0.0298 | 0.003082343 | Polar - Positive Charge |
| LysN - Asp | 0.0269 | 0.003149586 | Polar - Negative Charge |
| LysN - Glu | 0.0368 | 0.002911856 | Polar - Negative Charge |
| LysN - Tyr- | 0.0281 | 0.003121986 | Polar - Negative Charge |
| Arg - His+ | 0.0926 | 0.004071765 | Positive Charge - Positive Charge |
| Arg - Lys | 0.0033 | 0.002198924 | Positive Charge - Positive Charge |
| Arg - Asp | 0.0062 | 0.002292231 | Positive Charge - Negative Charge |
| Arg - Glu | 0.0037 | 0.001952776 | Positive Charge - Negative Charge |
| Arg - Tyr- | 0.0050 | 0.002254158 | Positive Charge - Negative Charge |
| His+ - Lys | 0.0893 | 0.004130279 | Positive Charge - Positive Charge |
| His+ - Asp | 0.0864 | 0.004180701 | Positive Charge - Negative Charge |
| His+ - Glu | 0.0963 | 0.004004656 | Positive Charge - Negative Charge |
| His+ - Tyr- | 0.0876 | 0.004159947 | Positive Charge - Negative Charge |
| Lys - Asp | 0.0029 | 0.002394631 | Positive Charge - Negative Charge |
| Lys - Glu | 0.0070 | 0.002072020 | Positive Charge - Negative Charge |
| Asp - Glu | 0.0099 | 0.002170788 | Negative Charge - Negative Charge |
| Glu - Tyr- | 0.0087 | 0.002130546 | Negative Charge - Negative Charge |

**Table S7.** Non-statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 0.0001 | 0.001755006 | Hydrophobic - Hydrophobic |
| Ala - Ile | 0.0010 | 0.001716799 | Hydrophobic - Hydrophobic |
| Ala - Thr | 0.0003 | 0.001746594 | Hydrophobic - Polar |
| Ala - Glu | 0.0006 | 0.001784111 | Hydrophobic - Negative Charge |
| Val - Ile | 0.0009 | 0.001712505 | Hydrophobic - Hydrophobic |
| Val - Thr | 0.0002 | 0.001742374 | Hydrophobic - Polar |
| Val - Glu | 0.0007 | 0.001779980 | Hydrophobic - Negative Charge |
| Leu - Arg | 0.0001 | 0.002090436 | Hydrophobic - Positive Charge |
| Ile - Thr | 0.0007 | 0.001703883 | Hydrophobic - Polar |
| Ile - Glu | 0.0016 | 0.001742320 | Hydrophobic - Negative Charge |
| Met - Phe | 0.0010 | 0.002743965 | Hydrophobic - Aromatic |
| Met - Tyr | 0.0002 | 0.002764682 | Hydrophobic - Aromatic |
| Met - Arg:NH | 0.0020 | 0.002717797 | Hydrophobic - Polar |
| Phe - Tyr | 0.0008 | 0.002738766 | Aromatic - Aromatic |
| Phe - Arg:NH | 0.0010 | 0.002691430 | Aromatic - Polar |
| Tyr - Arg:NH | 0.0018 | 0.002712548 | Aromatic - Polar |
| Ser - Gln | 0.0018 | 0.003093114 | Polar - Polar |
| Ser - Arg:NE | 0.0029 | 0.002984150 | Polar - Polar |
| Ser - Glu:H | 0.0015 | 0.003017134 | Polar - Polar |
| Thr - Glu | 0.0009 | 0.001771686 | Polar - Negative Charge |
| Cys - LysN | 0.0033 | 0.003638147 | Polar - Polar |
| Arg:NE - Glu:H | 0.0014 | 0.002948512 | Polar - Polar |
| Lys - Tyr- | 0.0017 | 0.002358211 | Positive Charge - Negative Charge |
| Asp - Tyr- | 0.0012 | 0.002445448 | Negative Charge - Negative Charge |

**Table S8.** Statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - His:ND1 | 0.0077 | 0.001107972 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 0.0225 | 0.001918007 | Hydrophobic - Aromatic |
| Ala - Phe | 0.0018 | 0.001310936 | Hydrophobic - Aromatic |
| Ala - Tyr | 0.0045 | 0.001222542 | Hydrophobic - Aromatic |
| Ala - Ser | 0.0100 | 0.001637942 | Hydrophobic - Polar |
| Ala - Asn | 0.0136 | 0.001724057 | Hydrophobic - Polar |
| Ala - Asp:H | 0.0054 | 0.001519780 | Hydrophobic - Polar |
| Ala - LysN | 0.0056 | 0.001184491 | Hydrophobic - Polar |
| Ala - Asp | 0.0044 | 0.001225938 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 0.0302 | 0.001743326 | Aromatic - Aromatic |
| His:ND1 - Phe | 0.0059 | 0.001038743 | Aromatic - Aromatic |
| His:ND1 - Tyr | 0.0032 | 0.000924685 | Aromatic - Aromatic |
| His:ND1 - Ser | 0.0177 | 0.001429436 | Aromatic - Polar |
| His:ND1 - Asn | 0.0213 | 0.001527353 | Aromatic - Polar |
| His:ND1 - Asp:H | 0.0131 | 0.001292349 | Aromatic - Polar |
| His:ND1 - LysN | 0.0021 | 0.000873758 | Aromatic - Polar |
| His:ND1 - Asp | 0.0033 | 0.000929171 | Aromatic - Negative Charge |
| His:NE2 - Phe | 0.0243 | 0.001878866 | Aromatic - Aromatic |
| His:NE2 - Tyr | 0.0270 | 0.001818294 | Aromatic - Aromatic |
| His:NE2 - Ser | 0.0125 | 0.002120009 | Aromatic - Polar |
| His:NE2 - Asn | 0.0089 | 0.002187226 | Aromatic - Polar |
| His:NE2 - Asp:H | 0.0171 | 0.002030102 | Aromatic - Polar |
| His:NE2 - LysN | 0.0281 | 0.001792931 | Aromatic - Polar |
| His:NE2 - Asp | 0.0269 | 0.001820579 | Aromatic - Negative Charge |
| Phe - Tyr | 0.0027 | 0.001160170 | Aromatic - Aromatic |
| Phe - Ser | 0.0118 | 0.001591930 | Aromatic - Polar |
| Phe - Asn | 0.0154 | 0.001680404 | Aromatic - Polar |
| Phe - Asp:H | 0.0072 | 0.001470074 | Aromatic - Polar |
| Phe - LysN | 0.0038 | 0.001120003 | Aromatic - Polar |
| Phe - Asp | 0.0026 | 0.001163749 | Aromatic - Negative Charge |
| Tyr - Ser | 0.0145 | 0.001519965 | Aromatic - Polar |
| Tyr - Asn | 0.0181 | 0.001612394 | Aromatic - Polar |
| Tyr - Asp:H | 0.0099 | 0.001391824 | Aromatic - Polar |
| Tyr - LysN | 0.0011 | 0.001015116 | Aromatic - Polar |
| Ser - Asn | 0.0036 | 0.001946294 | Polar - Polar |
| Ser - Asp:H | 0.0046 | 0.001767885 | Polar - Polar |
| Ser - LysN | 0.0156 | 0.001489532 | Polar - Polar |
| Ser - Asp | 0.0144 | 0.001522699 | Polar - Negative Charge |
| Asn - Asp:H | 0.0082 | 0.001847955 | Polar - Polar |
| Asn - LysN | 0.0192 | 0.001583738 | Polar - Polar |
| Asn - Asp | 0.0180 | 0.001614971 | Polar - Negative Charge |
| Asp:H - LysN | 0.0110 | 0.001358523 | Polar - Polar |
| Asp:H - Asp | 0.0098 | 0.001394808 | Polar - Negative Charge |
| LysN - Asp | 0.0012 | 0.001019204 | Polar - Negative Charge |

**Table S9.** Non-statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Tyr - Asp | 0.0001 | 0.001063187 | Aromatic - Negative Charge |

**Table S10.** Statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 0.0243 | 0.002906309 | Hydrophobic - Hydrophobic |
| Ala - Leu | 0.0053 | 0.003350345 | Hydrophobic - Hydrophobic |
| Ala - Ile | 0.0245 | 0.002901171 | Hydrophobic - Hydrophobic |
| Ala - Met | 0.0038 | 0.003537796 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 0.0060 | 0.003581107 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 0.0075 | 0.003302851 | Hydrophobic - Aromatic |
| Ala - Trp | 0.0085 | 0.003280961 | Hydrophobic - Aromatic |
| Ala - Ser | 0.0128 | 0.003710511 | Hydrophobic - Polar |
| Ala - Thr | 0.0111 | 0.003223126 | Hydrophobic - Polar |
| Ala - Asn | 0.0112 | 0.003220874 | Hydrophobic - Polar |
| Ala - Asp:H | 0.0080 | 0.003291930 | Hydrophobic - Polar |
| Ala - Glu:H | 0.0046 | 0.003365270 | Hydrophobic - Polar |
| Ala - Arg | 0.0038 | 0.003382219 | Hydrophobic - Positive Charge |
| Ala - His+ | 0.0559 | 0.004406463 | Hydrophobic - Positive Charge |
| Ala - Asp | 0.0085 | 0.003280961 | Hydrophobic - Negative Charge |
| Ala - Glu | 0.0127 | 0.003186851 | Hydrophobic - Negative Charge |
| Ala - Cys - | 0.0296 | 0.002766191 | Hydrophobic - Negative Charge |
| Val - Leu | 0.0190 | 0.002773358 | Hydrophobic - Hydrophobic |
| Val - Met | 0.0281 | 0.002997116 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 0.0303 | 0.003048119 | Hydrophobic - Aromatic |
| Val - His:NE2 | 0.0168 | 0.002715792 | Hydrophobic - Aromatic |
| Val - Phe | 0.0235 | 0.002886729 | Hydrophobic - Aromatic |
| Val - Tyr | 0.0220 | 0.002849562 | Hydrophobic - Aromatic |
| Val - Trp | 0.0158 | 0.002689127 | Hydrophobic - Aromatic |
| Val - Ser | 0.0371 | 0.003199155 | Hydrophobic - Polar |
| Val - Thr | 0.0132 | 0.002618251 | Hydrophobic - Polar |
| Val - Cys | 0.0240 | 0.002898986 | Hydrophobic - Polar |
| Val - Asn | 0.0131 | 0.002615479 | Hydrophobic - Polar |
| Val - Gln | 0.0240 | 0.002898986 | Hydrophobic - Polar |
| Val - Arg:NE | 0.0248 | 0.002918462 | Hydrophobic - Polar |
| Val - Arg:NH | 0.0227 | 0.002866982 | Hydrophobic - Polar |
| Val - Asp:H | 0.0163 | 0.002702500 | Hydrophobic - Polar |
| Val - Glu:H | 0.0197 | 0.002791370 | Hydrophobic - Polar |
| Val - LysN | 0.0248 | 0.002918462 | Hydrophobic - Polar |
| Val - Arg | 0.0205 | 0.002811780 | Hydrophobic - Positive Charge |
| Val - His+ | 0.0802 | 0.003985426 | Hydrophobic - Positive Charge |
| Val - Lys | 0.0237 | 0.002891640 | Hydrophobic - Positive Charge |
| Val - Asp | 0.0158 | 0.002689127 | Hydrophobic - Negative Charge |
| Val - Glu | 0.0116 | 0.002573464 | Hydrophobic - Negative Charge |
| Val - Cys - | 0.0053 | 0.002029412 | Hydrophobic - Negative Charge |
| Val - Tyr- | 0.0212 | 0.002829489 | Hydrophobic - Negative Charge |
| Leu - Ile | 0.0192 | 0.002767974 | Hydrophobic - Hydrophobic |
| Leu - Met | 0.0091 | 0.003429415 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 0.0113 | 0.003474077 | Hydrophobic - Aromatic |
| Leu - Phe | 0.0045 | 0.003333375 | Hydrophobic - Aromatic |
| Leu - Trp | 0.0032 | 0.003163793 | Hydrophobic - Aromatic |
| Leu - Ser | 0.0181 | 0.003607323 | Hydrophobic - Polar |
| Leu - Thr | 0.0058 | 0.003103776 | Hydrophobic - Polar |
| Leu - Cys | 0.0050 | 0.003343995 | Hydrophobic - Polar |
| Leu - Asn | 0.0059 | 0.003101437 | Hydrophobic - Polar |
| Leu - Gln | 0.0050 | 0.003343995 | Hydrophobic - Polar |
| Leu - Arg:NE | 0.0058 | 0.003360893 | Hydrophobic - Polar |
| Leu - Arg:NH | 0.0037 | 0.003316288 | Hydrophobic - Polar |
| Leu - LysN | 0.0058 | 0.003360893 | Hydrophobic - Polar |
| Leu - His+ | 0.0612 | 0.004319931 | Hydrophobic - Positive Charge |
| Leu - Lys | 0.0047 | 0.003337629 | Hydrophobic - Positive Charge |
| Leu - Asp | 0.0032 | 0.003163793 | Hydrophobic - Negative Charge |
| Leu - Glu | 0.0074 | 0.003066089 | Hydrophobic - Negative Charge |
| Leu - Cys - | 0.0243 | 0.002626156 | Hydrophobic - Negative Charge |
| Ile - Met | 0.0283 | 0.002992134 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 0.0305 | 0.003043220 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 0.0170 | 0.002710294 | Hydrophobic - Aromatic |
| Ile - Phe | 0.0237 | 0.002881557 | Hydrophobic - Aromatic |
| Ile - Tyr | 0.0222 | 0.002844322 | Hydrophobic - Aromatic |
| Ile - Trp | 0.0160 | 0.002683574 | Hydrophobic - Aromatic |
| Ile - Ser | 0.0373 | 0.003194488 | Hydrophobic - Polar |
| Ile - Thr | 0.0134 | 0.002612547 | Hydrophobic - Polar |
| Ile - Cys | 0.0242 | 0.002893835 | Hydrophobic - Polar |
| Ile - Asn | 0.0133 | 0.002609769 | Hydrophobic - Polar |
| Ile - Gln | 0.0242 | 0.002893835 | Hydrophobic - Polar |
| Ile - Arg:NE | 0.0250 | 0.002913346 | Hydrophobic - Polar |
| Ile - Arg:NH | 0.0229 | 0.002861774 | Hydrophobic - Polar |
| Ile - Asp:H | 0.0165 | 0.002696974 | Hydrophobic - Polar |
| Ile - Glu:H | 0.0199 | 0.002786020 | Hydrophobic - Polar |
| Ile - LysN | 0.0250 | 0.002913346 | Hydrophobic - Polar |
| Ile - Arg | 0.0207 | 0.002806469 | Hydrophobic - Positive Charge |
| Ile - His+ | 0.0804 | 0.003981681 | Hydrophobic - Positive Charge |
| Ile - Lys | 0.0239 | 0.002886476 | Hydrophobic - Positive Charge |
| Ile - Asp | 0.0160 | 0.002683574 | Hydrophobic - Negative Charge |
| Ile - Glu | 0.0118 | 0.002567661 | Hydrophobic - Negative Charge |
| Ile - Cys - | 0.0051 | 0.002022048 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 0.0214 | 0.002824212 | Hydrophobic - Negative Charge |
| Met - His:NE2 | 0.0113 | 0.003383031 | Hydrophobic - Aromatic |
| Met - Phe | 0.0046 | 0.003521729 | Hydrophobic - Aromatic |
| Met - Tyr | 0.0061 | 0.003491328 | Hydrophobic - Aromatic |
| Met - Trp | 0.0123 | 0.003361663 | Hydrophobic - Aromatic |
| Met - Ser | 0.0090 | 0.003782058 | Hydrophobic - Polar |
| Met - Thr | 0.0149 | 0.003305240 | Hydrophobic - Polar |
| Met - Cys | 0.0041 | 0.003531783 | Hydrophobic - Polar |
| Met - Asn | 0.0150 | 0.003303044 | Hydrophobic - Polar |
| Met - Gln | 0.0041 | 0.003531783 | Hydrophobic - Polar |
| Met - Arg:NH | 0.0054 | 0.003505561 | Hydrophobic - Polar |
| Met - Asp:H | 0.0118 | 0.003372370 | Hydrophobic - Polar |
| Met - Glu:H | 0.0084 | 0.003443997 | Hydrophobic - Polar |
| Met - Arg | 0.0076 | 0.003460560 | Hydrophobic - Positive Charge |
| Met - His+ | 0.0521 | 0.004466877 | Hydrophobic - Positive Charge |
| Met - Lys | 0.0044 | 0.003525756 | Hydrophobic - Positive Charge |
| Met - Asp | 0.0123 | 0.003361663 | Hydrophobic - Negative Charge |
| Met - Glu | 0.0165 | 0.003269876 | Hydrophobic - Negative Charge |
| Met - Cys - | 0.0334 | 0.002861448 | Hydrophobic - Negative Charge |
| Met - Tyr- | 0.0069 | 0.003474965 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 0.0135 | 0.003428297 | Aromatic - Aromatic |
| His:ND1 - Phe | 0.0068 | 0.003565235 | Aromatic - Aromatic |
| His:ND1 - Tyr | 0.0083 | 0.003535208 | Aromatic - Aromatic |
| His:ND1 - Trp | 0.0145 | 0.003407213 | Aromatic - Aromatic |
| His:ND1 - Ser | 0.0068 | 0.003822602 | Aromatic - Polar |
| His:ND1 - Thr | 0.0171 | 0.003351557 | Aromatic - Polar |
| His:ND1 - Cys | 0.0063 | 0.003575166 | Aromatic - Polar |
| His:ND1 - Asn | 0.0172 | 0.003349392 | Aromatic - Polar |
| His:ND1 - Gln | 0.0063 | 0.003575166 | Aromatic - Polar |
| His:ND1 - Arg:NE | 0.0055 | 0.003590977 | Aromatic - Polar |
| His:ND1 - Arg:NH | 0.0076 | 0.003549265 | Aromatic - Polar |
| His:ND1 - Asp:H | 0.0140 | 0.003417777 | Aromatic - Polar |
| His:ND1 - Glu:H | 0.0106 | 0.003488472 | Aromatic - Polar |
| His:ND1 - LysN | 0.0055 | 0.003590977 | Aromatic - Polar |
| His:ND1 - Arg | 0.0098 | 0.003504825 | Aromatic - Positive Charge |
| His:ND1 - His+ | 0.0499 | 0.004501257 | Aromatic - Positive Charge |
| His:ND1 - Lys | 0.0066 | 0.003569212 | Aromatic - Positive Charge |
| His:ND1 - Asp | 0.0145 | 0.003407213 | Aromatic - Negative Charge |
| His:ND1 - Glu | 0.0187 | 0.003316687 | Aromatic - Negative Charge |
| His:ND1 - Cys - | 0.0356 | 0.002914825 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 0.0091 | 0.003519049 | Aromatic - Negative Charge |
| His:NE2 - Phe | 0.0067 | 0.003285636 | Aromatic - Aromatic |
| His:NE2 - Tyr | 0.0052 | 0.003253029 | Aromatic - Aromatic |
| His:NE2 - Ser | 0.0203 | 0.003563255 | Aromatic - Polar |
| His:NE2 - Thr | 0.0036 | 0.003052448 | Aromatic - Polar |
| His:NE2 - Cys | 0.0072 | 0.003296410 | Aromatic - Polar |
| His:NE2 - Asn | 0.0037 | 0.003050070 | Aromatic - Polar |
| His:NE2 - Gln | 0.0072 | 0.003296410 | Aromatic - Polar |
| His:NE2 - Arg:NE | 0.0080 | 0.003313551 | Aromatic - Polar |
| His:NE2 - Arg:NH | 0.0059 | 0.003268299 | Aromatic - Polar |
| His:NE2 - LysN | 0.0080 | 0.003313551 | Aromatic - Polar |
| His:NE2 - Arg | 0.0037 | 0.003219985 | Aromatic - Positive Charge |
| His:NE2 - His+ | 0.0634 | 0.004283202 | Aromatic - Positive Charge |
| His:NE2 - Lys | 0.0069 | 0.003289951 | Aromatic - Positive Charge |
| His:NE2 - Glu | 0.0052 | 0.003014119 | Aromatic - Negative Charge |
| His:NE2 - Cys - | 0.0221 | 0.002565289 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 0.0044 | 0.003235461 | Aromatic - Negative Charge |
| Phe - Trp | 0.0077 | 0.003263630 | Aromatic - Aromatic |
| Phe - Ser | 0.0136 | 0.003695195 | Aromatic - Polar |
| Phe - Thr | 0.0103 | 0.003205482 | Aromatic - Polar |
| Phe - Asn | 0.0104 | 0.003203218 | Aromatic - Polar |
| Phe - Asp:H | 0.0072 | 0.003274657 | Aromatic - Polar |
| Phe - Glu:H | 0.0038 | 0.003348375 | Aromatic - Polar |
| Phe - His+ | 0.0567 | 0.004393574 | Aromatic - Positive Charge |
| Phe - Asp | 0.0077 | 0.003263630 | Aromatic - Negative Charge |
| Phe - Glu | 0.0119 | 0.003169005 | Aromatic - Negative Charge |
| Phe - Cys - | 0.0288 | 0.002745612 | Aromatic - Negative Charge |
| Tyr - Trp | 0.0062 | 0.003230801 | Aromatic - Aromatic |
| Tyr - Ser | 0.0151 | 0.003666233 | Aromatic - Polar |
| Tyr - Thr | 0.0088 | 0.003172051 | Aromatic - Polar |
| Tyr - Asn | 0.0089 | 0.003169764 | Aromatic - Polar |
| Tyr - Asp:H | 0.0057 | 0.003241940 | Aromatic - Polar |
| Tyr - His+ | 0.0582 | 0.004369244 | Aromatic - Positive Charge |
| Tyr - Asp | 0.0062 | 0.003230801 | Aromatic - Negative Charge |
| Tyr - Glu | 0.0104 | 0.003135186 | Aromatic - Negative Charge |
| Tyr - Cys - | 0.0273 | 0.002706508 | Aromatic - Negative Charge |
| Trp - Ser | 0.0213 | 0.003542974 | Aromatic - Polar |
| Trp - Cys | 0.0082 | 0.003274476 | Aromatic - Polar |
| Trp - Gln | 0.0082 | 0.003274476 | Aromatic - Polar |
| Trp - Arg:NE | 0.0090 | 0.003291731 | Aromatic - Polar |
| Trp - Arg:NH | 0.0069 | 0.003246176 | Aromatic - Polar |
| Trp - Glu:H | 0.0039 | 0.003179594 | Aromatic - Polar |
| Trp - LysN | 0.0090 | 0.003291731 | Aromatic - Polar |
| Trp - Arg | 0.0047 | 0.003197527 | Aromatic - Positive Charge |
| Trp - His+ | 0.0644 | 0.004266344 | Aromatic - Positive Charge |
| Trp - Lys | 0.0079 | 0.003267974 | Aromatic - Positive Charge |
| Trp - Glu | 0.0042 | 0.002990115 | Aromatic - Negative Charge |
| Trp - Cys - | 0.0211 | 0.002537043 | Aromatic - Negative Charge |
| Trp - Tyr- | 0.0054 | 0.003213111 | Aromatic - Negative Charge |
| Ser - Thr | 0.0239 | 0.003489484 | Polar - Polar |
| Ser - Cys | 0.0131 | 0.003704778 | Polar - Polar |
| Ser - Asn | 0.0240 | 0.003487405 | Polar - Polar |
| Ser - Gln | 0.0131 | 0.003704778 | Polar - Polar |
| Ser - Arg:NE | 0.0123 | 0.003720038 | Polar - Polar |
| Ser - Arg:NH | 0.0144 | 0.003679789 | Polar - Polar |
| Ser - Asp:H | 0.0208 | 0.003553135 | Polar - Polar |
| Ser - Glu:H | 0.0174 | 0.003621188 | Polar - Polar |
| Ser - LysN | 0.0123 | 0.003720038 | Polar - Polar |
| Ser - Arg | 0.0166 | 0.003636945 | Polar - Positive Charge |
| Ser - His+ | 0.0431 | 0.004604876 | Polar - Positive Charge |
| Ser - Lys | 0.0134 | 0.003699032 | Polar - Positive Charge |
| Ser - Asp | 0.0213 | 0.003542974 | Polar - Negative Charge |
| Ser - Glu | 0.0255 | 0.003456006 | Polar - Negative Charge |
| Ser - Cys - | 0.0424 | 0.003072421 | Polar - Negative Charge |
| Ser - Tyr- | 0.0159 | 0.003650654 | Polar - Negative Charge |
| Thr - Cys | 0.0108 | 0.003216524 | Polar - Polar |
| Thr - Gln | 0.0108 | 0.003216524 | Polar - Polar |
| Thr - Arg:NE | 0.0116 | 0.003234089 | Polar - Polar |
| Thr - Arg:NH | 0.0095 | 0.003187709 | Polar - Polar |
| Thr - Asp:H | 0.0031 | 0.003040627 | Polar - Polar |
| Thr - Glu:H | 0.0065 | 0.003119880 | Polar - Polar |
| Thr - LysN | 0.0116 | 0.003234089 | Polar - Polar |
| Thr - Arg | 0.0073 | 0.003138155 | Polar - Positive Charge |
| Thr - His+ | 0.0670 | 0.004222029 | Polar - Positive Charge |
| Thr - Lys | 0.0105 | 0.003209905 | Polar - Positive Charge |
| Thr - Cys - | 0.0185 | 0.002461792 | Polar - Negative Charge |
| Thr - Tyr- | 0.0080 | 0.003154032 | Polar - Negative Charge |
| Cys - Asn | 0.0109 | 0.003214268 | Polar - Polar |
| Cys - Asp:H | 0.0077 | 0.003285467 | Polar - Polar |
| Cys - Glu:H | 0.0043 | 0.003358948 | Polar - Polar |
| Cys - Arg | 0.0035 | 0.003375929 | Polar - Positive Charge |
| Cys - His+ | 0.0562 | 0.004401637 | Polar - Positive Charge |
| Cys - Asp | 0.0082 | 0.003274476 | Polar - Negative Charge |
| Cys - Glu | 0.0124 | 0.003180174 | Polar - Negative Charge |
| Cys - Cys - | 0.0293 | 0.002758496 | Polar - Negative Charge |
| Asn - Gln | 0.0109 | 0.003214268 | Polar - Polar |
| Asn - Arg:NE | 0.0117 | 0.003231845 | Polar - Polar |
| Asn - Arg:NH | 0.0096 | 0.003185433 | Polar - Polar |
| Asn - Asp:H | 0.0032 | 0.003038240 | Polar - Polar |
| Asn - Glu:H | 0.0066 | 0.003117554 | Polar - Polar |
| Asn - LysN | 0.0117 | 0.003231845 | Polar - Polar |
| Asn - Arg | 0.0074 | 0.003135842 | Polar - Positive Charge |
| Asn - His+ | 0.0671 | 0.004220310 | Polar - Positive Charge |
| Asn - Lys | 0.0106 | 0.003207644 | Polar - Positive Charge |
| Asn - Cys - | 0.0184 | 0.002458843 | Polar - Negative Charge |
| Asn - Tyr- | 0.0081 | 0.003151731 | Polar - Negative Charge |
| Gln - Asp:H | 0.0077 | 0.003285467 | Polar - Polar |
| Gln - Glu:H | 0.0043 | 0.003358948 | Polar - Polar |
| Gln - Arg | 0.0035 | 0.003375929 | Polar - Positive Charge |
| Gln - His+ | 0.0562 | 0.004401637 | Polar - Positive Charge |
| Gln - Asp | 0.0082 | 0.003274476 | Polar - Negative Charge |
| Gln - Glu | 0.0124 | 0.003180174 | Polar - Negative Charge |
| Gln - Cys - | 0.0293 | 0.002758496 | Polar - Negative Charge |
| Arg:NE - Asp:H | 0.0085 | 0.003302665 | Polar - Polar |
| Arg:NE - Glu:H | 0.0051 | 0.003375771 | Polar - Polar |
| Arg:NE - Arg | 0.0043 | 0.003392668 | Polar - Positive Charge |
| Arg:NE - His+ | 0.0554 | 0.004414489 | Polar - Positive Charge |
| Arg:NE - Asp | 0.0090 | 0.003291731 | Polar - Negative Charge |
| Arg:NE - Glu | 0.0132 | 0.003197938 | Polar - Negative Charge |
| Arg:NE - Cys - | 0.0301 | 0.002778957 | Polar - Negative Charge |
| Arg:NE - Tyr- | 0.0036 | 0.003407360 | Polar - Negative Charge |
| Arg:NH - Asp:H | 0.0064 | 0.003257262 | Polar - Polar |
| Arg:NH - His+ | 0.0575 | 0.004380625 | Polar - Positive Charge |
| Arg:NH - Asp | 0.0069 | 0.003246176 | Polar - Negative Charge |
| Arg:NH - Glu | 0.0111 | 0.003151027 | Polar - Negative Charge |
| Arg:NH - Cys - | 0.0280 | 0.002724842 | Polar - Negative Charge |
| Asp:H - Glu:H | 0.0034 | 0.003190912 | Polar - Polar |
| Asp:H - LysN | 0.0085 | 0.003302665 | Polar - Polar |
| Asp:H - Arg | 0.0042 | 0.003208782 | Polar - Positive Charge |
| Asp:H - His+ | 0.0639 | 0.004274786 | Polar - Positive Charge |
| Asp:H - Lys | 0.0074 | 0.003278987 | Polar - Positive Charge |
| Asp:H - Glu | 0.0047 | 0.003002148 | Polar - Negative Charge |
| Asp:H - Cys - | 0.0216 | 0.002551213 | Polar - Negative Charge |
| Asp:H - Tyr- | 0.0049 | 0.003224311 | Polar - Negative Charge |
| Glu:H - LysN | 0.0051 | 0.003375771 | Polar - Polar |
| Glu:H - His+ | 0.0605 | 0.004331516 | Polar - Positive Charge |
| Glu:H - Lys | 0.0040 | 0.003352610 | Polar - Positive Charge |
| Glu:H - Asp | 0.0039 | 0.003179594 | Polar - Negative Charge |
| Glu:H - Glu | 0.0081 | 0.003082390 | Polar - Negative Charge |
| Glu:H - Cys - | 0.0250 | 0.002645170 | Polar - Negative Charge |
| LysN - Arg | 0.0043 | 0.003392668 | Polar - Positive Charge |
| LysN - His+ | 0.0554 | 0.004414489 | Polar - Positive Charge |
| LysN - Asp | 0.0090 | 0.003291731 | Polar - Negative Charge |
| LysN - Glu | 0.0132 | 0.003197938 | Polar - Negative Charge |
| LysN - Cys - | 0.0301 | 0.002778957 | Polar - Negative Charge |
| LysN - Tyr- | 0.0036 | 0.003407360 | Polar - Negative Charge |
| Arg - His+ | 0.0597 | 0.004344697 | Positive Charge - Positive Charge |
| Arg - Asp | 0.0047 | 0.003197527 | Positive Charge - Negative Charge |
| Arg - Glu | 0.0089 | 0.003100886 | Positive Charge - Negative Charge |
| Arg - Cys - | 0.0258 | 0.002666700 | Positive Charge - Negative Charge |
| His+ - Lys | 0.0565 | 0.004396802 | Positive Charge - Positive Charge |
| His+ - Asp | 0.0644 | 0.004266344 | Positive Charge - Negative Charge |
| His+ - Glu | 0.0686 | 0.004194402 | Positive Charge - Negative Charge |
| His+ - Cys - | 0.0855 | 0.003884431 | Positive Charge - Negative Charge |
| His+ - Tyr- | 0.0590 | 0.004356179 | Positive Charge - Negative Charge |
| Lys - Asp | 0.0079 | 0.003267974 | Positive Charge - Negative Charge |
| Lys - Glu | 0.0121 | 0.003173479 | Positive Charge - Negative Charge |
| Lys - Cys - | 0.0290 | 0.002750775 | Positive Charge - Negative Charge |
| Asp - Glu | 0.0042 | 0.002990115 | Negative Charge - Negative Charge |
| Asp - Cys - | 0.0211 | 0.002537043 | Negative Charge - Negative Charge |
| Asp - Tyr- | 0.0054 | 0.003213111 | Negative Charge - Negative Charge |
| Glu - Cys - | 0.0169 | 0.002414104 | Negative Charge - Negative Charge |
| Glu - Tyr- | 0.0096 | 0.003116953 | Negative Charge - Negative Charge |
| Cys -  - Tyr- | 0.0265 | 0.002685366 | Negative Charge - Negative Charge |

**Table S11.** Non-statistically significant pairwise comparisons of the probability of the central Xaa residue f,y dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Phe | 0.0008 | 0.003444779 | Hydrophobic - Aromatic |
| Ala - Tyr | 0.0023 | 0.003413693 | Hydrophobic - Aromatic |
| Ala - Cys | 0.0003 | 0.003455057 | Hydrophobic - Polar |
| Ala - Gln | 0.0003 | 0.003455057 | Hydrophobic - Polar |
| Ala - Arg:NE | 0.0005 | 0.003471415 | Hydrophobic - Polar |
| Ala - Arg:NH | 0.0016 | 0.003428248 | Hydrophobic - Polar |
| Ala - LysN | 0.0005 | 0.003471415 | Hydrophobic - Polar |
| Ala - Lys | 0.0006 | 0.003448895 | Hydrophobic - Positive Charge |
| Ala - Tyr- | 0.0031 | 0.003396956 | Hydrophobic - Negative Charge |
| Val - Ile | 0.0002 | 0.002209863 | Hydrophobic - Hydrophobic |
| Leu - His:NE2 | 0.0022 | 0.003186489 | Hydrophobic - Aromatic |
| Leu - Tyr | 0.0030 | 0.003301240 | Hydrophobic - Aromatic |
| Leu - Asp:H | 0.0027 | 0.003175167 | Hydrophobic - Polar |
| Leu - Glu:H | 0.0007 | 0.003251143 | Hydrophobic - Polar |
| Leu - Arg | 0.0015 | 0.003268683 | Hydrophobic - Positive Charge |
| Leu - Tyr- | 0.0022 | 0.003283930 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 0.0022 | 0.003655188 | Hydrophobic - Aromatic |
| Met - Arg:NE | 0.0033 | 0.003547787 | Hydrophobic - Polar |
| Met - LysN | 0.0033 | 0.003547787 | Hydrophobic - Polar |
| His:NE2 - Trp | 0.0010 | 0.003113455 | Aromatic - Aromatic |
| His:NE2 - Asp:H | 0.0005 | 0.003125012 | Aromatic - Polar |
| His:NE2 - Glu:H | 0.0029 | 0.003202177 | Aromatic - Polar |
| His:NE2 - Asp | 0.0010 | 0.003113455 | Aromatic - Negative Charge |
| Phe - Tyr | 0.0015 | 0.003397039 | Aromatic - Aromatic |
| Phe - Cys | 0.0005 | 0.003438603 | Aromatic - Polar |
| Phe - Gln | 0.0005 | 0.003438603 | Aromatic - Polar |
| Phe - Arg:NE | 0.0013 | 0.003455039 | Aromatic - Polar |
| Phe - Arg:NH | 0.0008 | 0.003411665 | Aromatic - Polar |
| Phe - LysN | 0.0013 | 0.003455039 | Aromatic - Polar |
| Phe - Arg | 0.0030 | 0.003365409 | Aromatic - Positive Charge |
| Phe - Lys | 0.0002 | 0.003432412 | Aromatic - Positive Charge |
| Phe - Tyr- | 0.0023 | 0.003380220 | Aromatic - Negative Charge |
| Tyr - Cys | 0.0020 | 0.003407461 | Aromatic - Polar |
| Tyr - Gln | 0.0020 | 0.003407461 | Aromatic - Polar |
| Tyr - Arg:NE | 0.0028 | 0.003424046 | Aromatic - Polar |
| Tyr - Arg:NH | 0.0007 | 0.003380274 | Aromatic - Polar |
| Tyr - Glu:H | 0.0023 | 0.003316386 | Aromatic - Polar |
| Tyr - LysN | 0.0028 | 0.003424046 | Aromatic - Polar |
| Tyr - Arg | 0.0015 | 0.003333583 | Aromatic - Positive Charge |
| Tyr - Lys | 0.0017 | 0.003401213 | Aromatic - Positive Charge |
| Tyr - Tyr- | 0.0008 | 0.003348534 | Aromatic - Negative Charge |
| Trp - Thr | 0.0026 | 0.003028748 | Aromatic - Polar |
| Trp - Asn | 0.0027 | 0.003026351 | Aromatic - Polar |
| Trp - Asp:H | 0.0005 | 0.003101867 | Aromatic - Polar |
| Trp - Asp | 0.0000 | 0.003090223 | Aromatic - Negative Charge |
| Thr - Asn | 0.0001 | 0.002963552 | Polar - Polar |
| Thr - Asp | 0.0026 | 0.003028748 | Polar - Negative Charge |
| Thr - Glu | 0.0016 | 0.002926538 | Polar - Negative Charge |
| Cys - Gln | 0.0000 | 0.003448899 | Polar - Polar |
| Cys - Arg:NE | 0.0008 | 0.003465286 | Polar - Polar |
| Cys - Arg:NH | 0.0013 | 0.003422042 | Polar - Polar |
| Cys - LysN | 0.0008 | 0.003465286 | Polar - Polar |
| Cys - Lys | 0.0003 | 0.003442727 | Polar - Positive Charge |
| Cys - Tyr- | 0.0028 | 0.003390693 | Polar - Negative Charge |
| Asn - Asp | 0.0027 | 0.003026351 | Polar - Negative Charge |
| Asn - Glu | 0.0015 | 0.002924058 | Polar - Negative Charge |
| Gln - Arg:NE | 0.0008 | 0.003465286 | Polar - Polar |
| Gln - Arg:NH | 0.0013 | 0.003422042 | Polar - Polar |
| Gln - LysN | 0.0008 | 0.003465286 | Polar - Polar |
| Gln - Lys | 0.0003 | 0.003442727 | Polar - Positive Charge |
| Gln - Tyr- | 0.0028 | 0.003390693 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 0.0021 | 0.003438557 | Polar - Polar |
| Arg:NE - LysN | 0.0000 | 0.003481596 | Polar - Polar |
| Arg:NE - Lys | 0.0011 | 0.003459143 | Polar - Positive Charge |
| Arg:NH - Glu:H | 0.0030 | 0.003331365 | Polar - Polar |
| Arg:NH - LysN | 0.0021 | 0.003438557 | Polar - Polar |
| Arg:NH - Arg | 0.0022 | 0.003348486 | Polar - Positive Charge |
| Arg:NH - Lys | 0.0010 | 0.003415821 | Polar - Positive Charge |
| Arg:NH - Tyr- | 0.0015 | 0.003363371 | Polar - Negative Charge |
| Asp:H - Asp | 0.0005 | 0.003101867 | Polar - Negative Charge |
| Glu:H - Arg | 0.0008 | 0.003283979 | Polar - Positive Charge |
| Glu:H - Tyr- | 0.0015 | 0.003299155 | Polar - Negative Charge |
| LysN - Lys | 0.0011 | 0.003459143 | Polar - Positive Charge |
| Arg - Lys | 0.0032 | 0.003369622 | Positive Charge - Positive Charge |
| Arg - Tyr- | 0.0007 | 0.003316442 | Positive Charge - Negative Charge |
| Lys - Tyr- | 0.0025 | 0.003384414 | Positive Charge - Negative Charge |

**Table S12.** The f,y dihedral angles of the Xaa residue within the Ac-Ala-Xaa-Ala-NH2 peptides assigned by density clustering to the b, a, aL, e, and contiguous regions demonstrated in Figure S2 and expressed as a mean ± standard deviation(degrees). Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | b | | a | | aL | | e | | Cont. | |
| f | y | f | y | f | y | f | y | f | y |
| Gly | -68.60 ± 16.89 | 174.02 ± 22.49 | -81.50 ± 16.67 | -29.25 ± 13.98 | 85.47 ± 19.80 | 22.84 ± 15.52 | 68.06 ± 16.73 | -172.88 ± 22.81 | -4.96 ± 129.13 | -5.53 ± 118.90 |
| Ala | -83.50 ± 33.07 | 145.83 ± 15.01 | -87.54 ± 21.94 | -15.11 ± 23.29 | 72.71 ± 9.46 | 25.68 ± 9.45 | 53.16 ± 7.61 | -159.48 ± 13.71 | -50.89 ± 106.82 | 25.70 ± 84.93 |
| Val | -83.18 ± 27.57 | 134.76 ± 14.24 | -81.23 ± 20.28 | -25.50 ± 19.85 | 74.45 ± 7.91 | 112.81 ± 9.59 | N/S | N/S | -29.56 ± 95.73 | 10.72 ± 80.76 |
| Leu | -83.81 ± 27.87 | 138.89 ± 15.99 | -91.10 ± 20.57 | -12.43 ± 23.21 | 73.22 ± 9.58 | 26.43 ± 10.81 | N/S | N/S | -2.87 ± 96.39 | 31.07 ± 100.02 |
| Ile | -84.59 ± 27.75 | 133.96 ± 14.56 | -82.25 ± 20.82 | -25.98 ± 19.21 | 74.79 ± 7.85 | 112.74 ± 9.33 | N/S | N/S | -64.51 ± 93.90 | 16.99 ± 73.87 |
| Met | -84.42 ± 32.27 | 143.08 ± 15.58 | -93.89 ± 20.53 | -8.76 ± 21.99 | 70.09 ± 12.23 | 28.36 ± 12.88 | N/S | N/S | -3.53 ± 96.79 | 29.13 ± 103.27 |
| His:ND1 | -91.27 ± 34.70 | 140.73 ± 15.54 | -97.65 ± 21.88 | -5.20 ± 23.00 | 71.32 ± 13.60 | 32.73 ± 17.87 | 74.48 ± 5.35 | 148.12 ± 6.14 | -23.32 ± 114.76 | 42.76 ± 89.62 |
| His:NE2 | -89.14 ± 34.84 | 141.55 ± 15.83 | -95.36 ± 21.40 | -6.08 ± 22.81 | 70.89 ± 14.71 | 33.83 ± 18.92 | 70.72 ± 10.88 | 144.94 ± 30.32 | -33.96 ± 118.64 | 23.44 ± 90.37 |
| Phe | -84.80 ± 32.70 | 138.05 ± 14.62 | -90.72 ± 22.66 | -13.54 ± 23.69 | 69.36 ± 12.67 | 29.05 ± 12.85 | 74.31 ± 7.65 | 117.43 ± 10.65 | -0.26 ± 97.58 | 21.42 ± 106.11 |
| Tyr | -86.02 ± 33.26 | 137.66 ± 14.71 | -91.95 ± 23.16 | -12.84 ± 24.22 | 70.18 ± 11.87 | 28.54 ± 12.50 | 74.15 ± 7.02 | 116.62 ± 8.85 | -12.46 ± 102.46 | 23.16 ± 98.87 |
| Trp | -88.42 ± 35.27 | 136.78 ± 13.56 | -79.23 ± 21.73 | -27.04 ± 20.72 | 74.33 ± 6.70 | 117.63 ± 8.05 | N/S | N/S | -41.71 ± 113.75 | 23.43 ± 80.46 |
| Ser | -92.40 ± 36.49 | 140.99 ± 15.23 | -90.00 ± 21.50 | -12.35 ± 22.56 | 72.90 ± 12.06 | 32.39 ±1 6.67 | 70.54 ± 11.96 | 148.21 ± 38.40 | -25.81 ± 124.34 | 38.60 ± 84.54 |
| Thr | -93.20 ± 37.46 | 142.41 ± 15.70 | -89.18 ± 20.92 | -13.61 ± 21.61 | 76.55 ± 8.44 | 112.32 ± 9.77 | N/S | N/S | 9.46 ± 108.23 | 46.12 ± 77.62 |
| Cys:H | -85.30 ± 31.79 | 139.23 ± 14.46 | -89.85 ± 21.93 | -13.16 ± 23.57 | 70.17 ± 13.15 | 33.16 ± 17.70 | N/S | N/S | -4.18 ± 104.75 | 50.84 ± 91.96 |
| Asn | -86.35 ± 29.48 | 139.93 ± 16.20 | -96.48 ± 19.93 | -5.46 ± 22.51 | 70.14 ± 13.62 | 34.65 ± 19.31 | 70.80 ± 10.02 | 143.56 ± 30.05 | -43.33 ± 101.49 | 11.44 ± 94.00 |
| Gln | -84.41 ± 29.09 | 143.46 ± 15.33 | -93.84 ± 19.12 | -8.35 ± 21.68 | 70.94 ± 12.41 | 28.49 ± 13.60 | N/S | N/S | 3.00 ± 91.58 | 39.93 ± 99.93 |
| Arg:NE | -85.44 ± 32.33 | 144.87 ± 15.12 | -93.80 ± 20.58 | -9.07 ± 22.27 | 71.18 ± 11.97 | 28.05 ± 12.70 | N/S | N/S | 0.43 ± 93.43 | 27.57 ± 105.38 |
| Arg:NH | -83.73 ± 30.27 | 143.49 ± 15.36 | -92.18 ± 21.06 | -11.14 ± 22.62 | 71.42 ± 11.54 | 27.24 ± 12.31 | N/S | N/S | -17.15 ± 99.52 | 29.09 ± 94.48 |

**Table S12 (Cont.).** The f,y dihedral angles of the Xaa residue within the Ac-Ala-Xaa-Ala-NH2 peptides assigned by density clustering to the b, a, aL, e, and contiguous regions demonstrated in Figure S2 and expressed as a mean ± standard deviation(degrees). Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | b | | a | | aL | | e | | Cont. | |
| f | y | f | y | f | y | f | y | f | y |
| Asp:H | -95.52 ± 29.99 | 143.00 ± 16.23 | -102.61 ± 18.77 | -0.63 ± 20.93 | 69.99 ± 12.90 | 32.95 ± 17.86 | 65.98 ± 10.14 | 168.33 ± 22.79 | -32.18 ± 99.86 | 27.86 ± 88.66 |
| Glu:H | -85.64 ± 28.80 | 142.56 ± 15.19 | -95.83 ± 20.16 | -7.06 ± 22.04 | 70.21 ± 12.61 | 29.52 ± 13.25 | N/S | N/S | -1.89 ± 90.18 | 39.51 ± 98.61 |
| LysN | -83.45 ± 30.62 | 143.08 ± 15.33 | -92.71 ± 21.23 | -10.77 ± 22.65 | 68.83 ± 13.19 | 32.63 ± 17.92 | 73.41 ± 6.32 | 147.98 ± 8.46 | -11.57 ± 98.57 | 9.50 ± 107.89 |
| Arg | -91.93 ± 32.01 | 143.87 ± 15.61 | -98.29 ± 20.12 | -5.67 ± 21.50 | 73.19 ± 9.71 | 27.17 ± 10.67 | N/S | N/S | -10.73 ± 95.64 | 29.69 ± 99.88 |
| His+ | -100.73 ± 44.69 | 140.41 ± 16.33 | -125.43 ± 55.15 | 15.87 ± 28.84 | 60.99 ± 19.14 | 43.86 ± 19.57 | N/S | N/S | 21.02 ± 123.87 | 73.81 ± 71.74 |
| Lys | -86.09 ± 31.38 | 143.62 ± 15.36 | -94.09 ± 21.28 | -9.76 ± 22.35 | 72.60 ± 10.39 | 27.22 ± 11.28 | N/S | N/S | -27.72 ± 103.24 | 30.56 ± 88.32 |
| Asp | -72.87 ± 24.59 | 144.26 ± 14.82 | -80.68 ± 19.55 | -21.37 ± 22.49 | 67.25 ± 13.02 | 29.44 ± 12.74 | 56.80 ± 6.51 | -170.10 ± 10.73 | 0.61 ± 84.20 | 20.81 ± 105.32 |
| Glu | -77.49 ± 27.41 | 142.79 ± 14.28 | -88.38 ± 21.63 | -14.63 ± 22.97 | 73.00 ± 9.07 | 25.81 ± 10.01 | N/S | N/S | -12.01 ± 93.08 | 31.22 ± 92.06 |
| Cys- | -62.93 ± 17.66 | 143.32 ± 12.36 | -69.56 ± 14.27 | -32.25 ± 15.19 | N/S | N/S | N/S | N/S | -73.11 ± 74.66 | -15.68 ± 132.07 |
| Tyr- | -82.72 ± 33.80 | 142.44 ± 14.45 | -80.83 ± 21.75 | -22.90 ± 22.76 | 66.97 ± 12.52 | 28.84 ± 12.73 | N/S | N/S | -0.18 ± 93.03 | 29.76 ± 101.11 |
| Cys-Cys | -88.11 ± 32.76 | 141.92 ± 15.53 | -96.82 ± 25.22 | -9.12 ± 22.31 | 70.96 ± 12.79 | 33.16 ± 17.23 | N/S | N/S | -7.86 ± 107.88 | 47.55 ± 94.49 |
| Pro:cis | -52.76 ± 13.57 | 144.79 ± 13.17 | -83.83 ± 13.74 | -12.37 ± 22.44 | N/S | N/S | N/S | N/S | -86.44 ± 29.29 | 7.19 ± 89.32 |
| Pro:trans | -49.33 ± 11.53 | 141.80 ± 12.65 | -71.75 ± 5.76 | -36.07 ± 9.82 | N/S | N/S | N/S | N/S | -81.02 ± 15.85 | 38.89 ± 66.29 |
| F-statistic | 25645.83 | 14107.03 | 13580.16 | 14183.80 | 787.64 | 41746.72 | 3946.84 | 385381.87 | 625.58 | 663.60 |
| F-critical | 0.2769 | 0.2769 | 0.2769 | 0.2769 | 0.2682 | 0.2682 | 0.0734 | 0.0734 | 0.2769 | 0.2769 |
| p-value | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** | **< 0.0001** |

a The Gly, Cys-Cys, Pro:cis, and Pro:trans peptides were excluded from the ANOVA analysis.

b N/S: not sampled region secondary to low population density (<1000 conformations within 10°).

**Table S13.** Statistically significant pairwise comparisons of the f dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 16994.79173 | 61.657661 | Hydrophobic - Hydrophobic |
| Ala - Leu | 14441.3187 | 61.657661 | Hydrophobic - Hydrophobic |
| Ala - Ile | 194991.1733 | 61.657661 | Hydrophobic - Hydrophobic |
| Ala - Met | 126426.5854 | 61.657661 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 8877203.513 | 61.657661 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 4504564.46 | 61.657661 | Hydrophobic - Aromatic |
| Ala - Phe | 266655.8625 | 61.657661 | Hydrophobic - Aromatic |
| Ala - Tyr | 983215.5204 | 61.657661 | Hydrophobic - Aromatic |
| Ala - Trp | 3878362.222 | 61.657661 | Hydrophobic - Aromatic |
| Ala - Ser | 12002043.72 | 61.657661 | Hydrophobic - Polar |
| Ala - Thr | 15059499.6 | 61.657661 | Hydrophobic - Polar |
| Ala - Cys | 499896.5151 | 61.657661 | Hydrophobic - Polar |
| Ala - Asn | 1122412.823 | 61.657661 | Hydrophobic - Polar |
| Ala - Gln | 120645.5845 | 61.657661 | Hydrophobic - Polar |
| Ala - Arg:NE | 581089.3355 | 61.657661 | Hydrophobic - Polar |
| Ala - Arg:NH | 7960.353633 | 61.657661 | Hydrophobic - Polar |
| Ala - Asp:H | 19916672.2 | 61.657661 | Hydrophobic - Polar |
| Ala - Glu:H | 686288.7067 | 61.657661 | Hydrophobic - Polar |
| Ala - LysN | 373.3219587 | 61.657661 | Hydrophobic - Polar |
| Ala - Arg | 10954920.91 | 61.657661 | Hydrophobic - Positive Charge |
| Ala - His+ | 39683383.16 | 61.657661 | Hydrophobic - Positive Charge |
| Ala - Lys | 1017274.55 | 61.657661 | Hydrophobic - Positive Charge |
| Ala - Asp | 17300574.91 | 61.657661 | Hydrophobic - Negative Charge |
| Ala - Glu | 5680966.395 | 61.657661 | Hydrophobic - Negative Charge |
| Ala - Cys- | 65126068.88 | 61.657661 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 96229.38232 | 61.657661 | Hydrophobic - Negative Charge |
| Val - Leu | 64727.05681 | 61.657661 | Hydrophobic - Hydrophobic |
| Val - Ile | 356899.1074 | 61.657661 | Hydrophobic - Hydrophobic |
| Val - Met | 249117.8172 | 61.657661 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 10424531.64 | 61.657661 | Hydrophobic - Aromatic |
| Val - His:NE2 | 5432249.038 | 61.657661 | Hydrophobic - Aromatic |
| Val - Phe | 451304.5185 | 61.657661 | Hydrophobic - Aromatic |
| Val - Tyr | 1358715.872 | 61.657661 | Hydrophobic - Aromatic |
| Val - Trp | 4801301.289 | 61.657661 | Hydrophobic - Aromatic |
| Val - Ser | 13988328.61 | 61.657661 | Hydrophobic - Polar |
| Val - Thr | 17536363.5 | 61.657661 | Hydrophobic - Polar |
| Val - Cys | 754255.0648 | 61.657661 | Hydrophobic - Polar |
| Val - Asn | 1496702.189 | 61.657661 | Hydrophobic - Polar |
| Val - Gln | 238579.1438 | 61.657661 | Hydrophobic - Polar |
| Val - Arg:NE | 857816.5894 | 61.657661 | Hydrophobic - Polar |
| Val - Arg:NH | 49405.34789 | 61.657661 | Hydrophobic - Polar |
| Val - Asp:H | 22620912.08 | 61.657661 | Hydrophobic - Polar |
| Val - Glu:H | 983939.377 | 61.657661 | Hydrophobic - Polar |
| Val - LysN | 11807.54549 | 61.657661 | Hydrophobic - Polar |
| Val - Arg | 12836547.07 | 61.657661 | Hydrophobic - Positive Charge |
| Val - His+ | 44263258.15 | 61.657661 | Hydrophobic - Positive Charge |
| Val - Lys | 1394712.499 | 61.657661 | Hydrophobic - Positive Charge |
| Val - Asp | 17690126.58 | 61.657661 | Hydrophobic - Negative Charge |
| Val - Glu | 5548150.37 | 61.657661 | Hydrophobic - Negative Charge |
| Val - Cys- | 68636619.21 | 61.657661 | Hydrophobic - Negative Charge |
| Val - Tyr- | 36484.14998 | 61.657661 | Hydrophobic - Negative Charge |
| Leu - Ile | 98134.99323 | 61.657661 | Hydrophobic - Hydrophobic |
| Leu - Met | 54709.95591 | 61.657661 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 8056786.696 | 61.657661 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 3963204.366 | 61.657661 | Hydrophobic - Aromatic |
| Leu - Phe | 152088.2726 | 61.657661 | Hydrophobic - Aromatic |
| Leu - Tyr | 743922.4571 | 61.657661 | Hydrophobic - Aromatic |
| Leu - Trp | 3347881.655 | 61.657661 | Hydrophobic - Aromatic |
| Leu - Ser | 11002907.66 | 61.657661 | Hydrophobic - Polar |
| Leu - Thr | 13875732.14 | 61.657661 | Hydrophobic - Polar |
| Leu - Cys | 336998.2253 | 61.657661 | Hydrophobic - Polar |
| Leu - Asn | 878585.2207 | 61.657661 | Hydrophobic - Polar |
| Leu - Gln | 51646.71624 | 61.657661 | Hydrophobic - Polar |
| Leu - Arg:NE | 403580.0678 | 61.657661 | Hydrophobic - Polar |
| Leu - Arg:NH | 947.8728451 | 61.657661 | Hydrophobic - Polar |
| Leu - Asp:H | 18629040.13 | 61.657661 | Hydrophobic - Polar |
| Leu - Glu:H | 493972.9909 | 61.657661 | Hydrophobic - Polar |
| Leu - LysN | 19049.97179 | 61.657661 | Hydrophobic - Polar |
| Leu - Arg | 9999822.52 | 61.657661 | Hydrophobic - Positive Charge |
| Leu - His+ | 37730997.3 | 61.657661 | Hydrophobic - Positive Charge |
| Leu - Lys | 775797.7557 | 61.657661 | Hydrophobic - Positive Charge |
| Leu - Asp | 18030279.14 | 61.657661 | Hydrophobic - Negative Charge |
| Leu - Glu | 6178617.35 | 61.657661 | Hydrophobic - Negative Charge |
| Leu - Cys- | 66021317.54 | 61.657661 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 184805.5247 | 61.657661 | Hydrophobic - Negative Charge |
| Ile- Met | 4631.483823 | 61.657661 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 7031580.958 | 61.657661 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 3133540.677 | 61.657661 | Hydrophobic - Aromatic |
| Ile – Phe | 7496.3497 | 61.657661 | Hydrophobic - Aromatic |
| Ile - Tyr | 340594.4755 | 61.657661 | Hydrophobic - Aromatic |
| Ile - Trp | 2535019.471 | 61.657661 | Hydrophobic - Aromatic |
| Ile - Ser | 9926432.639 | 61.657661 | Hydrophobic - Polar |
| Ile - Thr | 12796863.07 | 61.657661 | Hydrophobic - Polar |
| Ile - Cys | 83647.94801 | 61.657661 | Hydrophobic - Polar |
| Ile - Asn | 456755.3533 | 61.657661 | Hydrophobic - Polar |
| Ile - Gln | 5055.380719 | 61.657661 | Hydrophobic - Polar |
| Ile - Arg:NE | 119978.5954 | 61.657661 | Hydrophobic - Polar |
| Ile - Arg:NH | 119472.6173 | 61.657661 | Hydrophobic - Polar |
| Ile - Asp:H | 17570045.95 | 61.657661 | Hydrophobic - Polar |
| Ile - Glu:H | 177304.9692 | 61.657661 | Hydrophobic - Polar |
| Ile - LysN | 208211.2035 | 61.657661 | Hydrophobic - Polar |
| Ile - Arg | 8931429.344 | 61.657661 | Hydrophobic - Positive Charge |
| Ile - His+ | 37075753.19 | 61.657661 | Hydrophobic - Positive Charge |
| Ile - Lys | 366491.6035 | 61.657661 | Hydrophobic - Positive Charge |
| Ile - Asp | 22604846.89 | 61.657661 | Hydrophobic - Negative Charge |
| Ile - Glu | 8539440.259 | 61.657661 | Hydrophobic - Negative Charge |
| Ile - Cys- | 77647524.7 | 61.657661 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 595977.8715 | 61.657661 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 6753677.473 | 61.657661 | Hydrophobic - Aromatic |
| Met - His:NE2 | 3090598.592 | 61.657661 | Hydrophobic - Aromatic |
| Met - Phe | 22268.27573 | 61.657661 | Hydrophobic - Aromatic |
| Met - Tyr | 387549.2364 | 61.657661 | Hydrophobic - Aromatic |
| Met - Trp | 2504617.107 | 61.657661 | Hydrophobic - Aromatic |
| Met - Ser | 9439008.192 | 61.657661 | Hydrophobic - Polar |
| Met - Thr | 12055067.96 | 61.657661 | Hydrophobic - Polar |
| Met - Cys | 116835.0847 | 61.657661 | Hydrophobic - Polar |
| Met - Asn | 504493.3781 | 61.657661 | Hydrophobic - Polar |
| Met - Arg:NE | 157074.5701 | 61.657661 | Hydrophobic - Polar |
| Met - Arg:NH | 70094.71717 | 61.657661 | Hydrophobic - Polar |
| Met - Asp:H | 16647641.04 | 61.657661 | Hydrophobic - Polar |
| Met - Glu:H | 218246.935 | 61.657661 | Hydrophobic - Polar |
| Met - LysN | 137489.3897 | 61.657661 | Hydrophobic - Polar |
| Met - Arg | 8501885.285 | 61.657661 | Hydrophobic - Positive Charge |
| Met - His+ | 34874356.07 | 61.657661 | Hydrophobic - Positive Charge |
| Met - Lys | 413722.4338 | 61.657661 | Hydrophobic - Positive Charge |
| Met - Asp | 19975816.14 | 61.657661 | Hydrophobic - Negative Charge |
| Met - Glu | 7382885.892 | 61.657661 | Hydrophobic - Negative Charge |
| Met - Cys- | 69511258.05 | 61.657661 | Hydrophobic - Negative Charge |
| Met - Tyr- | 446732.3568 | 61.657661 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 620257.8114 | 61.657661 | Aromatic - Aromatic |
| His:ND1 - Phe | 6351550.315 | 61.657661 | Aromatic - Aromatic |
| His:ND1 - Tyr | 4106628.812 | 61.657661 | Aromatic - Aromatic |
| His:ND1 - Trp | 1250712.299 | 61.657661 | Aromatic - Aromatic |
| His:ND1 - Ser | 186337.7276 | 61.657661 | Aromatic - Polar |
| His:ND1 - Thr | 572992.3006 | 61.657661 | Aromatic - Polar |
| His:ND1 - Cys | 5292487.717 | 61.657661 | Aromatic - Polar |
| His:ND1 - Asn | 3232025.846 | 61.657661 | Aromatic - Polar |
| His:ND1 - Gln | 6612458.594 | 61.657661 | Aromatic - Polar |
| His:ND1 - Arg:NE | 5050579.583 | 61.657661 | Aromatic - Polar |
| His:ND1 - Arg:NH | 8241350.658 | 61.657661 | Aromatic - Polar |
| His:ND1 - Asp:H | 2406040.897 | 61.657661 | Aromatic - Polar |
| His:ND1 - Glu:H | 4576578.022 | 61.657661 | Aromatic - Polar |
| His:ND1 - LysN | 8799495.888 | 61.657661 | Aromatic - Polar |
| His:ND1 - Arg | 64629.73397 | 61.657661 | Aromatic - Positive Charge |
| His:ND1 - His+ | 11571282.01 | 61.657661 | Aromatic - Positive Charge |
| His:ND1 - Lys | 3918803.331 | 61.657661 | Aromatic - Positive Charge |
| His:ND1 - Asp | 49903471.69 | 61.657661 | Aromatic - Negative Charge |
| His:ND1 - Glu | 28723129.85 | 61.657661 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 118987519.9 | 61.657661 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 11117751.88 | 61.657661 | Aromatic - Negative Charge |
| His:NE2 - Phe | 2749159.102 | 61.657661 | Aromatic - Aromatic |
| His:NE2 - Tyr | 1396122.299 | 61.657661 | Aromatic - Aromatic |
| His:NE2 - Trp | 76742.64459 | 61.657661 | Aromatic - Aromatic |
| His:NE2 - Ser | 1494034.459 | 61.657661 | Aromatic - Polar |
| His:NE2 - Thr | 2437850.278 | 61.657661 | Aromatic - Polar |
| His:NE2 - Cys | 2108023.394 | 61.657661 | Aromatic - Polar |
| His:NE2 - Asn | 1004362.477 | 61.657661 | Aromatic - Polar |
| His:NE2 - Gln | 3032563.472 | 61.657661 | Aromatic - Polar |
| His:NE2 - Arg:NE | 1958386.543 | 61.657661 | Aromatic - Polar |
| His:NE2 - Arg:NH | 4088248.339 | 61.657661 | Aromatic - Polar |
| His:NE2 - Asp:H | 5240083.589 | 61.657661 | Aromatic - Polar |
| His:NE2 - Glu:H | 1704551.607 | 61.657661 | Aromatic - Polar |
| His:NE2 - LysN | 4490269.482 | 61.657661 | Aromatic - Polar |
| His:NE2 - Arg | 1111906.703 | 61.657661 | Aromatic - Positive Charge |
| His:NE2 - His+ | 16802174.59 | 61.657661 | Aromatic - Positive Charge |
| His:NE2 - Lys | 1308766.886 | 61.657661 | Aromatic - Positive Charge |
| His:NE2 - Asp | 37574348.32 | 61.657661 | Aromatic - Negative Charge |
| His:NE2 - Glu | 19750825.45 | 61.657661 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 97988504.76 | 61.657661 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 6029279.561 | 61.657661 | Aromatic - Negative Charge |
| Phe – Tyr | 238198.323 | 61.657661 | Aromatic - Aromatic |
| Phe – Trp | 2172781.119 | 61.657661 | Aromatic - Aromatic |
| Phe – Ser | 9039864.576 | 61.657661 | Aromatic - Polar |
| Phe - Thr | 11686665.25 | 61.657661 | Aromatic - Polar |
| Phe - Cys | 39865.36126 | 61.657661 | Aromatic - Polar |
| Phe - Asn | 341924.2977 | 61.657661 | Aromatic - Polar |
| Phe - Gln | 22859.55334 | 61.657661 | Aromatic - Polar |
| Phe - Arg:NE | 65362.73198 | 61.657661 | Aromatic - Polar |
| Phe - Arg:NH | 177912.0995 | 61.657661 | Aromatic - Polar |
| Phe - Asp:H | 16314341.54 | 61.657661 | Aromatic - Polar |
| Phe - Glu:H | 109179.3549 | 61.657661 | Aromatic - Polar |
| Phe - LysN | 280972.5174 | 61.657661 | Aromatic - Polar |
| Phe - Arg | 8099178.797 | 61.657661 | Aromatic - Positive Charge |
| Phe - His+ | 34901898.87 | 61.657661 | Aromatic - Positive Charge |
| Phe - Lys | 260669.1195 | 61.657661 | Aromatic - Positive Charge |
| Phe - Asp | 22515620.86 | 61.657661 | Aromatic - Negative Charge |
| Phe - Glu | 8691824.499 | 61.657661 | Aromatic - Negative Charge |
| Phe - Cys- | 76079793.74 | 61.657661 | Aromatic - Negative Charge |
| Phe - Tyr- | 707834.8514 | 61.657661 | Aromatic - Negative Charge |
| Tyr - Trp | 936248.1205 | 61.657661 | Aromatic - Aromatic |
| Tyr - Ser | 6252089.695 | 61.657661 | Aromatic - Polar |
| Tyr - Thr | 8370660.706 | 61.657661 | Aromatic - Polar |
| Tyr - Cys | 81099.35557 | 61.657661 | Aromatic - Polar |
| Tyr - Asn | 15236.18168 | 61.657661 | Aromatic - Polar |
| Tyr - Gln | 382613.3582 | 61.657661 | Aromatic - Polar |
| Tyr - Arg:NE | 52664.38189 | 61.657661 | Aromatic - Polar |
| Tyr - Arg:NH | 799862.5713 | 61.657661 | Aromatic - Polar |
| Tyr - Asp:H | 12595843.78 | 61.657661 | Aromatic - Polar |
| Tyr - Glu:H | 21932.58504 | 61.657661 | Aromatic - Polar |
| Tyr - LysN | 999614.002 | 61.657661 | Aromatic - Polar |
| Tyr - Arg | 5459351.5 | 61.657661 | Aromatic - Positive Charge |
| Tyr - His+ | 29273311.36 | 61.657661 | Aromatic - Positive Charge |
| Tyr - Lys | 753.2659975 | 61.657661 | Aromatic - Positive Charge |
| Tyr - Asp | 26842093.83 | 61.657661 | Aromatic - Negative Charge |
| Tyr - Glu | 11606629.53 | 61.657661 | Aromatic - Negative Charge |
| Tyr - Cys- | 83202589.51 | 61.657661 | Aromatic - Negative Charge |
| Tyr - Tyr- | 1747093.073 | 61.657661 | Aromatic - Negative Charge |
| Trp - Ser | 2517099.278 | 61.657661 | Aromatic - Polar |
| Trp - Thr | 3845696.082 | 61.657661 | Aromatic - Polar |
| Trp - Cys | 1576485.132 | 61.657661 | Aromatic - Polar |
| Trp - Asn | 618307.2487 | 61.657661 | Aromatic - Polar |
| Trp - Gln | 2452238.842 | 61.657661 | Aromatic - Polar |
| Trp - Arg:NE | 1439238.218 | 61.657661 | Aromatic - Polar |
| Trp - Arg:NH | 3470050.77 | 61.657661 | Aromatic - Polar |
| Trp - Asp:H | 7255689.133 | 61.657661 | Aromatic - Polar |
| Trp - Glu:H | 1213935.482 | 61.657661 | Aromatic - Polar |
| Trp - LysN | 3865531.259 | 61.657661 | Aromatic - Polar |
| Trp - Arg | 1993402.569 | 61.657661 | Aromatic - Positive Charge |
| Trp - His+ | 21121645.89 | 61.657661 | Aromatic - Positive Charge |
| Trp - Lys | 863430.1674 | 61.657661 | Aromatic - Positive Charge |
| Trp - Asp | 38845002.98 | 61.657661 | Aromatic - Negative Charge |
| Trp - Glu | 19741375.35 | 61.657661 | Aromatic - Negative Charge |
| Trp - Cys- | 104958963.6 | 61.657661 | Aromatic - Negative Charge |
| Trp - Tyr- | 5400777.197 | 61.657661 | Aromatic - Negative Charge |
| Ser - Thr | 101593.7031 | 61.657661 | Polar - Polar |
| Ser - Cys | 7716138.067 | 61.657661 | Polar - Polar |
| Ser - Asn | 5022047.706 | 61.657661 | Polar - Polar |
| Ser - Gln | 9231283.066 | 61.657661 | Polar - Polar |
| Ser - Arg:NE | 7419996.625 | 61.657661 | Polar - Polar |
| Ser - Arg:NH | 11224008.37 | 61.657661 | Polar - Polar |
| Ser - Asp:H | 1332391.002 | 61.657661 | Polar - Polar |
| Ser - Glu:H | 6795472.309 | 61.657661 | Polar - Polar |
| Ser - LysN | 11869934.93 | 61.657661 | Polar - Polar |
| Ser - Arg | 33783.21847 | 61.657661 | Polar - Positive Charge |
| Ser - His+ | 9211620.003 | 61.657661 | Polar - Positive Charge |
| Ser - Lys | 5991070.145 | 61.657661 | Polar - Positive Charge |
| Ser - Asp | 57939272.21 | 61.657661 | Polar - Negative Charge |
| Ser - Glu | 34682477.59 | 61.657661 | Polar - Negative Charge |
| Ser - Cys- | 132618172.6 | 61.657661 | Polar - Negative Charge |
| Ser - Tyr- | 14700461.65 | 61.657661 | Polar - Negative Charge |
| Thr- Cys | 10096687.57 | 61.657661 | Polar - Polar |
| Thr - Asn | 6764543.673 | 61.657661 | Polar - Polar |
| Thr - Gln | 11771245.14 | 61.657661 | Polar - Polar |
| Thr - Arg:NE | 9749162.42 | 61.657661 | Polar - Polar |
| Thr - Arg:NH | 14133376.97 | 61.657661 | Polar - Polar |
| Thr - Asp:H | 773985.2484 | 61.657661 | Polar - Polar |
| Thr - Glu:H | 8968243.007 | 61.657661 | Polar - Polar |
| Thr - LysN | 14861581.98 | 61.657661 | Polar - Polar |
| Thr - Arg | 260694.9906 | 61.657661 | Polar - Positive Charge |
| Thr - His+ | 7896036.598 | 61.657661 | Polar - Positive Charge |
| Thr - Lys | 8031687.47 | 61.657661 | Polar - Positive Charge |
| Thr - Asp | 66327990.22 | 61.657661 | Polar - Negative Charge |
| Thr - Glu | 40740299.25 | 61.657661 | Polar - Negative Charge |
| Thr - Cys- | 147859727.7 | 61.657661 | Polar - Negative Charge |
| Thr - Tyr- | 18237324.2 | 61.657661 | Polar - Negative Charge |
| Cys - Asn | 153765.8239 | 61.657661 | Polar - Polar |
| Cys - Gln | 116532.2845 | 61.657661 | Polar - Polar |
| Cys - Arg:NE | 3057.64952 | 61.657661 | Polar - Polar |
| Cys - Arg:NH | 374674.0477 | 61.657661 | Polar - Polar |
| Cys - Asp:H | 14531758.05 | 61.657661 | Polar - Polar |
| Cys - Glu:H | 17498.32936 | 61.657661 | Polar - Polar |
| Cys - LysN | 516215.4099 | 61.657661 | Polar - Polar |
| Cys - Arg | 6846462.297 | 61.657661 | Polar - Positive Charge |
| Cys - His+ | 32111193.44 | 61.657661 | Polar - Positive Charge |
| Cys - Lys | 95610.29209 | 61.657661 | Polar - Positive Charge |
| Cys - Asp | 23899604.15 | 61.657661 | Polar - Negative Charge |
| Cys - Glu | 9695090.038 | 61.657661 | Polar - Negative Charge |
| Cys - Cys- | 77820925 | 61.657661 | Polar - Negative Charge |
| Cys - Tyr- | 1064045.954 | 61.657661 | Polar - Negative Charge |
| Asn - Gln | 498321.1827 | 61.657661 | Polar - Polar |
| Asn - Arg:NE | 115568.4029 | 61.657661 | Polar - Polar |
| Asn - Arg:NH | 935958.5149 | 61.657661 | Polar - Polar |
| Asn - Asp:H | 10586679.77 | 61.657661 | Polar - Polar |
| Asn - Glu:H | 68476.53628 | 61.657661 | Polar - Polar |
| Asn - LysN | 1138750.918 | 61.657661 | Polar - Polar |
| Asn - Arg | 4339155.331 | 61.657661 | Polar - Positive Charge |
| Asn - His+ | 25311167.25 | 61.657661 | Polar - Positive Charge |
| Asn - Lys | 9282.092366 | 61.657661 | Polar - Positive Charge |
| Asn - Asp | 25167478.11 | 61.657661 | Polar - Negative Charge |
| Asn - Glu | 11139841.32 | 61.657661 | Polar - Negative Charge |
| Asn - Cys- | 76332029.63 | 61.657661 | Polar - Negative Charge |
| Asn - Tyr- | 1879448.62 | 61.657661 | Polar - Negative Charge |
| Gln - Arg:NE | 156181.9687 | 61.657661 | Polar - Polar |
| Gln - Arg:NH | 66423.89818 | 61.657661 | Polar - Polar |
| Gln - Asp:H | 16305083.53 | 61.657661 | Polar - Polar |
| Gln - Glu:H | 216471.5267 | 61.657661 | Polar - Polar |
| Gln - LysN | 131421.539 | 61.657661 | Polar - Polar |
| Gln - Arg | 8312633.383 | 61.657661 | Polar - Positive Charge |
| Gln - His+ | 34159798.75 | 61.657661 | Polar - Positive Charge |
| Gln - Lys | 408445.3192 | 61.657661 | Polar - Positive Charge |
| Gln - Asp | 19448740.77 | 61.657661 | Polar - Negative Charge |
| Gln - Glu | 7175059.574 | 61.657661 | Polar - Negative Charge |
| Gln - Cys- | 67722763.68 | 61.657661 | Polar - Negative Charge |
| Gln - Tyr- | 430245.0594 | 61.657661 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 444781.1413 | 61.657661 | Polar - Polar |
| Arg:NE - Asp:H | 14145290.23 | 61.657661 | Polar - Polar |
| Arg:NE - Glu:H | 6058.949455 | 61.657661 | Polar - Polar |
| Arg:NE - LysN | 597710.9076 | 61.657661 | Polar - Polar |
| Arg:NE - Arg | 6565016.086 | 61.657661 | Polar - Positive Charge |
| Arg:NE - His+ | 31550453.07 | 61.657661 | Polar - Positive Charge |
| Arg:NE - Lys | 64770.81581 | 61.657661 | Polar - Positive Charge |
| Arg:NE - Asp | 24458179.81 | 61.657661 | Polar - Negative Charge |
| Arg:NE - Glu | 10053043.74 | 61.657661 | Polar - Negative Charge |
| Arg:NE - Cys- | 78853717.06 | 61.657661 | Polar - Negative Charge |
| Arg:NE - Tyr- | 1183515.926 | 61.657661 | Polar - Negative Charge |
| Arg:NH - Asp:H | 18907781.24 | 61.657661 | Polar - Polar |
| Arg:NH - Glu:H | 538827.8538 | 61.657661 | Polar - Polar |
| Arg:NH - LysN | 11539.46442 | 61.657661 | Polar - Polar |
| Arg:NH - Arg | 10211902.31 | 61.657661 | Polar - Positive Charge |
| Arg:NH - His+ | 38134287.96 | 61.657661 | Polar - Positive Charge |
| Arg:NH - Lys | 832323.128 | 61.657661 | Polar - Positive Charge |
| Arg:NH - Asp | 17791893.3 | 61.657661 | Polar - Negative Charge |
| Arg:NH - Glu | 6031661.843 | 61.657661 | Polar - Negative Charge |
| Arg:NH - Cys- | 65606621.77 | 61.657661 | Polar - Negative Charge |
| Arg:NH - Tyr- | 158898.1197 | 61.657661 | Polar - Negative Charge |
| Asp:H - Glu:H | 13228232.23 | 61.657661 | Polar - Polar |
| Asp:H - LysN | 19679471.67 | 61.657661 | Polar - Polar |
| Asp:H - Arg | 1791685.111 | 61.657661 | Polar - Positive Charge |
| Asp:H - His+ | 3315394.065 | 61.657661 | Polar - Positive Charge |
| Asp:H - Lys | 12180754.79 | 61.657661 | Polar - Positive Charge |
| Asp:H - Asp | 70882470.61 | 61.657661 | Polar - Negative Charge |
| Asp:H - Glu | 46017133.09 | 61.657661 | Polar - Negative Charge |
| Asp:H - Cys- | 147448111.5 | 61.657661 | Polar - Negative Charge |
| Asp:H - Tyr- | 23310317.07 | 61.657661 | Polar - Negative Charge |
| Glu:H - LysN | 703071.802 | 61.657661 | Polar - Polar |
| Glu:H - Arg | 5983650.904 | 61.657661 | Polar - Positive Charge |
| Glu:H - His+ | 29937793.2 | 61.657661 | Polar - Positive Charge |
| Glu:H - Lys | 30137.55279 | 61.657661 | Polar - Positive Charge |
| Glu:H - Asp | 24498665.94 | 61.657661 | Polar - Negative Charge |
| Glu:H - Glu | 10245493.44 | 61.657661 | Polar - Negative Charge |
| Glu:H - Cys- | 77883242.65 | 61.657661 | Polar - Negative Charge |
| Glu:H - Tyr- | 1322456.22 | 61.657661 | Polar - Negative Charge |
| LysN - Arg | 10836942.01 | 61.657661 | Polar - Positive Charge |
| LysN - His+ | 39136421.01 | 61.657661 | Polar - Positive Charge |
| LysN – Lys | 1033631.111 | 61.657661 | Polar - Positive Charge |
| LysN - Asp | 16756849.77 | 61.657661 | Polar - Negative Charge |
| LysN – Glu | 5459206.216 | 61.657661 | Polar - Negative Charge |
| LysN - Cys- | 63360251.04 | 61.657661 | Polar - Negative Charge |
| LysN - Tyr- | 82351.57381 | 61.657661 | Polar - Negative Charge |
| Arg - His+ | 10436547.77 | 61.657661 | Positive Charge - Positive Charge |
| Arg – Lys | 5220328.712 | 61.657661 | Positive Charge - Positive Charge |
| Arg - Asp | 56145152.25 | 61.657661 | Positive Charge - Negative Charge |
| Arg - Glu | 33112476.95 | 61.657661 | Positive Charge - Negative Charge |
| Arg - Cys- | 130670151.8 | 61.657661 | Positive Charge - Negative Charge |
| Arg - Tyr- | 13547073.84 | 61.657661 | Positive Charge - Negative Charge |
| His+ - Lys | 28473875.94 | 61.657661 | Positive Charge - Positive Charge |
| His+ - Asp | 103983580.5 | 61.657661 | Positive Charge - Negative Charge |
| His+ - Glu | 74075888.88 | 61.657661 | Positive Charge - Negative Charge |
| His+ - Cys- | 192305286.5 | 61.657661 | Positive Charge - Negative Charge |
| His+ - Tyr- | 44705770.28 | 61.657661 | Positive Charge - Negative Charge |
| Lys - Asp | 26570261.96 | 61.657661 | Positive Charge - Negative Charge |
| Lys - Glu | 11548510.22 | 61.657661 | Positive Charge - Negative Charge |
| Lys - Cys- | 81975895.29 | 61.657661 | Positive Charge - Negative Charge |
| Lys - Tyr- | 1783267.071 | 61.657661 | Positive Charge - Negative Charge |
| Asp - Glu | 3365830.094 | 61.657661 | Negative Charge - Negative Charge |
| Asp - Cys- | 15246484.34 | 61.657661 | Negative Charge - Negative Charge |
| Asp - Tyr- | 15386233.97 | 61.657661 | Negative Charge - Negative Charge |
| Glu - Cys- | 33611824.94 | 61.657661 | Negative Charge - Negative Charge |
| Glu - Tyr- | 4460322.21 | 61.657661 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 62449068.88 | 61.657661 | Negative Charge - Negative Charge |

**Table S14.** Non-statistically significant pairwise comparisons of the f dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Met - Gln | 14.26388857 | 61.657661 | Hydrophobic - Polar |

**Table S15.** Statistically significant pairwise comparisons of the y dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 20338135.31 | 61.65766093 | Hydrophobic - Hydrophobic |
| Ala - Leu | 7237730.469 | 61.65766093 | Hydrophobic - Hydrophobic |
| Ala - Ile | 23124023.13 | 61.65766093 | Hydrophobic - Hydrophobic |
| Ala - Met | 1129608.995 | 61.65766093 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 3824498.469 | 61.65766093 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 2594072.66 | 61.65766093 | Hydrophobic - Aromatic |
| Ala - Phe | 9550445.4 | 61.65766093 | Hydrophobic - Aromatic |
| Ala - Tyr | 10334554.44 | 61.65766093 | Hydrophobic - Aromatic |
| Ala - Trp | 13122461.92 | 61.65766093 | Hydrophobic - Aromatic |
| Ala - Ser | 3549489.656 | 61.65766093 | Hydrophobic - Polar |
| Ala - Thr | 1872057.937 | 61.65766093 | Hydrophobic - Polar |
| Ala - Cys | 6720830.933 | 61.65766093 | Hydrophobic - Polar |
| Ala - Asn | 4810241.972 | 61.65766093 | Hydrophobic - Polar |
| Ala - Gln | 818324.0968 | 61.65766093 | Hydrophobic - Polar |
| Ala - Arg:NE | 142292.4679 | 61.65766093 | Hydrophobic - Polar |
| Ala - Arg:NH | 823964.3176 | 61.65766093 | Hydrophobic - Polar |
| Ala - Asp:H | 1104029.586 | 61.65766093 | Hydrophobic - Polar |
| Ala - Glu:H | 1602414.298 | 61.65766093 | Hydrophobic - Polar |
| Ala - LysN | 1129298.926 | 61.65766093 | Hydrophobic - Polar |
| Ala - Arg | 592197.0513 | 61.65766093 | Hydrophobic - Positive Charge |
| Ala - His+ | 3926781.253 | 61.65766093 | Hydrophobic - Positive Charge |
| Ala - Lys | 740667.3479 | 61.65766093 | Hydrophobic - Positive Charge |
| Ala - Asp | 377392.5403 | 61.65766093 | Hydrophobic - Negative Charge |
| Ala - Glu | 1453518.099 | 61.65766093 | Hydrophobic - Negative Charge |
| Ala - Cys- | 969691.8026 | 61.65766093 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 1817681.929 | 61.65766093 | Hydrophobic - Negative Charge |
| Val - Leu | 2781665.247 | 61.65766093 | Hydrophobic - Hydrophobic |
| Val - Ile | 114891.3178 | 61.65766093 | Hydrophobic - Hydrophobic |
| Val - Met | 11215227.11 | 61.65766093 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 5676859.833 | 61.65766093 | Hydrophobic - Aromatic |
| Val - His:NE2 | 7050610.14 | 61.65766093 | Hydrophobic - Aromatic |
| Val - Phe | 1861364.595 | 61.65766093 | Hydrophobic - Aromatic |
| Val - Tyr | 1416732.853 | 61.65766093 | Hydrophobic - Aromatic |
| Val - Trp | 713508.4568 | 61.65766093 | Hydrophobic - Aromatic |
| Val - Ser | 6386752.367 | 61.65766093 | Hydrophobic - Polar |
| Val - Thr | 10221790.29 | 61.65766093 | Hydrophobic - Polar |
| Val - Cys | 3353216.234 | 61.65766093 | Hydrophobic - Polar |
| Val - Asn | 3981052.969 | 61.65766093 | Hydrophobic - Polar |
| Val - Gln | 11936053.55 | 61.65766093 | Hydrophobic - Polar |
| Val - Arg:NE | 17166425.55 | 61.65766093 | Hydrophobic - Polar |
| Val - Arg:NH | 12447354.85 | 61.65766093 | Hydrophobic - Polar |
| Val - Asp:H | 10086354.23 | 61.65766093 | Hydrophobic - Polar |
| Val - Glu:H | 9892073.462 | 61.65766093 | Hydrophobic - Polar |
| Val - LysN | 11211888.04 | 61.65766093 | Hydrophobic - Polar |
| Val - Arg | 13914540.4 | 61.65766093 | Hydrophobic - Positive Charge |
| Val - His+ | 4587605.165 | 61.65766093 | Hydrophobic - Positive Charge |
| Val - Lys | 12929036.43 | 61.65766093 | Hydrophobic - Positive Charge |
| Val - Asp | 15019684.87 | 61.65766093 | Hydrophobic - Negative Charge |
| Val - Glu | 11049809.26 | 61.65766093 | Hydrophobic - Negative Charge |
| Val - Cys- | 12264599.14 | 61.65766093 | Hydrophobic - Negative Charge |
| Val - Tyr- | 10169767.16 | 61.65766093 | Hydrophobic - Negative Charge |
| Leu - Ile | 3920383.3 | 61.65766093 | Hydrophobic - Hydrophobic |
| Leu - Met | 2581277.769 | 61.65766093 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 490139.6737 | 61.65766093 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 987086.7524 | 61.65766093 | Hydrophobic - Aromatic |
| Leu - Phe | 109492.3837 | 61.65766093 | Hydrophobic - Aromatic |
| Leu - Tyr | 230437.6009 | 61.65766093 | Hydrophobic - Aromatic |
| Leu - Trp | 701347.3459 | 61.65766093 | Hydrophobic - Aromatic |
| Leu - Ser | 657596.8593 | 61.65766093 | Hydrophobic - Polar |
| Leu - Thr | 1949889.724 | 61.65766093 | Hydrophobic - Polar |
| Leu - Cys | 17547.40547 | 61.65766093 | Hydrophobic - Polar |
| Leu - Asn | 147293.3498 | 61.65766093 | Hydrophobic - Polar |
| Leu - Gln | 2996212.514 | 61.65766093 | Hydrophobic - Polar |
| Leu - Arg:NE | 5431963.82 | 61.65766093 | Hydrophobic - Polar |
| Leu - Arg:NH | 3133904.598 | 61.65766093 | Hydrophobic - Polar |
| Leu - Asp:H | 2294881.856 | 61.65766093 | Hydrophobic - Polar |
| Leu - Glu:H | 1986703.94 | 61.65766093 | Hydrophobic - Polar |
| Leu - LysN | 2580580.325 | 61.65766093 | Hydrophobic - Polar |
| Leu - Arg | 3761308.19 | 61.65766093 | Hydrophobic - Positive Charge |
| Leu - His+ | 304498.2097 | 61.65766093 | Hydrophobic - Positive Charge |
| Leu - Lys | 3338882.277 | 61.65766093 | Hydrophobic - Positive Charge |
| Leu - Asp | 4344265.689 | 61.65766093 | Hydrophobic - Negative Charge |
| Leu - Glu | 2352807.293 | 61.65766093 | Hydrophobic - Negative Charge |
| Leu - Cys- | 2971875.771 | 61.65766093 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 1960282.491 | 61.65766093 | Hydrophobic - Negative Charge |
| Ile - Met | 13329442.51 | 61.65766093 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 7222331.099 | 61.65766093 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 8719590.622 | 61.65766093 | Hydrophobic - Aromatic |
| Ile - Phe | 2843530.33 | 61.65766093 | Hydrophobic - Aromatic |
| Ile - Tyr | 2280179.165 | 61.65766093 | Hydrophobic - Aromatic |
| Ile - Trp | 1374301.336 | 61.65766093 | Hydrophobic - Aromatic |
| Ile - Ser | 8042698.391 | 61.65766093 | Hydrophobic - Polar |
| Ile - Thr | 12325672.91 | 61.65766093 | Hydrophobic - Polar |
| Ile - Cys | 4608502.475 | 61.65766093 | Hydrophobic - Polar |
| Ile - Asn | 5255414.479 | 61.65766093 | Hydrophobic - Polar |
| Ile - Gln | 14081731.8 | 61.65766093 | Hydrophobic - Polar |
| Ile - Arg:NE | 19765846.74 | 61.65766093 | Hydrophobic - Polar |
| Ile - Arg:NH | 14670917.58 | 61.65766093 | Hydrophobic - Polar |
| Ile - Asp:H | 12019030.43 | 61.65766093 | Hydrophobic - Polar |
| Ile - Glu:H | 11894308.88 | 61.65766093 | Hydrophobic - Polar |
| Ile - LysN | 13325517.04 | 61.65766093 | Hydrophobic - Polar |
| Ile - Arg | 16280815.57 | 61.65766093 | Hydrophobic - Positive Charge |
| Ile - His+ | 5921099.395 | 61.65766093 | Hydrophobic - Positive Charge |
| Ile - Lys | 15199726.18 | 61.65766093 | Hydrophobic - Positive Charge |
| Ile - Asp | 17459057.54 | 61.65766093 | Hydrophobic - Negative Charge |
| Ile - Glu | 13207910.42 | 61.65766093 | Hydrophobic - Negative Charge |
| Ile - Cys- | 14499813.25 | 61.65766093 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 12255714.26 | 61.65766093 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 794867.7902 | 61.65766093 | Hydrophobic - Aromatic |
| Met - His:NE2 | 324744.2479 | 61.65766093 | Hydrophobic - Aromatic |
| Met - Phe | 3901713.422 | 61.65766093 | Hydrophobic - Aromatic |
| Met - Tyr | 4447188.047 | 61.65766093 | Hydrophobic - Aromatic |
| Met - Trp | 6213015.819 | 61.65766093 | Hydrophobic - Aromatic |
| Met - Ser | 647460.3132 | 61.65766093 | Hydrophobic - Polar |
| Met - Thr | 70198.88874 | 61.65766093 | Hydrophobic - Polar |
| Met - Cys | 2236296.545 | 61.65766093 | Hydrophobic - Polar |
| Met - Asn | 1343884.547 | 61.65766093 | Hydrophobic - Polar |
| Met - Gln | 20597.05511 | 61.65766093 | Hydrophobic - Polar |
| Met - Arg:NE | 483739.5528 | 61.65766093 | Hydrophobic - Polar |
| Met - Arg:NH | 24748.83842 | 61.65766093 | Hydrophobic - Polar |
| Met - Asp:H | 864.7423323 | 61.65766093 | Hydrophobic - Polar |
| Met - Glu:H | 39649.26853 | 61.65766093 | Hydrophobic - Polar |
| Met - Arg | 94078.31922 | 61.65766093 | Hydrophobic - Positive Charge |
| Met - His+ | 934589.2872 | 61.65766093 | Hydrophobic - Positive Charge |
| Met - Lys | 43257.72233 | 61.65766093 | Hydrophobic - Positive Charge |
| Met - Asp | 208499.2891 | 61.65766093 | Hydrophobic - Negative Charge |
| Met - Glu | 12928.72456 | 61.65766093 | Hydrophobic - Negative Charge |
| Met - Cys- | 8669.71461 | 61.65766093 | Hydrophobic - Negative Charge |
| Met - Tyr- | 63315.42338 | 61.65766093 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 91926.50331 | 61.65766093 | Aromatic - Aromatic |
| His:ND1 - Phe | 1089784.86 | 61.65766093 | Aromatic - Aromatic |
| His:ND1 - Tyr | 1404247.29 | 61.65766093 | Aromatic - Aromatic |
| His:ND1 - Trp | 2402491.679 | 61.65766093 | Aromatic - Aromatic |
| His:ND1 - Ser | 9864.852688 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Thr | 434162.9227 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Cys | 334113.2625 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Asn | 85452.4648 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Gln | 1047225.066 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Arg:NE | 2546858.354 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Arg:NH | 1104266.421 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Asp:H | 686399.344 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Glu:H | 483533.158 | 61.65766093 | Aromatic - Polar |
| His:ND1 - LysN | 794657.5456 | 61.65766093 | Aromatic - Polar |
| His:ND1 - Arg | 1462863.466 | 61.65766093 | Aromatic - Positive Charge |
| His:ND1 - His+ | 13240.34076 | 61.65766093 | Aromatic - Positive Charge |
| His:ND1 - Lys | 1219802.826 | 61.65766093 | Aromatic - Positive Charge |
| His:ND1 - Asp | 1836726.639 | 61.65766093 | Aromatic - Negative Charge |
| His:ND1 - Glu | 641900.5794 | 61.65766093 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 993805.1642 | 61.65766093 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 444710.0758 | 61.65766093 | Aromatic - Negative Charge |
| His:NE2 - Phe | 1787954.673 | 61.65766093 | Aromatic - Aromatic |
| His:NE2 - Tyr | 2170268.559 | 61.65766093 | Aromatic - Aromatic |
| His:NE2 - Trp | 3368282.639 | 61.65766093 | Aromatic - Aromatic |
| His:NE2 - Ser | 44086.07841 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Thr | 109383.5126 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Cys | 769465.1374 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Asn | 338619.6076 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Gln | 494486.4017 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Arg:NE | 1576780.121 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Arg:NH | 525709.9526 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Asp:H | 270665.475 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Glu:H | 141943.9262 | 61.65766093 | Aromatic - Polar |
| His:NE2 - LysN | 324661.4584 | 61.65766093 | Aromatic - Polar |
| His:NE2 - Arg | 768839.8973 | 61.65766093 | Aromatic - Positive Charge |
| His:NE2 - His+ | 162557.9913 | 61.65766093 | Aromatic - Positive Charge |
| His:NE2 - Lys | 602841.7345 | 61.65766093 | Aromatic - Positive Charge |
| His:NE2 - Asp | 1042449.279 | 61.65766093 | Aromatic - Negative Charge |
| His:NE2 - Glu | 223757.0723 | 61.65766093 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 446876.6081 | 61.65766093 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 115871.1665 | 61.65766093 | Aromatic - Negative Charge |
| Phe - Tyr | 24341.55131 | 61.65766093 | Aromatic - Aromatic |
| Phe - Trp | 267427.6327 | 61.65766093 | Aromatic - Aromatic |
| Phe - Ser | 1352786.938 | 61.65766093 | Aromatic - Polar |
| Phe - Thr | 3148509.524 | 61.65766093 | Aromatic - Polar |
| Phe - Cys | 222034.1163 | 61.65766093 | Aromatic - Polar |
| Phe - Asn | 503016.5407 | 61.65766093 | Aromatic - Polar |
| Phe - Gln | 4398788.257 | 61.65766093 | Aromatic - Polar |
| Phe - Arg:NE | 7422308.443 | 61.65766093 | Aromatic - Polar |
| Phe - Arg:NH | 4598706.885 | 61.65766093 | Aromatic - Polar |
| Phe - Asp:H | 3478486.945 | 61.65766093 | Aromatic - Polar |
| Phe - Glu:H | 3147277.493 | 61.65766093 | Aromatic - Polar |
| Phe - LysN | 3900607.721 | 61.65766093 | Aromatic - Polar |
| Phe - Arg | 5396446.758 | 61.65766093 | Aromatic - Positive Charge |
| Phe - His+ | 766022.4726 | 61.65766093 | Aromatic - Positive Charge |
| Phe - Lys | 4859824.154 | 61.65766093 | Aromatic - Positive Charge |
| Phe - Asp | 6100792.309 | 61.65766093 | Aromatic - Negative Charge |
| Phe - Glu | 3654541.337 | 61.65766093 | Aromatic - Negative Charge |
| Phe - Cys- | 4417667.156 | 61.65766093 | Aromatic - Negative Charge |
| Phe - Tyr- | 3153075.087 | 61.65766093 | Aromatic - Negative Charge |
| Tyr - Trp | 125873.3586 | 61.65766093 | Aromatic - Aromatic |
| Tyr - Ser | 1703226.125 | 61.65766093 | Aromatic - Polar |
| Tyr - Thr | 3663515.809 | 61.65766093 | Aromatic - Polar |
| Tyr - Cys | 385613.0435 | 61.65766093 | Aromatic - Polar |
| Tyr - Asn | 720941.4203 | 61.65766093 | Aromatic - Polar |
| Tyr - Gln | 4965515.753 | 61.65766093 | Aromatic - Polar |
| Tyr - Arg:NE | 8138259.506 | 61.65766093 | Aromatic - Polar |
| Tyr - Arg:NH | 5184197.285 | 61.65766093 | Aromatic - Polar |
| Tyr - Asp:H | 3979812.115 | 61.65766093 | Aromatic - Polar |
| Tyr - Glu:H | 3646823.874 | 61.65766093 | Aromatic - Polar |
| Tyr - LysN | 4445950.855 | 61.65766093 | Aromatic - Polar |
| Tyr - Arg | 6027667.62 | 61.65766093 | Aromatic - Positive Charge |
| Tyr - His+ | 1023085.418 | 61.65766093 | Aromatic - Positive Charge |
| Tyr - Lys | 5460655.814 | 61.65766093 | Aromatic - Positive Charge |
| Tyr - Asp | 6761651.079 | 61.65766093 | Aromatic - Negative Charge |
| Tyr - Glu | 4198003.446 | 61.65766093 | Aromatic - Negative Charge |
| Tyr - Cys- | 4999445.519 | 61.65766093 | Aromatic - Negative Charge |
| Tyr - Tyr- | 3665590.579 | 61.65766093 | Aromatic - Negative Charge |
| Trp - Ser | 2816426.312 | 61.65766093 | Aromatic - Polar |
| Trp - Thr | 5335018.832 | 61.65766093 | Aromatic - Polar |
| Trp - Cys | 972104.2918 | 61.65766093 | Aromatic - Polar |
| Trp - Asn | 1431807.903 | 61.65766093 | Aromatic - Polar |
| Trp - Gln | 6804981.477 | 61.65766093 | Aromatic - Polar |
| Trp - Arg:NE | 10607113.07 | 61.65766093 | Aromatic - Polar |
| Trp - Arg:NH | 7102891.561 | 61.65766093 | Aromatic - Polar |
| Trp - Asp:H | 5568557.9 | 61.65766093 | Aromatic - Polar |
| Trp - Glu:H | 5247611.691 | 61.65766093 | Aromatic - Polar |
| Trp - LysN | 6211228.572 | 61.65766093 | Aromatic - Polar |
| Trp - Arg | 8133420.978 | 61.65766093 | Aromatic - Positive Charge |
| Trp - His+ | 1836643.652 | 61.65766093 | Aromatic - Positive Charge |
| Trp - Lys | 7440936.19 | 61.65766093 | Aromatic - Positive Charge |
| Trp - Asp | 8988300.193 | 61.65766093 | Aromatic - Negative Charge |
| Trp - Glu | 5968786.252 | 61.65766093 | Aromatic - Negative Charge |
| Trp - Cys- | 6909320.835 | 61.65766093 | Aromatic - Negative Charge |
| Trp - Tyr- | 5325242.788 | 61.65766093 | Aromatic - Negative Charge |
| Ser - Thr | 320083.661 | 61.65766093 | Polar - Polar |
| Ser - Cys | 474142.2198 | 61.65766093 | Polar - Polar |
| Ser - Asn | 154163.5902 | 61.65766093 | Polar - Polar |
| Ser - Gln | 882190.5811 | 61.65766093 | Polar - Polar |
| Ser - Arg:NE | 2305943.596 | 61.65766093 | Polar - Polar |
| Ser - Arg:NH | 933232.3924 | 61.65766093 | Polar - Polar |
| Ser - Asp:H | 552986.6136 | 61.65766093 | Polar - Polar |
| Ser - Glu:H | 366543.5321 | 61.65766093 | Polar - Polar |
| Ser - LysN | 647283.9528 | 61.65766093 | Polar - Polar |
| Ser - Arg | 1268499.446 | 61.65766093 | Polar - Positive Charge |
| Ser - His+ | 44658.28068 | 61.65766093 | Polar - Positive Charge |
| Ser - Lys | 1040775.795 | 61.65766093 | Polar - Positive Charge |
| Ser - Asp | 1624291.811 | 61.65766093 | Polar - Negative Charge |
| Ser - Glu | 505475.1829 | 61.65766093 | Polar - Negative Charge |
| Ser - Cys- | 829000.1517 | 61.65766093 | Polar - Negative Charge |
| Ser - Tyr- | 329849.8293 | 61.65766093 | Polar - Negative Charge |
| Thr - Cys | 1635983.713 | 61.65766093 | Polar - Polar |
| Thr - Asn | 886667.3654 | 61.65766093 | Polar - Polar |
| Thr - Gln | 167966.7243 | 61.65766093 | Polar - Polar |
| Thr - Arg:NE | 979747.3059 | 61.65766093 | Polar - Polar |
| Thr - Arg:NH | 183820.3108 | 61.65766093 | Polar - Polar |
| Thr - Asp:H | 50056.52966 | 61.65766093 | Polar - Polar |
| Thr - Glu:H | 3530.581938 | 61.65766093 | Polar - Polar |
| Thr - LysN | 70178.71568 | 61.65766093 | Polar - Polar |
| Thr - Arg | 344533.1034 | 61.65766093 | Polar - Positive Charge |
| Thr - His+ | 557030.7777 | 61.65766093 | Polar - Positive Charge |
| Thr - Lys | 232615.3342 | 61.65766093 | Polar - Positive Charge |
| Thr - Asp | 549244.2741 | 61.65766093 | Polar - Negative Charge |
| Thr - Glu | 23836.31074 | 61.65766093 | Polar - Negative Charge |
| Thr - Cys- | 133631.1929 | 61.65766093 | Polar - Negative Charge |
| Thr - Tyr- | 149.4448877 | 61.65766093 | Polar - Negative Charge |
| Cys - Asn | 68340.36626 | 61.65766093 | Polar - Polar |
| Cys - Gln | 2632370.3 | 61.65766093 | Polar - Polar |
| Cys - Arg:NE | 4962377.973 | 61.65766093 | Polar - Polar |
| Cys - Arg:NH | 2758503.289 | 61.65766093 | Polar - Polar |
| Cys - Asp:H | 1977420.661 | 61.65766093 | Polar - Polar |
| Cys - Glu:H | 1678522.705 | 61.65766093 | Polar - Polar |
| Cys - LysN | 2235676.529 | 61.65766093 | Polar - Polar |
| Cys - Arg | 3353320.976 | 61.65766093 | Polar - Positive Charge |
| Cys - His+ | 187796.9825 | 61.65766093 | Polar - Positive Charge |
| Cys - Lys | 2952429.278 | 61.65766093 | Polar - Positive Charge |
| Cys - Asp | 3913671.962 | 61.65766093 | Polar - Negative Charge |
| Cys - Glu | 2014418.844 | 61.65766093 | Polar - Negative Charge |
| Cys - Cys- | 2601423.367 | 61.65766093 | Polar - Negative Charge |
| Cys - Tyr- | 1647141.987 | 61.65766093 | Polar - Negative Charge |
| Asn - Gln | 1649891.177 | 61.65766093 | Polar - Polar |
| Asn - Arg:NE | 3405730.082 | 61.65766093 | Polar - Polar |
| Asn - Arg:NH | 1728040.884 | 61.65766093 | Polar - Polar |
| Asn - Asp:H | 1186582.275 | 61.65766093 | Polar - Polar |
| Asn - Glu:H | 939586.1026 | 61.65766093 | Polar - Polar |
| Asn - LysN | 1343550.059 | 61.65766093 | Polar - Polar |
| Asn - Arg | 2163362.231 | 61.65766093 | Polar - Positive Charge |
| Asn - His+ | 28201.80314 | 61.65766093 | Polar - Positive Charge |
| Asn - Lys | 1869613.876 | 61.65766093 | Polar - Positive Charge |
| Asn - Asp | 2596783.293 | 61.65766093 | Polar - Negative Charge |
| Asn - Glu | 1160763.191 | 61.65766093 | Polar - Negative Charge |
| Asn - Cys- | 1599309.163 | 61.65766093 | Polar - Negative Charge |
| Asn - Tyr- | 898596.3517 | 61.65766093 | Polar - Negative Charge |
| Gln - Arg:NE | 292681.0936 | 61.65766093 | Polar - Polar |
| Gln - Arg:NH | 129.2852691 | 61.65766093 | Polar - Polar |
| Gln - Asp:H | 27951.85109 | 61.65766093 | Polar - Polar |
| Gln - Glu:H | 115897.9026 | 61.65766093 | Polar - Polar |
| Gln - LysN | 20591.65609 | 61.65766093 | Polar - Polar |
| Gln - Arg | 24709.88133 | 61.65766093 | Polar - Positive Charge |
| Gln - His+ | 1193094.033 | 61.65766093 | Polar - Positive Charge |
| Gln - Lys | 3704.719453 | 61.65766093 | Polar - Positive Charge |
| Gln - Asp | 93467.33168 | 61.65766093 | Polar - Negative Charge |
| Gln - Glu | 67260.93935 | 61.65766093 | Polar - Negative Charge |
| Gln - Cys- | 2876.882938 | 61.65766093 | Polar - Negative Charge |
| Gln - Tyr- | 156726.6413 | 61.65766093 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 289675.8683 | 61.65766093 | Polar - Polar |
| Arg:NE - Asp:H | 486826.2773 | 61.65766093 | Polar - Polar |
| Arg:NE - Glu:H | 808279.0055 | 61.65766093 | Polar - Polar |
| Arg:NE - LysN | 483605.3436 | 61.65766093 | Polar - Polar |
| Arg:NE - Arg | 155864.2096 | 61.65766093 | Polar - Positive Charge |
| Arg:NE - His+ | 2684481.079 | 61.65766093 | Polar - Positive Charge |
| Arg:NE - Lys | 239537.041 | 61.65766093 | Polar - Positive Charge |
| Arg:NE - Asp | 57598.77521 | 61.65766093 | Polar - Negative Charge |
| Arg:NE - Glu | 688160.8873 | 61.65766093 | Polar - Negative Charge |
| Arg:NE - Cys- | 373882.0171 | 61.65766093 | Polar - Negative Charge |
| Arg:NE - Tyr- | 944601.9678 | 61.65766093 | Polar - Negative Charge |
| Arg:NH - Asp:H | 32659.16818 | 61.65766093 | Polar - Polar |
| Arg:NH - Glu:H | 127746.5561 | 61.65766093 | Polar - Polar |
| Arg:NH - LysN | 24742.1425 | 61.65766093 | Polar - Polar |
| Arg:NH - Arg | 21930.37916 | 61.65766093 | Polar - Positive Charge |
| Arg:NH - His+ | 1251754.705 | 61.65766093 | Polar - Positive Charge |
| Arg:NH - Lys | 2525.542387 | 61.65766093 | Polar - Positive Charge |
| Arg:NH - Asp | 89442.50745 | 61.65766093 | Polar - Negative Charge |
| Arg:NH - Glu | 75903.86429 | 61.65766093 | Polar - Negative Charge |
| Arg:NH - Cys- | 4382.468961 | 61.65766093 | Polar - Negative Charge |
| Arg:NH - Tyr- | 171733.3371 | 61.65766093 | Polar - Negative Charge |
| Asp:H - Glu:H | 26235.73738 | 61.65766093 | Polar - Polar |
| Asp:H - LysN | 864.5276129 | 61.65766093 | Polar - Polar |
| Asp:H - Arg | 105223.1487 | 61.65766093 | Polar - Positive Charge |
| Asp:H - His+ | 819330.7184 | 61.65766093 | Polar - Positive Charge |
| Asp:H - Lys | 52654.34255 | 61.65766093 | Polar - Positive Charge |
| Asp:H - Asp | 219352.9728 | 61.65766093 | Polar - Negative Charge |
| Asp:H - Glu | 6242.617057 | 61.65766093 | Polar - Negative Charge |
| Asp:H - Cys- | 14215.77204 | 61.65766093 | Polar - Negative Charge |
| Asp:H - Tyr- | 44617.40382 | 61.65766093 | Polar - Negative Charge |
| Glu:H - LysN | 39638.58457 | 61.65766093 | Polar - Polar |
| Glu:H - Arg | 259541.9415 | 61.65766093 | Polar - Positive Charge |
| Glu:H - His+ | 607740.5644 | 61.65766093 | Polar - Positive Charge |
| Glu:H - Lys | 167222.4906 | 61.65766093 | Polar - Positive Charge |
| Glu:H - Asp | 434168.6732 | 61.65766093 | Polar - Negative Charge |
| Glu:H - Glu | 8159.683896 | 61.65766093 | Polar - Negative Charge |
| Glu:H - Cys- | 87224.1893 | 61.65766093 | Polar - Negative Charge |
| Glu:H - Tyr- | 2233.45956 | 61.65766093 | Polar - Negative Charge |
| LysN - Arg | 94052.25827 | 61.65766093 | Polar - Positive Charge |
| LysN - His+ | 934364.1226 | 61.65766093 | Polar - Positive Charge |
| LysN – Lys | 43245.9298 | 61.65766093 | Polar - Positive Charge |
| LysN - Asp | 208441.9157 | 61.65766093 | Polar - Negative Charge |
| LysN – Glu | 12925.07216 | 61.65766093 | Polar - Negative Charge |
| LysN - Cys- | 8667.31659 | 61.65766093 | Polar - Negative Charge |
| LysN - Tyr- | 63297.43792 | 61.65766093 | Polar - Negative Charge |
| Arg - His+ | 1613406.191 | 61.65766093 | Positive Charge - Positive Charge |
| Arg – Lys | 9566.480134 | 61.65766093 | Positive Charge - Positive Charge |
| Arg - Asp | 23506.91764 | 61.65766093 | Positive Charge - Negative Charge |
| Arg - Glu | 185227.2137 | 61.65766093 | Positive Charge - Negative Charge |
| Arg - Cys- | 47000.85726 | 61.65766093 | Positive Charge - Negative Charge |
| Arg - Tyr- | 326586.5635 | 61.65766093 | Positive Charge - Negative Charge |
| His+ - Lys | 1368908.753 | 61.65766093 | Positive Charge - Positive Charge |
| His+ - Asp | 1985747.402 | 61.65766093 | Positive Charge - Negative Charge |
| His+ - Glu | 776888.2243 | 61.65766093 | Positive Charge - Negative Charge |
| His+ - Cys- | 1139708.014 | 61.65766093 | Positive Charge - Negative Charge |
| His+ - Tyr- | 567973.7087 | 61.65766093 | Positive Charge - Negative Charge |
| Lys - Asp | 62272.00863 | 61.65766093 | Positive Charge - Negative Charge |
| Lys - Glu | 107568.533 | 61.65766093 | Positive Charge - Negative Charge |
| Lys - Cys- | 13754.71412 | 61.65766093 | Positive Charge - Negative Charge |
| Lys - Tyr- | 218635.4615 | 61.65766093 | Positive Charge - Negative Charge |
| Asp - Glu | 340755.5265 | 61.65766093 | Negative Charge - Negative Charge |
| Asp - Cys- | 136349.2178 | 61.65766093 | Negative Charge - Negative Charge |
| Asp - Tyr- | 525294.2508 | 61.65766093 | Negative Charge - Negative Charge |
| Glu - Cys- | 44537.0126 | 61.65766093 | Negative Charge - Negative Charge |
| Glu - Tyr- | 19975.55913 | 61.65766093 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 123480.8822 | 61.65766093 | Negative Charge - Negative Charge |

**Table S16.** Non-statistically significant pairwise comparisons of the y dihedral angles populating the b conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Met - LysN | 0 | 61.65766093 | Hydrophobic - Polar |

**Table S17.** Statistically significant pairwise comparisons of the f dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 753363.6154 | 61.65926145 | Hydrophobic - Hydrophobic |
| Ala - Leu | 483244.1663 | 61.65926145 | Hydrophobic - Hydrophobic |
| Ala - Ile | 653466.9029 | 61.65926145 | Hydrophobic - Hydrophobic |
| Ala - Met | 1497408.486 | 61.65926145 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 3559483.294 | 61.65926145 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 1981273.225 | 61.65926145 | Hydrophobic - Aromatic |
| Ala - Phe | 272200.2636 | 61.65926145 | Hydrophobic - Aromatic |
| Ala - Tyr | 613664.5664 | 61.65926145 | Hydrophobic - Aromatic |
| Ala - Trp | 1961818.592 | 61.65926145 | Hydrophobic - Aromatic |
| Ala - Ser | 189285.0926 | 61.65926145 | Hydrophobic - Polar |
| Ala - Thr | 76392.94755 | 61.65926145 | Hydrophobic - Polar |
| Ala - Cys | 163024.4238 | 61.65926145 | Hydrophobic - Polar |
| Ala - Asn | 3076113.976 | 61.65926145 | Hydrophobic - Polar |
| Ala - Gln | 1572757.589 | 61.65926145 | Hydrophobic - Polar |
| Ala - Arg:NE | 1260557.238 | 61.65926145 | Hydrophobic - Polar |
| Ala - Arg:NH | 793111.9596 | 61.65926145 | Hydrophobic - Polar |
| Ala - Asp:H | 9205360.82 | 61.65926145 | Hydrophobic - Polar |
| Ala - Glu:H | 2548729.343 | 61.65926145 | Hydrophobic - Polar |
| Ala - LysN | 933741.9746 | 61.65926145 | Hydrophobic - Polar |
| Ala - Arg | 3983693.341 | 61.65926145 | Hydrophobic - Positive Charge |
| Ala - His+ | 53720121.71 | 61.65926145 | Hydrophobic - Positive Charge |
| Ala - Lys | 1556623.541 | 61.65926145 | Hydrophobic - Positive Charge |
| Ala - Asp | 1633352.807 | 61.65926145 | Hydrophobic - Negative Charge |
| Ala - Glu | 22799.32091 | 61.65926145 | Hydrophobic - Negative Charge |
| Ala - Cys- | 12404473.07 | 61.65926145 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 1297118.448 | 61.65926145 | Hydrophobic - Negative Charge |
| Val - Leu | 1933519.823 | 61.65926145 | Hydrophobic - Hydrophobic |
| Val - Ile | 15532.72519 | 61.65926145 | Hydrophobic - Hydrophobic |
| Val - Met | 3137411.229 | 61.65926145 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 5099364.998 | 61.65926145 | Hydrophobic - Aromatic |
| Val - His:NE2 | 3628653.215 | 61.65926145 | Hydrophobic - Aromatic |
| Val - Phe | 1468985.12 | 61.65926145 | Hydrophobic - Aromatic |
| Val - Tyr | 2057667.948 | 61.65926145 | Hydrophobic - Aromatic |
| Val - Trp | 67388.67374 | 61.65926145 | Hydrophobic - Aromatic |
| Val - Ser | 1370314.109 | 61.65926145 | Hydrophobic - Polar |
| Val - Thr | 1064650.526 | 61.65926145 | Hydrophobic - Polar |
| Val - Cys | 1306129.081 | 61.65926145 | Hydrophobic - Polar |
| Val - Asn | 4638344.802 | 61.65926145 | Hydrophobic - Polar |
| Val - Gln | 3219321.875 | 61.65926145 | Hydrophobic - Polar |
| Val - Arg:NE | 2860095.004 | 61.65926145 | Hydrophobic - Polar |
| Val - Arg:NH | 2337151.399 | 61.65926145 | Hydrophobic - Polar |
| Val - Asp:H | 9361512.183 | 61.65926145 | Hydrophobic - Polar |
| Val - Glu:H | 4169700.663 | 61.65926145 | Hydrophobic - Polar |
| Val - LysN | 2496849.057 | 61.65926145 | Hydrophobic - Polar |
| Val - Arg | 5474243.289 | 61.65926145 | Hydrophobic - Positive Charge |
| Val - His+ | 38395673.73 | 61.65926145 | Hydrophobic - Positive Charge |
| Val - Lys | 3197695.634 | 61.65926145 | Hydrophobic - Positive Charge |
| Val - Asp | 5710.912451 | 61.65926145 | Hydrophobic - Negative Charge |
| Val - Glu | 927722.1082 | 61.65926145 | Hydrophobic - Negative Charge |
| Val - Cys- | 2711915.493 | 61.65926145 | Hydrophobic - Negative Charge |
| Val - Tyr- | 2717.94641 | 61.65926145 | Hydrophobic - Negative Charge |
| Leu - Ile | 1940782.877 | 61.65926145 | Hydrophobic - Hydrophobic |
| Leu - Met | 318234.3485 | 61.65926145 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 1634535.501 | 61.65926145 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 639061.0034 | 61.65926145 | Hydrophobic - Aromatic |
| Leu - Phe | 4163.462052 | 61.65926145 | Hydrophobic - Aromatic |
| Leu - Tyr | 24722.97471 | 61.65926145 | Hydrophobic - Aromatic |
| Leu - Trp | 4304544.221 | 61.65926145 | Hydrophobic - Aromatic |
| Leu - Ser | 41012.90607 | 61.65926145 | Hydrophobic - Polar |
| Leu - Thr | 112597.8475 | 61.65926145 | Hydrophobic - Polar |
| Leu - Cys | 51629.01275 | 61.65926145 | Hydrophobic - Polar |
| Leu - Asn | 1230938.645 | 61.65926145 | Hydrophobic - Polar |
| Leu - Gln | 329743.2698 | 61.65926145 | Hydrophobic - Polar |
| Leu - Arg:NE | 254720.4748 | 61.65926145 | Hydrophobic - Polar |
| Leu - Arg:NH | 47265.1299 | 61.65926145 | Hydrophobic - Polar |
| Leu - Asp:H | 5966758.857 | 61.65926145 | Hydrophobic - Polar |
| Leu - Glu:H | 913323.1249 | 61.65926145 | Hydrophobic - Polar |
| Leu - LysN | 99095.25488 | 61.65926145 | Hydrophobic - Polar |
| Leu - Arg | 1947784.831 | 61.65926145 | Hydrophobic - Positive Charge |
| Leu - His+ | 48586434.12 | 61.65926145 | Hydrophobic - Positive Charge |
| Leu - Lys | 356273.7849 | 61.65926145 | Hydrophobic - Positive Charge |
| Leu - Asp | 4121525.233 | 61.65926145 | Hydrophobic - Negative Charge |
| Leu - Glu | 259771.8481 | 61.65926145 | Hydrophobic - Negative Charge |
| Leu - Cys- | 19665075.71 | 61.65926145 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 3271192.763 | 61.65926145 | Hydrophobic - Negative Charge |
| Ile- Met | 3299936.277 | 61.65926145 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 5535238.444 | 61.65926145 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 3819782.319 | 61.65926145 | Hydrophobic - Aromatic |
| Ile - Phe | 1398985.884 | 61.65926145 | Hydrophobic - Aromatic |
| Ile - Tyr | 2053389.391 | 61.65926145 | Hydrophobic - Aromatic |
| Ile - Trp | 184885.0862 | 61.65926145 | Hydrophobic - Aromatic |
| Ile - Ser | 1302849.33 | 61.65926145 | Hydrophobic - Polar |
| Ile - Thr | 973395.5695 | 61.65926145 | Hydrophobic - Polar |
| Ile - Cys | 1232556.14 | 61.65926145 | Hydrophobic - Polar |
| Ile - Asn | 5048180.063 | 61.65926145 | Hydrophobic - Polar |
| Ile - Gln | 3412288.358 | 61.65926145 | Hydrophobic - Polar |
| Ile - Arg:NE | 2950235.361 | 61.65926145 | Hydrophobic - Polar |
| Ile - Arg:NH | 2388928.602 | 61.65926145 | Hydrophobic - Polar |
| Ile - Asp:H | 10683478.05 | 61.65926145 | Hydrophobic - Polar |
| Ile - Glu:H | 4487658.943 | 61.65926145 | Hydrophobic - Polar |
| Ile - LysN | 2558998.571 | 61.65926145 | Hydrophobic - Polar |
| Ile - Arg | 5964022.018 | 61.65926145 | Hydrophobic - Positive Charge |
| Ile - His+ | 45637625.66 | 61.65926145 | Hydrophobic - Positive Charge |
| Ile - Lys | 3362465.415 | 61.65926145 | Hydrophobic - Positive Charge |
| Ile - Asp | 57401.06228 | 61.65926145 | Hydrophobic - Negative Charge |
| Ile - Glu | 833590.8899 | 61.65926145 | Hydrophobic - Negative Charge |
| Ile - Cys- | 4006704.746 | 61.65926145 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 41285.05365 | 61.65926145 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 524593.5079 | 61.65926145 | Hydrophobic - Aromatic |
| Met - His:NE2 | 74259.26513 | 61.65926145 | Hydrophobic - Aromatic |
| Met - Phe | 283989.2916 | 61.65926145 | Hydrophobic - Aromatic |
| Met - Tyr | 125763.8031 | 61.65926145 | Hydrophobic - Aromatic |
| Met - Trp | 6428009.138 | 61.65926145 | Hydrophobic - Aromatic |
| Met - Ser | 500979.6661 | 61.65926145 | Hydrophobic - Polar |
| Met - Thr | 663367.689 | 61.65926145 | Hydrophobic - Polar |
| Met - Cys | 527079.5849 | 61.65926145 | Hydrophobic - Polar |
| Met - Asn | 277008.7962 | 61.65926145 | Hydrophobic - Polar |
| Met - Gln | 106.5183882 | 61.65926145 | Hydrophobic - Polar |
| Met - Arg:NE | 276.2457539 | 61.65926145 | Hydrophobic - Polar |
| Met - Arg:NH | 115213.1181 | 61.65926145 | Hydrophobic - Polar |
| Met - Asp:H | 3319709.626 | 61.65926145 | Hydrophobic - Polar |
| Met - Glu:H | 149359.5198 | 61.65926145 | Hydrophobic - Polar |
| Met - LysN | 51839.60926 | 61.65926145 | Hydrophobic - Polar |
| Met - Arg | 710639.1569 | 61.65926145 | Hydrophobic - Positive Charge |
| Met - His+ | 39856454.28 | 61.65926145 | Hydrophobic - Positive Charge |
| Met - Lys | 1550.660922 | 61.65926145 | Hydrophobic - Positive Charge |
| Met - Asp | 6452157.419 | 61.65926145 | Hydrophobic - Negative Charge |
| Met - Glu | 1040353.43 | 61.65926145 | Hydrophobic - Negative Charge |
| Met - Cys- | 24364253.04 | 61.65926145 | Hydrophobic - Negative Charge |
| Met - Tyr- | 5177213.409 | 61.65926145 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 169785.3763 | 61.65926145 | Aromatic - Aromatic |
| His:ND1 - Phe | 1291963.446 | 61.65926145 | Aromatic - Aromatic |
| His:ND1 - Tyr | 1024495.12 | 61.65926145 | Aromatic - Aromatic |
| His:ND1 - Trp | 9633223.28 | 61.65926145 | Aromatic - Aromatic |
| His:ND1 - Ser | 1829270.561 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Thr | 2036423.142 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Cys | 1857520.278 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Asn | 52643.03387 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Gln | 574727.3412 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Arg:NE | 476470.4498 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Arg:NH | 1101362.643 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Asp:H | 996323.6484 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Glu:H | 122747.3927 | 61.65926145 | Aromatic - Polar |
| His:ND1 - LysN | 851872.4289 | 61.65926145 | Aromatic - Polar |
| His:ND1 - Arg | 14109.38494 | 61.65926145 | Aromatic - Positive Charge |
| His:ND1 - His+ | 28853866.07 | 61.65926145 | Aromatic - Positive Charge |
| His:ND1 - Lys | 459476.5042 | 61.65926145 | Aromatic - Positive Charge |
| His:ND1 - Asp | 9987859.494 | 61.65926145 | Aromatic - Negative Charge |
| His:ND1 - Glu | 2774738.559 | 61.65926145 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 30251388.92 | 61.65926145 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 8145512.785 | 61.65926145 | Aromatic - Negative Charge |
| His:NE2 - Phe | 547523.2861 | 61.65926145 | Aromatic - Aromatic |
| His:NE2 - Tyr | 343387.066 | 61.65926145 | Aromatic - Aromatic |
| His:NE2 - Trp | 6961952.824 | 61.65926145 | Aromatic - Aromatic |
| His:NE2 - Ser | 841473.0725 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Thr | 1021770.509 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Cys | 869839.2771 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Asn | 44556.19565 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Gln | 84299.20375 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Arg:NE | 73171.76432 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Arg:NH | 344933.734 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Asp:H | 1958207.605 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Glu:H | 7581.875096 | 61.65926145 | Aromatic - Polar |
| His:NE2 - LysN | 228027.0612 | 61.65926145 | Aromatic - Polar |
| His:NE2 - Arg | 275332.7186 | 61.65926145 | Aromatic - Positive Charge |
| His:NE2 - His+ | 31291837.05 | 61.65926145 | Aromatic - Positive Charge |
| His:NE2 - Lys | 54247.09922 | 61.65926145 | Aromatic - Positive Charge |
| His:NE2 - Asp | 6955534.754 | 61.65926145 | Aromatic - Negative Charge |
| His:NE2 - Glu | 1471048.798 | 61.65926145 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 23576825.86 | 61.65926145 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 5724214.773 | 61.65926145 | Aromatic - Negative Charge |
| Phe – Tyr | 37682.75492 | 61.65926145 | Aromatic - Aromatic |
| Phe – Trp | 3024055.54 | 61.65926145 | Aromatic - Aromatic |
| Phe - Ser | 12822.98099 | 61.65926145 | Aromatic - Polar |
| Phe - Thr | 54314.72563 | 61.65926145 | Aromatic - Polar |
| Phe - Cys | 18376.48843 | 61.65926145 | Aromatic - Polar |
| Phe - Asn | 963384.1876 | 61.65926145 | Aromatic - Polar |
| Phe - Gln | 288918.6864 | 61.65926145 | Aromatic - Polar |
| Phe - Arg:NE | 239894.0949 | 61.65926145 | Aromatic - Polar |
| Phe - Arg:NH | 59872.50081 | 61.65926145 | Aromatic - Polar |
| Phe - Asp:H | 4267510.452 | 61.65926145 | Aromatic - Polar |
| Phe - Glu:H | 737199.731 | 61.65926145 | Aromatic - Polar |
| Phe - LysN | 106792.5664 | 61.65926145 | Aromatic - Polar |
| Phe - Arg | 1529538.677 | 61.65926145 | Aromatic - Positive Charge |
| Phe - His+ | 34245055.41 | 61.65926145 | Aromatic - Positive Charge |
| Phe - Lys | 315313.092 | 61.65926145 | Aromatic - Positive Charge |
| Phe - Asp | 2704757.96 | 61.65926145 | Aromatic - Negative Charge |
| Phe - Glu | 138957.3898 | 61.65926145 | Aromatic - Negative Charge |
| Phe - Cys- | 12971292.83 | 61.65926145 | Aromatic - Negative Charge |
| Phe - Tyr- | 2265875.864 | 61.65926145 | Aromatic - Negative Charge |
| Tyr - Trp | 4235804.872 | 61.65926145 | Aromatic - Aromatic |
| Tyr - Ser | 108740.5002 | 61.65926145 | Aromatic - Polar |
| Tyr - Thr | 200833.9789 | 61.65926145 | Aromatic - Polar |
| Tyr - Cys | 123426.8837 | 61.65926145 | Aromatic - Polar |
| Tyr - Asn | 708111.6474 | 61.65926145 | Aromatic - Polar |
| Tyr - Gln | 126519.1092 | 61.65926145 | Aromatic - Polar |
| Tyr - Arg:NE | 100409.9388 | 61.65926145 | Aromatic - Polar |
| Tyr - Arg:NH | 1754.940273 | 61.65926145 | Aromatic - Polar |
| Tyr - Asp:H | 4107010.57 | 61.65926145 | Aromatic - Polar |
| Tyr - Glu:H | 502452.8974 | 61.65926145 | Aromatic - Polar |
| Tyr - LysN | 18264.99963 | 61.65926145 | Aromatic - Polar |
| Tyr - Arg | 1255852.129 | 61.65926145 | Aromatic - Positive Charge |
| Tyr - His+ | 37712632.45 | 61.65926145 | Aromatic - Positive Charge |
| Tyr - Lys | 149860.8954 | 61.65926145 | Aromatic - Positive Charge |
| Tyr - Asp | 3992935.245 | 61.65926145 | Aromatic - Negative Charge |
| Tyr - Glu | 375445.8531 | 61.65926145 | Aromatic - Negative Charge |
| Tyr - Cys- | 17251319.2 | 61.65926145 | Aromatic - Negative Charge |
| Tyr - Tyr- | 3279208.443 | 61.65926145 | Aromatic - Negative Charge |
| Trp - Ser | 3014613.551 | 61.65926145 | Aromatic - Polar |
| Trp - Thr | 2373392.958 | 61.65926145 | Aromatic - Polar |
| Trp - Cys | 2874369.953 | 61.65926145 | Aromatic - Polar |
| Trp - Asn | 9159136.336 | 61.65926145 | Aromatic - Polar |
| Trp - Gln | 6724599.447 | 61.65926145 | Aromatic - Polar |
| Trp - Arg:NE | 5646840.459 | 61.65926145 | Aromatic - Polar |
| Trp - Arg:NH | 4983466.523 | 61.65926145 | Aromatic - Polar |
| Trp - Asp:H | 17532943.58 | 61.65926145 | Aromatic - Polar |
| Trp - Glu:H | 8233016.559 | 61.65926145 | Aromatic - Polar |
| Trp - LysN | 5172274.4 | 61.65926145 | Aromatic - Polar |
| Trp - Arg | 10229037.56 | 61.65926145 | Aromatic - Positive Charge |
| Trp - His+ | 64230943.59 | 61.65926145 | Aromatic - Positive Charge |
| Trp - Lys | 6481862.669 | 61.65926145 | Aromatic - Positive Charge |
| Trp - Asp | 59531.04557 | 61.65926145 | Aromatic - Negative Charge |
| Trp - Glu | 2235321.709 | 61.65926145 | Aromatic - Negative Charge |
| Trp - Cys- | 2871220.468 | 61.65926145 | Aromatic - Negative Charge |
| Trp - Tyr- | 62110.42612 | 61.65926145 | Aromatic - Negative Charge |
| Ser - Thr | 17472.07505 | 61.65926145 | Polar - Polar |
| Ser - Cys | 624.8484088 | 61.65926145 | Polar - Polar |
| Ser - Asn | 1435135.96 | 61.65926145 | Polar - Polar |
| Ser - Gln | 517157.9647 | 61.65926145 | Polar - Polar |
| Ser - Arg:NE | 420202.9165 | 61.65926145 | Polar - Polar |
| Ser - Arg:NH | 156213.0489 | 61.65926145 | Polar - Polar |
| Ser - Asp:H | 5689617.149 | 61.65926145 | Polar - Polar |
| Ser - Glu:H | 1123938.406 | 61.65926145 | Polar - Polar |
| Ser - LysN | 230205.2331 | 61.65926145 | Polar - Polar |
| Ser - Arg | 2128622.653 | 61.65926145 | Polar - Positive Charge |
| Ser - His+ | 41840751.13 | 61.65926145 | Polar - Positive Charge |
| Ser - Lys | 542449.3854 | 61.65926145 | Polar - Positive Charge |
| Ser - Asp | 2706964.823 | 61.65926145 | Polar - Negative Charge |
| Ser - Glu | 76680.52299 | 61.65926145 | Polar - Negative Charge |
| Ser - Cys- | 14240490.69 | 61.65926145 | Polar - Negative Charge |
| Ser - Tyr- | 2213582.822 | 61.65926145 | Polar - Negative Charge |
| Thr - Cys | 11438.29771 | 61.65926145 | Polar - Polar |
| Thr - Asn | 1639922.042 | 61.65926145 | Polar - Polar |
| Thr - Gln | 683969.3764 | 61.65926145 | Polar - Polar |
| Thr - Arg:NE | 567655.625 | 61.65926145 | Polar - Polar |
| Thr - Arg:NH | 267386.2643 | 61.65926145 | Polar - Polar |
| Thr - Asp:H | 5783821.073 | 61.65926145 | Polar - Polar |
| Thr - Glu:H | 1320961.504 | 61.65926145 | Polar - Polar |
| Thr - LysN | 354617.1854 | 61.65926145 | Polar - Polar |
| Thr - Arg | 2336336.082 | 61.65926145 | Polar - Positive Charge |
| Thr - His+ | 39534817.63 | 61.65926145 | Polar - Positive Charge |
| Thr - Lys | 707507.3086 | 61.65926145 | Polar - Positive Charge |
| Thr - Asp | 2045287.828 | 61.65926145 | Polar - Negative Charge |
| Thr - Glu | 17084.09921 | 61.65926145 | Polar - Negative Charge |
| Thr - Cys- | 11817156.82 | 61.65926145 | Polar - Negative Charge |
| Thr - Tyr- | 1691295.851 | 61.65926145 | Polar - Negative Charge |
| Cys - Asn | 1464258.028 | 61.65926145 | Polar - Polar |
| Cys - Gln | 543833.6474 | 61.65926145 | Polar - Polar |
| Cys - Arg:NE | 444193.8114 | 61.65926145 | Polar - Polar |
| Cys - Arg:NH | 174094.5051 | 61.65926145 | Polar - Polar |
| Cys - Asp:H | 5671338.025 | 61.65926145 | Polar - Polar |
| Cys - Glu:H | 1153487.789 | 61.65926145 | Polar - Polar |
| Cys - LysN | 250420.3027 | 61.65926145 | Polar - Polar |
| Cys - Arg | 2155537.239 | 61.65926145 | Polar - Positive Charge |
| Cys - His+ | 41151836.17 | 61.65926145 | Polar - Positive Charge |
| Cys - Lys | 568926.3747 | 61.65926145 | Polar - Positive Charge |
| Cys - Asp | 2559817.509 | 61.65926145 | Polar - Negative Charge |
| Cys - Glu | 61764.34929 | 61.65926145 | Polar - Negative Charge |
| Cys - Cys- | 13677435.03 | 61.65926145 | Polar - Negative Charge |
| Cys - Tyr- | 2099689.646 | 61.65926145 | Polar - Negative Charge |
| Asn - Gln | 309430.7879 | 61.65926145 | Polar - Polar |
| Asn - Arg:NE | 253119.5016 | 61.65926145 | Polar - Polar |
| Asn - Arg:NH | 756740.6378 | 61.65926145 | Polar - Polar |
| Asn - Asp:H | 1711234.059 | 61.65926145 | Polar - Polar |
| Asn - Glu:H | 17421.19173 | 61.65926145 | Polar - Polar |
| Asn - LysN | 548472.9836 | 61.65926145 | Polar - Polar |
| Asn - Arg | 124581.2569 | 61.65926145 | Polar - Positive Charge |
| Asn - His+ | 34902510.81 | 61.65926145 | Polar - Positive Charge |
| Asn - Lys | 229869.9808 | 61.65926145 | Polar - Positive Charge |
| Asn - Asp | 9564873.674 | 61.65926145 | Polar - Negative Charge |
| Asn - Glu | 2323604.815 | 61.65926145 | Polar - Negative Charge |
| Asn - Cys- | 31036341.94 | 61.65926145 | Polar - Negative Charge |
| Asn - Tyr- | 7654098.153 | 61.65926145 | Polar - Negative Charge |
| Gln - Arg:NH | 116330.6014 | 61.65926145 | Polar - Polar |
| Gln - Asp:H | 3625764.889 | 61.65926145 | Polar - Polar |
| Gln - Glu:H | 168471.8811 | 61.65926145 | Polar - Polar |
| Gln - LysN | 50736.04773 | 61.65926145 | Polar - Polar |
| Gln - Arg | 775024.0286 | 61.65926145 | Polar - Positive Charge |
| Gln - His+ | 42891018.58 | 61.65926145 | Polar - Positive Charge |
| Gln - Lys | 2593.017527 | 61.65926145 | Polar - Positive Charge |
| Gln - Asp | 6830811.004 | 61.65926145 | Polar - Negative Charge |
| Gln - Glu | 1084443.596 | 61.65926145 | Polar - Negative Charge |
| Gln - Cys- | 26080805.53 | 61.65926145 | Polar - Negative Charge |
| Gln - Tyr- | 5415838.178 | 61.65926145 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 88844.49187 | 61.65926145 | Polar - Polar |
| Arg:NE - Asp:H | 2867822.933 | 61.65926145 | Polar - Polar |
| Arg:NE - Glu:H | 140369.1451 | 61.65926145 | Polar - Polar |
| Arg:NE - LysN | 38302.20512 | 61.65926145 | Polar - Polar |
| Arg:NE - Arg | 641992.0806 | 61.65926145 | Polar - Positive Charge |
| Arg:NE - His+ | 34358485.34 | 61.65926145 | Polar - Positive Charge |
| Arg:NE - Lys | 2807.56491 | 61.65926145 | Polar - Positive Charge |
| Arg:NE - Asp | 5516211.616 | 61.65926145 | Polar - Negative Charge |
| Arg:NE - Glu | 881067.7329 | 61.65926145 | Polar - Negative Charge |
| Arg:NE - Cys- | 20649270.31 | 61.65926145 | Polar - Negative Charge |
| Arg:NE - Tyr- | 4533719.569 | 61.65926145 | Polar - Negative Charge |
| Arg:NH - Asp:H | 4704685.499 | 61.65926145 | Polar - Polar |
| Arg:NH - Glu:H | 524181.8882 | 61.65926145 | Polar - Polar |
| Arg:NH - LysN | 10374.0008 | 61.65926145 | Polar - Polar |
| Arg:NH - Arg | 1359477.827 | 61.65926145 | Polar - Positive Charge |
| Arg:NH - His+ | 43912661.66 | 61.65926145 | Polar - Positive Charge |
| Arg:NH - Lys | 140241.4791 | 61.65926145 | Polar - Positive Charge |
| Arg:NH - Asp | 4850827.598 | 61.65926145 | Polar - Negative Charge |
| Arg:NH - Glu | 491156.0822 | 61.65926145 | Polar - Negative Charge |
| Arg:NH - Cys- | 20872903.53 | 61.65926145 | Polar - Negative Charge |
| Arg:NH - Tyr- | 3884572.365 | 61.65926145 | Polar - Negative Charge |
| Asp:H - Glu:H | 2003765.348 | 61.65926145 | Polar - Polar |
| Asp:H - LysN | 3983738.25 | 61.65926145 | Polar - Polar |
| Asp:H - Arg | 746919.3391 | 61.65926145 | Polar - Positive Charge |
| Asp:H - His+ | 22939009.34 | 61.65926145 | Polar - Positive Charge |
| Asp:H - Lys | 3083939.879 | 61.65926145 | Polar - Positive Charge |
| Asp:H - Asp | 19401049.34 | 61.65926145 | Polar - Negative Charge |
| Asp:H - Glu | 7520561.693 | 61.65926145 | Polar - Negative Charge |
| Asp:H - Cys- | 49563277.05 | 61.65926145 | Polar - Negative Charge |
| Asp:H - Tyr- | 15457878.04 | 61.65926145 | Polar - Negative Charge |
| Glu:H - LysN | 361932.214 | 61.65926145 | Polar - Polar |
| Glu:H - Arg | 221841.3462 | 61.65926145 | Polar - Positive Charge |
| Glu:H - His+ | 35053786.34 | 61.65926145 | Polar - Positive Charge |
| Glu:H - Lys | 117206.5262 | 61.65926145 | Polar - Positive Charge |
| Glu:H - Asp | 8475179.738 | 61.65926145 | Polar - Negative Charge |
| Glu:H - Glu | 1899576.14 | 61.65926145 | Polar - Negative Charge |
| Glu:H - Cys- | 28362744.26 | 61.65926145 | Polar - Negative Charge |
| Glu:H - Tyr- | 6822123.668 | 61.65926145 | Polar - Negative Charge |
| LysN - Arg | 1075877.669 | 61.65926145 | Polar - Positive Charge |
| LysN - His+ | 40163139.9 | 61.65926145 | Polar - Positive Charge |
| LysN - Lys | 69268.9529 | 61.65926145 | Polar - Positive Charge |
| LysN - Asp | 5034954.834 | 61.65926145 | Polar - Negative Charge |
| LysN - Glu | 607156.0396 | 61.65926145 | Polar - Negative Charge |
| LysN - Cys- | 20617812.64 | 61.65926145 | Polar - Negative Charge |
| LysN - Tyr- | 4074031.394 | 61.65926145 | Polar - Negative Charge |
| Arg - His+ | 27240820.07 | 61.65926145 | Positive Charge - Positive Charge |
| Arg - Lys | 632799.0729 | 61.65926145 | Positive Charge - Positive Charge |
| Arg - Asp | 10647060.05 | 61.65926145 | Positive Charge - Negative Charge |
| Arg - Glu | 3141334.191 | 61.65926145 | Positive Charge - Negative Charge |
| Arg - Cys- | 31293508.27 | 61.65926145 | Positive Charge - Negative Charge |
| Arg - Tyr- | 8703641.475 | 61.65926145 | Positive Charge - Negative Charge |
| His+ - Lys | 38379122.1 | 61.65926145 | Positive Charge - Positive Charge |
| His+ - Asp | 74604658.71 | 61.65926145 | Positive Charge - Negative Charge |
| His+ - Glu | 47368937.93 | 61.65926145 | Positive Charge - Negative Charge |
| His+ - Cys- | 129562604.3 | 61.65926145 | Positive Charge - Negative Charge |
| His+ - Tyr- | 60753420.49 | 61.65926145 | Positive Charge - Negative Charge |
| Lys - Asp | 6496933.635 | 61.65926145 | Positive Charge - Negative Charge |
| Lys - Glu | 1093526.599 | 61.65926145 | Positive Charge - Negative Charge |
| Lys - Cys- | 24137520.47 | 61.65926145 | Positive Charge - Negative Charge |
| Lys - Tyr- | 5236373.389 | 61.65926145 | Positive Charge - Negative Charge |
| Asp - Glu | 1908520.226 | 61.65926145 | Negative Charge - Negative Charge |
| Asp - Cys- | 4723372.31 | 61.65926145 | Negative Charge - Negative Charge |
| Asp - Tyr- | 646.0221828 | 61.65926145 | Negative Charge - Negative Charge |
| Glu - Cys- | 12508606.71 | 61.65926145 | Negative Charge - Negative Charge |
| Glu - Tyr- | 1542060.182 | 61.65926145 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 3959444.114 | 61.65926145 | Negative Charge - Negative Charge |

**Table S18.** Non-statistically significant pairwise comparisons of the f dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Gln - Arg:NE | 57.90920791 | 61.65926145 | Polar - Polar |

**Table S19.** Statistically significant pairwise comparisons of the y dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 2042570.4 | 61.65925894 | Hydrophobic - Hydrophobic |
| Ala - Leu | 273864.8076 | 61.65925894 | Hydrophobic - Hydrophobic |
| Ala - Ile | 2759124.87 | 61.65925894 | Hydrophobic - Hydrophobic |
| Ala - Met | 1497408.54 | 61.65925894 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 3420046.197 | 61.65925894 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 2641839.204 | 61.65925894 | Hydrophobic - Aromatic |
| Ala - Phe | 66348.88394 | 61.65925894 | Hydrophobic - Aromatic |
| Ala - Tyr | 162594.4055 | 61.65925894 | Hydrophobic - Aromatic |
| Ala - Trp | 4043316.159 | 61.65925894 | Hydrophobic - Aromatic |
| Ala - Ser | 238267.2637 | 61.65925894 | Hydrophobic - Polar |
| Ala - Thr | 63906.95203 | 61.65925894 | Hydrophobic - Polar |
| Ala - Cys | 116171.0601 | 61.65925894 | Hydrophobic - Polar |
| Ala - Asn | 3584115.757 | 61.65925894 | Hydrophobic - Polar |
| Ala - Gln | 1810815.062 | 61.65925894 | Hydrophobic - Polar |
| Ala - Arg:NE | 1173512.708 | 61.65925894 | Hydrophobic - Polar |
| Ala - Arg:NH | 580603.3895 | 61.65925894 | Hydrophobic - Polar |
| Ala - Asp:H | 8498679.487 | 61.65925894 | Hydrophobic - Polar |
| Ala - Glu:H | 2403291.41 | 61.65925894 | Hydrophobic - Polar |
| Ala - LysN | 657999.0561 | 61.65925894 | Hydrophobic - Polar |
| Ala - Arg | 3071941.744 | 61.65925894 | Hydrophobic - Positive Charge |
| Ala - His+ | 35912911.88 | 61.65925894 | Hydrophobic - Positive Charge |
| Ala - Lys | 1038504.957 | 61.65925894 | Hydrophobic - Positive Charge |
| Ala - Asp | 1360130.107 | 61.65925894 | Hydrophobic - Negative Charge |
| Ala - Glu | 7444.676483 | 61.65925894 | Hydrophobic - Negative Charge |
| Ala - Cys- | 11272509.15 | 61.65925894 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 1748274.112 | 61.65925894 | Hydrophobic - Negative Charge |
| Val - Leu | 3390513.785 | 61.65925894 | Hydrophobic - Hydrophobic |
| Val - Ile | 3439.773177 | 61.65925894 | Hydrophobic - Hydrophobic |
| Val - Met | 5485484.071 | 61.65925894 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 7794026.616 | 61.65925894 | Hydrophobic - Aromatic |
| Val - His:NE2 | 6854244.755 | 61.65925894 | Hydrophobic - Aromatic |
| Val - Phe | 2333175.174 | 61.65925894 | Hydrophobic - Aromatic |
| Val - Tyr | 2869810.03 | 61.65925894 | Hydrophobic - Aromatic |
| Val - Trp | 39954.7461 | 61.65925894 | Hydrophobic - Aromatic |
| Val - Ser | 3080863.55 | 61.65925894 | Hydrophobic - Polar |
| Val - Thr | 2381422.984 | 61.65925894 | Hydrophobic - Polar |
| Val - Cys | 2676713.582 | 61.65925894 | Hydrophobic - Polar |
| Val - Asn | 8009746.89 | 61.65925894 | Hydrophobic - Polar |
| Val - Gln | 5954735.724 | 61.65925894 | Hydrophobic - Polar |
| Val - Arg:NE | 4886355.346 | 61.65925894 | Hydrophobic - Polar |
| Val - Arg:NH | 4019458.081 | 61.65925894 | Hydrophobic - Polar |
| Val - Asp:H | 12667245.61 | 61.65925894 | Hydrophobic - Polar |
| Val - Glu:H | 6651521.76 | 61.65925894 | Hydrophobic - Polar |
| Val - LysN | 4110683.329 | 61.65925894 | Hydrophobic - Polar |
| Val - Arg | 7396248.344 | 61.65925894 | Hydrophobic - Positive Charge |
| Val - His+ | 33636346.01 | 61.65925894 | Hydrophobic - Positive Charge |
| Val - Lys | 4790321.463 | 61.65925894 | Hydrophobic - Positive Charge |
| Val - Asp | 322018.0698 | 61.65925894 | Hydrophobic - Negative Charge |
| Val - Glu | 2144198.197 | 61.65925894 | Hydrophobic - Negative Charge |
| Val - Cys- | 907281.3871 | 61.65925894 | Hydrophobic - Negative Charge |
| Val - Tyr- | 114833.24 | 61.65925894 | Hydrophobic - Negative Charge |
| Leu - Ile | 4549556.015 | 61.65925894 | Hydrophobic - Hydrophobic |
| Leu - Met | 550643.8473 | 61.65925894 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 1991536.947 | 61.65925894 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 1419941.934 | 61.65925894 | Hydrophobic - Aromatic |
| Leu - Phe | 35524.94307 | 61.65925894 | Hydrophobic - Aromatic |
| Leu - Tyr | 5752.155293 | 61.65925894 | Hydrophobic - Aromatic |
| Leu - Trp | 6521179.932 | 61.65925894 | Hydrophobic - Aromatic |
| Leu - Ser | 216.9277755 | 61.65925894 | Hydrophobic - Polar |
| Leu - Thr | 42529.63557 | 61.65925894 | Hydrophobic - Polar |
| Leu - Cys | 17608.38521 | 61.65925894 | Hydrophobic - Polar |
| Leu - Asn | 2066033.822 | 61.65925894 | Hydrophobic - Polar |
| Leu - Gln | 731130.9292 | 61.65925894 | Hydrophobic - Polar |
| Leu - Arg:NE | 394470.8336 | 61.65925894 | Hydrophobic - Polar |
| Leu - Arg:NH | 67433.04655 | 61.65925894 | Hydrophobic - Polar |
| Leu - Asp:H | 6271217.589 | 61.65925894 | Hydrophobic - Polar |
| Leu - Glu:H | 1177201.372 | 61.65925894 | Hydrophobic - Polar |
| Leu - LysN | 105345.8178 | 61.65925894 | Hydrophobic - Polar |
| Leu - Arg | 1721775.826 | 61.65925894 | Hydrophobic - Positive Charge |
| Leu - His+ | 33017205 | 61.65925894 | Hydrophobic - Positive Charge |
| Leu - Lys | 284095.2871 | 61.65925894 | Hydrophobic - Positive Charge |
| Leu - Asp | 3033874.268 | 61.65925894 | Hydrophobic - Negative Charge |
| Leu - Glu | 169941.5806 | 61.65925894 | Hydrophobic - Negative Charge |
| Leu - Cys- | 16649896.6 | 61.65925894 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 3399841.169 | 61.65925894 | Hydrophobic - Negative Charge |
| Ile - Met | 7222139.999 | 61.65925894 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 10078270.12 | 61.65925894 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 8801149.522 | 61.65925894 | Hydrophobic - Aromatic |
| Ile - Phe | 3017778 | 61.65925894 | Hydrophobic - Aromatic |
| Ile - Tyr | 3768066.785 | 61.65925894 | Hydrophobic - Aromatic |
| Ile - Trp | 22777.1688 | 61.65925894 | Hydrophobic - Aromatic |
| Ile - Ser | 4029790.943 | 61.65925894 | Hydrophobic - Polar |
| Ile - Thr | 3101432.338 | 61.65925894 | Hydrophobic - Polar |
| Ile - Cys | 3507160.094 | 61.65925894 | Hydrophobic - Polar |
| Ile - Asn | 10497352.13 | 61.65925894 | Hydrophobic - Polar |
| Ile - Gln | 7895570.084 | 61.65925894 | Hydrophobic - Polar |
| Ile - Arg:NE | 6323826.214 | 61.65925894 | Hydrophobic - Polar |
| Ile - Arg:NH | 5335467.647 | 61.65925894 | Hydrophobic - Polar |
| Ile - Asp:H | 16562010.58 | 61.65925894 | Hydrophobic - Polar |
| Ile - Glu:H | 8710891.083 | 61.65925894 | Hydrophobic - Polar |
| Ile - LysN | 5410845.31 | 61.65925894 | Hydrophobic - Polar |
| Ile - Arg | 9562035.962 | 61.65925894 | Hydrophobic - Positive Charge |
| Ile - His+ | 42869528.42 | 61.65925894 | Hydrophobic - Positive Charge |
| Ile - Lys | 6310389.07 | 61.65925894 | Hydrophobic - Positive Charge |
| Ile - Asp | 494905.7405 | 61.65925894 | Hydrophobic - Negative Charge |
| Ile - Glu | 2857746.815 | 61.65925894 | Hydrophobic - Negative Charge |
| Ile - Cys- | 978135.8882 | 61.65925894 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 194230.5828 | 61.65925894 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 470269.9554 | 61.65925894 | Hydrophobic - Aromatic |
| Met - His:NE2 | 246822.9743 | 61.65925894 | Hydrophobic - Aromatic |
| Met - Phe | 645712.5819 | 61.65925894 | Hydrophobic - Aromatic |
| Met - Tyr | 556253.2277 | 61.65925894 | Hydrophobic - Aromatic |
| Met - Trp | 9994497.032 | 61.65925894 | Hydrophobic - Aromatic |
| Met - Ser | 426687.3909 | 61.65925894 | Hydrophobic - Polar |
| Met - Thr | 703389.6812 | 61.65925894 | Hydrophobic - Polar |
| Met - Cys | 625199.8047 | 61.65925894 | Hydrophobic - Polar |
| Met - Asn | 449699.0057 | 61.65925894 | Hydrophobic - Polar |
| Met - Gln | 7162.29668 | 61.65925894 | Hydrophobic - Polar |
| Met - Arg:NE | 3277.43431 | 61.65925894 | Hydrophobic - Polar |
| Met - Arg:NH | 223184.2994 | 61.65925894 | Hydrophobic - Polar |
| Met - Asp:H | 2885680.434 | 61.65925894 | Hydrophobic - Polar |
| Met - Glu:H | 114690.4633 | 61.65925894 | Hydrophobic - Polar |
| Met - LysN | 150414.5453 | 61.65925894 | Hydrophobic - Polar |
| Met - Arg | 350477.9948 | 61.65925894 | Hydrophobic - Positive Charge |
| Met - His+ | 24305475.49 | 61.65925894 | Hydrophobic - Positive Charge |
| Met - Lys | 38766.52445 | 61.65925894 | Hydrophobic - Positive Charge |
| Met - Asp | 5879352.621 | 61.65925894 | Hydrophobic - Negative Charge |
| Met - Glu | 1180739.043 | 61.65925894 | Hydrophobic - Negative Charge |
| Met - Cys- | 22710930.73 | 61.65925894 | Hydrophobic - Negative Charge |
| Met - Tyr- | 6068879.968 | 61.65925894 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 25072.32894 | 61.65925894 | Aromatic - Aromatic |
| His:ND1 - Phe | 1871181.323 | 61.65925894 | Aromatic - Aromatic |
| His:ND1 - Tyr | 1840547.016 | 61.65925894 | Aromatic - Aromatic |
| His:ND1 - Trp | 13542463.03 | 61.65925894 | Aromatic - Aromatic |
| His:ND1 - Ser | 1597964.674 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Thr | 2007674.072 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Cys | 1934507.908 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Asn | 2599.656088 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Gln | 392855.6739 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Arg:NE | 481433.6675 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Arg:NH | 1298759.073 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Asp:H | 845803.5459 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Glu:H | 128202.1782 | 61.65925894 | Aromatic - Polar |
| His:ND1 - LysN | 1083006.518 | 61.65925894 | Aromatic - Polar |
| His:ND1 - Arg | 7609.285269 | 61.65925894 | Aromatic - Positive Charge |
| His:ND1 - His+ | 16598491.32 | 61.65925894 | Aromatic - Positive Charge |
| His:ND1 - Lys | 753864.0151 | 61.65925894 | Aromatic - Positive Charge |
| His:ND1 - Asp | 9068360.886 | 61.65925894 | Aromatic - Negative Charge |
| His:ND1 - Glu | 2871349.132 | 61.65925894 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 28052811.61 | 61.65925894 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 9020134.122 | 61.65925894 | Aromatic - Negative Charge |
| His:NE2 - Phe | 1415286.304 | 61.65925894 | Aromatic - Aromatic |
| His:NE2 - Tyr | 1349486.619 | 61.65925894 | Aromatic - Aromatic |
| His:NE2 - Trp | 11755603.07 | 61.65925894 | Aromatic - Aromatic |
| His:NE2 - Ser | 1151451.741 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Thr | 1516932.939 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Cys | 1436158.416 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Asn | 13653.86019 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Gln | 188013.0638 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Arg:NE | 268804.6161 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Arg:NH | 873338.2452 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Asp:H | 1106561.969 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Glu:H | 32963.48169 | 61.65925894 | Aromatic - Polar |
| His:NE2 - LysN | 714233.709 | 61.65925894 | Aromatic - Polar |
| His:NE2 - Arg | 5391.26043 | 61.65925894 | Aromatic - Positive Charge |
| His:NE2 - His+ | 16673749.35 | 61.65925894 | Aromatic - Positive Charge |
| His:NE2 - Lys | 455475.1956 | 61.65925894 | Aromatic - Positive Charge |
| His:NE2 - Asp | 7545593.419 | 61.65925894 | Aromatic - Negative Charge |
| His:NE2 - Glu | 2207234.519 | 61.65925894 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 24257910.24 | 61.65925894 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 7670729.89 | 61.65925894 | Aromatic - Negative Charge |
| Phe - Tyr | 12204.73962 | 61.65925894 | Aromatic - Aromatic |
| Phe - Trp | 4174622.971 | 61.65925894 | Aromatic - Aromatic |
| Phe - Ser | 35028.20994 | 61.65925894 | Aromatic - Polar |
| Phe - Thr | 112.2205115 | 61.65925894 | Aromatic - Polar |
| Phe - Cys | 3505.833036 | 61.65925894 | Aromatic - Polar |
| Phe - Asn | 1895733.498 | 61.65925894 | Aromatic - Polar |
| Phe - Gln | 799468.1655 | 61.65925894 | Aromatic - Polar |
| Phe - Arg:NE | 505281.2545 | 61.65925894 | Aromatic - Polar |
| Phe - Arg:NH | 161787.2101 | 61.65925894 | Aromatic - Polar |
| Phe - Asp:H | 5031105.038 | 61.65925894 | Aromatic - Polar |
| Phe - Glu:H | 1185477.717 | 61.65925894 | Aromatic - Polar |
| Phe - LysN | 206916.1668 | 61.65925894 | Aromatic - Polar |
| Phe - Arg | 1653172.547 | 61.65925894 | Aromatic - Positive Charge |
| Phe - His+ | 24585481.07 | 61.65925894 | Aromatic - Positive Charge |
| Phe - Lys | 396703.3035 | 61.65925894 | Aromatic - Positive Charge |
| Phe - Asp | 1645070.528 | 61.65925894 | Aromatic - Negative Charge |
| Phe - Glu | 30151.08495 | 61.65925894 | Aromatic - Negative Charge |
| Phe - Cys- | 10141437.72 | 61.65925894 | Aromatic - Negative Charge |
| Phe - Tyr- | 2029528.916 | 61.65925894 | Aromatic - Negative Charge |
| Tyr - Trp | 5278839.131 | 61.65925894 | Aromatic - Aromatic |
| Tyr - Ser | 6866.165688 | 61.65925894 | Aromatic - Polar |
| Tyr - Thr | 15518.83517 | 61.65925894 | Aromatic - Polar |
| Tyr - Cys | 2865.966745 | 61.65925894 | Aromatic - Polar |
| Tyr - Asn | 1879395.027 | 61.65925894 | Aromatic - Polar |
| Tyr - Gln | 714044.3956 | 61.65925894 | Aromatic - Polar |
| Tyr - Arg:NE | 416980.7074 | 61.65925894 | Aromatic - Polar |
| Tyr - Arg:NH | 95874.81232 | 61.65925894 | Aromatic - Polar |
| Tyr - Asp:H | 5388188.179 | 61.65925894 | Aromatic - Polar |
| Tyr - Glu:H | 1115032.68 | 61.65925894 | Aromatic - Polar |
| Tyr - LysN | 135498.0951 | 61.65925894 | Aromatic - Polar |
| Tyr - Arg | 1606195.177 | 61.65925894 | Aromatic - Positive Charge |
| Tyr - His+ | 27732074.01 | 61.65925894 | Aromatic - Positive Charge |
| Tyr - Lys | 310428.9566 | 61.65925894 | Aromatic - Positive Charge |
| Tyr - Asp | 2287402.087 | 61.65925894 | Aromatic - Negative Charge |
| Tyr - Glu | 94388.03767 | 61.65925894 | Aromatic - Negative Charge |
| Tyr - Cys- | 12964781.75 | 61.65925894 | Aromatic - Negative Charge |
| Tyr - Tyr- | 2683832.614 | 61.65925894 | Aromatic - Negative Charge |
| Trp - Ser | 5608462.853 | 61.65925894 | Aromatic - Polar |
| Trp - Thr | 4323898.881 | 61.65925894 | Aromatic - Polar |
| Trp - Cys | 4909899.229 | 61.65925894 | Aromatic - Polar |
| Trp - Asn | 14334390.16 | 61.65925894 | Aromatic - Polar |
| Trp - Gln | 11004862.16 | 61.65925894 | Aromatic - Polar |
| Trp - Arg:NE | 8589790.743 | 61.65925894 | Aromatic - Polar |
| Trp - Arg:NH | 7512530.924 | 61.65925894 | Aromatic - Polar |
| Trp - Asp:H | 22371888.17 | 61.65925894 | Aromatic - Polar |
| Trp - Glu:H | 11927070.77 | 61.65925894 | Aromatic - Polar |
| Trp - LysN | 7534889.612 | 61.65925894 | Aromatic - Polar |
| Trp - Arg | 12858728.92 | 61.65925894 | Aromatic - Positive Charge |
| Trp - His+ | 55408627.9 | 61.65925894 | Aromatic - Positive Charge |
| Trp - Lys | 8764955.158 | 61.65925894 | Aromatic - Positive Charge |
| Trp - Asp | 910277.1462 | 61.65925894 | Aromatic - Negative Charge |
| Trp - Glu | 4111889.418 | 61.65925894 | Aromatic - Negative Charge |
| Trp - Cys- | 833468.24 | 61.65925894 | Aromatic - Negative Charge |
| Trp - Tyr- | 415839.0226 | 61.65925894 | Aromatic - Negative Charge |
| Ser - Thr | 41253.22329 | 61.65925894 | Polar - Polar |
| Ser - Cys | 18220.58026 | 61.65925894 | Polar - Polar |
| Ser - Asn | 1622488.004 | 61.65925894 | Polar - Polar |
| Ser - Gln | 561152.3257 | 61.65925894 | Polar - Polar |
| Ser - Arg:NE | 313068.644 | 61.65925894 | Polar - Polar |
| Ser - Arg:NH | 48125.48041 | 61.65925894 | Polar - Polar |
| Ser - Asp:H | 4914825.578 | 61.65925894 | Polar - Polar |
| Ser - Glu:H | 925372.8685 | 61.65925894 | Polar - Polar |
| Ser - LysN | 78251.16279 | 61.65925894 | Polar - Polar |
| Ser - Arg | 1382109.841 | 61.65925894 | Polar - Positive Charge |
| Ser - His+ | 26544295.43 | 61.65925894 | Polar - Positive Charge |
| Ser - Lys | 217526.4886 | 61.65925894 | Polar - Positive Charge |
| Ser - Asp | 2535501.537 | 61.65925894 | Polar - Negative Charge |
| Ser - Glu | 151888.4488 | 61.65925894 | Polar - Negative Charge |
| Ser - Cys- | 13497997.39 | 61.65925894 | Polar - Negative Charge |
| Ser - Tyr- | 2929962.348 | 61.65925894 | Polar - Negative Charge |
| Thr - Cys | 5159.847117 | 61.65925894 | Polar - Polar |
| Thr - Asn | 2044055.654 | 61.65925894 | Polar - Polar |
| Thr - Gln | 871437.667 | 61.65925894 | Polar - Polar |
| Thr - Arg:NE | 548166.7839 | 61.65925894 | Polar - Polar |
| Thr - Arg:NH | 181255.2132 | 61.65925894 | Polar - Polar |
| Thr - Asp:H | 5402717.064 | 61.65925894 | Polar - Polar |
| Thr - Glu:H | 1281532.093 | 61.65925894 | Polar - Polar |
| Thr - LysN | 229534.0203 | 61.65925894 | Polar - Polar |
| Thr - Arg | 1774759.799 | 61.65925894 | Polar - Positive Charge |
| Thr - His+ | 26146808.85 | 61.65925894 | Polar - Positive Charge |
| Thr - Lys | 435000.1643 | 61.65925894 | Polar - Positive Charge |
| Thr - Asp | 1704668.91 | 61.65925894 | Polar - Negative Charge |
| Thr - Glu | 27772.33978 | 61.65925894 | Polar - Negative Charge |
| Thr - Cys- | 10666128.82 | 61.65925894 | Polar - Negative Charge |
| Thr - Tyr- | 2093524.637 | 61.65925894 | Polar - Negative Charge |
| Cys - Asn | 1975022.388 | 61.65925894 | Polar - Polar |
| Cys - Gln | 790333.6099 | 61.65925894 | Polar - Polar |
| Cys - Arg:NE | 476238.9851 | 61.65925894 | Polar - Polar |
| Cys - Arg:NH | 130850.6777 | 61.65925894 | Polar - Polar |
| Cys - Asp:H | 5468728.235 | 61.65925894 | Polar - Polar |
| Cys - Glu:H | 1200246.143 | 61.65925894 | Polar - Polar |
| Cys - LysN | 174877.2388 | 61.65925894 | Polar - Polar |
| Cys - Arg | 1697595.784 | 61.65925894 | Polar - Positive Charge |
| Cys - His+ | 27395007.13 | 61.65925894 | Polar - Positive Charge |
| Cys - Lys | 365832.432 | 61.65925894 | Polar - Positive Charge |
| Cys - Asp | 2051902.232 | 61.65925894 | Polar - Negative Charge |
| Cys - Glu | 61764.35152 | 61.65925894 | Polar - Negative Charge |
| Cys - Cys- | 12107443.16 | 61.65925894 | Polar - Negative Charge |
| Cys - Tyr- | 2448273.665 | 61.65925894 | Polar - Negative Charge |
| Asn - Gln | 370809.9428 | 61.65925894 | Polar - Polar |
| Asn - Arg:NE | 459272.496 | 61.65925894 | Polar - Polar |
| Asn - Arg:NH | 1320404.004 | 61.65925894 | Polar - Polar |
| Asn - Asp:H | 1062386.99 | 61.65925894 | Polar - Polar |
| Asn - Glu:H | 105557.994 | 61.65925894 | Polar - Polar |
| Asn - LysN | 1088081.929 | 61.65925894 | Polar - Polar |
| Asn - Arg | 1677.004251 | 61.65925894 | Polar - Positive Charge |
| Asn - His+ | 18947035.14 | 61.65925894 | Polar - Positive Charge |
| Asn - Lys | 744086.4301 | 61.65925894 | Polar - Positive Charge |
| Asn - Asp | 9698519.417 | 61.65925894 | Polar - Negative Charge |
| Asn - Glu | 2978042.676 | 61.65925894 | Polar - Negative Charge |
| Asn - Cys- | 30737310.18 | 61.65925894 | Polar - Negative Charge |
| Asn - Tyr- | 9505135.674 | 61.65925894 | Polar - Negative Charge |
| Gln - Arg:NE | 18762.58404 | 61.65925894 | Polar - Polar |
| Gln - Arg:NH | 328614.1193 | 61.65925894 | Polar - Polar |
| Gln - Asp:H | 2809539.023 | 61.65925894 | Polar - Polar |
| Gln - Glu:H | 70794.69395 | 61.65925894 | Polar - Polar |
| Gln - LysN | 232696.8444 | 61.65925894 | Polar - Polar |
| Gln - Arg | 281102.5267 | 61.65925894 | Polar - Positive Charge |
| Gln - His+ | 25212470.41 | 61.65925894 | Polar - Positive Charge |
| Gln - Lys | 82482.8533 | 61.65925894 | Polar - Positive Charge |
| Gln - Asp | 6686247.907 | 61.65925894 | Polar - Negative Charge |
| Gln - Glu | 1434633.561 | 61.65925894 | Polar - Negative Charge |
| Gln - Cys- | 25270826.94 | 61.65925894 | Polar - Negative Charge |
| Gln - Tyr- | 6773873.602 | 61.65925894 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 145057.833 | 61.65925894 | Polar - Polar |
| Arg:NE - Asp:H | 2631997.215 | 61.65925894 | Polar - Polar |
| Arg:NE - Glu:H | 137616.8807 | 61.65925894 | Polar - Polar |
| Arg:NE - LysN | 93168.40064 | 61.65925894 | Polar - Polar |
| Arg:NE - Arg | 368124.5986 | 61.65925894 | Polar - Positive Charge |
| Arg:NE - His+ | 21361342.34 | 61.65925894 | Polar - Positive Charge |
| Arg:NE - Lys | 15893.95602 | 61.65925894 | Polar - Positive Charge |
| Arg:NE - Asp | 4848233.041 | 61.65925894 | Polar - Negative Charge |
| Arg:NE - Glu | 927172.031 | 61.65925894 | Polar - Negative Charge |
| Arg:NE - Cys- | 18882798.44 | 61.65925894 | Polar - Negative Charge |
| Arg:NE - Tyr- | 5154886.142 | 61.65925894 | Polar - Negative Charge |
| Arg:NH - Asp:H | 4777134.046 | 61.65925894 | Polar - Polar |
| Arg:NH - Glu:H | 654962.7846 | 61.65925894 | Polar - Polar |
| Arg:NH - LysN | 5055.894485 | 61.65925894 | Polar - Polar |
| Arg:NH - Arg | 1089593.181 | 61.65925894 | Polar - Positive Charge |
| Arg:NH - His+ | 28977148.5 | 61.65925894 | Polar - Positive Charge |
| Arg:NH - Lys | 73209.58377 | 61.65925894 | Polar - Positive Charge |
| Arg:NH - Asp | 3838587.477 | 61.65925894 | Polar - Negative Charge |
| Arg:NH - Glu | 414288.8098 | 61.65925894 | Polar - Negative Charge |
| Arg:NH - Cys- | 18179174.03 | 61.65925894 | Polar - Negative Charge |
| Arg:NH - Tyr- | 4170288.998 | 61.65925894 | Polar - Negative Charge |
| Asp:H - Glu:H | 1802226.767 | 61.65925894 | Polar - Polar |
| Asp:H - LysN | 4179230.57 | 61.65925894 | Polar - Polar |
| Asp:H - Arg | 1016640.248 | 61.65925894 | Polar - Positive Charge |
| Asp:H - His+ | 11992542.94 | 61.65925894 | Polar - Positive Charge |
| Asp:H - Lys | 3541345.377 | 61.65925894 | Polar - Positive Charge |
| Asp:H - Asp | 17352636.79 | 61.65925894 | Polar - Negative Charge |
| Asp:H - Glu | 7279416.439 | 61.65925894 | Polar - Negative Charge |
| Asp:H - Cys- | 45367080.58 | 61.65925894 | Polar - Negative Charge |
| Asp:H - Tyr- | 16161236.12 | 61.65925894 | Polar - Negative Charge |
| Glu:H - LysN | 511759.4681 | 61.65925894 | Polar - Polar |
| Glu:H - Arg | 70827.49695 | 61.65925894 | Polar - Positive Charge |
| Glu:H - His+ | 21035829.31 | 61.65925894 | Polar - Positive Charge |
| Glu:H - Lys | 282215.4865 | 61.65925894 | Polar - Positive Charge |
| Glu:H - Asp | 7561412.568 | 61.65925894 | Polar - Negative Charge |
| Glu:H - Glu | 1961263.451 | 61.65925894 | Polar - Negative Charge |
| Glu:H - Cys- | 26078610.87 | 61.65925894 | Polar - Negative Charge |
| Glu:H - Tyr- | 7607595.973 | 61.65925894 | Polar - Negative Charge |
| LysN - Arg | 898741.639 | 61.65925894 | Polar - Positive Charge |
| LysN - His+ | 26623768.28 | 61.65925894 | Polar - Positive Charge |
| LysN - Lys | 37104.21204 | 61.65925894 | Polar - Positive Charge |
| LysN - Asp | 3909093.611 | 61.65925894 | Polar - Negative Charge |
| LysN - Glu | 482502.0376 | 61.65925894 | Polar - Negative Charge |
| LysN - Cys- | 17750441.84 | 61.65925894 | Polar - Negative Charge |
| LysN - Tyr- | 4247301.66 | 61.65925894 | Polar - Negative Charge |
| Arg - His+ | 17158997.25 | 61.65925894 | Positive Charge - Positive Charge |
| Arg - Lys | 600086.5393 | 61.65925894 | Positive Charge - Positive Charge |
| Arg - Asp | 8462726.63 | 61.65925894 | Positive Charge - Negative Charge |
| Arg - Glu | 2567928.145 | 61.65925894 | Positive Charge - Negative Charge |
| Arg - Cys- | 26785081.42 | 61.65925894 | Positive Charge - Negative Charge |
| Arg - Tyr- | 8475846.538 | 61.65925894 | Positive Charge - Negative Charge |
| His+ - Lys | 25668132.95 | 61.65925894 | Positive Charge - Positive Charge |
| His+ - Asp | 51665332.53 | 61.65925894 | Positive Charge - Negative Charge |
| His+ - Glu | 32100878.45 | 61.65925894 | Positive Charge - Negative Charge |
| His+ - Cys- | 96111106.98 | 61.65925894 | Positive Charge - Negative Charge |
| His+ - Tyr- | 45908450.48 | 61.65925894 | Positive Charge - Negative Charge |
| Lys - Asp | 4869847.148 | 61.65925894 | Positive Charge - Negative Charge |
| Lys - Glu | 795454.0053 | 61.65925894 | Positive Charge - Negative Charge |
| Lys - Cys- | 20289740.16 | 61.65925894 | Positive Charge - Negative Charge |
| Lys - Tyr- | 5142026.436 | 61.65925894 | Positive Charge - Negative Charge |
| Asp - Glu | 1462295.439 | 61.65925894 | Negative Charge - Negative Charge |
| Asp - Cys- | 4521686.114 | 61.65925894 | Negative Charge - Negative Charge |
| Asp - Tyr- | 67212.15033 | 61.65925894 | Negative Charge - Negative Charge |
| Glu - Cys- | 10964315.49 | 61.65925894 | Negative Charge - Negative Charge |
| Glu - Tyr- | 1850199.055 | 61.65925894 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 2725270.547 | 61.65925894 | Negative Charge - Negative Charge |

**Table S20.** Non-statistically significant pairwise comparisons of the y dihedral angles populating the a conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| None Exist | None Exist | None Exist | None Exist |

**Table S21.** Statistically significant pairwise comparisons of the f dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 6268.222051 | 60.15599251 | Hydrophobic - Hydrophobic |
| Ala - Leu | 637.6065654 | 60.15599251 | Hydrophobic - Hydrophobic |
| Ala - Ile | 8564.345771 | 60.15599251 | Hydrophobic - Hydrophobic |
| Ala - Met | 20500.04148 | 60.15599251 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 6987.343615 | 60.15599251 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 12749.59023 | 60.15599251 | Hydrophobic - Aromatic |
| Ala - Phe | 33167.36966 | 60.15599251 | Hydrophobic - Aromatic |
| Ala - Tyr | 19074.96105 | 60.15599251 | Hydrophobic - Aromatic |
| Ala - Trp | 3851.062116 | 60.15599251 | Hydrophobic - Aromatic |
| Ala - Ser | 113.714625 | 60.15599251 | Hydrophobic - Polar |
| Ala - Thr | 30278.97998 | 60.15599251 | Hydrophobic - Polar |
| Ala - Cys | 21834.25419 | 60.15599251 | Hydrophobic - Polar |
| Ala - Asn | 24994.34223 | 60.15599251 | Hydrophobic - Polar |
| Ala - Gln | 9998.210405 | 60.15599251 | Hydrophobic - Polar |
| Ala - Arg:NE | 7200.384465 | 60.15599251 | Hydrophobic - Polar |
| Ala - Arg:NH | 4858.988392 | 60.15599251 | Hydrophobic - Polar |
| Ala - Asp:H | 27371.254 | 60.15599251 | Hydrophobic - Polar |
| Ala - Glu:H | 19445.65699 | 60.15599251 | Hydrophobic - Polar |
| Ala - LysN | 51625.69152 | 60.15599251 | Hydrophobic - Polar |
| Ala - Arg | 562.7823059 | 60.15599251 | Hydrophobic - Positive Charge |
| Ala - His+ | 523104.9163 | 60.15599251 | Hydrophobic - Positive Charge |
| Ala - Asp | 83062.93385 | 60.15599251 | Hydrophobic - Negative Charge |
| Ala - Glu | 179.9955513 | 60.15599251 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 89950.76629 | 60.15599251 | Hydrophobic - Negative Charge |
| Val - Leu | 3668.854214 | 60.15599251 | Hydrophobic - Hydrophobic |
| Val - Ile | 226.8466489 | 60.15599251 | Hydrophobic - Hydrophobic |
| Val - Met | 56029.34292 | 60.15599251 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 34871.17575 | 60.15599251 | Hydrophobic - Aromatic |
| Val - His:NE2 | 47963.2403 | 60.15599251 | Hydrophobic - Aromatic |
| Val - Phe | 75579.88852 | 60.15599251 | Hydrophobic - Aromatic |
| Val - Tyr | 53626.67729 | 60.15599251 | Hydrophobic - Aromatic |
| Val - Ser | 7463.668904 | 60.15599251 | Hydrophobic - Polar |
| Val - Thr | 8973.946805 | 60.15599251 | Hydrophobic - Polar |
| Val - Cys | 61079.26388 | 60.15599251 | Hydrophobic - Polar |
| Val - Asn | 69136.56152 | 60.15599251 | Hydrophobic - Polar |
| Val - Gln | 38769.59883 | 60.15599251 | Hydrophobic - Polar |
| Val - Arg:NE | 32448.06568 | 60.15599251 | Hydrophobic - Polar |
| Val - Arg:NH | 26464.79232 | 60.15599251 | Hydrophobic - Polar |
| Val - Asp:H | 72404.32654 | 60.15599251 | Hydrophobic - Polar |
| Val - Glu:H | 55173.12621 | 60.15599251 | Hydrophobic - Polar |
| Val - LysN | 106690.3531 | 60.15599251 | Hydrophobic - Polar |
| Val - Arg | 3836.396877 | 60.15599251 | Hydrophobic - Positive Charge |
| Val - His+ | 678509.3531 | 60.15599251 | Hydrophobic - Positive Charge |
| Val - Lys | 8939.480823 | 60.15599251 | Hydrophobic - Positive Charge |
| Val - Asp | 142678.2317 | 60.15599251 | Hydrophobic - Negative Charge |
| Val - Glu | 4457.612604 | 60.15599251 | Hydrophobic - Negative Charge |
| Val - Tyr- | 150925.2034 | 60.15599251 | Hydrophobic - Negative Charge |
| Leu - Ile | 5672.704225 | 60.15599251 | Hydrophobic - Hydrophobic |
| Leu - Met | 37080.90064 | 60.15599251 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 17535.37744 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 28700.08409 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - Phe | 55654.71601 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - Tyr | 34884.38057 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - Trp | 2017.092711 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - Ser | 414.8828517 | 60.15599251 | Hydrophobic - Polar |
| Leu - Thr | 26633.8189 | 60.15599251 | Hydrophobic - Polar |
| Leu - Cys | 41374.6086 | 60.15599251 | Hydrophobic - Polar |
| Leu - Asn | 48997.1907 | 60.15599251 | Hydrophobic - Polar |
| Leu - Gln | 21418.91471 | 60.15599251 | Hydrophobic - Polar |
| Leu - Arg:NE | 16354.44462 | 60.15599251 | Hydrophobic - Polar |
| Leu - Arg:NH | 11919.03924 | 60.15599251 | Hydrophobic - Polar |
| Leu - Asp:H | 52255.03938 | 60.15599251 | Hydrophobic - Polar |
| Leu - Glu:H | 36130.01199 | 60.15599251 | Hydrophobic - Polar |
| Leu - LysN | 87219.05196 | 60.15599251 | Hydrophobic - Polar |
| Leu - His+ | 779276.4112 | 60.15599251 | Hydrophobic - Positive Charge |
| Leu - Lys | 1248.959295 | 60.15599251 | Hydrophobic - Positive Charge |
| Leu - Asp | 123641.9052 | 60.15599251 | Hydrophobic - Negative Charge |
| Leu - Glu | 122.0406817 | 60.15599251 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 132128.5515 | 60.15599251 | Hydrophobic - Negative Charge |
| Ile - Met | 61117.37382 | 60.15599251 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 39725.59416 | 60.15599251 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 53109.02312 | 60.15599251 | Hydrophobic - Aromatic |
| Ile - Phe | 80792.22487 | 60.15599251 | Hydrophobic - Aromatic |
| Ile - Tyr | 58682.63276 | 60.15599251 | Hydrophobic - Aromatic |
| Ile - Trp | 298.8439201 | 60.15599251 | Hydrophobic - Aromatic |
| Ile - Ser | 10382.53428 | 60.15599251 | Hydrophobic - Polar |
| Ile - Thr | 6031.400553 | 60.15599251 | Hydrophobic - Polar |
| Ile - Cys | 66272.90924 | 60.15599251 | Hydrophobic - Polar |
| Ile - Asn | 74344.13466 | 60.15599251 | Hydrophobic - Polar |
| Ile - Gln | 43604.09612 | 60.15599251 | Hydrophobic - Polar |
| Ile - Arg:NE | 37055.09518 | 60.15599251 | Hydrophobic - Polar |
| Ile - Arg:NH | 30771.97963 | 60.15599251 | Hydrophobic - Polar |
| Ile - Asp:H | 77605.60859 | 60.15599251 | Hydrophobic - Polar |
| Ile - Glu:H | 60277.68483 | 60.15599251 | Hydrophobic - Polar |
| Ile - LysN | 111634.9239 | 60.15599251 | Hydrophobic - Polar |
| Ile – Arg | 5871.800454 | 60.15599251 | Hydrophobic - Positive Charge |
| Ile - His+ | 658573.4643 | 60.15599251 | Hydrophobic - Positive Charge |
| Ile – Lys | 11841.97277 | 60.15599251 | Hydrophobic - Positive Charge |
| Ile – Asp | 147478.2757 | 60.15599251 | Hydrophobic - Negative Charge |
| Ile – Glu | 6488.378791 | 60.15599251 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 155654.6089 | 60.15599251 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 11393.53512 | 60.15599251 | Hydrophobic - Aromatic |
| Met - His:NE2 | 5513.628147 | 60.15599251 | Hydrophobic - Aromatic |
| Met - Phe | 2737.998107 | 60.15599251 | Hydrophobic - Aromatic |
| Met – Trp | 33431.40156 | 60.15599251 | Hydrophobic - Aromatic |
| Met – Ser | 45449.63874 | 60.15599251 | Hydrophobic - Polar |
| Met - Thr | 121573.2913 | 60.15599251 | Hydrophobic - Polar |
| Met - Gln | 4259.579893 | 60.15599251 | Hydrophobic - Polar |
| Met - Arg:NE | 6550.364128 | 60.15599251 | Hydrophobic - Polar |
| Met - Arg:NH | 8900.113063 | 60.15599251 | Hydrophobic - Polar |
| Met - Asp:H | 79.00781065 | 60.15599251 | Hydrophobic - Polar |
| Met - Glu:H | 81.04452051 | 60.15599251 | Hydrophobic - Polar |
| Met - LysN | 10735.85237 | 60.15599251 | Hydrophobic - Polar |
| Met - Arg | 36173.22319 | 60.15599251 | Hydrophobic - Positive Charge |
| Met - His+ | 696734.3682 | 60.15599251 | Hydrophobic - Positive Charge |
| Met - Lys | 26844.05768 | 60.15599251 | Hydrophobic - Positive Charge |
| Met - Asp | 37483.84598 | 60.15599251 | Hydrophobic - Negative Charge |
| Met - Glu | 26176.07327 | 60.15599251 | Hydrophobic - Negative Charge |
| Met - Tyr- | 43739.02384 | 60.15599251 | Hydrophobic - Negative Charge |
| His :ND1 - His:NE2 | 3202.166672 | 60.15599251 | Aromatic - Aromatic |
| His:ND1 - Phe | 28185.42645 | 60.15599251 | Aromatic - Aromatic |
| His:ND1 - Tyr | 9734.591836 | 60.15599251 | Aromatic - Aromatic |
| His:ND1 - Trp | 18898.35638 | 60.15599251 | Aromatic - Aromatic |
| His:ND1 - Ser | 21632.75296 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Thr | 95998.99273 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Cys | 14156.74108 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Asn | 22388.18111 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Gln | 1297.583276 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Arg:NE | 159.2908431 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Arg:NH | 71.21674243 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Asp:H | 25923.30418 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Glu:H | 10323.74254 | 60.15599251 | Aromatic - Polar |
| His:ND1 - LysN | 69240.45428 | 60.15599251 | Aromatic - Polar |
| His:ND1 - Arg | 16866.16451 | 60.15599251 | Aromatic - Positive Charge |
| His:ND1 - His+ | 1763182.702 | 60.15599251 | Aromatic - Positive Charge |
| His:ND1 - Lys | 9290.158376 | 60.15599251 | Aromatic - Positive Charge |
| His:ND1 - Asp | 105615.5457 | 60.15599251 | Aromatic - Negative Charge |
| His:ND1 - Glu | 10643.67795 | 60.15599251 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 115224.7412 | 60.15599251 | Aromatic - Negative Charge |
| His:NE2 - Phe | 19574.77568 | 60.15599251 | Aromatic - Aromatic |
| His:NE2 - Tyr | 4316.165753 | 60.15599251 | Aromatic - Aromatic |
| His:NE2 - Trp | 25574.97822 | 60.15599251 | Aromatic - Aromatic |
| His:NE2 - Ser | 40937.57733 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Thr | 119438.122 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Cys | 6758.044326 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Asn | 12367.06263 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Arg:NE | 790.8925673 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Arg:NH | 2270.695169 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Asp:H | 15720.19152 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Glu:H | 4505.222356 | 60.15599251 | Aromatic - Polar |
| His:NE2 - LysN | 58263.46749 | 60.15599251 | Aromatic - Polar |
| His:NE2 - Arg | 27751.19102 | 60.15599251 | Aromatic - Positive Charge |
| His:NE2 - His+ | 2237119.428 | 60.15599251 | Aromatic - Positive Charge |
| His:NE2 - Lys | 18315.82111 | 60.15599251 | Aromatic - Positive Charge |
| His:NE2 - Asp | 94551.06546 | 60.15599251 | Aromatic - Negative Charge |
| His:NE2 - Glu | 17918.65817 | 60.15599251 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 104169.991 | 60.15599251 | Aromatic - Negative Charge |
| Phe - Tyr | 3442.049862 | 60.15599251 | Aromatic - Aromatic |
| Phe - Trp | 45636.13559 | 60.15599251 | Aromatic - Aromatic |
| Phe - Ser | 70702.32956 | 60.15599251 | Aromatic - Polar |
| Phe - Thr | 149077.0132 | 60.15599251 | Aromatic - Polar |
| Phe - Cys | 4225.710887 | 60.15599251 | Aromatic - Polar |
| Phe - Asn | 4904.910796 | 60.15599251 | Aromatic - Polar |
| Phe - Gln | 14419.28706 | 60.15599251 | Aromatic - Polar |
| Phe - Arg:NE | 17915.44087 | 60.15599251 | Aromatic - Polar |
| Phe - Arg:NH | 20980.72443 | 60.15599251 | Aromatic - Polar |
| Phe - Asp:H | 3051.168206 | 60.15599251 | Aromatic - Polar |
| Phe - Glu:H | 3987.489983 | 60.15599251 | Aromatic - Polar |
| Phe - LysN | 1855.473885 | 60.15599251 | Aromatic - Polar |
| Phe - Arg | 54495.23086 | 60.15599251 | Aromatic - Positive Charge |
| Phe - His+ | 572519.1502 | 60.15599251 | Aromatic - Positive Charge |
| Phe - Lys | 44069.7711 | 60.15599251 | Aromatic - Positive Charge |
| Phe - Asp | 20358.32798 | 60.15599251 | Aromatic - Negative Charge |
| Phe - Glu | 40516.55809 | 60.15599251 | Aromatic - Negative Charge |
| Phe - Tyr- | 25267.17999 | 60.15599251 | Aromatic - Negative Charge |
| Tyr - Trp | 31984.53324 | 60.15599251 | Aromatic - Aromatic |
| Tyr - Ser | 42409.75945 | 60.15599251 | Aromatic - Polar |
| Tyr - Thr | 117962.8418 | 60.15599251 | Aromatic - Polar |
| Tyr - Gln | 3390.962399 | 60.15599251 | Aromatic - Polar |
| Tyr - Arg:NE | 5491.58809 | 60.15599251 | Aromatic - Polar |
| Tyr - Arg:NH | 7708.5146 | 60.15599251 | Aromatic - Polar |
| Tyr - Asp:H | 283.6105568 | 60.15599251 | Aromatic - Polar |
| Tyr - LysN | 12264.81542 | 60.15599251 | Aromatic - Polar |
| Tyr - Arg | 34011.48051 | 60.15599251 | Aromatic - Positive Charge |
| Tyr - His+ | 706320.4183 | 60.15599251 | Aromatic - Positive Charge |
| Tyr - Lys | 24877.44842 | 60.15599251 | Aromatic - Positive Charge |
| Tyr - Asp | 39764.63946 | 60.15599251 | Aromatic - Negative Charge |
| Tyr - Glu | 24527.57663 | 60.15599251 | Aromatic - Negative Charge |
| Tyr - Tyr- | 46150.04987 | 60.15599251 | Aromatic - Negative Charge |
| Trp - Ser | 3929.78552 | 60.15599251 | Aromatic - Polar |
| Trp - Thr | 7143.756573 | 60.15599251 | Aromatic - Polar |
| Trp - Cys | 34723.80997 | 60.15599251 | Aromatic - Polar |
| Trp - Asn | 37580.99901 | 60.15599251 | Aromatic - Polar |
| Trp - Gln | 22260.98945 | 60.15599251 | Aromatic - Polar |
| Trp - Arg:NE | 18792.41919 | 60.15599251 | Aromatic - Polar |
| Trp - Arg:NH | 15527.07117 | 60.15599251 | Aromatic - Polar |
| Trp - Asp:H | 39805.07037 | 60.15599251 | Aromatic - Polar |
| Trp - Glu:H | 32374.9654 | 60.15599251 | Aromatic - Polar |
| Trp - LysN | 61172.33648 | 60.15599251 | Aromatic - Polar |
| Trp - Arg | 2122.515469 | 60.15599251 | Aromatic - Positive Charge |
| Trp - His+ | 382304.9923 | 60.15599251 | Aromatic - Positive Charge |
| Trp - Lys | 5148.46613 | 60.15599251 | Aromatic - Positive Charge |
| Trp - Asp | 89224.38227 | 60.15599251 | Aromatic - Negative Charge |
| Trp - Glu | 2639.63081 | 60.15599251 | Aromatic - Negative Charge |
| Trp - Tyr- | 95170.85754 | 60.15599251 | Aromatic - Negative Charge |
| Ser - Thr | 40882.09499 | 60.15599251 | Polar - Polar |
| Ser - Cys | 55467.35564 | 60.15599251 | Polar - Polar |
| Ser - Asn | 73856.42453 | 60.15599251 | Polar - Polar |
| Ser - Gln | 25235.34519 | 60.15599251 | Polar - Polar |
| Ser - Arg:NE | 18039.85038 | 60.15599251 | Polar - Polar |
| Ser - Arg:NH | 12077.39954 | 60.15599251 | Polar - Polar |
| Ser - Asp:H | 77558.75907 | 60.15599251 | Polar - Polar |
| Ser - Glu:H | 45142.85005 | 60.15599251 | Polar - Polar |
| Ser - LysN | 126942.2718 | 60.15599251 | Polar - Polar |
| Ser - Arg | 338.7313042 | 60.15599251 | Polar - Positive Charge |
| Ser - His+ | 1397962.548 | 60.15599251 | Polar - Positive Charge |
| Ser - Lys | 414.1629019 | 60.15599251 | Polar - Positive Charge |
| Ser - Asp | 161397.0512 | 60.15599251 | Polar - Negative Charge |
| Ser - Tyr- | 171394.243 | 60.15599251 | Polar - Negative Charge |
| Thr - Cys | 133942.1129 | 60.15599251 | Polar - Polar |
| Thr - Asn | 150687.6815 | 60.15599251 | Polar - Polar |
| Thr - Gln | 97812.08048 | 60.15599251 | Polar - Polar |
| Thr - Arg:NE | 86461.65052 | 60.15599251 | Polar - Polar |
| Thr - Arg:NH | 74999.6822 | 60.15599251 | Polar - Polar |
| Thr - Asp:H | 154401.1404 | 60.15599251 | Polar - Polar |
| Thr - Glu:H | 121870.0966 | 60.15599251 | Polar - Polar |
| Thr - LysN | 198647.0703 | 60.15599251 | Polar - Polar |
| Thr - Arg | 27020.9382 | 60.15599251 | Polar - Positive Charge |
| Thr - His+ | 893415.7624 | 60.15599251 | Polar - Positive Charge |
| Thr - Lys | 40333.65689 | 60.15599251 | Polar - Positive Charge |
| Thr - Asp | 235463.1895 | 60.15599251 | Polar - Negative Charge |
| Thr - Glu | 26495.40226 | 60.15599251 | Polar - Negative Charge |
| Thr - Tyr- | 244933.2681 | 60.15599251 | Polar - Negative Charge |
| Cys - Gln | 4552.0073 | 60.15599251 | Polar - Polar |
| Cys - Arg:NE | 7183.206199 | 60.15599251 | Polar - Polar |
| Cys - Arg:NH | 9803.438793 | 60.15599251 | Polar - Polar |
| Cys - Asp:H | 371.5497092 | 60.15599251 | Polar - Polar |
| Cys - LysN | 16547.64608 | 60.15599251 | Polar - Polar |
| Cys - Arg | 40302.48722 | 60.15599251 | Polar - Positive Charge |
| Cys - His+ | 1060202.983 | 60.15599251 | Polar - Positive Charge |
| Cys - Lys | 30231.13751 | 60.15599251 | Polar - Positive Charge |
| Cys - Asp | 48498.3831 | 60.15599251 | Polar - Negative Charge |
| Cys - Glu | 28186.6633 | 60.15599251 | Polar - Negative Charge |
| Cys - Tyr- | 55898.56153 | 60.15599251 | Polar - Negative Charge |
| Asn - Gln | 6462.990439 | 60.15599251 | Polar - Polar |
| Asn - Arg:NE | 9762.88443 | 60.15599251 | Polar - Polar |
| Asn - Arg:NH | 12784.22098 | 60.15599251 | Polar - Polar |
| Asn - Asp:H | 401.9474584 | 60.15599251 | Polar - Polar |
| Asn - LysN | 22204.52796 | 60.15599251 | Polar - Polar |
| Asn - Arg | 47687.07438 | 60.15599251 | Polar - Positive Charge |
| Asn - His+ | 1734743.459 | 60.15599251 | Polar - Positive Charge |
| Asn - Lys | 36877.46025 | 60.15599251 | Polar - Positive Charge |
| Asn - Asp | 57766.79531 | 60.15599251 | Polar - Negative Charge |
| Asn - Glu | 32341.54843 | 60.15599251 | Polar - Negative Charge |
| Asn - Tyr- | 66126.79881 | 60.15599251 | Polar - Negative Charge |
| Gln - Arg:NE | 360.2765055 | 60.15599251 | Polar - Polar |
| Gln - Arg:NH | 1299.871736 | 60.15599251 | Polar - Polar |
| Gln - Asp:H | 8589.696685 | 60.15599251 | Polar - Polar |
| Gln - Glu:H | 3412.130308 | 60.15599251 | Polar - Polar |
| Gln - LysN | 35228.91255 | 60.15599251 | Polar - Polar |
| Gln - Arg | 20734.00658 | 60.15599251 | Polar - Positive Charge |
| Gln - His+ | 1016949.221 | 60.15599251 | Polar - Positive Charge |
| Gln - Lys | 12925.52842 | 60.15599251 | Polar - Positive Charge |
| Gln - Asp | 70304.46511 | 60.15599251 | Polar - Negative Charge |
| Gln - Glu | 14051.50055 | 60.15599251 | Polar - Negative Charge |
| Gln - Tyr- | 78391.22911 | 60.15599251 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 304.7460692 | 60.15599251 | Polar - Polar |
| Arg:NE - Asp:H | 12121.10302 | 60.15599251 | Polar - Polar |
| Arg:NE - Glu:H | 5602.607665 | 60.15599251 | Polar - Polar |
| Arg:NE - LysN | 39978.17415 | 60.15599251 | Polar - Polar |
| Arg:NE - Arg | 15786.22474 | 60.15599251 | Polar - Positive Charge |
| Arg:NE - His+ | 951629.3541 | 60.15599251 | Polar - Positive Charge |
| Arg:NE - Lys | 8963.687087 | 60.15599251 | Polar - Positive Charge |
| Arg:NE - Asp | 75181.48251 | 60.15599251 | Polar - Negative Charge |
| Arg:NE - Glu | 10556.94896 | 60.15599251 | Polar - Negative Charge |
| Arg:NE - Tyr- | 83283.70356 | 60.15599251 | Polar - Negative Charge |
| Arg:NH - Asp:H | 15237.6645 | 60.15599251 | Polar - Polar |
| Arg:NH - Glu:H | 7900.784594 | 60.15599251 | Polar - Polar |
| Arg:NH - LysN | 43136.42987 | 60.15599251 | Polar - Polar |
| Arg:NH - Arg | 11463.365 | 60.15599251 | Polar - Positive Charge |
| Arg:NH - His+ | 860061.1929 | 60.15599251 | Polar - Positive Charge |
| Arg:NH - Lys | 5746.046652 | 60.15599251 | Polar - Positive Charge |
| Arg:NH - Asp | 78045.04329 | 60.15599251 | Polar - Negative Charge |
| Arg:NH - Glu | 7538.89752 | 60.15599251 | Polar - Negative Charge |
| Arg:NH - Tyr- | 86027.88226 | 60.15599251 | Polar - Negative Charge |
| Asp:H - Glu:H | 427.8256751 | 60.15599251 | Polar - Polar |
| Asp:H - LysN | 16148.15417 | 60.15599251 | Polar - Polar |
| Asp:H - Arg | 50915.83975 | 60.15599251 | Polar - Positive Charge |
| Asp:H - His+ | 1491587.713 | 60.15599251 | Polar - Positive Charge |
| Asp:H - Lys | 40037.58992 | 60.15599251 | Polar - Positive Charge |
| Asp:H - Asp | 49842.84514 | 60.15599251 | Polar - Negative Charge |
| Asp:H - Glu | 34987.10162 | 60.15599251 | Polar - Negative Charge |
| Asp:H - Tyr- | 57721.68368 | 60.15599251 | Polar - Negative Charge |
| Glu:H - LysN | 14165.55729 | 60.15599251 | Polar - Polar |
| Glu:H - Arg | 35208.0303 | 60.15599251 | Polar - Positive Charge |
| Glu:H - His+ | 806417.2781 | 60.15599251 | Polar - Positive Charge |
| Glu:H - Lys | 25817.05544 | 60.15599251 | Polar - Positive Charge |
| Glu:H - Asp | 43431.06523 | 60.15599251 | Polar - Negative Charge |
| Glu:H - Glu | 25104.67252 | 60.15599251 | Polar - Negative Charge |
| Glu:H - Tyr- | 50199.68915 | 60.15599251 | Polar - Negative Charge |
| LysN - Arg | 85465.30186 | 60.15599251 | Polar - Positive Charge |
| LysN - His+ | 812895.9289 | 60.15599251 | Polar - Positive Charge |
| LysN - Lys | 74237.72409 | 60.15599251 | Polar - Positive Charge |
| LysN - Asp | 14519.52466 | 60.15599251 | Polar - Negative Charge |
| LysN - Glu | 62044.714 | 60.15599251 | Polar - Negative Charge |
| LysN - Tyr- | 19293.41661 | 60.15599251 | Polar - Negative Charge |
| Arg - His+ | 769593.0707 | 60.15599251 | Positive Charge - Positive Charge |
| Arg - Lys | 1125.666671 | 60.15599251 | Positive Charge - Positive Charge |
| Arg - Asp | 121784.4195 | 60.15599251 | Positive Charge - Negative Charge |
| Arg - Glu | 90.69171605 | 60.15599251 | Positive Charge - Negative Charge |
| Arg - Tyr- | 130218.8838 | 60.15599251 | Positive Charge - Negative Charge |
| His+ - Lys | 829860.9975 | 60.15599251 | Positive Charge - Positive Charge |
| His+ - Asp | 274211.4649 | 60.15599251 | Positive Charge - Negative Charge |
| His+ - Glu | 574112.4682 | 60.15599251 | Positive Charge - Negative Charge |
| His+ - Tyr- | 237940.7557 | 60.15599251 | Positive Charge - Negative Charge |
| Lys - Asp | 110619.1258 | 60.15599251 | Positive Charge - Negative Charge |
| Lys - Glu | 435.8744221 | 60.15599251 | Positive Charge - Negative Charge |
| Lys - Tyr- | 119103.405 | 60.15599251 | Positive Charge - Negative Charge |
| Asp - Glu | 95127.17933 | 60.15599251 | Negative Charge - Negative Charge |
| Asp - Tyr- | 317.9081992 | 60.15599251 | Negative Charge - Negative Charge |
| Glu - Tyr- | 102441.786 | 60.15599251 | Negative Charge - Negative Charge |

**Table S22.** Non-statistically significant pairwise comparisons of the f dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Lys | 31.97497414 | 60.15599251 | Hydrophobic - Positive Charge |
| Val - Trp | 20.99414262 | 60.15599251 | Hydrophobic - Aromatic |
| Leu - Arg | 2.656827897 | 60.15599251 | Hydrophobic - Positive Charge |
| Met - Tyr | 42.22331272 | 60.15599251 | Hydrophobic - Aromatic |
| Met - Cys | 42.174002 | 60.15599251 | Hydrophobic - Polar |
| Met - Asn | 20.74217257 | 60.15599251 | Hydrophobic - Polar |
| His:NE2 - Gln | 26.43432901 | 60.15599251 | Aromatic - Polar |
| Tyr - Cys | 0.655867954 | 60.15599251 | Aromatic - Polar |
| Tyr - Asn | 13.19643664 | 60.15599251 | Aromatic - Polar |
| Tyr - Glu:H | 5.044911594 | 60.15599251 | Aromatic - Polar |
| Ser - Glu | 32.66707516 | 60.15599251 | Polar - Negative Charge |
| Cys - Asn | 11.08921223 | 60.15599251 | Polar - Polar |
| Cys - Glu:H | 11.56799194 | 60.15599251 | Polar - Polar |
| Asn - Glu:H | 45.75683802 | 60.15599251 | Polar - Polar |

**Table S23.** Statistically significant pairwise comparisons of the y dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 15717437.62 | 60.1559216 | Hydrophobic - Hydrophobic |
| Ala - Leu | 1378.908332 | 60.1559216 | Hydrophobic - Hydrophobic |
| Ala - Ile | 15003938.99 | 60.1559216 | Hydrophobic - Hydrophobic |
| Ala - Met | 21449.7476 | 60.1559216 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 179746.8033 | 60.1559216 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 255663.7234 | 60.1559216 | Hydrophobic - Aromatic |
| Ala - Phe | 33564.61422 | 60.1559216 | Hydrophobic - Aromatic |
| Ala - Tyr | 24375.58935 | 60.1559216 | Hydrophobic - Aromatic |
| Ala - Trp | 12406646.35 | 60.1559216 | Hydrophobic - Aromatic |
| Ala - Ser | 141825.5914 | 60.1559216 | Hydrophobic - Polar |
| Ala - Thr | 15414027.18 | 60.1559216 | Hydrophobic - Polar |
| Ala - Cys | 189354.0356 | 60.1559216 | Hydrophobic - Polar |
| Ala - Asn | 304481.4173 | 60.1559216 | Hydrophobic - Polar |
| Ala - Gln | 25199.31991 | 60.1559216 | Hydrophobic - Polar |
| Ala - Arg:NE | 17277.06462 | 60.1559216 | Hydrophobic - Polar |
| Ala - Arg:NH | 7105.850706 | 60.1559216 | Hydrophobic - Polar |
| Ala - Asp:H | 195535.7401 | 60.1559216 | Hydrophobic - Polar |
| Ala - Glu:H | 45878.10735 | 60.1559216 | Hydrophobic - Polar |
| Ala - LysN | 165642.7687 | 60.1559216 | Hydrophobic - Polar |
| Ala - Arg | 5422.89178 | 60.1559216 | Hydrophobic - Positive Charge |
| Ala - His+ | 1258698.681 | 60.1559216 | Hydrophobic - Positive Charge |
| Ala - Lys | 6267.101296 | 60.1559216 | Hydrophobic - Positive Charge |
| Ala - Asp | 39391.10031 | 60.1559216 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 27261.87291 | 60.1559216 | Hydrophobic - Negative Charge |
| Val - Leu | 18094520.23 | 60.1559216 | Hydrophobic - Hydrophobic |
| Val - Met | 21020464.07 | 60.1559216 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 22825825.12 | 60.1559216 | Hydrophobic - Aromatic |
| Val - His:NE2 | 23607131.51 | 60.1559216 | Hydrophobic - Aromatic |
| Val - Phe | 20466541.51 | 60.1559216 | Hydrophobic - Aromatic |
| Val - Tyr | 20886783.63 | 60.1559216 | Hydrophobic - Aromatic |
| Val - Trp | 33871.16766 | 60.1559216 | Hydrophobic - Aromatic |
| Val - Ser | 20091739.92 | 60.1559216 | Hydrophobic - Polar |
| Val - Thr | 488.5820445 | 60.1559216 | Hydrophobic - Polar |
| Val - Cys | 21153306.28 | 60.1559216 | Hydrophobic - Polar |
| Val - Asn | 22736456.4 | 60.1559216 | Hydrophobic - Polar |
| Val - Gln | 22373746.39 | 60.1559216 | Hydrophobic - Polar |
| Val - Arg:NE | 21800961.31 | 60.1559216 | Hydrophobic - Polar |
| Val - Arg:NH | 21107011.09 | 60.1559216 | Hydrophobic - Polar |
| Val - Asp:H | 23214207.05 | 60.1559216 | Hydrophobic - Polar |
| Val - Glu:H | 21290312.92 | 60.1559216 | Hydrophobic - Polar |
| Val - LysN | 21716261.68 | 60.1559216 | Hydrophobic - Polar |
| Val - Arg | 17722957.53 | 60.1559216 | Hydrophobic - Positive Charge |
| Val - His+ | 17804701.66 | 60.1559216 | Hydrophobic - Positive Charge |
| Val - Lys | 19134421.39 | 60.1559216 | Hydrophobic - Positive Charge |
| Val - Asp | 19129903.07 | 60.1559216 | Hydrophobic - Negative Charge |
| Val - Glu | 16047421.67 | 60.1559216 | Hydrophobic - Negative Charge |
| Val - Tyr- | 19019860.25 | 60.1559216 | Hydrophobic - Negative Charge |
| Leu- Ile | 17144053.35 | 60.1559216 | Hydrophobic - Hydrophobic |
| Leu - Met | 14098.62171 | 60.1559216 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 192792.1987 | 60.1559216 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 289491.0941 | 60.1559216 | Hydrophobic - Aromatic |
| Leu - Phe | 25640.72999 | 60.1559216 | Hydrophobic - Aromatic |
| Leu - Tyr | 16805.4134 | 60.1559216 | Hydrophobic - Aromatic |
| Leu - Trp | 13616642.02 | 60.1559216 | Hydrophobic - Aromatic |
| Leu - Ser | 143919.1179 | 60.1559216 | Hydrophobic - Polar |
| Leu - Thr | 17718649.69 | 60.1559216 | Hydrophobic - Polar |
| Leu - Cys | 201448.8485 | 60.1559216 | Hydrophobic - Polar |
| Leu - Asn | 348990.6753 | 60.1559216 | Hydrophobic - Polar |
| Leu - Gln | 17484.87973 | 60.1559216 | Hydrophobic - Polar |
| Leu - Arg:NE | 10313.49675 | 60.1559216 | Hydrophobic - Polar |
| Leu - Arg:NH | 2413.607896 | 60.1559216 | Hydrophobic - Polar |
| Leu - Asp:H | 212921.1324 | 60.1559216 | Hydrophobic - Polar |
| Leu - Glu:H | 38076.10488 | 60.1559216 | Hydrophobic - Polar |
| Leu - LysN | 173966.7064 | 60.1559216 | Hydrophobic - Polar |
| Leu - Arg | 1616.533815 | 60.1559216 | Hydrophobic - Positive Charge |
| Leu - His+ | 1582828.391 | 60.1559216 | Hydrophobic - Positive Charge |
| Leu - Lys | 2027.7739 | 60.1559216 | Hydrophobic - Positive Charge |
| Leu - Asp | 31430.43983 | 60.1559216 | Hydrophobic - Negative Charge |
| Leu - Glu | 969.2662331 | 60.1559216 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 19645.86546 | 60.1559216 | Hydrophobic - Negative Charge |
| Ile - Met | 19699193.76 | 60.1559216 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 21120317.07 | 60.1559216 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 21742207.04 | 60.1559216 | Hydrophobic - Aromatic |
| Ile - Phe | 19191878.5 | 60.1559216 | Hydrophobic - Aromatic |
| Ile - Tyr | 19576378.95 | 60.1559216 | Hydrophobic - Aromatic |
| Ile - Trp | 33771.23327 | 60.1559216 | Hydrophobic - Aromatic |
| Ile - Ser | 18765146.9 | 60.1559216 | Hydrophobic - Polar |
| Ile - Thr | 343.4724103 | 60.1559216 | Hydrophobic - Polar |
| Ile - Cys | 19663480.65 | 60.1559216 | Hydrophobic - Polar |
| Ile – Asn | 20966797.06 | 60.1559216 | Hydrophobic - Polar |
| Ile – Gln | 20880749.8 | 60.1559216 | Hydrophobic - Polar |
| Ile - Arg:NE | 20393803.77 | 60.1559216 | Hydrophobic - Polar |
| Ile - Arg:NH | 19807437.99 | 60.1559216 | Hydrophobic - Polar |
| Ile - Asp:H | 21444108.97 | 60.1559216 | Hydrophobic - Polar |
| Ile - Glu:H | 19901301.14 | 60.1559216 | Hydrophobic - Polar |
| Ile - LysN | 20168865.3 | 60.1559216 | Hydrophobic - Polar |
| Ile – Arg | 16794799.67 | 60.1559216 | Hydrophobic - Positive Charge |
| Ile - His+ | 16407135.81 | 60.1559216 | Hydrophobic - Positive Charge |
| Ile – Lys | 18058083.38 | 60.1559216 | Hydrophobic - Positive Charge |
| Ile – Asp | 18000136.7 | 60.1559216 | Hydrophobic - Negative Charge |
| Ile – Glu | 15302765.9 | 60.1559216 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 17917311.38 | 60.1559216 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 143817.4511 | 60.1559216 | Hydrophobic - Aromatic |
| Met - His:NE2 | 257770.1312 | 60.1559216 | Hydrophobic - Aromatic |
| Met - Phe | 2446.166678 | 60.1559216 | Hydrophobic - Aromatic |
| Met - Tyr | 168.8934224 | 60.1559216 | Hydrophobic - Aromatic |
| Met – Trp | 14819528.34 | 60.1559216 | Hydrophobic - Aromatic |
| Met – Ser | 93482.07183 | 60.1559216 | Hydrophobic - Polar |
| Met - Thr | 20536122.17 | 60.1559216 | Hydrophobic - Polar |
| Met - Cys | 151826.5614 | 60.1559216 | Hydrophobic - Polar |
| Met - Asn | 328258.4892 | 60.1559216 | Hydrophobic - Polar |
| Met - Gln | 99.6359492 | 60.1559216 | Hydrophobic - Polar |
| Met - Arg:NE | 529.8296709 | 60.1559216 | Hydrophobic - Polar |
| Met - Arg:NH | 6311.443928 | 60.1559216 | Hydrophobic - Polar |
| Met - Asp:H | 166454.6146 | 60.1559216 | Hydrophobic - Polar |
| Met - Glu:H | 7573.167886 | 60.1559216 | Hydrophobic - Polar |
| Met - LysN | 123296.7507 | 60.1559216 | Hydrophobic - Polar |
| Met - Arg | 5330.380164 | 60.1559216 | Hydrophobic - Positive Charge |
| Met - His+ | 2021381.499 | 60.1559216 | Hydrophobic - Positive Charge |
| Met - Lys | 5537.46334 | 60.1559216 | Hydrophobic - Positive Charge |
| Met - Asp | 5420.70055 | 60.1559216 | Hydrophobic - Negative Charge |
| Met - Glu | 20100.15107 | 60.1559216 | Hydrophobic - Negative Charge |
| Met - Tyr- | 1035.244219 | 60.1559216 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 20955.24937 | 60.1559216 | Aromatic - Aromatic |
| His:ND1- Phe | 99359.30517 | 60.1559216 | Aromatic - Aromatic |
| His:ND1 - Tyr | 131503.2635 | 60.1559216 | Aromatic - Aromatic |
| His:ND1 - Trp | 15035118.83 | 60.1559216 | Aromatic - Aromatic |
| His:ND1 - Ser | 1001.742021 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Thr | 22232113.4 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Cys | 1979.269628 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Asn | 59273.10735 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Gln | 161547.4847 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Arg:NE | 178002.8217 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Arg:NH | 214648.1918 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Asp:H | 709.3047638 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Glu:H | 86337.94623 | 60.1559216 | Aromatic - Polar |
| His:ND1 - LysN | 111.6764642 | 60.1559216 | Aromatic - Polar |
| His:ND1 - Arg | 149101.8881 | 60.1559216 | Aromatic - Positive Charge |
| His:ND1 - His+ | 2046856.72 | 60.1559216 | Aromatic - Positive Charge |
| His:ND1 - Lys | 172149.9168 | 60.1559216 | Aromatic - Positive Charge |
| His:ND1 - Asp | 69013.05707 | 60.1559216 | Aromatic - Negative Charge |
| His:ND1 - Glu | 180586.7126 | 60.1559216 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 92143.95969 | 60.1559216 | Aromatic - Negative Charge |
| His:NE2 - Phe | 191060.1729 | 60.1559216 | Aromatic - Aromatic |
| His:NE2 - Tyr | 239603.5245 | 60.1559216 | Aromatic - Aromatic |
| His:NE2 - Trp | 15177032.55 | 60.1559216 | Aromatic - Aromatic |
| His:NE2 - Ser | 21011.42213 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Thr | 22968847.42 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Cys | 5852.023879 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Asn | 14783.32686 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Gln | 301516.6071 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Arg:NE | 314179.3351 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Arg:NH | 351057.5899 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Asp:H | 15029.29466 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Glu:H | 180989.5026 | 60.1559216 | Aromatic - Polar |
| His:NE2 - LysN | 19770.82628 | 60.1559216 | Aromatic - Polar |
| His:NE2 - Arg | 232688.4647 | 60.1559216 | Aromatic - Positive Charge |
| His:NE2 - His+ | 2296260.141 | 60.1559216 | Aromatic - Positive Charge |
| His:NE2 - Lys | 273676.516 | 60.1559216 | Aromatic - Positive Charge |
| His:NE2 - Asp | 137528.6378 | 60.1559216 | Aromatic - Negative Charge |
| His:NE2 - Glu | 258874.7852 | 60.1559216 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 168799.8378 | 60.1559216 | Aromatic - Negative Charge |
| Phe - Tyr | 1331.466506 | 60.1559216 | Aromatic - Aromatic |
| Phe - Trp | 14496657.46 | 60.1559216 | Aromatic - Aromatic |
| Phe - Ser | 62939.10663 | 60.1559216 | Aromatic - Polar |
| Phe - Thr | 19995417.32 | 60.1559216 | Aromatic - Polar |
| Phe - Cys | 108796.2252 | 60.1559216 | Aromatic - Polar |
| Phe - Asn | 252824.0611 | 60.1559216 | Aromatic - Polar |
| Phe - Gln | 1811.365572 | 60.1559216 | Aromatic - Polar |
| Phe - Arg:NE | 5408.603752 | 60.1559216 | Aromatic - Polar |
| Phe - Arg:NH | 16197.33743 | 60.1559216 | Aromatic - Polar |
| Phe - Asp:H | 116926.9729 | 60.1559216 | Aromatic - Polar |
| Phe - Glu:H | 1219.152155 | 60.1559216 | Aromatic - Polar |
| Phe - LysN | 84658.31131 | 60.1559216 | Aromatic - Polar |
| Phe - Arg | 13130.37375 | 60.1559216 | Aromatic - Positive Charge |
| Phe - His+ | 1792460.773 | 60.1559216 | Aromatic - Positive Charge |
| Phe - Lys | 14058.96646 | 60.1559216 | Aromatic - Positive Charge |
| Phe - Asp | 695.5155613 | 60.1559216 | Aromatic - Negative Charge |
| Phe - Glu | 32101.12397 | 60.1559216 | Aromatic - Negative Charge |
| Phe - Tyr- | 195.0742755 | 60.1559216 | Aromatic - Negative Charge |
| Tyr - Trp | 14740159.49 | 60.1559216 | Aromatic - Aromatic |
| Tyr - Ser | 84966.92499 | 60.1559216 | Aromatic - Polar |
| Tyr - Thr | 20405512.88 | 60.1559216 | Aromatic - Polar |
| Tyr - Cys | 139991.2218 | 60.1559216 | Aromatic - Polar |
| Tyr - Asn | 307906.9954 | 60.1559216 | Aromatic - Polar |
| Tyr - Arg:NE | 1318.531639 | 60.1559216 | Aromatic - Polar |
| Tyr - Arg:NH | 8472.556519 | 60.1559216 | Aromatic - Polar |
| Tyr - Asp:H | 152789.254 | 60.1559216 | Aromatic - Polar |
| Tyr - Glu:H | 5383.486684 | 60.1559216 | Aromatic - Polar |
| Tyr - LysN | 112574.6322 | 60.1559216 | Aromatic - Polar |
| Tyr - Arg | 7045.861812 | 60.1559216 | Aromatic - Positive Charge |
| Tyr - His+ | 1962857.22 | 60.1559216 | Aromatic - Positive Charge |
| Tyr - Lys | 7401.562418 | 60.1559216 | Aromatic - Positive Charge |
| Tyr - Asp | 3751.865563 | 60.1559216 | Aromatic - Negative Charge |
| Tyr - Glu | 22986.99279 | 60.1559216 | Aromatic - Negative Charge |
| Tyr - Tyr- | 403.0928181 | 60.1559216 | Aromatic - Negative Charge |
| Trp - Ser | 13963172.27 | 60.1559216 | Aromatic - Polar |
| Trp - Thr | 40870.52173 | 60.1559216 | Aromatic - Polar |
| Trp - Cys | 14316805.96 | 60.1559216 | Aromatic - Polar |
| Trp - Asn | 14739663.77 | 60.1559216 | Aromatic - Polar |
| Trp - Gln | 15391848.07 | 60.1559216 | Aromatic - Polar |
| Trp - Arg:NE | 15197919.55 | 60.1559216 | Aromatic - Polar |
| Trp - Arg:NH | 14981137.13 | 60.1559216 | Aromatic - Polar |
| Trp - Asp:H | 15153783.45 | 60.1559216 | Aromatic - Polar |
| Trp - Glu:H | 14806953.91 | 60.1559216 | Aromatic - Polar |
| Trp - LysN | 14610597.68 | 60.1559216 | Aromatic - Polar |
| Trp - Arg | 13364563.2 | 60.1559216 | Aromatic - Positive Charge |
| Trp - His+ | 11691179.22 | 60.1559216 | Aromatic - Positive Charge |
| Trp - Lys | 14061091.47 | 60.1559216 | Aromatic - Positive Charge |
| Trp - Asp | 13843826.91 | 60.1559216 | Aromatic - Negative Charge |
| Trp - Glu | 12580993.12 | 60.1559216 | Aromatic - Negative Charge |
| Trp - Tyr- | 13850865.34 | 60.1559216 | Aromatic - Negative Charge |
| Ser - Thr | 19605028.64 | 60.1559216 | Polar - Polar |
| Ser - Cys | 4412.594904 | 60.1559216 | Polar - Polar |
| Ser - Asn | 49520.77518 | 60.1559216 | Polar - Polar |
| Ser - Gln | 99914.09573 | 60.1559216 | Polar - Polar |
| Ser - Arg:NE | 114856.5951 | 60.1559216 | Polar - Polar |
| Ser - Arg:NH | 146239.5703 | 60.1559216 | Polar - Polar |
| Ser - Asp:H | 2872.244251 | 60.1559216 | Polar - Polar |
| Ser - Glu:H | 51386.45391 | 60.1559216 | Polar - Polar |
| Ser - LysN | 441.4081753 | 60.1559216 | Polar - Polar |
| Ser - Arg | 109749.054 | 60.1559216 | Polar - Positive Charge |
| Ser - His+ | 1296579.917 | 60.1559216 | Polar - Positive Charge |
| Ser - Lys | 123001.4448 | 60.1559216 | Polar - Positive Charge |
| Ser - Asp | 43999.03719 | 60.1559216 | Polar - Negative Charge |
| Ser - Glu | 141436.8189 | 60.1559216 | Polar - Negative Charge |
| Ser - Tyr- | 61424.83387 | 60.1559216 | Polar - Negative Charge |
| Thr - Cys | 20619959.13 | 60.1559216 | Polar - Polar |
| Thr - Asn | 22124259.47 | 60.1559216 | Polar - Polar |
| Thr - Gln | 21840679.58 | 60.1559216 | Polar - Polar |
| Thr - Arg:NE | 21292241.3 | 60.1559216 | Polar - Polar |
| Thr - Arg:NH | 20629091.23 | 60.1559216 | Polar - Polar |
| Thr - Asp:H | 22602476.51 | 60.1559216 | Polar - Polar |
| Thr - Glu:H | 20786422.68 | 60.1559216 | Polar - Polar |
| Thr - LysN | 21166822.04 | 60.1559216 | Polar - Polar |
| Thr - Arg | 17353681.21 | 60.1559216 | Polar - Positive Charge |
| Thr - His+ | 17294525.69 | 60.1559216 | Polar - Positive Charge |
| Thr - Lys | 18721169.25 | 60.1559216 | Polar - Positive Charge |
| Thr - Asp | 18700665.03 | 60.1559216 | Polar - Negative Charge |
| Thr - Glu | 15734280.08 | 60.1559216 | Polar - Negative Charge |
| Thr - Tyr- | 18598678.23 | 60.1559216 | Polar - Negative Charge |
| Cys - Asn | 27354.65008 | 60.1559216 | Polar - Polar |
| Cys - Gln | 167438.6453 | 60.1559216 | Polar - Polar |
| Cys - Arg:NE | 183872.9429 | 60.1559216 | Polar - Polar |
| Cys - Arg:NH | 219888.3752 | 60.1559216 | Polar - Polar |
| Cys - Asp:H | 505.7209511 | 60.1559216 | Polar - Polar |
| Cys - Glu:H | 95794.63856 | 60.1559216 | Polar - Polar |
| Cys - LysN | 2588.682615 | 60.1559216 | Polar - Polar |
| Cys - Arg | 158552.1184 | 60.1559216 | Polar - Positive Charge |
| Cys - His+ | 1440362.002 | 60.1559216 | Polar - Positive Charge |
| Cys - Lys | 180640.5607 | 60.1559216 | Polar - Positive Charge |
| Cys - Asp | 78713.25604 | 60.1559216 | Polar - Negative Charge |
| Cys - Glu | 190127.9283 | 60.1559216 | Polar - Negative Charge |
| Cys - Tyr- | 101875.2319 | 60.1559216 | Polar - Negative Charge |
| Asn - Gln | 383191.0923 | 60.1559216 | Polar - Polar |
| Asn - Arg:NE | 393187.5718 | 60.1559216 | Polar - Polar |
| Asn - Arg:NH | 428441.1601 | 60.1559216 | Polar - Polar |
| Asn - Asp:H | 51627.97042 | 60.1559216 | Polar - Polar |
| Asn - Glu:H | 245750.8884 | 60.1559216 | Polar - Polar |
| Asn - LysN | 52796.13536 | 60.1559216 | Polar - Polar |
| Asn - Arg | 286816.8338 | 60.1559216 | Polar - Positive Charge |
| Asn - His+ | 1757570.57 | 60.1559216 | Polar - Positive Charge |
| Asn - Lys | 336409.9698 | 60.1559216 | Polar - Positive Charge |
| Asn - Asp | 187740.7192 | 60.1559216 | Polar - Negative Charge |
| Asn - Glu | 308982.3798 | 60.1559216 | Polar - Negative Charge |
| Asn - Tyr- | 222132.2831 | 60.1559216 | Polar - Negative Charge |
| Gln - Arg:NE | 1210.930595 | 60.1559216 | Polar - Polar |
| Gln - Arg:NH | 8815.328342 | 60.1559216 | Polar - Polar |
| Gln - Asp:H | 189321.866 | 60.1559216 | Polar - Polar |
| Gln - Glu:H | 6792.893076 | 60.1559216 | Polar - Polar |
| Gln - LysN | 135623.6569 | 60.1559216 | Polar - Polar |
| Gln - Arg | 7136.191556 | 60.1559216 | Polar - Positive Charge |
| Gln - His+ | 2426617.262 | 60.1559216 | Polar - Positive Charge |
| Gln - Lys | 7565.541431 | 60.1559216 | Polar - Positive Charge |
| Gln - Asp | 4659.913206 | 60.1559216 | Polar - Negative Charge |
| Gln - Glu | 23782.54313 | 60.1559216 | Polar - Negative Charge |
| Gln - Tyr- | 609.2885126 | 60.1559216 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 3471.25172 | 60.1559216 | Polar - Polar |
| Arg:NE - Asp:H | 205513.7201 | 60.1559216 | Polar - Polar |
| Arg:NE - Glu:H | 12867.13487 | 60.1559216 | Polar - Polar |
| Arg:NE - LysN | 151851.3398 | 60.1559216 | Polar - Polar |
| Arg:NE - Arg | 3025.881748 | 60.1559216 | Polar - Positive Charge |
| Arg:NE - His+ | 2290781.371 | 60.1559216 | Polar - Positive Charge |
| Arg:NE - Lys | 3062.433201 | 60.1559216 | Polar - Positive Charge |
| Arg:NE - Asp | 9404.935602 | 60.1559216 | Polar - Negative Charge |
| Arg:NE - Glu | 15991.60757 | 60.1559216 | Polar - Negative Charge |
| Arg:NE - Tyr- | 2932.584006 | 60.1559216 | Polar - Negative Charge |
| Arg:NH - Asp:H | 242951.1672 | 60.1559216 | Polar - Polar |
| Arg:NH - Glu:H | 28052.37371 | 60.1559216 | Polar - Polar |
| Arg:NH - LysN | 186819.6877 | 60.1559216 | Polar - Polar |
| Arg:NH - His+ | 2183852.063 | 60.1559216 | Polar - Positive Charge |
| Arg:NH - Asp | 21722.9608 | 60.1559216 | Polar - Negative Charge |
| Arg:NH - Glu | 6175.415476 | 60.1559216 | Polar - Negative Charge |
| Arg:NH - Tyr- | 11121.40398 | 60.1559216 | Polar - Negative Charge |
| Asp:H - Glu:H | 103994.4504 | 60.1559216 | Polar - Polar |
| Asp:H - LysN | 1228.87386 | 60.1559216 | Polar - Polar |
| Asp:H - Arg | 166115.0848 | 60.1559216 | Polar - Positive Charge |
| Asp:H - His+ | 2191864.589 | 60.1559216 | Polar - Positive Charge |
| Asp:H - Lys | 192973.0217 | 60.1559216 | Polar - Positive Charge |
| Asp:H - Asp | 81793.04438 | 60.1559216 | Polar - Negative Charge |
| Asp:H - Glu | 196866.5089 | 60.1559216 | Polar - Negative Charge |
| Asp:H - Tyr- | 106907.75 | 60.1559216 | Polar - Negative Charge |
| Glu:H - LysN | 71944.35298 | 60.1559216 | Polar - Polar |
| Glu:H - Arg | 21895.02103 | 60.1559216 | Polar - Positive Charge |
| Glu:H - His+ | 1950728.037 | 60.1559216 | Polar - Positive Charge |
| Glu:H - Lys | 23909.30866 | 60.1559216 | Polar - Positive Charge |
| Glu:H - Glu | 44390.94744 | 60.1559216 | Polar - Negative Charge |
| Glu:H - Tyr- | 2211.206356 | 60.1559216 | Polar - Negative Charge |
| LysN - Arg | 134030.1732 | 60.1559216 | Polar - Positive Charge |
| LysN - His+ | 1667872.226 | 60.1559216 | Polar - Positive Charge |
| LysN - Lys | 152875.1584 | 60.1559216 | Polar - Positive Charge |
| LysN - Asp | 59186.14203 | 60.1559216 | Polar - Negative Charge |
| LysN - Glu | 165959.4044 | 60.1559216 | Polar - Negative Charge |
| LysN - Tyr- | 80105.4593 | 60.1559216 | Polar - Negative Charge |
| Arg - His+ | 1440305.443 | 60.1559216 | Positive Charge - Positive Charge |
| Arg - Asp | 17785.70137 | 60.1559216 | Positive Charge - Negative Charge |
| Arg - Glu | 4646.636242 | 60.1559216 | Positive Charge - Negative Charge |
| Arg - Tyr- | 9386.994911 | 60.1559216 | Positive Charge - Negative Charge |
| His+ - Lys | 1704700.149 | 60.1559216 | Positive Charge - Positive Charge |
| His+ - Asp | 1455016.453 | 60.1559216 | Positive Charge - Negative Charge |
| His+ - Glu | 1296778.548 | 60.1559216 | Positive Charge - Negative Charge |
| His+ - Tyr- | 1501090.149 | 60.1559216 | Positive Charge - Negative Charge |
| Lys - Asp | 19047.10817 | 60.1559216 | Positive Charge - Negative Charge |
| Lys - Glu | 5416.017616 | 60.1559216 | Positive Charge - Negative Charge |
| Lys - Tyr- | 9861.383715 | 60.1559216 | Positive Charge - Negative Charge |
| Asp - Glu | 37912.51727 | 60.1559216 | Negative Charge - Negative Charge |
| Asp - Tyr- | 1459.78403 | 60.1559216 | Negative Charge - Negative Charge |
| Glu - Tyr- | 25865.93699 | 60.1559216 | Negative Charge - Negative Charge |

**Table S24.** Non-statistically significant pairwise comparisons of the y dihedral angles populating the aL conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Glu | 36.17036749 | 60.1559216 | Hydrophobic - Negative Charge |
| Val - Ile | 9.615481907 | 60.1559216 | Hydrophobic - Hydrophobic |
| Tyr - Gln | 14.67696435 | 60.1559216 | Aromatic - Polar |
| Arg:NH - Arg | 17.92924942 | 60.1559216 | Polar - Positive Charge |
| Arg:NH - Lys | 1.650690172 | 60.1559216 | Polar - Positive Charge |
| Glu:H - Asp | 31.72469638 | 60.1559216 | Polar - Negative Charge |
| Arg - Lys | 8.084370975 | 60.1559216 | Positive Charge - Positive Charge |

**Table S25.** Statistically significant pairwise comparisons of the f dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - His:ND1 | 479970.7673 | 33.75234691 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 1033482.765 | 33.75234691 | Hydrophobic - Aromatic |
| Ala - Phe | 911759.9373 | 33.75234691 | Hydrophobic - Aromatic |
| Ala - Tyr | 734988.3221 | 33.75234691 | Hydrophobic - Aromatic |
| Ala - Ser | 882430.2069 | 33.75234691 | Hydrophobic - Polar |
| Ala - Asn | 957579.4264 | 33.75234691 | Hydrophobic - Polar |
| Ala - Asp:H | 438541.9189 | 33.75234691 | Hydrophobic - Polar |
| Ala - LysN | 614384.2597 | 33.75234691 | Hydrophobic - Polar |
| Ala - Asp | 22350.8111 | 33.75234691 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 17738.89236 | 33.75234691 | Aromatic - Aromatic |
| His:ND1 - Tyr | 99.17509688 | 33.75234691 | Aromatic - Aromatic |
| His:ND1 - Ser | 18460.05233 | 33.75234691 | Aromatic - Polar |
| His:ND1 - Asn | 16443.45192 | 33.75234691 | Aromatic - Polar |
| His:ND1 - Asp:H | 82723.66042 | 33.75234691 | Aromatic - Polar |
| His:ND1 - LysN | 981.8566079 | 33.75234691 | Aromatic - Polar |
| His:ND1 - Asp | 286399.3595 | 33.75234691 | Aromatic - Negative Charge |
| His:NE2 - Phe | 37842.00342 | 33.75234691 | Aromatic - Aromatic |
| His:NE2 - Tyr | 26179.10043 | 33.75234691 | Aromatic - Aromatic |
| His:NE2 - Ser | 168.5113501 | 33.75234691 | Aromatic - Polar |
| His:NE2 - Asn | 36.58886851 | 33.75234691 | Aromatic - Polar |
| His:NE2 - Asp:H | 99974.93027 | 33.75234691 | Aromatic - Polar |
| His:NE2 - LysN | 13985.5377 | 33.75234691 | Aromatic - Polar |
| His:NE2 - Asp | 437629.0855 | 33.75234691 | Aromatic - Negative Charge |
| Phe - Tyr | 39.89706272 | 33.75234691 | Aromatic - Aromatic |
| Phe - Ser | 36962.44795 | 33.75234691 | Aromatic - Polar |
| Phe - Asn | 33554.45282 | 33.75234691 | Aromatic - Polar |
| Phe - Asp:H | 166406.9771 | 33.75234691 | Aromatic - Polar |
| Phe - LysN | 1141.408465 | 33.75234691 | Aromatic - Polar |
| Phe - Asp | 482823.5749 | 33.75234691 | Aromatic - Negative Charge |
| Tyr - Ser | 26415.70942 | 33.75234691 | Aromatic - Polar |
| Tyr - Asn | 23577.1138 | 33.75234691 | Aromatic - Polar |
| Tyr - Asp:H | 126945.6263 | 33.75234691 | Aromatic - Polar |
| Tyr - LysN | 669.0504228 | 33.75234691 | Aromatic - Polar |
| Tyr - Asp | 404687.8937 | 33.75234691 | Aromatic - Negative Charge |
| Ser - Asn | 308.8694389 | 33.75234691 | Polar - Polar |
| Ser - Asp:H | 77392.13778 | 33.75234691 | Polar - Polar |
| Ser - LysN | 14673.51039 | 33.75234691 | Polar - Polar |
| Ser - Asp | 387885.1046 | 33.75234691 | Polar - Negative Charge |
| Asn - Asp:H | 92440.35875 | 33.75234691 | Polar - Polar |
| Asn - LysN | 12522.48304 | 33.75234691 | Polar - Polar |
| Asn - Asp | 417594.5567 | 33.75234691 | Polar - Negative Charge |
| Asp:H - LysN | 92968.01345 | 33.75234691 | Polar - Polar |
| Asp:H - Asp | 162321.232 | 33.75234691 | Polar - Negative Charge |
| LysN - Asp | 339836.8314 | 33.75234691 | Polar - Negative Charge |

**Table S26.** Non-statistically significant pairwise comparisons of the f dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| His:ND1 - Phe | 29.21452289 | 33.75234691 | Aromatic - Aromatic |

**Table S27.** Statistically significant pairwise comparisons of the y dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - His:ND1 | 99914039.85 | 33.74972341 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 310609009.6 | 33.74972341 | Hydrophobic - Aromatic |
| Ala - Phe | 156296953 | 33.74972341 | Hydrophobic - Aromatic |
| Ala - Tyr | 127175029 | 33.74972341 | Hydrophobic - Aromatic |
| Ala - Ser | 276580180.6 | 33.74972341 | Hydrophobic - Polar |
| Ala - Asn | 282612280.8 | 33.74972341 | Hydrophobic - Polar |
| Ala - Asp:H | 286743068.3 | 33.74972341 | Hydrophobic - Polar |
| Ala - LysN | 141638311.8 | 33.74972341 | Hydrophobic - Polar |
| Ala - Asp | 190262.4236 | 33.74972341 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 12688.74059 | 33.74972341 | Aromatic - Aromatic |
| His:ND1 - Phe | 952156.2064 | 33.74972341 | Aromatic - Aromatic |
| His:ND1 - Tyr | 903668.8903 | 33.74972341 | Aromatic - Aromatic |
| His:ND1 - Asn | 25248.78656 | 33.74972341 | Aromatic - Polar |
| His:ND1 - Asp:H | 467668.3603 | 33.74972341 | Aromatic - Polar |
| His:ND1 - Asp | 92784607.33 | 33.74972341 | Aromatic - Negative Charge |
| His:NE2 - Phe | 2222183.275 | 33.74972341 | Aromatic - Aromatic |
| His:NE2 - Tyr | 1784705.029 | 33.74972341 | Aromatic - Aromatic |
| His:NE2 - Ser | 55615.15137 | 33.74972341 | Aromatic - Polar |
| His:NE2 - Asn | 10887.81288 | 33.74972341 | Aromatic - Polar |
| His:NE2 - Asp:H | 2434491.937 | 33.74972341 | Aromatic - Polar |
| His:NE2 - LysN | 17862.21226 | 33.74972341 | Aromatic - Polar |
| His:NE2 - Asp | 224167462.4 | 33.74972341 | Aromatic - Negative Charge |
| Phe - Tyr | 1022.549796 | 33.74972341 | Aromatic - Aromatic |
| Phe - Ser | 2463932.05 | 33.74972341 | Aromatic - Polar |
| Phe - Asn | 1859637.169 | 33.74972341 | Aromatic - Polar |
| Phe - Asp:H | 6213417.89 | 33.74972341 | Aromatic - Polar |
| Phe - LysN | 1315200.513 | 33.74972341 | Aromatic - Polar |
| Phe - Asp | 130195500.1 | 33.74972341 | Aromatic - Negative Charge |
| Tyr - Ser | 2022835.641 | 33.74972341 | Aromatic - Polar |
| Tyr - Asn | 1524788.749 | 33.74972341 | Aromatic - Polar |
| Tyr - Asp:H | 5085529.47 | 33.74972341 | Aromatic - Polar |
| Tyr - LysN | 1201602.957 | 33.74972341 | Aromatic - Polar |
| Tyr - Asp | 110522500.2 | 33.74972341 | Aromatic - Negative Charge |
| Ser - Asn | 98797.87857 | 33.74972341 | Polar - Polar |
| Ser - Asp:H | 1506733.974 | 33.74972341 | Polar - Polar |
| Ser - LysN | 94.24088867 | 33.74972341 | Polar - Polar |
| Ser - Asp | 208182237.7 | 33.74972341 | Polar - Negative Charge |
| Asn- Asp:H | 2441366.771 | 33.74972341 | Polar - Polar |
| Asn- LysN | 35914.30335 | 33.74972341 | Polar - Polar |
| Asn- Asp | 209618932.2 | 33.74972341 | Polar - Negative Charge |
| Asp:H- LysN | 697426.1398 | 33.74972341 | Polar - Polar |
| Asp:H- Asp | 220618103.1 | 33.74972341 | Polar - Negative Charge |
| LysN- Asp | 124628502.5 | 33.74972341 | Polar - Negative Charge |

**Table S28.** Non-statistically significant pairwise comparisons of the y dihedral angles populating the e conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| His:ND1 – Ser | 9.632499017 | 33.74972341 | Aromatic - Polar |
| His:ND1 - LysN | 16.80931646 | 33.74972341 | Aromatic - Polar |

**Table S29.** Statistically significant pairwise comparisons of the f dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 2103373.46 | 61.66679419 | Hydrophobic - Hydrophobic |
| Ala - Leu | 17369900.2 | 61.66679419 | Hydrophobic - Hydrophobic |
| Ala - Ile | 850761.8356 | 61.66679419 | Hydrophobic - Hydrophobic |
| Ala - Met | 18987330.37 | 61.66679419 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 6585844.642 | 61.66679419 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 2085308.909 | 61.66679419 | Hydrophobic - Aromatic |
| Ala - Phe | 20574744.74 | 61.66679419 | Hydrophobic - Aromatic |
| Ala - Tyr | 11623625.05 | 61.66679419 | Hydrophobic - Aromatic |
| Ala - Trp | 602361.8073 | 61.66679419 | Hydrophobic - Aromatic |
| Ala - Ser | 5790670.898 | 61.66679419 | Hydrophobic - Polar |
| Ala - Thr | 24824583.01 | 61.66679419 | Hydrophobic - Polar |
| Ala - Cys | 17605071.4 | 61.66679419 | Hydrophobic - Polar |
| Ala - Asn | 388421.8819 | 61.66679419 | Hydrophobic - Polar |
| Ala - Gln | 23455314.21 | 61.66679419 | Hydrophobic - Polar |
| Ala - Arg:NE | 21458886.86 | 61.66679419 | Hydrophobic - Polar |
| Ala - Arg:NH | 9038556.381 | 61.66679419 | Hydrophobic - Polar |
| Ala - Asp:H | 2524894.211 | 61.66679419 | Hydrophobic - Polar |
| Ala - Glu:H | 18279064.67 | 61.66679419 | Hydrophobic - Polar |
| Ala - LysN | 12609813.98 | 61.66679419 | Hydrophobic - Polar |
| Ala - Arg | 12424974.72 | 61.66679419 | Hydrophobic - Positive Charge |
| Ala - His+ | 59026395.32 | 61.66679419 | Hydrophobic - Positive Charge |
| Ala - Lys | 4315365.84 | 61.66679419 | Hydrophobic - Positive Charge |
| Ala - Asp | 18964369.4 | 61.66679419 | Hydrophobic - Negative Charge |
| Ala - Glu | 9974517.355 | 61.66679419 | Hydrophobic - Negative Charge |
| Ala - Cys- | 1697507.833 | 61.66679419 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 20016074.16 | 61.66679419 | Hydrophobic - Negative Charge |
| Val - Leu | 3156119.202 | 61.66679419 | Hydrophobic - Hydrophobic |
| Val - Ile | 3927691.47 | 61.66679419 | Hydrophobic - Hydrophobic |
| Val - Met | 3209936.605 | 61.66679419 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 186869.8577 | 61.66679419 | Hydrophobic - Aromatic |
| Val - His:NE2 | 84026.99758 | 61.66679419 | Hydrophobic - Aromatic |
| Val - Phe | 3946318.143 | 61.66679419 | Hydrophobic - Aromatic |
| Val - Tyr | 1329077.781 | 61.66679419 | Hydrophobic - Aromatic |
| Val - Trp | 633965.2586 | 61.66679419 | Hydrophobic - Aromatic |
| Val - Ser | 69762.55311 | 61.66679419 | Hydrophobic - Polar |
| Val - Thr | 6352819.512 | 61.66679419 | Hydrophobic - Polar |
| Val - Cys | 2969993.716 | 61.66679419 | Hydrophobic - Polar |
| Val - Asn | 789739.0786 | 61.66679419 | Hydrophobic - Polar |
| Val - Gln | 4890728.02 | 61.66679419 | Hydrophobic - Polar |
| Val - Arg:NE | 4169934.378 | 61.66679419 | Hydrophobic - Polar |
| Val - Arg:NH | 703553.0734 | 61.66679419 | Hydrophobic - Polar |
| Val - Asp:H | 29639.34204 | 61.66679419 | Hydrophobic - Polar |
| Val - Glu:H | 3413338.818 | 61.66679419 | Hydrophobic - Polar |
| Val - LysN | 1501389.438 | 61.66679419 | Hydrophobic - Polar |
| Val - Arg | 1591724.773 | 61.66679419 | Hydrophobic - Positive Charge |
| Val - His+ | 14169038.85 | 61.66679419 | Hydrophobic - Positive Charge |
| Val - Lys | 15576.24966 | 61.66679419 | Hydrophobic - Positive Charge |
| Val - Asp | 3909802.057 | 61.66679419 | Hydrophobic - Negative Charge |
| Val - Glu | 1259702.488 | 61.66679419 | Hydrophobic - Negative Charge |
| Val - Cys- | 4941547.69 | 61.66679419 | Hydrophobic - Negative Charge |
| Val - Tyr- | 3898324.187 | 61.66679419 | Hydrophobic - Negative Charge |
| Leu - Ile | 16704945.35 | 61.66679419 | Hydrophobic - Hydrophobic |
| Leu - Met | 3415.619893 | 61.66679419 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 3350527.923 | 61.66679419 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 6582075.636 | 61.66679419 | Hydrophobic - Aromatic |
| Leu - Phe | 50839.8151 | 61.66679419 | Hydrophobic - Aromatic |
| Leu - Tyr | 673960.8092 | 61.66679419 | Hydrophobic - Aromatic |
| Leu - Trp | 10103768.34 | 61.66679419 | Hydrophobic - Aromatic |
| Leu - Ser | 4458707.232 | 61.66679419 | Hydrophobic - Polar |
| Leu - Thr | 973818.2398 | 61.66679419 | Hydrophobic - Polar |
| Leu - Cys | 12870.73201 | 61.66679419 | Hydrophobic - Polar |
| Leu - Asn | 10457127.67 | 61.66679419 | Hydrophobic - Polar |
| Leu - Gln | 258651.4934 | 61.66679419 | Hydrophobic - Polar |
| Leu - Arg:NE | 82414.90293 | 61.66679419 | Hydrophobic - Polar |
| Leu - Arg:NH | 1506601.814 | 61.66679419 | Hydrophobic - Polar |
| Leu - Asp:H | 5802725.164 | 61.66679419 | Hydrophobic - Polar |
| Leu - Glu:H | 6823.23224 | 61.66679419 | Hydrophobic - Polar |
| Leu - LysN | 573366.4388 | 61.66679419 | Hydrophobic - Polar |
| Leu - Arg | 443796.3505 | 61.66679419 | Hydrophobic - Positive Charge |
| Leu - His+ | 5883372.563 | 61.66679419 | Hydrophobic - Positive Charge |
| Leu - Lys | 4615059.002 | 61.66679419 | Hydrophobic - Positive Charge |
| Leu - Asp | 81138.2698 | 61.66679419 | Hydrophobic - Negative Charge |
| Leu - Glu | 519029.1331 | 61.66679419 | Hydrophobic - Negative Charge |
| Leu - Cys- | 16431459.45 | 61.66679419 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 52483.46383 | 61.66679419 | Hydrophobic - Negative Charge |
| Ile - Met | 17472550.42 | 61.66679419 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 8074966.411 | 61.66679419 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 4020381.036 | 61.66679419 | Hydrophobic - Aromatic |
| Ile - Phe | 18825301.82 | 61.66679419 | Hydrophobic - Aromatic |
| Ile - Tyr | 12217353.6 | 61.66679419 | Hydrophobic - Aromatic |
| Ile - Trp | 2215890.046 | 61.66679419 | Hydrophobic - Aromatic |
| Ile - Ser | 7366269.991 | 61.66679419 | Hydrophobic - Polar |
| Ile - Thr | 22665245.08 | 61.66679419 | Hydrophobic - Polar |
| Ile - Cys | 16648201.29 | 61.66679419 | Hydrophobic - Polar |
| Ile - Asn | 1854942.48 | 61.66679419 | Hydrophobic - Polar |
| Ile - Gln | 20857749.97 | 61.66679419 | Hydrophobic - Polar |
| Ile - Arg:NE | 19395904.52 | 61.66679419 | Hydrophobic - Polar |
| Ile - Arg:NH | 10165691.22 | 61.66679419 | Hydrophobic - Polar |
| Ile - Asp:H | 4479458.198 | 61.66679419 | Hydrophobic - Polar |
| Ile - Glu:H | 17347224.26 | 61.66679419 | Hydrophobic - Polar |
| Ile - LysN | 12897515.05 | 61.66679419 | Hydrophobic - Polar |
| Ile - Arg | 12883340.56 | 61.66679419 | Hydrophobic - Positive Charge |
| Ile - His+ | 40128502.57 | 61.66679419 | Hydrophobic - Positive Charge |
| Ile - Lys | 6177641.733 | 61.66679419 | Hydrophobic - Positive Charge |
| Ile - Asp | 18079976.7 | 61.66679419 | Hydrophobic - Negative Charge |
| Ile - Glu | 11193128.89 | 61.66679419 | Hydrophobic - Negative Charge |
| Ile - Cys- | 191830.8268 | 61.66679419 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 18543886.22 | 61.66679419 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 3554168.437 | 61.66679419 | Hydrophobic - Aromatic |
| Met - His:NE2 | 7002964.501 | 61.66679419 | Hydrophobic - Aromatic |
| Met - Phe | 89579.70877 | 61.66679419 | Hydrophobic - Aromatic |
| Met - Tyr | 654531.3228 | 61.66679419 | Hydrophobic - Aromatic |
| Met - Trp | 10823425.8 | 61.66679419 | Hydrophobic - Aromatic |
| Met - Ser | 4800663.304 | 61.66679419 | Hydrophobic - Polar |
| Met - Thr | 1192574.483 | 61.66679419 | Hydrophobic - Polar |
| Met - Cys | 3559.108139 | 61.66679419 | Hydrophobic - Polar |
| Met - Asn | 11161417.06 | 61.66679419 | Hydrophobic - Polar |
| Met - Gln | 359555.1966 | 61.66679419 | Hydrophobic - Polar |
| Met - Arg:NE | 133446.4666 | 61.66679419 | Hydrophobic - Polar |
| Met - Arg:NH | 1536575.107 | 61.66679419 | Hydrophobic - Polar |
| Met - Asp:H | 6152031.361 | 61.66679419 | Hydrophobic - Polar |
| Met - Glu:H | 21323.96299 | 61.66679419 | Hydrophobic - Polar |
| Met - LysN | 550676.4201 | 61.66679419 | Hydrophobic - Polar |
| Met - Arg | 416107.8417 | 61.66679419 | Hydrophobic - Positive Charge |
| Met - His+ | 7315803.493 | 61.66679419 | Hydrophobic - Positive Charge |
| Met - Lys | 4909770.056 | 61.66679419 | Hydrophobic - Positive Charge |
| Met - Asp | 127306.7266 | 61.66679419 | Hydrophobic - Negative Charge |
| Met - Glu | 491427.637 | 61.66679419 | Hydrophobic - Negative Charge |
| Met - Cys- | 16949651.14 | 61.66679419 | Hydrophobic - Negative Charge |
| Met - Tyr- | 91054.84211 | 61.66679419 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 874119.6744 | 61.66679419 | Aromatic - Aromatic |
| His:ND1 - Phe | 4558524.26 | 61.66679419 | Aromatic - Aromatic |
| His:ND1 - Tyr | 990088.5141 | 61.66679419 | Aromatic - Aromatic |
| His:ND1 - Trp | 2562714.051 | 61.66679419 | Aromatic - Aromatic |
| His:ND1 - Ser | 61577.8453 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Thr | 7742817.748 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Cys | 3158245.472 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Asn | 2876309.603 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Gln | 5978172.853 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Arg:NE | 4913546.277 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Arg:NH | 322587.6321 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Asp:H | 600571.5998 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Glu:H | 3721126.923 | 61.66679419 | Aromatic - Polar |
| His:ND1 - LysN | 1203988.387 | 61.66679419 | Aromatic - Polar |
| His:ND1 - Arg | 1300651.526 | 61.66679419 | Aromatic - Positive Charge |
| His:ND1 - His+ | 24677616.72 | 61.66679419 | Aromatic - Positive Charge |
| His:ND1 - Lys | 166227.1738 | 61.66679419 | Aromatic - Positive Charge |
| His:ND1 - Asp | 4340933.253 | 61.66679419 | Aromatic - Negative Charge |
| His:ND1 - Glu | 890689.3215 | 61.66679419 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 8762413.707 | 61.66679419 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 4442356.34 | 61.66679419 | Aromatic - Negative Charge |
| His:NE2 - Phe | 8188857.002 | 61.66679419 | Aromatic - Aromatic |
| His:NE2 - Tyr | 3274770.608 | 61.66679419 | Aromatic - Aromatic |
| His:NE2 - Trp | 390013.5801 | 61.66679419 | Aromatic - Aromatic |
| His:NE2 - Ser | 541244.2722 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Thr | 11723597.69 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Cys | 6425072.432 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Asn | 544507.7765 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Gln | 9905076.368 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Arg:NE | 8643235.794 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Arg:NH | 2017742.061 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Asp:H | 20743.36568 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Glu:H | 7071044.476 | 61.66679419 | Aromatic - Polar |
| His:NE2 - LysN | 3667092.028 | 61.66679419 | Aromatic - Polar |
| His:NE2 - Arg | 3749979.406 | 61.66679419 | Aromatic - Positive Charge |
| His:NE2 - His+ | 29721710.8 | 61.66679419 | Aromatic - Positive Charge |
| His:NE2 - Lys | 281134.2824 | 61.66679419 | Aromatic - Positive Charge |
| His:NE2 - Asp | 7762704.601 | 61.66679419 | Aromatic - Negative Charge |
| His:NE2 - Glu | 2908567.924 | 61.66679419 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 5026100.551 | 61.66679419 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 8003722.722 | 61.66679419 | Aromatic - Negative Charge |
| Phe - Tyr | 1160140.545 | 61.66679419 | Aromatic - Aromatic |
| Phe - Trp | 12172957.77 | 61.66679419 | Aromatic - Aromatic |
| Phe - Ser | 5942037.403 | 61.66679419 | Aromatic - Polar |
| Phe - Thr | 638574.7651 | 61.66679419 | Aromatic - Polar |
| Phe - Cys | 122765.0264 | 61.66679419 | Aromatic - Polar |
| Phe - Asn | 12501791.04 | 61.66679419 | Aromatic - Polar |
| Phe - Gln | 84984.65873 | 61.66679419 | Aromatic - Polar |
| Phe - Arg:NE | 3840.384086 | 61.66679419 | Aromatic - Polar |
| Phe - Arg:NH | 2242959.535 | 61.66679419 | Aromatic - Polar |
| Phe - Asp:H | 7283863.496 | 61.66679419 | Aromatic - Polar |
| Phe - Glu:H | 20038.4516 | 61.66679419 | Aromatic - Polar |
| Phe - LysN | 1032868.385 | 61.66679419 | Aromatic - Polar |
| Phe - Arg | 836527.6308 | 61.66679419 | Aromatic - Positive Charge |
| Phe - His+ | 5097044.929 | 61.66679419 | Aromatic - Positive Charge |
| Phe - Lys | 6001604.846 | 61.66679419 | Aromatic - Positive Charge |
| Phe - Asp | 5364.584638 | 61.66679419 | Aromatic - Negative Charge |
| Phe - Glu | 903613.878 | 61.66679419 | Aromatic - Negative Charge |
| Phe - Cys- | 18169322.03 | 61.66679419 | Aromatic - Negative Charge |
| Tyr - Trp | 5957599.102 | 61.66679419 | Aromatic - Aromatic |
| Tyr - Ser | 1586605.848 | 61.66679419 | Aromatic - Polar |
| Tyr - Thr | 3194305.832 | 61.66679419 | Aromatic - Polar |
| Tyr - Cys | 537136.2838 | 61.66679419 | Aromatic - Polar |
| Tyr - Asn | 6317314.686 | 61.66679419 | Aromatic - Polar |
| Tyr - Gln | 1874294.418 | 61.66679419 | Aromatic - Polar |
| Tyr - Arg:NE | 1314082.176 | 61.66679419 | Aromatic - Polar |
| Tyr - Arg:NH | 169653.2761 | 61.66679419 | Aromatic - Polar |
| Tyr - Asp:H | 2731839.763 | 61.66679419 | Aromatic - Polar |
| Tyr - Glu:H | 827237.8723 | 61.66679419 | Aromatic - Polar |
| Tyr - LysN | 6270.921178 | 61.66679419 | Aromatic - Polar |
| Tyr - Arg | 22416.97106 | 61.66679419 | Aromatic - Positive Charge |
| Tyr - His+ | 12275742.87 | 61.66679419 | Aromatic - Positive Charge |
| Tyr - Lys | 1817725.347 | 61.66679419 | Aromatic - Positive Charge |
| Tyr - Asp | 1189922.49 | 61.66679419 | Aromatic - Negative Charge |
| Tyr - Glu | 1304.289463 | 61.66679419 | Aromatic - Negative Charge |
| Tyr - Cys- | 12487847.49 | 61.66679419 | Aromatic - Negative Charge |
| Tyr - Tyr- | 1140880.02 | 61.66679419 | Aromatic - Negative Charge |
| Trp - Ser | 2019643.879 | 61.66679419 | Aromatic - Polar |
| Trp - Thr | 16037462.61 | 61.66679419 | Aromatic - Polar |
| Trp - Cys | 10026130.29 | 61.66679419 | Aromatic - Polar |
| Trp - Asn | 16032.3005 | 61.66679419 | Aromatic - Polar |
| Trp - Gln | 14241129.47 | 61.66679419 | Aromatic - Polar |
| Trp - Arg:NE | 12749180.86 | 61.66679419 | Aromatic - Polar |
| Trp - Arg:NH | 4232955.937 | 61.66679419 | Aromatic - Polar |
| Trp - Asp:H | 585199.4376 | 61.66679419 | Aromatic - Polar |
| Trp - Glu:H | 10720694.37 | 61.66679419 | Aromatic - Polar |
| Trp - LysN | 6527911.377 | 61.66679419 | Aromatic - Polar |
| Trp - Arg | 6557685.461 | 61.66679419 | Aromatic - Positive Charge |
| Trp - His+ | 37779968.06 | 61.66679419 | Aromatic - Positive Charge |
| Trp - Lys | 1388524.376 | 61.66679419 | Aromatic - Positive Charge |
| Trp - Asp | 11450868.78 | 61.66679419 | Aromatic - Negative Charge |
| Trp - Glu | 5247316.434 | 61.66679419 | Aromatic - Negative Charge |
| Trp - Cys- | 3207351.373 | 61.66679419 | Aromatic - Negative Charge |
| Trp - Tyr- | 11892846.63 | 61.66679419 | Aromatic - Negative Charge |
| Ser - Thr | 9424994.706 | 61.66679419 | Polar - Polar |
| Ser - Cys | 4284254.409 | 61.66679419 | Polar - Polar |
| Ser - Asn | 2318087.89 | 61.66679419 | Polar - Polar |
| Ser - Gln | 7608699.954 | 61.66679419 | Polar - Polar |
| Ser - Arg:NE | 6374959.446 | 61.66679419 | Polar - Polar |
| Ser - Arg:NH | 674298.4591 | 61.66679419 | Polar - Polar |
| Ser - Asp:H | 327451.4603 | 61.66679419 | Polar - Polar |
| Ser - Glu:H | 4906048.411 | 61.66679419 | Polar - Polar |
| Ser - LysN | 1879656.989 | 61.66679419 | Polar - Polar |
| Ser - Arg | 1976117.243 | 61.66679419 | Polar - Positive Charge |
| Ser - His+ | 30092084.94 | 61.66679419 | Polar - Positive Charge |
| Ser - Lys | 33262.43655 | 61.66679419 | Polar - Positive Charge |
| Ser - Asp | 5578480.662 | 61.66679419 | Polar - Negative Charge |
| Ser - Glu | 1391862.351 | 61.66679419 | Polar - Negative Charge |
| Ser - Cys- | 8102391.996 | 61.66679419 | Polar - Negative Charge |
| Ser - Tyr- | 5775212.67 | 61.66679419 | Polar - Negative Charge |
| Thr - Cys | 1263116.796 | 61.66679419 | Polar - Polar |
| Thr - Asn | 16344238.75 | 61.66679419 | Polar - Polar |
| Thr - Gln | 283545.059 | 61.66679419 | Polar - Polar |
| Thr - Arg:NE | 558129.1332 | 61.66679419 | Polar - Polar |
| Thr - Arg:NH | 4742415.324 | 61.66679419 | Polar - Polar |
| Thr - Asp:H | 10702523.59 | 61.66679419 | Polar - Polar |
| Thr - Glu:H | 832644.1886 | 61.66679419 | Polar - Polar |
| Thr - LysN | 3029799.365 | 61.66679419 | Polar - Polar |
| Thr - Arg | 2661372.333 | 61.66679419 | Polar - Positive Charge |
| Thr - His+ | 1204251.509 | 61.66679419 | Polar - Positive Charge |
| Thr - Lys | 9354976.967 | 61.66679419 | Polar - Positive Charge |
| Thr - Asp | 479867.6909 | 61.66679419 | Polar - Negative Charge |
| Thr - Glu | 2635355.493 | 61.66679419 | Polar - Negative Charge |
| Thr - Cys- | 21697735.38 | 61.66679419 | Polar - Negative Charge |
| Thr - Tyr- | 612045.5845 | 61.66679419 | Polar - Negative Charge |
| Cys - Asn | 10375665.61 | 61.66679419 | Polar - Polar |
| Cys - Gln | 414424.221 | 61.66679419 | Polar - Polar |
| Cys - Arg:NE | 172341.2625 | 61.66679419 | Polar - Polar |
| Cys - Arg:NH | 1329518.818 | 61.66679419 | Polar - Polar |
| Cys - Asp:H | 5631181.956 | 61.66679419 | Polar - Polar |
| Cys - Glu:H | 39748.45697 | 61.66679419 | Polar - Polar |
| Cys - LysN | 443324.7288 | 61.66679419 | Polar - Polar |
| Cys - Arg | 329045.1233 | 61.66679419 | Polar - Positive Charge |
| Cys - His+ | 7201191.899 | 61.66679419 | Polar - Positive Charge |
| Cys - Lys | 4433629.485 | 61.66679419 | Polar - Positive Charge |
| Cys - Asp | 163379.8519 | 61.66679419 | Polar - Negative Charge |
| Cys - Glu | 402999.7891 | 61.66679419 | Polar - Negative Charge |
| Cys - Cys- | 16303298.9 | 61.66679419 | Polar - Negative Charge |
| Cys - Tyr- | 123981.3551 | 61.66679419 | Polar - Negative Charge |
| Asn - Gln | 14541805.07 | 61.66679419 | Polar - Polar |
| Asn - Arg:NE | 13068963.75 | 61.66679419 | Polar - Polar |
| Asn - Arg:NH | 4577241.3 | 61.66679419 | Polar - Polar |
| Asn - Asp:H | 765361.558 | 61.66679419 | Polar - Polar |
| Asn - Glu:H | 11068922.69 | 61.66679419 | Polar - Polar |
| Asn - LysN | 6890052.74 | 61.66679419 | Polar - Polar |
| Asn - Arg | 6919173.233 | 61.66679419 | Polar - Positive Charge |
| Asn - His+ | 37172679.15 | 61.66679419 | Polar - Positive Charge |
| Asn - Lys | 1644263.637 | 61.66679419 | Polar - Positive Charge |
| Asn - Asp | 11798199.23 | 61.66679419 | Polar - Negative Charge |
| Asn - Glu | 5594423.977 | 61.66679419 | Polar - Negative Charge |
| Asn - Cys- | 2818558.352 | 61.66679419 | Polar - Negative Charge |
| Asn - Tyr- | 12228316.22 | 61.66679419 | Polar - Negative Charge |
| Gln - Arg:NE | 53612.06505 | 61.66679419 | Polar - Polar |
| Gln - Arg:NH | 3211908.154 | 61.66679419 | Polar - Polar |
| Gln - Asp:H | 8896870.979 | 61.66679419 | Polar - Polar |
| Gln - Glu:H | 181404.9684 | 61.66679419 | Polar - Polar |
| Gln - LysN | 1724890.275 | 61.66679419 | Polar - Polar |
| Gln - Arg | 1447106.919 | 61.66679419 | Polar - Positive Charge |
| Gln - His+ | 3687098.386 | 61.66679419 | Polar - Positive Charge |
| Gln - Lys | 7557746.268 | 61.66679419 | Polar - Positive Charge |
| Gln - Asp | 40708.23546 | 61.66679419 | Polar - Negative Charge |
| Gln - Glu | 1482088.269 | 61.66679419 | Polar - Negative Charge |
| Gln - Cys- | 19884530.22 | 61.66679419 | Polar - Negative Charge |
| Gln - Tyr- | 78429.8383 | 61.66679419 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 2465932.607 | 61.66679419 | Polar - Polar |
| Arg:NE - Asp:H | 7704347.044 | 61.66679419 | Polar - Polar |
| Arg:NE - Glu:H | 41170.32475 | 61.66679419 | Polar - Polar |
| Arg:NE - LysN | 1180421.189 | 61.66679419 | Polar - Polar |
| Arg:NE - Arg | 964067.5419 | 61.66679419 | Polar - Positive Charge |
| Arg:NE - His+ | 4873628.93 | 61.66679419 | Polar - Positive Charge |
| Arg:NE - Lys | 6401525.118 | 61.66679419 | Polar - Positive Charge |
| Arg:NE - Asp | 232.6970009 | 61.66679419 | Polar - Negative Charge |
| Arg:NE - Glu | 1025305.601 | 61.66679419 | Polar - Negative Charge |
| Arg:NE - Cys- | 18633479.38 | 61.66679419 | Polar - Negative Charge |
| Arg:NE - Tyr- | 2910.340883 | 61.66679419 | Polar - Negative Charge |
| Arg:NH - Asp:H | 1599398.677 | 61.66679419 | Polar - Polar |
| Arg:NH - Glu:H | 1738485.51 | 61.66679419 | Polar - Polar |
| Arg:NH - LysN | 248685.4331 | 61.66679419 | Polar - Polar |
| Arg:NH - Arg | 311299.2231 | 61.66679419 | Polar - Positive Charge |
| Arg:NH - His+ | 16152108.33 | 61.66679419 | Polar - Positive Charge |
| Arg:NH - Lys | 879722.8035 | 61.66679419 | Polar - Positive Charge |
| Arg:NH - Asp | 2214226.586 | 61.66679419 | Polar - Negative Charge |
| Arg:NH - Glu | 171391.4396 | 61.66679419 | Polar - Negative Charge |
| Arg:NH - Cys- | 10671363.09 | 61.66679419 | Polar - Negative Charge |
| Arg:NH - Tyr- | 2197186.294 | 61.66679419 | Polar - Negative Charge |
| Asp:H - Glu:H | 6256469.767 | 61.66679419 | Polar - Polar |
| Asp:H - LysN | 3080266.949 | 61.66679419 | Polar - Polar |
| Asp:H - Arg | 3170970.085 | 61.66679419 | Polar - Positive Charge |
| Asp:H - His+ | 27505058.57 | 61.66679419 | Polar - Positive Charge |
| Asp:H - Lys | 142390.7979 | 61.66679419 | Polar - Positive Charge |
| Asp:H - Asp | 6930073.582 | 61.66679419 | Polar - Negative Charge |
| Asp:H - Glu | 2438366.782 | 61.66679419 | Polar - Negative Charge |
| Asp:H - Cys- | 5472074.231 | 61.66679419 | Polar - Negative Charge |
| Asp:H - Tyr- | 7122727.537 | 61.66679419 | Polar - Negative Charge |
| Glu:H - LysN | 717429.7622 | 61.66679419 | Polar - Polar |
| Glu:H - Arg | 567070.7225 | 61.66679419 | Polar - Positive Charge |
| Glu:H - His+ | 5489891.012 | 61.66679419 | Polar - Positive Charge |
| Glu:H - Lys | 5039014.977 | 61.66679419 | Polar - Positive Charge |
| Glu:H - Asp | 42271.1523 | 61.66679419 | Polar - Negative Charge |
| Glu:H - Glu | 641886.354 | 61.66679419 | Polar - Negative Charge |
| Glu:H - Cys- | 16972380.13 | 61.66679419 | Polar - Negative Charge |
| Glu:H - Tyr- | 21426.28704 | 61.66679419 | Polar - Negative Charge |
| LysN - Arg | 5467.175724 | 61.66679419 | Polar - Positive Charge |
| LysN - His+ | 12227576.53 | 61.66679419 | Polar - Positive Charge |
| LysN - Lys | 2109189.827 | 61.66679419 | Polar - Positive Charge |
| LysN - Asp | 1066436.56 | 61.66679419 | Polar - Negative Charge |
| LysN - Glu | 1283.754549 | 61.66679419 | Polar - Negative Charge |
| LysN - Cys- | 13054221.68 | 61.66679419 | Polar - Negative Charge |
| LysN - Tyr- | 1015690.674 | 61.66679419 | Polar - Negative Charge |
| Arg - His+ | 10717345.12 | 61.66679419 | Positive Charge - Positive Charge |
| Arg - Lys | 2205914.896 | 61.66679419 | Positive Charge - Positive Charge |
| Arg - Asp | 878939.6348 | 61.66679419 | Positive Charge - Negative Charge |
| Arg - Glu | 10369.29744 | 61.66679419 | Positive Charge - Negative Charge |
| Arg - Cys- | 13088320.95 | 61.66679419 | Positive Charge - Negative Charge |
| Arg - Tyr- | 824919.8086 | 61.66679419 | Positive Charge - Negative Charge |
| His+ - Lys | 26795001.65 | 61.66679419 | Positive Charge - Positive Charge |
| His+ - Asp | 4001299.328 | 61.66679419 | Positive Charge - Negative Charge |
| His+ - Glu | 9420806.49 | 61.66679419 | Positive Charge - Negative Charge |
| His+ - Cys- | 34732085.48 | 61.66679419 | Positive Charge - Negative Charge |
| His+ - Tyr- | 4846979.731 | 61.66679419 | Positive Charge - Negative Charge |
| Lys - Asp | 5695895.031 | 61.66679419 | Positive Charge - Negative Charge |
| Lys - Glu | 1617286.651 | 61.66679419 | Positive Charge - Negative Charge |
| Lys - Cys- | 7057905.007 | 61.66679419 | Positive Charge - Negative Charge |
| Lys - Tyr- | 5855678.263 | 61.66679419 | Positive Charge - Negative Charge |
| Asp - Glu | 947696.9134 | 61.66679419 | Negative Charge - Negative Charge |
| Asp - Cys- | 17681821.99 | 61.66679419 | Negative Charge - Negative Charge |
| Asp - Tyr- | 4304.895943 | 61.66679419 | Negative Charge - Negative Charge |
| Glu - Cys- | 11700848.64 | 61.66679419 | Negative Charge - Negative Charge |
| Glu - Tyr- | 893261.9907 | 61.66679419 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 17970388.53 | 61.66679419 | Negative Charge - Negative Charge |

**Table S30.** Non-statistically significant pairwise comparisons of the f dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Phe - Tyr- | 49.34099622 | 61.66679419 | Aromatic - Negative Charge |

**Table S31.** Statistically significant pairwise comparisons of the y dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Ala - Val | 1037428.006 | 61.66684837 | Hydrophobic - Hydrophobic |
| Ala - Leu | 217220.7183 | 61.66684837 | Hydrophobic - Hydrophobic |
| Ala - Ile | 347928.3014 | 61.66684837 | Hydrophobic - Hydrophobic |
| Ala - Met | 99592.90993 | 61.66684837 | Hydrophobic - Hydrophobic |
| Ala - His:ND1 | 2521713.047 | 61.66684837 | Hydrophobic - Aromatic |
| Ala - His:NE2 | 37159.77048 | 61.66684837 | Hydrophobic - Aromatic |
| Ala - Phe | 147029.9473 | 61.66684837 | Hydrophobic - Aromatic |
| Ala - Tyr | 50777.10296 | 61.66684837 | Hydrophobic - Aromatic |
| Ala - Trp | 36831.84225 | 61.66684837 | Hydrophobic - Aromatic |
| Ala - Ser | 1531979.317 | 61.66684837 | Hydrophobic - Polar |
| Ala - Thr | 2842094.742 | 61.66684837 | Hydrophobic - Polar |
| Ala - Cys | 5099742.704 | 61.66684837 | Hydrophobic - Polar |
| Ala - Asn | 1381970.62 | 61.66684837 | Hydrophobic - Polar |
| Ala - Gln | 1635439.001 | 61.66684837 | Hydrophobic - Polar |
| Ala - Arg:NE | 28491.59549 | 61.66684837 | Hydrophobic - Polar |
| Ala - Arg:NH | 91244.7685 | 61.66684837 | Hydrophobic - Polar |
| Ala - Asp:H | 33651.37206 | 61.66684837 | Hydrophobic - Polar |
| Ala - Glu:H | 1451940.531 | 61.66684837 | Hydrophobic - Polar |
| Ala - LysN | 2140480.88 | 61.66684837 | Hydrophobic - Polar |
| Ala - Arg | 122646.0481 | 61.66684837 | Hydrophobic - Positive Charge |
| Ala - His+ | 26420319.23 | 61.66684837 | Hydrophobic - Positive Charge |
| Ala - Lys | 189861.8694 | 61.66684837 | Hydrophobic - Positive Charge |
| Ala - Asp | 170978.4315 | 61.66684837 | Hydrophobic - Negative Charge |
| Ala - Glu | 201056.0729 | 61.66684837 | Hydrophobic - Negative Charge |
| Ala - Cys- | 5887139.307 | 61.66684837 | Hydrophobic - Negative Charge |
| Ala - Tyr- | 128304.9494 | 61.66684837 | Hydrophobic - Negative Charge |
| Val - Leu | 1834783.134 | 61.66684837 | Hydrophobic - Hydrophobic |
| Val - Ile | 126408.9283 | 61.66684837 | Hydrophobic - Hydrophobic |
| Val - Met | 1605666.544 | 61.66684837 | Hydrophobic - Hydrophobic |
| Val - His:ND1 | 4926684.513 | 61.66684837 | Hydrophobic - Aromatic |
| Val - His:NE2 | 702242.9336 | 61.66684837 | Hydrophobic - Aromatic |
| Val - Phe | 526288.7313 | 61.66684837 | Hydrophobic - Aromatic |
| Val - Tyr | 703393.9037 | 61.66684837 | Hydrophobic - Aromatic |
| Val - Trp | 693751.0712 | 61.66684837 | Hydrophobic - Aromatic |
| Val - Ser | 3856071.089 | 61.66684837 | Hydrophobic - Polar |
| Val - Thr | 5228753.558 | 61.66684837 | Hydrophobic - Polar |
| Val - Cys | 7421536.128 | 61.66684837 | Hydrophobic - Polar |
| Val - Asn | 2159.138012 | 61.66684837 | Hydrophobic - Polar |
| Val - Gln | 3936112.436 | 61.66684837 | Hydrophobic - Polar |
| Val - Arg:NE | 1316363.288 | 61.66684837 | Hydrophobic - Polar |
| Val - Arg:NH | 1541598.491 | 61.66684837 | Hydrophobic - Polar |
| Val - Asp:H | 1268490.659 | 61.66684837 | Hydrophobic - Polar |
| Val - Glu:H | 3695252.109 | 61.66684837 | Hydrophobic - Polar |
| Val - LysN | 6904.78807 | 61.66684837 | Hydrophobic - Polar |
| Val - Arg | 1615480.275 | 61.66684837 | Hydrophobic - Positive Charge |
| Val - His+ | 22044662.7 | 61.66684837 | Hydrophobic - Positive Charge |
| Val - Lys | 1810965.812 | 61.66684837 | Hydrophobic - Positive Charge |
| Val - Asp | 437306.714 | 61.66684837 | Hydrophobic - Negative Charge |
| Val - Glu | 1718783.318 | 61.66684837 | Hydrophobic - Negative Charge |
| Val - Cys- | 1815909.449 | 61.66684837 | Hydrophobic - Negative Charge |
| Val - Tyr- | 1637223.312 | 61.66684837 | Hydrophobic - Negative Charge |
| Leu - Ile | 871615.1513 | 61.66684837 | Hydrophobic - Hydrophobic |
| Leu - Met | 29511.05839 | 61.66684837 | Hydrophobic - Hydrophobic |
| Leu - His:ND1 | 1094851.712 | 61.66684837 | Hydrophobic - Aromatic |
| Leu - His:NE2 | 396433.332 | 61.66684837 | Hydrophobic - Aromatic |
| Leu - Phe | 694987.8893 | 61.66684837 | Hydrophobic - Aromatic |
| Leu - Tyr | 458511.3155 | 61.66684837 | Hydrophobic - Aromatic |
| Leu - Trp | 390941.0879 | 61.66684837 | Hydrophobic - Aromatic |
| Leu - Ser | 480409.6739 | 61.66684837 | Hydrophobic - Polar |
| Leu - Thr | 1450856.346 | 61.66684837 | Hydrophobic - Polar |
| Leu - Cys | 2931390.373 | 61.66684837 | Hydrophobic - Polar |
| Leu - Asn | 2461506.093 | 61.66684837 | Hydrophobic - Polar |
| Leu - Gln | 589258.5516 | 61.66684837 | Hydrophobic - Polar |
| Leu - Arg:NE | 92707.23378 | 61.66684837 | Hydrophobic - Polar |
| Leu - Arg:NH | 28964.90538 | 61.66684837 | Hydrophobic - Polar |
| Leu - Asp:H | 69600.13655 | 61.66684837 | Hydrophobic - Polar |
| Leu - Glu:H | 506083.9423 | 61.66684837 | Hydrophobic - Polar |
| Leu - LysN | 3524469.169 | 61.66684837 | Hydrophobic - Polar |
| Leu - Arg | 13680.32672 | 61.66684837 | Hydrophobic - Positive Charge |
| Leu - His+ | 18830538.91 | 61.66684837 | Hydrophobic - Positive Charge |
| Leu - Lys | 1943.857775 | 61.66684837 | Hydrophobic - Positive Charge |
| Leu - Asp | 705280.1137 | 61.66684837 | Hydrophobic - Negative Charge |
| Leu - Glu | 139.7917444 | 61.66684837 | Hydrophobic - Negative Charge |
| Leu - Cys- | 7278971.622 | 61.66684837 | Hydrophobic - Negative Charge |
| Leu - Tyr- | 12446.87086 | 61.66684837 | Hydrophobic - Negative Charge |
| Ile - Met | 692497.9594 | 61.66684837 | Hydrophobic - Hydrophobic |
| Ile - His:ND1 | 3160717.202 | 61.66684837 | Hydrophobic - Aromatic |
| Ile - His:NE2 | 179210.6761 | 61.66684837 | Hydrophobic - Aromatic |
| Ile - Phe | 89495.82968 | 61.66684837 | Hydrophobic - Aromatic |
| Ile - Tyr | 171674.4507 | 61.66684837 | Hydrophobic - Aromatic |
| Ile - Trp | 176786.8305 | 61.66684837 | Hydrophobic - Aromatic |
| Ile - Ser | 2296861.979 | 61.66684837 | Hydrophobic - Polar |
| Ile - Thr | 3515036.293 | 61.66684837 | Hydrophobic - Polar |
| Ile - Cys | 5241042.434 | 61.66684837 | Hydrophobic - Polar |
| Ile - Asn | 127369.1246 | 61.66684837 | Hydrophobic - Polar |
| Ile - Gln | 2408339.621 | 61.66684837 | Hydrophobic - Polar |
| Ile - Arg:NE | 514821.2522 | 61.66684837 | Hydrophobic - Polar |
| Ile - Arg:NH | 663565.7005 | 61.66684837 | Hydrophobic - Polar |
| Ile - Asp:H | 506375.6684 | 61.66684837 | Hydrophobic - Polar |
| Ile - Glu:H | 2243573.497 | 61.66684837 | Hydrophobic - Polar |
| Ile - LysN | 258167.4393 | 61.66684837 | Hydrophobic - Polar |
| Ile - Arg | 718445.7756 | 61.66684837 | Hydrophobic - Positive Charge |
| Ile - His+ | 17709982.46 | 61.66684837 | Hydrophobic - Positive Charge |
| Ile - Lys | 840470.5494 | 61.66684837 | Hydrophobic - Positive Charge |
| Ile - Asp | 62215.05233 | 61.66684837 | Hydrophobic - Negative Charge |
| Ile - Glu | 822322.8544 | 61.66684837 | Hydrophobic - Negative Charge |
| Ile - Cys- | 2768339.997 | 61.66684837 | Hydrophobic - Negative Charge |
| Ile - Tyr- | 730726.9215 | 61.66684837 | Hydrophobic - Negative Charge |
| Met - His:ND1 | 1685923.217 | 61.66684837 | Hydrophobic - Aromatic |
| Met - His:NE2 | 244851.1878 | 61.66684837 | Hydrophobic - Aromatic |
| Met - Phe | 497992.2215 | 61.66684837 | Hydrophobic - Aromatic |
| Met - Tyr | 292533.6578 | 61.66684837 | Hydrophobic - Aromatic |
| Met - Trp | 241236.084 | 61.66684837 | Hydrophobic - Aromatic |
| Met - Ser | 867302.2937 | 61.66684837 | Hydrophobic - Polar |
| Met - Thr | 2040110.216 | 61.66684837 | Hydrophobic - Polar |
| Met - Cys | 3970395.588 | 61.66684837 | Hydrophobic - Polar |
| Met - Asn | 2204999.627 | 61.66684837 | Hydrophobic - Polar |
| Met - Gln | 983527.2127 | 61.66684837 | Hydrophobic - Polar |
| Met - Arg:NE | 20709.307 | 61.66684837 | Hydrophobic - Polar |
| Met - Asp:H | 12088.61071 | 61.66684837 | Hydrophobic - Polar |
| Met - Glu:H | 854229.5553 | 61.66684837 | Hydrophobic - Polar |
| Met - LysN | 3282650.485 | 61.66684837 | Hydrophobic - Polar |
| Met - Arg | 2517.193628 | 61.66684837 | Hydrophobic - Positive Charge |
| Met - His+ | 24231763.95 | 61.66684837 | Hydrophobic - Positive Charge |
| Met - Lys | 17157.78231 | 61.66684837 | Hydrophobic - Positive Charge |
| Met - Asp | 514158.4575 | 61.66684837 | Hydrophobic - Negative Charge |
| Met - Glu | 29851.08401 | 61.66684837 | Hydrophobic - Negative Charge |
| Met - Cys- | 7029775.651 | 61.66684837 | Hydrophobic - Negative Charge |
| Met - Tyr- | 3220.284137 | 61.66684837 | Hydrophobic - Negative Charge |
| His:ND1 - His:NE2 | 2882050.231 | 61.66684837 | Aromatic - Aromatic |
| His:ND1 - Phe | 3903859.302 | 61.66684837 | Aromatic - Aromatic |
| His:ND1 – Tyr | 3224973.697 | 61.66684837 | Aromatic - Aromatic |
| His:ND1 - Trp | 2831392.4 | 61.66684837 | Aromatic - Aromatic |
| His:ND1 - Ser | 171874.7651 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Thr | 81350.33683 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Cys | 562839.2804 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Asn | 7046681.184 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Gln | 69114.50971 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Arg:NE | 2009939.721 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Arg:NH | 1583485.446 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Asp:H | 1698515.626 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Glu:H | 85584.77745 | 61.66684837 | Aromatic - Polar |
| His:ND1 - LysN | 9646965.31 | 61.66684837 | Aromatic - Polar |
| His:ND1 - Arg | 1401716.972 | 61.66684837 | Aromatic - Positive Charge |
| His:ND1 - His+ | 12101374.7 | 61.66684837 | Aromatic - Positive Charge |
| His:ND1 - Lys | 1277956.266 | 61.66684837 | Aromatic - Positive Charge |
| His:ND1 - Asp | 3652299.823 | 61.66684837 | Aromatic - Negative Charge |
| His:ND1 - Glu | 927283.038 | 61.66684837 | Aromatic - Negative Charge |
| His:ND1 - Cys- | 12071453.85 | 61.66684837 | Aromatic - Negative Charge |
| His:ND1 - Tyr- | 1402080.825 | 61.66684837 | Aromatic - Negative Charge |
| His:NE2 - Phe | 29421.5729 | 61.66684837 | Aromatic - Aromatic |
| His:NE2 - Tyr | 555.4176658 | 61.66684837 | Aromatic - Aromatic |
| His:NE2 - Ser | 1872734.282 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Thr | 3198652.279 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Cys | 5439129.876 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Asn | 893073.2048 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Gln | 1971672.943 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Arg:NE | 124655.5947 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Arg:NH | 227943.2721 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Asp:H | 127903.7919 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Glu:H | 1775485.234 | 61.66684837 | Aromatic - Polar |
| His:NE2 - LysN | 1421473.709 | 61.66684837 | Aromatic - Polar |
| His:NE2 - Arg | 271450.1963 | 61.66684837 | Aromatic - Positive Charge |
| His:NE2 - His+ | 24946400.88 | 61.66684837 | Aromatic - Positive Charge |
| His:NE2 - Lys | 366019.5463 | 61.66684837 | Aromatic - Positive Charge |
| His:NE2 - Asp | 44928.86631 | 61.66684837 | Aromatic - Negative Charge |
| His:NE2 - Glu | 365400.3992 | 61.66684837 | Aromatic - Negative Charge |
| His:NE2 - Cys- | 5018396.764 | 61.66684837 | Aromatic - Negative Charge |
| His:NE2 - Tyr- | 280160.2802 | 61.66684837 | Aromatic - Negative Charge |
| Phe - Tyr | 23598.7556 | 61.66684837 | Aromatic - Aromatic |
| Phe - Trp | 28624.5602 | 61.66684837 | Aromatic - Aromatic |
| Phe - Ser | 2686578.615 | 61.66684837 | Aromatic - Polar |
| Phe - Thr | 4123564.492 | 61.66684837 | Aromatic - Polar |
| Phe - Cys | 6914925.836 | 61.66684837 | Aromatic - Polar |
| Phe - Asn | 671248.3589 | 61.66684837 | Aromatic - Polar |
| Phe - Gln | 2739793.522 | 61.66684837 | Aromatic - Polar |
| Phe - Arg:NE | 305088.8766 | 61.66684837 | Aromatic - Polar |
| Phe - Arg:NH | 462543.4438 | 61.66684837 | Aromatic - Polar |
| Phe - Asp:H | 296488.2112 | 61.66684837 | Aromatic - Polar |
| Phe - Glu:H | 2468117.021 | 61.66684837 | Aromatic - Polar |
| Phe - LysN | 1147286.67 | 61.66684837 | Aromatic - Polar |
| Phe - Arg | 521912.3918 | 61.66684837 | Aromatic - Positive Charge |
| Phe - His+ | 30893824.41 | 61.66684837 | Aromatic - Positive Charge |
| Phe - Lys | 664903.1424 | 61.66684837 | Aromatic - Positive Charge |
| Phe - Asp | 2637.284174 | 61.66684837 | Aromatic - Negative Charge |
| Phe - Glu | 628577.7047 | 61.66684837 | Aromatic - Negative Charge |
| Phe - Cys- | 4712236.638 | 61.66684837 | Aromatic - Negative Charge |
| Phe - Tyr- | 536240.6137 | 61.66684837 | Aromatic - Negative Charge |
| Tyr - Trp | 507.6293513 | 61.66684837 | Aromatic - Aromatic |
| Tyr - Ser | 2122270.677 | 61.66684837 | Aromatic - Polar |
| Tyr - Thr | 3504602.969 | 61.66684837 | Aromatic - Polar |
| Tyr - Cys | 6002824.556 | 61.66684837 | Aromatic - Polar |
| Tyr - Asn | 910571.6773 | 61.66684837 | Aromatic - Polar |
| Tyr - Gln | 2205386.034 | 61.66684837 | Aromatic - Polar |
| Tyr - Arg:NE | 153813.173 | 61.66684837 | Aromatic - Polar |
| Tyr - Arg:NH | 271222.4372 | 61.66684837 | Aromatic - Polar |
| Tyr - Asp:H | 155180.3686 | 61.66684837 | Aromatic - Polar |
| Tyr - Glu:H | 1979318.166 | 61.66684837 | Aromatic - Polar |
| Tyr - LysN | 1477244.527 | 61.66684837 | Aromatic - Polar |
| Tyr - Arg | 319382.2306 | 61.66684837 | Aromatic - Positive Charge |
| Tyr - His+ | 28095414.65 | 61.66684837 | Aromatic - Positive Charge |
| Tyr - Lys | 427447.024 | 61.66684837 | Aromatic - Positive Charge |
| Tyr - Asp | 38468.2903 | 61.66684837 | Aromatic - Negative Charge |
| Tyr - Glu | 418426.0399 | 61.66684837 | Aromatic - Negative Charge |
| Tyr - Cys- | 5121345.561 | 61.66684837 | Aromatic - Negative Charge |
| Tyr - Tyr- | 329557.1772 | 61.66684837 | Aromatic - Negative Charge |
| Trp - Ser | 1838448.095 | 61.66684837 | Aromatic - Polar |
| Trp - Thr | 3153359.439 | 61.66684837 | Aromatic - Polar |
| Trp - Cys | 5348031.402 | 61.66684837 | Aromatic - Polar |
| Trp - Asn | 878221.0529 | 61.66684837 | Aromatic - Polar |
| Trp - Gln | 1939557.44 | 61.66684837 | Aromatic - Polar |
| Trp - Arg:NE | 123053.3848 | 61.66684837 | Aromatic - Polar |
| Trp - Arg:NH | 224812.0301 | 61.66684837 | Aromatic - Polar |
| Trp - Asp:H | 126451.8576 | 61.66684837 | Aromatic - Polar |
| Trp - Glu:H | 1748204.182 | 61.66684837 | Aromatic - Polar |
| Trp - LysN | 1394407.304 | 61.66684837 | Aromatic - Polar |
| Trp - Arg | 267754.0717 | 61.66684837 | Aromatic - Positive Charge |
| Trp - His+ | 24368399.16 | 61.66684837 | Aromatic - Positive Charge |
| Trp - Lys | 360659.0225 | 61.66684837 | Aromatic - Positive Charge |
| Trp - Asp | 43888.36122 | 61.66684837 | Aromatic - Negative Charge |
| Trp - Glu | 360993.1272 | 61.66684837 | Aromatic - Negative Charge |
| Trp - Cys- | 4975795.679 | 61.66684837 | Aromatic - Negative Charge |
| Trp - Tyr- | 276292.4633 | 61.66684837 | Aromatic - Negative Charge |
| Ser - Thr | 428455.3194 | 61.66684837 | Polar - Polar |
| Ser - Cys | 1371907.124 | 61.66684837 | Polar - Polar |
| Ser - Asn | 5570842.602 | 61.66684837 | Polar - Polar |
| Ser - Gln | 16215.37086 | 61.66684837 | Polar - Polar |
| Ser - Arg:NE | 1126420.257 | 61.66684837 | Polar - Polar |
| Ser - Arg:NH | 813162.0075 | 61.66684837 | Polar - Polar |
| Ser - Asp:H | 930842.6886 | 61.66684837 | Polar - Polar |
| Ser - Glu:H | 7100.548949 | 61.66684837 | Polar - Polar |
| Ser - LysN | 7849541.059 | 61.66684837 | Polar - Polar |
| Ser - Arg | 689866.5619 | 61.66684837 | Polar - Positive Charge |
| Ser - His+ | 17011228.41 | 61.66684837 | Polar - Positive Charge |
| Ser - Lys | 589385.0077 | 61.66684837 | Polar - Positive Charge |
| Ser - Asp | 2529308.851 | 61.66684837 | Polar - Negative Charge |
| Ser - Glu | 398061.7982 | 61.66684837 | Polar - Negative Charge |
| Ser - Cys- | 10670144.71 | 61.66684837 | Polar - Negative Charge |
| Ser - Tyr- | 687028.8295 | 61.66684837 | Polar - Negative Charge |
| Thr - Cys | 151251.0608 | 61.66684837 | Polar - Polar |
| Thr - Asn | 7053736.199 | 61.66684837 | Polar - Polar |
| Thr - Gln | 260338.2661 | 61.66684837 | Polar - Polar |
| Thr - Arg:NE | 2355302.44 | 61.66684837 | Polar - Polar |
| Thr - Arg:NH | 1942400.559 | 61.66684837 | Polar - Polar |
| Thr - Asp:H | 2058097.575 | 61.66684837 | Polar - Polar |
| Thr - Glu:H | 282403.6551 | 61.66684837 | Polar - Polar |
| Thr - LysN | 9186956.65 | 61.66684837 | Polar - Polar |
| Thr - Arg | 1762413.412 | 61.66684837 | Polar - Positive Charge |
| Thr - His+ | 6909507.697 | 61.66684837 | Polar - Positive Charge |
| Thr - Lys | 1638486.243 | 61.66684837 | Polar - Positive Charge |
| Thr - Asp | 3924812.567 | 61.66684837 | Polar - Negative Charge |
| Thr - Glu | 1269250.425 | 61.66684837 | Polar - Negative Charge |
| Thr - Cys- | 12154761.78 | 61.66684837 | Polar - Negative Charge |
| Thr - Tyr- | 1762771.265 | 61.66684837 | Polar - Negative Charge |
| Cys - Asn | 10508592.22 | 61.66684837 | Polar - Polar |
| Cys - Gln | 956853.401 | 61.66684837 | Polar - Polar |
| Cys - Arg:NE | 4391165.93 | 61.66684837 | Polar - Polar |
| Cys - Arg:NH | 3738804.196 | 61.66684837 | Polar - Polar |
| Cys - Asp:H | 3793003.198 | 61.66684837 | Polar - Polar |
| Cys - Glu:H | 972990.929 | 61.66684837 | Polar - Polar |
| Cys - LysN | 13873105.44 | 61.66684837 | Polar - Polar |
| Cys - Arg | 3430783.118 | 61.66684837 | Polar - Positive Charge |
| Cys - His+ | 5983082.005 | 61.66684837 | Polar - Positive Charge |
| Cys - Lys | 3290652.659 | 61.66684837 | Polar - Positive Charge |
| Cys - Asp | 6421519.385 | 61.66684837 | Polar - Negative Charge |
| Cys - Glu | 2530340.479 | 61.66684837 | Polar - Negative Charge |
| Cys - Cys- | 15183191.77 | 61.66684837 | Polar - Negative Charge |
| Cys - Tyr- | 3443319.1 | 61.66684837 | Polar - Negative Charge |
| Asn - Gln | 5498931.111 | 61.66684837 | Polar - Polar |
| Asn - Arg:NE | 1775640.016 | 61.66684837 | Polar - Polar |
| Asn - Arg:NH | 2080432.383 | 61.66684837 | Polar - Polar |
| Asn - Asp:H | 1659827.203 | 61.66684837 | Polar - Polar |
| Asn - Glu:H | 5078674.138 | 61.66684837 | Polar - Polar |
| Asn - LysN | 25707.78629 | 61.66684837 | Polar - Polar |
| Asn - Arg | 2168424.99 | 61.66684837 | Polar - Positive Charge |
| Asn - His+ | 34920295.58 | 61.66684837 | Polar - Positive Charge |
| Asn - Lys | 2466840.582 | 61.66684837 | Polar - Positive Charge |
| Asn - Asp | 536505.8533 | 61.66684837 | Polar - Negative Charge |
| Asn - Glu | 2231331.552 | 61.66684837 | Polar - Negative Charge |
| Asn - Cys- | 2337527.217 | 61.66684837 | Polar - Negative Charge |
| Asn - Tyr- | 2204223.67 | 61.66684837 | Polar - Negative Charge |
| Gln - Arg:NE | 1240032.001 | 61.66684837 | Polar - Polar |
| Gln - Arg:NH | 929546.7648 | 61.66684837 | Polar - Polar |
| Gln - Asp:H | 1047272.802 | 61.66684837 | Polar - Polar |
| Gln - Glu:H | 1338.226736 | 61.66684837 | Polar - Polar |
| Gln - LysN | 7523950.63 | 61.66684837 | Polar - Polar |
| Gln - Arg | 804931.8666 | 61.66684837 | Polar - Positive Charge |
| Gln - His+ | 13033516.88 | 61.66684837 | Polar - Positive Charge |
| Gln - Lys | 703118.8301 | 61.66684837 | Polar - Positive Charge |
| Gln - Asp | 2605325.044 | 61.66684837 | Polar - Negative Charge |
| Gln - Glu | 499055.2833 | 61.66684837 | Polar - Negative Charge |
| Gln - Cys- | 10615423.96 | 61.66684837 | Polar - Negative Charge |
| Gln - Tyr- | 802174.1223 | 61.66684837 | Polar - Negative Charge |
| Arg:NE - Arg:NH | 18434.45489 | 61.66684837 | Polar - Polar |
| Arg:NE - Asp:H | 609.2982039 | 61.66684837 | Polar - Polar |
| Arg:NE - Glu:H | 1090477.323 | 61.66684837 | Polar - Polar |
| Arg:NE - LysN | 2676643.133 | 61.66684837 | Polar - Polar |
| Arg:NE - Arg | 34789.68178 | 61.66684837 | Polar - Positive Charge |
| Arg:NE - His+ | 24579615.2 | 61.66684837 | Polar - Positive Charge |
| Arg:NE - Lys | 72221.86423 | 61.66684837 | Polar - Positive Charge |
| Arg:NE - Asp | 328200.1914 | 61.66684837 | Polar - Negative Charge |
| Arg:NE - Glu | 88266.91755 | 61.66684837 | Polar - Negative Charge |
| Arg:NE - Cys- | 6444935.747 | 61.66684837 | Polar - Negative Charge |
| Arg:NE - Tyr- | 37512.16086 | 61.66684837 | Polar - Negative Charge |
| Arg:NH - Asp:H | 10711.45965 | 61.66684837 | Polar - Polar |
| Arg:NH - Glu:H | 810582.285 | 61.66684837 | Polar - Polar |
| Arg:NH - LysN | 3065141.184 | 61.66684837 | Polar - Polar |
| Arg:NH - Arg | 2719.005861 | 61.66684837 | Polar - Positive Charge |
| Arg:NH - His+ | 22171146.45 | 61.66684837 | Polar - Positive Charge |
| Arg:NH - Lys | 17014.93157 | 61.66684837 | Polar - Positive Charge |
| Arg:NH - Asp | 481278.5143 | 61.66684837 | Polar - Negative Charge |
| Arg:NH - Glu | 29432.13438 | 61.66684837 | Polar - Negative Charge |
| Arg:NH - Cys- | 6830277.305 | 61.66684837 | Polar - Negative Charge |
| Arg:NH - Tyr- | 3424.93603 | 61.66684837 | Polar - Negative Charge |
| Asp:H - Glu:H | 925512.5595 | 61.66684837 | Polar - Polar |
| Asp:H - LysN | 2444428.78 | 61.66684837 | Polar - Polar |
| Asp:H - Arg | 23080.19074 | 61.66684837 | Polar - Positive Charge |
| Asp:H - His+ | 20519180.09 | 61.66684837 | Polar - Positive Charge |
| Asp:H - Lys | 52184.24409 | 61.66684837 | Polar - Positive Charge |
| Asp:H - Asp | 320356.0343 | 61.66684837 | Polar - Negative Charge |
| Asp:H - Glu | 67665.2131 | 61.66684837 | Polar - Negative Charge |
| Asp:H - Cys- | 6192200.392 | 61.66684837 | Polar - Negative Charge |
| Asp:H - Tyr- | 25110.37736 | 61.66684837 | Polar - Negative Charge |
| Glu:H - LysN | 6895413.706 | 61.66684837 | Polar - Polar |
| Glu:H - Arg | 699770.0219 | 61.66684837 | Polar - Positive Charge |
| Glu:H - His+ | 12305561.83 | 61.66684837 | Polar - Positive Charge |
| Glu:H - Lys | 604982.1623 | 61.66684837 | Polar - Positive Charge |
| Glu:H - Asp | 2365086.04 | 61.66684837 | Polar - Negative Charge |
| Glu:H - Glu | 430730.7144 | 61.66684837 | Polar - Negative Charge |
| Glu:H - Cys- | 10191996.41 | 61.66684837 | Polar - Negative Charge |
| Glu:H - Tyr- | 696568.1158 | 61.66684837 | Polar - Negative Charge |
| LysN - Arg | 3158470.036 | 61.66684837 | Polar - Positive Charge |
| LysN - His+ | 47613307.41 | 61.66684837 | Polar - Positive Charge |
| LysN - Lys | 3586633.583 | 61.66684837 | Polar - Positive Charge |
| LysN - Asp | 919528.7681 | 61.66684837 | Polar - Negative Charge |
| LysN - Glu | 3128210.337 | 61.66684837 | Polar - Negative Charge |
| LysN - Cys- | 2185481.394 | 61.66684837 | Polar - Negative Charge |
| LysN - Tyr- | 3213605.494 | 61.66684837 | Polar - Negative Charge |
| Arg - His+ | 20695238.07 | 61.66684837 | Positive Charge - Positive Charge |
| Arg - Lys | 5784.158208 | 61.66684837 | Positive Charge - Positive Charge |
| Arg - Asp | 538962.4812 | 61.66684837 | Positive Charge - Negative Charge |
| Arg - Glu | 14815.35004 | 61.66684837 | Positive Charge - Negative Charge |
| Arg - Cys- | 6923575.238 | 61.66684837 | Positive Charge - Negative Charge |
| His+ - Lys | 21098647.89 | 61.66684837 | Positive Charge - Positive Charge |
| His+ - Asp | 26981521.32 | 61.66684837 | Positive Charge - Negative Charge |
| His+ - Glu | 15663394.21 | 61.66684837 | Positive Charge - Negative Charge |
| His+ - Cys- | 31392320.69 | 61.66684837 | Positive Charge - Negative Charge |
| His+ - Tyr- | 20926228.8 | 61.66684837 | Positive Charge - Negative Charge |
| Lys - Asp | 674648.7528 | 61.66684837 | Positive Charge - Negative Charge |
| Lys - Glu | 2854.448193 | 61.66684837 | Positive Charge - Negative Charge |
| Lys - Cys- | 7324715.426 | 61.66684837 | Positive Charge - Negative Charge |
| Lys - Tyr- | 4941.160615 | 61.66684837 | Positive Charge - Negative Charge |
| Asp - Glu | 644839.8639 | 61.66684837 | Negative Charge - Negative Charge |
| Asp - Cys- | 4332152.638 | 61.66684837 | Negative Charge - Negative Charge |
| Asp - Tyr- | 552527.8948 | 61.66684837 | Negative Charge - Negative Charge |
| Glu - Cys- | 6894143.023 | 61.66684837 | Negative Charge - Negative Charge |
| Glu - Tyr- | 13605.50729 | 61.66684837 | Negative Charge - Negative Charge |
| Cys- - Tyr- | 6976238.948 | 61.66684837 | Negative Charge - Negative Charge |

**Table S32.** Non-statistically significant pairwise comparisons of the y dihedral angles populating the contiguous conformation region.

|  |  |  |  |
| --- | --- | --- | --- |
| Pairwise Interaction | Calculated Value | Critical Value | Chemical Properties |
| Met - Arg:NH | 13.25315335 | 61.66684837 | Hydrophobic - Polar |
| His:NE2 - Trp | 0.649345726 | 61.66684837 | Aromatic - Aromatic |
| Arg - Tyr- | 36.31638031 | 61.66684837 | Positive Charge - Negative Charge |

**Table S33.** The mean standard ± deviation distances between the *i-1* (Ala 1) carbonyl oxygen and *i+1* (Ala 3) amide nitrogen of the Ac-Ala-Xaa-Ala-NH2 peptides. The probability () and number of conformations (n) with distances between 0.27 and 0.33 nm indicating possible hydrogen bond formation.a

|  |  |  |  |
| --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | Distance/nm | H-Bond  Distance/nm | r (n) |
| Gly | 0.421 ± 0.041 | 0.317 ± 0.011 | 0.0132 (5262) |
| Ala | 0.400 ± 0.048 | 0.318 ± 0.011 | 0.0322 (12898) |
| Val | 0.389 ± 0.043 | 0.319 ± 0.010 | 0.0497 (19898) |
| Leu | 0.392 ± 0.043 | 0.318 ± 0.010 | 0.0479 (19178) |
| Ile | 0.389 ± 0.044 | 0.320 ± 0.009 | 0.0519 (20743) |
| Met | 0.398 ± 0.047 | 0.318 ± 0.011 | 0.0392 (15670) |
| His:ND1 | 0.402 ± 0.051 | 0.318 ± 0.011 | 0.0444 (17763) |
| His:NE2 | 0.399 ± 0.051 | 0.318 ± 0.011 | 0.0526 (21051) |
| Phe | 0.395 ± 0.049 | 0.391 ± 0.010 | 0.0481 (19260) |
| Tyr | 0.396 ± 0.049 | 0.319 ± 0.010 | 0.0491 (19632) |
| Trp | 0.398 ± 0.053 | 0.320 ± 0.009 | 0.0430 (17212) |
| Ser | 0.406 ± 0.054 | 0.318 ± 0.011 | 0.0399 (15964) |
| Thr | 0.409 ± 0.056 | 0.319 ± 0.010 | 0.0379 (15152) |
| Cys:H | 0.395 ± 0.048 | 0.318 ± 0.011 | 0.0464 (18551) |
| Asn | 0.394 ± 0.046 | 0.317 ± 0.011 | 0.0550 (21996) |
| Gln | 0.396 ± 0.044 | 0.317 ± 0.011 | 0.0372 (14879) |
| Arg:NE | 0.402 ± 0.047 | 0.318 ± 0.011 | 0.0321 (12822) |
| Arg:NH | 0.397 ± 0.045 | 0.318 ± 0.011 | 0.0368 (14735) |
| Asp:H | 0.405 ± 0.047 | 0.317 ± 0.012 | 0.0385 (15418) |
| Glu:H | 0.398 ± 0.044 | 0.318 ± 0.011 | 0.0354 (14172) |
| LysN | 0.397 ± 0.046 | 0.317 ± 0.011 | 0.0413 (16511) |
| Arg | 0.407 ± 0.048 | 0.318 ± 0.011 | 0.0277 (11097) |
| His+ | 0.420 ± 0.062 | 0.317 ± 0.011 | 0.0539 (21549) |
| Lys | 0.401 ± 0.047 | 0.318 ± 0.011 | 0.0332 (13273) |
| Asp | 0.386 ± 0.040 | 0.318 ± 0.011 | 0.0459 (18355) |
| Glu | 0.392 ± 0.041 | 0.319 ± 0.011 | 0.0358 (14321) |
| Cys- | 0.378 ± 0.030 | 0.321 ± 0.008 | 0.0358 (14325) |
| Tyr- | 0.397 ± 0.049 | 0.319 ± 0.010 | 0.0413 (16537) |
| Cys-Cys | 0.400 ± 0.050 | 0.318 ± 0.011 | 0.0422 (33778) |
| Pro:cis | 0.510 ± 0.046 | 0.320 ± 0.003 | 0.0000 (2) |
| Pro:trans | 0.364 ± 0.025 | 0.315 ± 0.014 | 0.0868 (34724) |

aTotal sample size nTot = 400,000 for all Ac-Ala-Xaa-Ala-NH2 peptides except for the Cys-Cys system where nTot = 800,000.

**Table S34.** The mean standard ± deviation distances between the *i-1* (Ala 1) amide nitrogen and *i+1* (Ala 3) carbonyl oxygen of the Ac-Ala-Xaa-Ala-NH2 peptides. The probability () and number of conformations (n) with distances between 0.27 and 0.33 nm indicating possible hydrogen bond formation.a,b

|  |  |  |  |
| --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | Distance/nm | H-Bond  Distance/nm | r (n) |
| Gly | 0.844 ± 0.100 | N/S | N/S |
| Ala | 0.870 ± 0.111 | 0.315 ± 0.010 | 0.0000 (4) |
| Val | 0.897 ± 0.085 | N/S | N/S |
| Leu | 0.862 ± 0.116 | N/S | N/S |
| Ile | 0.892 ± 0.090 | 0.305 ± 0.012 | 0.0000 (3) |
| Met | 0.862 ± 0.114 | 0.312 ± 0.015 | 0.0000 (3) |
| His:ND1 | 0.865 ± 0.113 | 0.328 ± 0.000 | 0.0000 (1) |
| His:NE2 | 0.862 ± 0.111 | 0.307 ± 0.019 | 0.0000 (2) |
| Phe | 0.888 ± 0.101 | N/S | N/S |
| Tyr | 0.880 ± 0.108 | 0.294 ± 0.019 | 0.0000 (2) |
| Trp | 0.889 ± 0.105 | 0.322 ± 0.006 | 0.0000 (2) |
| Ser | 0.877 ± 0.111 | N/S | N/S |
| Thr | 0.889 ± 0.102 | N/S | N/S |
| Cys:H | 0.877 ± 0.105 | N/S | N/S |
| Asn | 0.849 ± 0.118 | 0.317 ± 0.014 | 0.0000 (6) |
| Gln | 0.856 ± 0.118 | 0.309 ± 0.001 | 0.0000 (2) |
| Arg:NE | 0.873 ± 0.107 | 0.324 ± 0.006 | 0.0000 (2) |
| Arg:NH | 0.866 ± 0.114 | 0.316 ± 0.006 | 0.0000 (2) |
| Asp:H | 0.843 ± 0.120 | 0.325 ± 0.000 | 0.0000 (1) |
| Glu:H | 0.863 ± 0.114 | 0.330 ± 0.000 | 0.0000 (1) |
| LysN | 0.872 ± 0.107 | 0.322 ± 0.007 | 0.0000 (2) |
| Arg | 0.880 ± 0.109 | N/S | N/S |
| His+ | 0.875 ± 0.099 | 0.304 ± 0.000 | 0.0000 (1) |
| Lys | 0.872 ± 0.112 | N/S | N/S |
| Asp | 0.863 ± 0.110 | 0.294 ± 0.002 | 0.0000 (3) |
| Glu | 0.876 ± 0.105 | N/S | N/S |
| Cys- | 0.863 ± 0.114 | 0.304 ± 0.010 | 0.0000 (3) |
| Tyr- | 0.875 ± 0.102 | 0.294 ± 0.007 | 0.0000 (2) |
| Cys-Cys | 0.874 ± 0.108 | 0.314 ± 0.009 | 0.0000 (5) |
| Pro:cis | 0.693 ± 0.093 | 0.311 ± 0.016 | 0.0011 (456) |
| Pro:trans | 0.890 ± 0.069 | N/S | N/S |

a Total sample size nTot = 400,000 for all Ac-Ala-Xaa-Ala-NH2 peptides except for the Cys-Cys system where nTot = 800,000.

b N/S: not sampled

**Table S35.** The solvent accessible surface area (SASA) for the whole Xaa residue of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Gly | 0.788 ± 0.065 | 0.773 ± 0.049 | 0.899 ± 0.047 | 0.895 ± 0.050 | 0.776 ± 0.056 | 0.799 ± 0.083 | 47654.32 | 5.8783 | **< 0.0001** |
| Ala | 1.093 ± 0.075 | 1.068 ± 0.0059 | 1.188 ± 0.053 | 1.182 ± 0.058 | 1.105 ± 0.058 | 1.111 ± 0.070 | 272666.02 | 5.8783 | **< 0.0001** |
| Val | 1.523 ± 0.077 | 1.514 ± 0.070 | 1.643 ± 0.061 | 1.516 ± 0.060 | N/S | 1.585 ± 0.087 | 29422.26 | 7.0360 | **< 0.0001** |
| Leu | 1.857 ± 0.087 | 1.829 ± 0.075 | 1.946 ± 0.060 | 1.940 ± 0.077 | N/S | 1.861 ± 0.090 | 59206.60 | 7.0360 | **< 0.0001** |
| Ile | 1.749 ± 0.084 | 1.736 ± 0.075 | 1.873 ± 0.069 | 1.727 ± 0.072 | N/S | 1.790 ± 0.084 | 36666.56 | 7.0360 | **< 0.0001** |
| Met | 1.895 ± 0.117 | 1.864 ± 0.108 | 1.990 ± 0.087 | 2.006 ± 0.096 | N/S | 1.913 ± 0.107 | 35044.55 | 7.0360 | **< 0.0001** |
| His:ND1 | 1.898 ± 0.100 | 1.864 ± 0.086 | 1.992 ± 0.071 | 2.003 ± 0.075 | 1.890 ± 0.069 | 1.901 ± 0.096 | 44617.81 | 5.8783 | **< 0.0001** |
| His:NE2 | 1.902 ± 0.101 | 1.867 ± 0.087 | 1.973 ± 0.087 | 2.003 ± 0.079 | 1.887 ± 0.071 | 1.914 ± 0.099 | 38227.92 | 5.8783 | **< 0.0001** |
| Phe | 2.116 ± 0.099 | 2.097 ± 0.087 | 2.225 ± 0.090 | 2.240 ± 0.086 | 2.094 ± 0.070 | 2.140 ± 0.105 | 26018.50 | 5.8783 | **< 0.0001** |
| Tyr | 2.258 ± 0.101 | 2.233 ± 0.087 | 2.368 ± 0.087 | 2.384 ± 0.083 | 2.243 ± 0.069 | 2.284 ± 0.102 | 34998.835 | 5.8783 | **< 0.0001** |
| Trp | 2.513 ± 0.108 | 2.491 ± 0.093 | 2.655 ± 0.099 | 2.486 ± 0.069 | N/S | 2.555 ± 0.108 | 43418.25 | 7.0360 | **< 0.0001** |
| Ser | 1.209 ± 0.075 | 1.187 ± 0.063 | 1.298 ± 0.055 | 1.299 ± 0.062 | 1.211 ± 0.060 | 1.224 ± 0.074 | 45051.92 | 5.8783 | **< 0.0001** |
| Thr | 1.415 ± 0.081 | 1.397 ± 0.068 | 1.532 ± 0.059 | 1.401 ± 0.061 | N/S | 1.454 ± 0.088 | 57179.05 | 7.0360 | **< 0.0001** |
| Cys:H | 1.360 ± 0.080 | 1.338 ± 0.067 | 1.456 ± 0.062 | 1.445 ± 0.072 | N/S | 1.370 ± 0.081 | 57758.14 | 7.0360 | **< 0.0001** |
| Asn | 1.584 ± 0.085 | 1.549 ± 0.072 | 1.654 ± 0.063 | 1.656 ± 0.068 | 1.551 ± 0.064 | 1.600 ± 0.084 | 48613.03 | 5.8783 | **< 0.0001** |
| Gln | 1.800 ± 0.105 | 1.767 ± 0.095 | 1.884 ± 0.076 | 1.902 ± 0.089 | N/S | 1.808 ± 0.106 | 43730.18 | 7.0360 | **< 0.0001** |
| Arg:NE | 2.419 ± 0.128 | 2.392 ± 0.120 | 2.523 ± 0.102 | 2.552 ± 0.100 | N/S | 2.449 ± 0.125 | 26582.73 | 7.0360 | **< 0.0001** |
| Arg:NH | 2.421 ± 0.124 | 2.394 ± 0.116 | 2.508 ± 0.104 | 2.524 ± 0.102 | N/S | 2.434 ± 0.120 | 23588.57 | 7.0360 | **< 0.0001** |

**Table S35 (Cont.).** The solvent accessible surface area (SASA) for the whole Xaa residue of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Asp:H | 1.516 ± 0.090 | 1.476 ± 0.075 | 1.590 ± 0.060 | 1.603 ± 0.067 | 1.496 ± 0.068 | 1.537 ± 0.082 | 58520.06 | 5.8783 | **< 0.0001** |
| Glu:H | 1.810 ± 0.092 | 1.786 ± 0.083 | 1.888 ± 0.077 | 1.890 ± 0.080 | N/S | 1.820 ± 0.092 | 36146.44 | 7.0360 | **< 0.0001** |
| LysN | 2.092 ± 0.112 | 2.065 ± 0.103 | 2.182 ± 0.092 | 2.194 ± 0.091 | 2.085 ± 0.091 | 2.116 ± 0.107 | 24335.38 | 5.8783 | **< 0.0001** |
| Arg | 2.409 ± 0.125 | 2.386 ± 0.119 | 2.503 ± 0.105 | 2.499 ± 0.112 | N/S | 2.425 ± 0.123 | 20010.14 | 7.0360 | **< 0.0001** |
| His+ | 1.879 ± 0.108 | 1.845 ± 0.092 | 1.928 ± 0.106 | 1.985 ± 0.086 | N/S | 1.872 ± 0.111 | 34228.51 | 7.0360 | **< 0.0001** |
| Lys | 2.127 ± 0.106 | 2.100 ± 0.096 | 2.217 ± 0.087 | 2.232 ± 0.090 | N/S | 2.144 ± 0.104 | 34130.37 | 7.0360 | **< 0.0001** |
| Asp | 1.480 ± 0.079 | 1.455 ± 0.063 | 1.574 ± 0.065 | 1.575 ± 0.057 | 1.477 ± 0.055 | 1.502 ± 0.079 | 54399.16 | 5.8783 | **< 0.0001** |
| Glu | 1.774 ± 0.084 | 1.753 ± 0.072 | 1.871 ± 0.069 | 1.878 ± 0.064 | N/S | 1.807 ± 0.084 | 49692.14 | 7.0360 | **< 0.0001** |
| Cys- | 1.375 ± 0.082 | 1.350 ± 0.065 | 1.469 ± 0.067 | N/S | N/S | 1.379 ± 0.083 | 109975.82 | 9.2106 | **< 0.0001** |
| Tyr- | 2.205 ± 0.109 | 2.181 ± 0.097 | 2.320 ± 0.094 | 2.358 ± 0.065 | N/S | 2.255 ± 0.093 | 38372.66 | 7.0360 | **< 0.0001** |
| Cys-Cys | 0.753 ± 0.141 | 0.735 ± 0.134 | 0.796 ± 0.145 | 0.819 ± 0.148 | N/S | 0.761 ± 0.135 | 10624.17 | 7.0359 | **< 0.0001** |
| Pro:cis | 1.476 ± 0.060 | 1.461 ± 0.055 | 1.533 ± 0.040 | N/S | N/S | 1.482 ± 0.090 | 62719.94 | 9.2106 | **< 0.0001** |
| Pro:trans | 1.415 ± 0.056 | 1.407 ± 0.047 | 1.534 ± 0.043 | N/S | N/S | 1.489 ± 0.074 | 66358.99 | 9.2106 | **< 0.0001** |

a Only the b, a, aL, e, and contiguous regions of the f,y space are compared with the Welch’s ANOVA.

b N/S: not sampled region secondary to low population density (<1000 conformations within 10°).

**Table S36.** The solvent accessible surface area (SASA) for the Xaa residue backbone of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Gly\* | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |
| Ala | 0.418 ± 0.062 | 0.398 ± 0.051 | 0.478 ± 0.048 | 0.539 ± 0.052 | 0.515 ± 0.055 | 0.469 ± 0.057 | 50207.06 | 5.8783 | **< 0.0001** |
| Val | 0.300 ± 0.054 | 0.294 ± 0.052 | 0.350 ± 0.039 | 0.360 ± 0.046 | N/S | 0.364 ± 0.065 | 15012.58 | 7.0360 | **< 0.0001** |
| Leu | 0.327 ± 0.061 | 0.309 ± 0.056 | 0.373 ± 0.043 | 0.429 ± 0.052 | N/S | 0.371 ± 0.058 | 42184.12 | 7.0360 | **< 0.0001** |
| Ile | 0.284 ± 0.054 | 0.279 ± 0.053 | 0.325 ± 0.049 | 0.328 ± 0.050 | N/S | 0.320 ± 0.053 | 10042.64 | 7.0360 | **< 0.0001** |
| Met | 0.334 ± 0.064 | 0.313 ± 0.056 | 0.383 ± 0.045 | 0.439 ± 0.059 | N/S | 0.389 ± 0.062 | 55113.31 | 7.0360 | **< 0.0001** |
| His:ND1 | 0.352 ± 0.067 | 0.331 ± 0.058 | 0.386 ± 0.046 | 0.455 ± 0.059 | 0.409 ± 0.054 | 0.390 ± 0.062 | 41089.47 | 5.8783 | **< 0.0001** |
| His:NE2 | 0.364 ± 0.072 | 0.336 ± 0.059 | 0.393 ± 0.048 | 0.458 ± 0.061 | 0.409 ± 0.058 | 0.400 ± 0.074 | 54000.27 | 5.8783 | **< 0.0001** |
| Phe | 0.335 ± 0.060 | 0.323 ± 0.055 | 0.375 ± 0.045 | 0.439 ± 0.053 | 0.360 ± 0.048 | 0.380 ± 0.062 | 22198.68 | 5.8783 | **< 0.0001** |
| Tyr | 0.338 ± 0.060 | 0.326 ± 0.055 | 0.372 ± 0.046 | 0.444 ± 0.050 | 0.369 ± 0.049 | 0.379 ± 0.060 | 22158.11 | 5.8783 | **< 0.0001** |
| Trp | 0.321 ± 0.057 | 0.315 ± 0.054 | 0.348 ± 0.060 | 0.348 ± 0.051 | N/S | 0.355 ± 0.067 | 6935.44 | 7.0360 | **< 0.0001** |
| Ser | 0.391 ± 0.062 | 0.375 ± 0.055 | 0.430 ± 0.046 | 0.492 ± 0.055 | 0.452 ± 0.062 | 0.436 ± 0.058 | 31416.90 | 5.8783 | **< 0.0001** |
| Thr | 0.325 ± 0.059 | 0.315 ± 0.056 | 0.378 ± 0.040 | 0.377 ± 0.048 | N/S | 0.394 ± 0.062 | 26436.53 | 7.0360 | **< 0.0001** |
| Cys:H | 0.375 ± 0.063 | 0.358 ± 0.054 | 0.423 ± 0.042 | 0.484 ± 0.055 | N/S | 0.424 ± 0.060 | 55579.45 | 7.0360 | **< 0.0001** |
| Asn | 0.361 ± 0.069 | 0.330 ± 0.056 | 0.396 ± 0.042 | 0.454 ± 0.058 | 0.401 ± 0.056 | 0.404 ± 0.064 | 63252.00 | 5.8783 | **< 0.0001** |
| Gln | 0.323 ± 0.065 | 0.299 ± 0.056 | 0.373 ± 0.043 | 0.418 ± 0.059 | N/S | 0.367 ± 0.062 | 62841.70 | 7.0360 | **< 0.0001** |
| Arg:NE | 0.332 ± 0.067 | 0.313 ± 0.057 | 0.389 ± 0.045 | 0.451 ± 0.059 | N/S | 0.396 ± 0.067 | 57507.71 | 7.0360 | **< 0.0001** |
| Arg:NH | 0.331 ± 0.065 | 0.312 ± 0.057 | 0.380 ± 0.052 | 0.428 ± 0.059 | N/S | 0.382 ± 0.063 | 44743.70 | 7.0360 | **< 0.0001** |

**Table S36 (Cont.).** The solvent accessible surface area (SASA) for the Xaa residue backbone of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Asp:H | 0.360 ± 0.072 | 0.324 ± 0.056 | 0.405 ± 0.038 | 0.472 ± 0.055 | 0.426 ± 0.058 | 0.411 ± 0.061 | 90243.53 | 5.8783 | **< 0.0001** |
| Glu:H | 0.344 ± 0.066 | 0.322 ± 0.057 | 0.398 ± 0.044 | 0.454 ± 0.057 | N/S | 0.399 ± 0.060 | 62670.99 | 7.0360 | **< 0.0001** |
| LysN | 0.363 ± 0.070 | 0.340 ± 0.058 | 0.419 ± 0.048 | 0.469 ± 0.065 | 0.421 ± 0.060 | 0.426 ± 0.067 | 50608.30 | 5.8783 | **< 0.0001** |
| Arg | 0.336 ± 0.063 | 0.321 ± 0.057 | 0.387 ± 0.048 | 0.434 ± 0.066 | N/S | 0.392 ± 0.061 | 37357.67 | 7.0360 | **< 0.0001** |
| His+ | 0.337 ± 0.066 | 0.322 ± 0.061 | 0.339 ± 0.061 | 0.394 ± 0.066 | N/S | 0.363 ± 0.067 | 18928.90 | 7.0360 | **< 0.0001** |
| Lys | 0.337 ± 0.064 | 0.318 ± 0.055 | 0.389 ± 0.047 | 0.448 ± 0.058 | N/S | 0.397 ± 0.060 | 52803.79 | 7.0360 | **< 0.0001** |
| Asp | 0.348 ± 0.064 | 0.327 ± 0.051 | 0.416 ± 0.042 | 0.465 ± 0.049 | 0.437 ± 0.055 | 0.408 ± 0.064 | 63622.07 | 5.8783 | **< 0.0001** |
| Glu | 0.347 ± 0.063 | 0.330 ± 0.054 | 0.416 ± 0.040 | 0.484 ± 0.052 | N/S | 0.420 ± 0.061 | 63571.10 | 7.0360 | **< 0.0001** |
| Cys- | 0.400 ± 0.064 | 0.377 ± 0.050 | 0.479 ± 0.039 | N/S | N/S | 0.439 ± 0.067 | 152072.74 | 9.2106 | **< 0.0001** |
| Tyr- | 0.323 ± 0.063 | 0.310 ± 0.056 | 0.375 ± 0.046 | 0.449 ± 0.050 | N/S | 0.379 ± 0.062 | 39693.13 | 7.0360 | **< 0.0001** |
| Cys-Cys | 0.316 ± 0.079 | 0.300 ± 0.069 | 0.395 ± 0.109 | 0.353 ± 0.077 | N/S | 0.360 ± 0.093 | 58860.66 | 7.0359 | **< 0.0001** |
| Pro:cis | 0.248 ± 0.056 | 0.226 ± 0.039 | 0.330 ± 0.031 | N/S | N/S | 0.284 ± 0.061 | 255061.36 | 9.2106 | **< 0.0001** |
| Pro:trans | 0.294 ± 0.047 | 0.286 ± 0.034 | 0.423 ± 0.032 | N/S | N/S | 0.374 ± 0.058 | 144055.39 | 9.2106 | **< 0.0001** |

a Only the b, a, aL, e, and contiguous regions of the f,y space are compared with the Welch’s ANOVA.

b N/A: not applicable, Gly is reported as the whole residue.

b N/S: not sampled region secondary to low population density (<1000 conformations within 10°).

**Table S37.** The solvent accessible surface area (SASA) for the Xaa residue side chain of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b,c Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Gly | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |
| Ala | 0.675 ± 0.043 | 0.670 ± 0.041 | 0.710 ± 0.025 | 0.643 ± 0.028 | 0.589 ± 0.037 | 0.643 ± 0.049 | 24262.90 | 5.8783 | **< 0.0001** |
| Val | 1.224 ± 0.068 | 1.219 ± 0.065 | 1.293 ± 0.057 | 1.157 ± 0.052 | N/S | 1.221 ± 0.072 | 12092.08 | 7.0360 | **< 0.0001** |
| Leu | 1.530 ± 0.076 | 1.520 ± 0.076 | 1.573 ± 0.058 | 1.511 ± 0.059 | N/S | 1.490 ± 0.083 | 13267.08 | 7.0360 | **< 0.0001** |
| Ile | 1.465 ± 0.076 | 1.457 ± 0.072 | 1.548 ± 0.067 | 1.400 ± 0.060 | N/S | 1.470 ± 0.079 | 18252.51 | 7.0360 | **< 0.0001** |
| Met | 1.561 ± 0.102 | 1.551 ± 0.104 | 1.607 ± 0.083 | 1.567 ± 0.074 | N/S | 1.524 ± 0.098 | 7518.82 | 7.0360 | **< 0.0001** |
| His:ND1 | 1.546 ± 0.090 | 1.533 ± 0.089 | 1.606 ± 0.072 | 1.548 ± 0.059 | 1.482 ± 0.064 | 1.511 ± 0.093 | 11404.51 | 5.8783 | **< 0.0001** |
| His:NE2 | 1.538 ± 0.088 | 1.531 ± 0.087 | 1.580 ± 0.096 | 1.545 ± 0.061 | 1.478 ± 0.068 | 1.514 ± 0.100 | 6079.75 | 5.8783 | **< 0.0001** |
| Phe | 1.782 ± 0.089 | 1.774 ± 0.084 | 1.851 ± 0.094 | 1.801 ± 0.067 | 1.733 ± 0.061 | 1.760 ± 0.097 | 8623.07 | 5.8783 | **< 0.0001** |
| Tyr | 1.921 ± 0.091 | 1.908 ± 0.084 | 1.996 ± 0.091 | 1.940 ± 0.064 | 1.873 ± 0.059 | 1.904 ± 0.098 | 13545.08 | 5.8783 | **< 0.0001** |
| Trp | 2.192 ± 0.096 | 2.176 ± 0.081 | 2.307 ± 0.112 | 2.138 ± 0.060 | N/S | 2.200 ± 0.117 | 32396.00 | 7.0360 | **< 0.0001** |
| Ser | 0.818 ± 0.054 | 0.813 ± 0.051 | 0.868 ± 0.033 | 0.807 ± 0.037 | 0.760 ± 0.042 | 0.788 ± 0.062 | 20723.45 | 5.8783 | **< 0.0001** |
| Thr | 1.089 ± 0.073 | 1.082 ± 0.071 | 1.154 ± 0.048 | 1.025 ± 0.052 | N/S | 1.060 ± 0.080 | 17295.09 | 7.0360 | **< 0.0001** |
| Cys:H | 0.986 ± 0.063 | 0.981 ± 0.061 | 1.034 ± 0.049 | 0.961 ± 0.054 | N/S | 0.946 ± 0.072 | 15892.50 | 7.0360 | **< 0.0001** |
| Asn | 1.223 ± 0.067 | 1.219 ± 0.068 | 1.258 ± 0.053 | 1.202 ± 0.051 | 1.149 ± 0.058 | 1.196 ± 0.076 | 11767.18 | 5.8783 | **< 0.0001** |
| Gln | 1.478 ± 0.090 | 1.468 ± 0.093 | 1.511 ± 0.072 | 1.484 ± 0.068 | N/S | 1.441 ± 0.093 | 6487.70 | 7.0360 | **< 0.0001** |
| Arg:NE | 2.087 ± 0.114 | 2.079 ± 0.116 | 2.134 ± 0.094 | 2.101 ± 0.077 | N/S | 2.053 ± 0.113 | 4610.30 | 7.0360 | **< 0.0001** |
| Arg:NH | 2.090 ± 0.110 | 2.082 ± 0.112 | 2.129 ± 0.096 | 2.096 ± 0.081 | N/S | 2.053 ± 0.108 | 4536.09 | 7.0360 | **< 0.0001** |

**Table S37 (Cont.).** The solvent accessible surface area (SASA) for the Xaa residue side chain of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y space assigned by density clustering and demonstrated in Figure S2. Results are compared using a Welch’s analysis of variance (ANOVA).a,b,c Results are considered statistically significant for an a = 0.0001 using a right-tailed F distribution.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | All | b | a | aL | e | Cont. | F-statistic | F-critical | p-value |
| SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 | SASA/nm2 |  |  |  |
| Asp:H | 1.156 ± 0.068 | 1.151 ± 0.071 | 1.185 ± 0.052 | 1.131 ± 0.048 | 1.070 ± 0.056 | 1.126 ± 0.070 | 9993.86 | 5.8783 | **< 0.0001** |
| Glu:H | 1.466 ± 0.074 | 1.463 ± 0.076 | 1.490 ± 0.061 | 1.436 ± 0.060 | N/S | 1.421 ± 0.078 | 5541.15 | 7.0360 | **< 0.0001** |
| LysN | 1.730 ± 0.098 | 1.725 ± 0.102 | 1.763 ± 0.082 | 1.725 ± 0.071 | 1.664 ± 0.076 | 1.690 ± 0.094 | 3190.83 | 5.8783 | **< 0.0001** |
| Arg | 2.073 ± 0.120 | 2.065 ± 0.123 | 2.116 ± 0.096 | 2.065 ± 0.087 | N/S | 2.033 ± 0.113 | 4065.32 | 7.0360 | **< 0.0001** |
| His+ | 1.542 ± 0.111 | 1.523 ± 0.100 | 1.589 ± 0.124 | 1.591 ±0.079 | N/S | 1.508 ± 0.121 | 12337.66 | 7.0360 | **< 0.0001** |
| Lys | 1.789 ± 0.097 | 1.782 ± 0.099 | 1.829 ± 0.078 | 1.783 ± 0.070 | N/S | 1.747 ± 0.095 | 6092.93 | 7.0360 | **< 0.0001** |
| Asp | 1.131 ± 0.057 | 1.128 ± 0.056 | 1.158 ± 0.050 | 1.110 ± 0.040 | 1.039 ± 0.047 | 1.094 ± 0.065 | 8050.45 | 5.8783 | **< 0.0001** |
| Glu | 1.427 ± 0.066 | 1.423 ± 0.067 | 1.455 ± 0.056 | 1.394 ± 0.045 | N/S | 1.388 ± 0.069 | 5784.73 | 7.0360 | **< 0.0001** |
| Cys- | 0.976 ± 0.056 | 0.972 ± 0.054 | 0.990 ± 0.059 | N/S | N/S | 0.940 ± 0.061 | 4473.81 | 9.2106 | **< 0.0001** |
| Tyr- | 1.882 ± 0.099 | 1.872 ± 0.097 | 1.946 ± 0.096 | 1.909 ± 0.053 | N/S | 1.876 ± 0.091 | 8691.59 | 7.0360 | **< 0.0001** |
| Cys-Cys | 0.437 ± 0.129 | 0.435 ± 0.127 | 0.401 ± 0.118 | 0.465 ± 0.133 | N/S | 0.401 ± 0.123 | 4275.94 | 7.0359 | **< 0.0001** |
| Pro:cis | 1.228 ± 0.036 | 1.235 ± 0.033 | 1.203 ± 0.036 | N/S | N/S | 1.198 ± 0.057 | 30389.47 | 9.2106 | **< 0.0001** |
| Pro:trans | 1.121 ± 0.036 | 1.122 ± 0.036 | 1.110 ± 0.036 | N/S | N/S | 1.115 ± 0.042 | 985.94 | 9.2106 | **< 0.0001** |

a Only the b, a, aL, e, and contiguous regions of the f,y space are compared with the Welch’s ANOVA.

b N/A: not applicable, Gly does not have a side chain.

c N/S: not sampled region secondary to low population density (<1000 conformations within 10°)

**Table S38.** Scheffe’s pairwise comparison of the solvent accessible surface area (SASA) for the whole Xaa residue of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y dihedral space assigned by density clustering and demonstrated in Figure S2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | Pairwise Interaction | Scheffe LSD | Difference | Statistically Significant |
| Gly | b - a | 0.002066222 | 0.126 | Yes |
|  | b - aL | 0.001795867 | 0.122 | Yes |
|  | b - e | 0.000901919 | 0.003 | Yes |
|  | b - Contig. | 0.001983122 | 0.026 | Yes |
|  | a - aL | 0.00260905 | 0.004 | Yes |
|  | a - e | 0.002096536 | 0.123 | Yes |
|  | a - Contig. | 0.002741309 | 0.1 | Yes |
|  | aL - e | 0.001830663 | 0.119 | Yes |
|  | aL – Contig. | 0.002543745 | 0.096 | Yes |
|  | e – Contig. | 0.002014686 | 0.023 | Yes |
| Ala | b - a | 0.000571158 | 0.12 | Yes |
|  | b - aL | 0.002118898 | 0.114 | Yes |
|  | b - e | 0.002051781 | 0.037 | Yes |
|  | b - Contig. | 0.001096498 | 0.043 | Yes |
|  | a - aL | 0.002166731 | 0.006 | Yes |
|  | a - e | 0.002101143 | 0.083 | Yes |
|  | a - Contig. | 0.001186298 | 0.077 | Yes |
|  | aL - e | 0.002928875 | 0.077 | Yes |
|  | aL – Contig. | 0.002360256 | 0.071 | Yes |
|  | e – Contig. | 0.002300193 | 0.006 | Yes |
| Val | b - a | 0.002055777 | 0.129 | Yes |
|  | b - aL | 0.0050243 | 0.002 | **No** |
|  | b - Contig. | 0.004015008 | 0.071 | Yes |
|  | a - aL | 0.005376439 | 0.127 | Yes |
|  | a - Contig. | 0.004447785 | 0.058 | Yes |
|  | aL – Contig. | 0.006387501 | 0.069 | Yes |
| Leu | b - a | 0.001305372 | 0.117 | Yes |
|  | b - aL | 0.004382424 | 0.111 | Yes |
|  | b - Contig. | 0.002883341 | 0.032 | Yes |
|  | a - aL | 0.004489391 | 0.006 | Yes |
|  | a - Contig. | 0.003043461 | 0.085 | Yes |
|  | aL – Contig. | 0.005173422 | 0.079 | Yes |
| Ile | b - a | 0.001917824 | 0.137 | Yes |
|  | b - aL | 0.005618888 | 0.009 | Yes |
|  | b - Contig. | 0.00432509 | 0.054 | Yes |
|  | a - aL | 0.005881098 | 0.146 | Yes |
|  | a - Contig. | 0.004660667 | 0.083 | Yes |
|  | aL – Contig. | 0.007043839 | 0.063 | Yes |
| Met | b - a | 0.001907869 | 0.126 | Yes |
|  | b - aL | 0.004744546 | 0.142 | Yes |
|  | b - Contig. | 0.003690287 | 0.049 | Yes |
|  | a - aL | 0.004959274 | 0.016 | Yes |
|  | a - Contig. | 0.003962563 | 0.077 | Yes |
|  | aL – Contig. | 0.005879851 | 0.093 | Yes |
| His:ND1 | b - a | 0.001709192 | 0.128 | Yes |
|  | b - aL | 0.002579055 | 0.139 | Yes |
|  | b - e | 0.010887182 | 0.026 | Yes |
|  | b - Contig. | 0.003057358 | 0.037 | Yes |
|  | a - aL | 0.002901954 | 0.011 | Yes |
|  | a - e | 0.01096816 | 0.102 | Yes |
|  | a - Contig. | 0.003334254 | 0.091 | Yes |
|  | aL - e | 0.011136908 | 0.113 | Yes |
|  | aL – Contig. | 0.003853237 | 0.102 | Yes |
|  | e – Contig. | 0.011257293 | 0.011 | **No** |
| His:NE2 | b - a | 0.001879091 | 0.106 | Yes |
|  | b - aL | 0.002055598 | 0.136 | Yes |
|  | b - e | 0.003681059 | 0.02 | Yes |
|  | b - Contig. | 0.003719334 | 0.047 | Yes |
|  | a - aL | 0.002537553 | 0.03 | Yes |
|  | a - e | 0.003970376 | 0.086 | Yes |
|  | a - Contig. | 0.004005887 | 0.059 | Yes |
|  | aL - e | 0.004056894 | 0.116 | Yes |
|  | aL – Contig. | 0.004091655 | 0.089 | Yes |
|  | e – Contig. | 0.005105521 | 0.027 | Yes |
| Phe | b - a | 0.002169012 | 0.128 | Yes |
|  | b - aL | 0.00430955 | 0.143 | Yes |
|  | b - e | 0.006999557 | 0.003 | **No** |
|  | b - Contig. | 0.003463862 | 0.043 | Yes |
|  | a - aL | 0.004707693 | 0.015 | Yes |
|  | a - e | 0.00725148 | 0.131 | Yes |
|  | a - Contig. | 0.003948227 | 0.085 | Yes |
|  | aL - e | 0.008151783 | 0.146 | Yes |
|  | aL – Contig. | 0.005427347 | 0.1 | Yes |
|  | e – Contig. | 0.007738067 | 0.046 | Yes |
| Tyr | b - a | 0.001920517 | 0.135 | Yes |
|  | b - aL | 0.004226836 | 0.151 | Yes |
|  | b - e | 0.008244032 | 0.01 | Yes |
|  | b - Contig. | 0.003509619 | 0.051 | Yes |
|  | a - aL | 0.004517756 | 0.016 | Yes |
|  | a - e | 0.008396907 | 0.125 | Yes |
|  | a - Contig. | 0.00385505 | 0.084 | Yes |
|  | aL - e | 0.009202489 | 0.141 | Yes |
|  | aL – Contig. | 0.0053888 | 0.1 | Yes |
|  | e – Contig. | 0.008895903 | 0.041 | Yes |
| Trp | b - a | 0.002110799 | 0.164 | Yes |
|  | b - aL | 0.00912397 | 0.005 | No |
|  | b - Contig. | 0.003896842 | 0.064 | Yes |
|  | a - aL | 0.009305494 | 0.169 | Yes |
|  | a - Contig. | 0.004304737 | 0.1 | Yes |
|  | aL – Contig. | 0.009865198 | 0.069 | Yes |
| Ser | b - a | 0.001386654 | 0.111 | Yes |
|  | b - aL | 0.002734734 | 0.112 | Yes |
|  | b - e | 0.003337927 | 0.024 | Yes |
|  | b - Contig. | 0.002147978 | 0.037 | Yes |
|  | a - aL | 0.002964976 | 0.001 | **No** |
|  | a - e | 0.003529032 | 0.087 | Yes |
|  | a - Contig. | 0.002434362 | 0.074 | Yes |
|  | aL - e | 0.004243823 | 0.088 | Yes |
|  | aL – Contig. | 0.003388522 | 0.075 | Yes |
|  | e – Contig. | 0.003891666 | 0.013 | Yes |
| Thr | b - a | 0.001516214 | 0.135 | Yes |
|  | b - aL | 0.004916697 | 0.004 | **No** |
|  | b - Contig. | 0.00291345 | 0.057 | Yes |
|  | a - aL | 0.005089118 | 0.131 | Yes |
|  | a - Contig. | 0.003195841 | 0.078 | Yes |
|  | aL – Contig. | 0.005664663 | 0.053 | Yes |
| Cys | b - a | 0.001434554 | 0.118 | Yes |
|  | b - aL | 0.002379137 | 0.107 | Yes |
|  | b - Contig. | 0.002497715 | 0.032 | Yes |
|  | a - aL | 0.002665867 | 0.011 | Yes |
|  | a - Contig. | 0.002772207 | 0.086 | Yes |
|  | aL – Contig. | 0.003359685 | 0.075 | Yes |
| Asn | b - a | 0.001339802 | 0.105 | Yes |
|  | b - aL | 0.001824523 | 0.107 | Yes |
|  | b - e | 0.003470908 | 0.002 | **No** |
|  | b - Contig. | 0.003207959 | 0.051 | Yes |
|  | a - aL | 0.002052279 | 0.002 | **No** |
|  | a - e | 0.003595854 | 0.103 | Yes |
|  | a - Contig. | 0.003342748 | 0.054 | Yes |
|  | aL - e | 0.003803154 | 0.105 | Yes |
|  | aL – Contig. | 0.003564797 | 0.056 | Yes |
|  | e – Contig. | 0.004628833 | 0.049 | Yes |
| Gln | b - a | 0.001595612 | 0.117 | Yes |
|  | b - aL | 0.003694734 | 0.135 | Yes |
|  | b - Contig. | 0.003399519 | 0.041 | Yes |
|  | a - aL | 0.003864519 | 0.018 | Yes |
|  | a - Contig. | 0.003583319 | 0.076 | Yes |
|  | aL – Contig. | 0.004893389 | 0.094 | Yes |
| Arg:NE | b - a | 0.00240368 | 0.131 | Yes |
|  | b - aL | 0.005077914 | 0.16 | Yes |
|  | b - Contig. | 0.00431449 | 0.057 | Yes |
|  | a - aL | 0.005450423 | 0.029 | Yes |
|  | a - Contig. | 0.004747287 | 0.074 | Yes |
|  | aL – Contig. | 0.006522596 | 0.103 | Yes |
| Arg:NH | b - a | 0.002098567 | 0.114 | Yes |
|  | b - aL | 0.005386719 | 0.13 | Yes |
|  | b - Contig. | 0.004291957 | 0.04 | Yes |
|  | a - aL | 0.005619987 | 0.016 | Yes |
|  | a - Contig. | 0.00458131 | 0.074 | Yes |
|  | aL – Contig. | 0.006752863 | 0.09 | Yes |
| Asp:H | b - a | 0.001304816 | 0.114 | Yes |
|  | b - aL | 0.002040573 | 0.127 | Yes |
|  | b - e | 0.004288204 | 0.02 | Yes |
|  | b - Contig. | 0.003103851 | 0.061 | Yes |
|  | a - aL | 0.002217876 | 0.013 | Yes |
|  | a - e | 0.004375355 | 0.094 | Yes |
|  | a - Contig. | 0.003223187 | 0.053 | Yes |
|  | aL - e | 0.004648131 | 0.107 | Yes |
|  | aL – Contig. | 0.003584735 | 0.066 | Yes |
|  | e – Contig. | 0.005203372 | 0.041 | Yes |
| Glu:H | b - a | 0.001509523 | 0.102 | Yes |
|  | b - aL | 0.003487803 | 0.104 | Yes |
|  | b - Contig. | 0.003224219 | 0.034 | Yes |
|  | a - aL | 0.003671 | 0.002 | **No** |
|  | a - Contig. | 0.003421557 | 0.068 | Yes |
|  | aL – Contig. | 0.004646845 | 0.07 | Yes |
| LysN | b - a | 0.002054697 | 0.117 | Yes |
|  | b - aL | 0.003645805 | 0.129 | Yes |
|  | b - e | 0.010319453 | 0.02 | Yes |
|  | b - Contig. | 0.003917536 | 0.051 | Yes |
|  | a - aL | 0.003985101 | 0.012 | Yes |
|  | a - e | 0.010444148 | 0.097 | Yes |
|  | a - Contig. | 0.004235118 | 0.066 | Yes |
|  | aL - e | 0.010869699 | 0.109 | Yes |
|  | aL – Contig. | 0.005196762 | 0.078 | Yes |
|  | e – Contig. | 0.010963829 | 0.031 | Yes |
| Arg | b - a | 0.002268384 | 0.117 | Yes |
|  | b - aL | 0.007062773 | 0.113 | Yes |
|  | b - Contig. | 0.004531528 | 0.039 | Yes |
|  | a - aL | 0.007292356 | 0.004 | **No** |
|  | a - Contig. | 0.004881643 | 0.078 | Yes |
|  | aL – Contig. | 0.008280558 | 0.074 | Yes |
| His+ | b - a | 0.001802496 | 0.083 | Yes |
|  | b - aL | 0.002320937 | 0.14 | Yes |
|  | b - Contig. | 0.002429675 | 0.027 | Yes |
|  | a - aL | 0.002643363 | 0.057 | Yes |
|  | a - Contig. | 0.002739332 | 0.056 | Yes |
|  | aL – Contig. | 0.003105108 | 0.113 | Yes |
| Lys | b - a | 0.001767175 | 0.117 | Yes |
|  | b - aL | 0.005186539 | 0.132 | Yes |
|  | b - Contig. | 0.003531769 | 0.044 | Yes |
|  | a - aL | 0.005363663 | 0.015 | Yes |
|  | a - Contig. | 0.003787095 | 0.073 | Yes |
|  | aL – Contig. | 0.006174089 | 0.088 | Yes |
| Asp | b - a | 0.001301399 | 0.119 | Yes |
|  | b - aL | 0.003426408 | 0.12 | Yes |
|  | b - e | 0.005960256 | 0.022 | Yes |
|  | b - Contig. | 0.002789573 | 0.047 | Yes |
|  | a - aL | 0.003579288 | 0.001 | **No** |
|  | a - e | 0.006049436 | 0.097 | Yes |
|  | a - Contig. | 0.002975357 | 0.072 | Yes |
|  | aL - e | 0.006829518 | 0.098 | Yes |
|  | aL – Contig. | 0.004347342 | 0.073 | Yes |
|  | e – Contig. | 0.006533281 | 0.025 | Yes |
| Glu | b - a | 0.001464313 | 0.118 | Yes |
|  | b - aL | 0.005015948 | 0.125 | Yes |
|  | b - Contig. | 0.003181898 | 0.054 | Yes |
|  | a - aL | 0.005160627 | 0.007 | Yes |
|  | a - Contig. | 0.003405409 | 0.064 | Yes |
|  | aL – Contig. | 0.005883224 | 0.071 | Yes |
| Cys- | b - a | 0.001089061 | 0.119 | Yes |
|  | b - Contig. | 0.004295435 | 0.029 | Yes |
|  | a – Contig. | 0.004373212 | 0.09 | Yes |
| Tyr- | b - a | 0.002133174 | 0.139 | Yes |
|  | b - aL | 0.005027003 | 0.177 | Yes |
|  | b - Contig. | 0.003684236 | 0.074 | Yes |
|  | a - aL | 0.005351279 | 0.038 | Yes |
|  | a - Contig. | 0.004115704 | 0.065 | Yes |
|  | aL – Contig. | 0.006136721 | 0.103 | Yes |
| Cys-Cys | b - a | 0.001891939 | 0.061 | Yes |
|  | b - aL | 0.00340897 | 0.084 | Yes |
|  | b - Contig. | 0.003389664 | 0.026 | Yes |
|  | a - aL | 0.003724329 | 0.023 | Yes |
|  | a - Contig. | 0.003706666 | 0.035 | Yes |
|  | aL – Contig. | 0.004667013 | 0.058 | Yes |
| Pro:cis | b - a | 0.000872577 | 0.072 | Yes |
|  | b - Contig. | 0.005877482 | 0.021 | Yes |
|  | a - Contig. | 0.005914781 | 0.051 | Yes |
| Pro:trans | b - a | 0.001848992 | 0.127 | Yes |
|  | b - Contig. | 0.001558011 | 0.082 | Yes |
|  | a - Contig. | 0.002368747 | 0.045 | Yes |

**Table S39.** Scheffe’s pairwise comparison of the solvent accessible surface area (SASA) for the backbone Xaa residue of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y dihedral space assigned by density clustering and demonstrated in Figure S2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | Pairwise Interaction | Calculated Value | Critical Value | Statistically Significant |
| Ala | b - a | 0.001034161 | 0.08 | Yes |
|  | b - aL | 0.003836558 | 0.141 | Yes |
|  | b - e | 0.003715034 | 0.117 | Yes |
|  | b - Contig. | 0.00198536 | 0.071 | Yes |
|  | a - aL | 0.003923166 | 0.061 | Yes |
|  | a - e | 0.00380441 | 0.037 | Yes |
|  | a - Contig. | 0.002147956 | 0.009 | Yes |
|  | aL - e | 0.005303133 | 0.024 | Yes |
|  | aL – Contig. | 0.00427357 | 0.07 | Yes |
|  | e – Contig. | 0.004164817 | 0.046 | Yes |
| Val | b - a | 0.001517866 | 0.056 | Yes |
|  | b - aL | 0.00370965 | 0.066 | Yes |
|  | b - Contig. | 0.002964447 | 0.07 | Yes |
|  | a - aL | 0.003969648 | 0.01 | Yes |
|  | a - Contig. | 0.003283984 | 0.014 | Yes |
|  | aL – Contig. | 0.004716157 | 0.004 | **No** |
| Leu | b - a | 0.000960917 | 0.064 | Yes |
|  | b - aL | 0.003226012 | 0.12 | Yes |
|  | b - Contig. | 0.0021225 | 0.062 | Yes |
|  | a - aL | 0.003304753 | 0.056 | Yes |
|  | a - Contig. | 0.002240368 | 0.002 | **No** |
|  | aL – Contig. | 0.003808285 | 0.058 | Yes |
| Ile | b - a | 0.001352774 | 0.046 | Yes |
|  | b - aL | 0.003963391 | 0.049 | Yes |
|  | b - Contig. | 0.003050786 | 0.041 | Yes |
|  | a - aL | 0.004148346 | 0.003 | **No** |
|  | a - Contig. | 0.003287491 | 0.005 | Yes |
|  | aL – Contig. | 0.004968508 | 0.008 | Yes |
| Met | b - a | 0.000999147 | 0.07 | Yes |
|  | b - aL | 0.002484709 | 0.126 | Yes |
|  | b - Contig. | 0.001932596 | 0.076 | Yes |
|  | a - aL | 0.002597162 | 0.056 | Yes |
|  | a - Contig. | 0.002075186 | 0.006 | Yes |
|  | aL – Contig. | 0.003079267 | 0.05 | Yes |
| His:ND1 | b - a | 0.00115592 | 0.055 | Yes |
|  | b - aL | 0.001744205 | 0.124 | Yes |
|  | b - e | 0.00736296 | 0.078 | Yes |
|  | b - Contig. | 0.00206768 | 0.059 | Yes |
|  | a - aL | 0.001962581 | 0.069 | Yes |
|  | a - e | 0.007417725 | 0.023 | Yes |
|  | a - Contig. | 0.002254944 | 0.004 | Yes |
|  | aL - e | 0.007531849 | 0.046 | Yes |
|  | aL – Contig. | 0.00260593 | 0.065 | Yes |
|  | e – Contig. | 0.007613265 | 0.019 | Yes |
| His:NE2 | b - a | 0.00127297 | 0.057 | Yes |
|  | b - aL | 0.001392543 | 0.122 | Yes |
|  | b - e | 0.002493694 | 0.073 | Yes |
|  | b - Contig. | 0.002519622 | 0.064 | Yes |
|  | a - aL | 0.001719038 | 0.065 | Yes |
|  | a - e | 0.002689689 | 0.016 | Yes |
|  | a - Contig. | 0.002713745 | 0.007 | Yes |
|  | aL - e | 0.002748299 | 0.049 | Yes |
|  | aL – Contig. | 0.002771847 | 0.058 | Yes |
|  | e – Contig. | 0.00345868 | 0.009 | Yes |
| Phe | b - a | 0.001336237 | 0.052 | Yes |
|  | b - aL | 0.002654931 | 0.116 | Yes |
|  | b - e | 0.004312131 | 0.037 | Yes |
|  | b - Contig. | 0.002133939 | 0.057 | Yes |
|  | a - aL | 0.00290021 | 0.064 | Yes |
|  | a - e | 0.004467329 | 0.015 | Yes |
|  | a - Contig. | 0.002432335 | 0.005 | Yes |
|  | aL - e | 0.005021968 | 0.079 | Yes |
|  | aL – Contig. | 0.003343559 | 0.059 | Yes |
|  | e – Contig. | 0.004767095 | 0.02 | Yes |
| Tyr | b - a | 0.00118278 | 0.046 | Yes |
|  | b - aL | 0.002603162 | 0.118 | Yes |
|  | b - e | 0.005077215 | 0.043 | Yes |
|  | b - Contig. | 0.002161453 | 0.053 | Yes |
|  | a - aL | 0.00278233 | 0.072 | Yes |
|  | a - e | 0.005171365 | 0.003 | **No** |
|  | a - Contig. | 0.002374192 | 0.007 | Yes |
|  | aL - e | 0.005667496 | 0.075 | Yes |
|  | aL – Contig. | 0.003318776 | 0.065 | Yes |
|  | e – Contig. | 0.00547868 | 0.01 | Yes |
| Trp | b - a | 0.001237638 | 0.033 | Yes |
|  | b - aL | 0.005349716 | 0.033 | Yes |
|  | b - Contig. | 0.002284861 | 0.04 | Yes |
|  | a - aL | 0.00545615 | 0 | **No** |
|  | a - Contig. | 0.002524024 | 0.007 | Yes |
|  | aL – Contig. | 0.005784325 | 0.007 | Yes |
| Ser | b - a | 0.001201656 | 0.055 | Yes |
|  | b - aL | 0.002369885 | 0.117 | Yes |
|  | b - e | 0.002892604 | 0.077 | Yes |
|  | b - Contig. | 0.001861409 | 0.061 | Yes |
|  | a - aL | 0.002569409 | 0.062 | Yes |
|  | a - e | 0.003058213 | 0.022 | Yes |
|  | a - Contig. | 0.002109586 | 0.006 | Yes |
|  | aL - e | 0.003677641 | 0.04 | Yes |
|  | aL – Contig. | 0.002936448 | 0.056 | Yes |
|  | e – Contig. | 0.003372467 | 0.016 | Yes |
| Thr | b - a | 0.001221191 | 0.063 | Yes |
|  | b - aL | 0.003960012 | 0.062 | Yes |
|  | b - Contig. | 0.002346554 | 0.079 | Yes |
|  | a - aL | 0.004098883 | 0.001 | **No** |
|  | a - Contig. | 0.002573998 | 0.016 | Yes |
|  | aL – Contig. | 0.00456244 | 0.017 | Yes |
| Cys | b - a | 0.001127977 | 0.065 | Yes |
|  | b - aL | 0.001870695 | 0.126 | Yes |
|  | b - Contig. | 0.001963932 | 0.066 | Yes |
|  | a - aL | 0.002096148 | 0.061 | Yes |
|  | a - Contig. | 0.002179763 | 0.001 | **No** |
|  | aL – Contig. | 0.002641691 | 0.06 | Yes |
| Asn | b - a | 0.001029887 | 0.066 | Yes |
|  | b - aL | 0.001402485 | 0.124 | Yes |
|  | b - e | 0.002668037 | 0.071 | Yes |
|  | b - Contig. | 0.002465912 | 0.074 | Yes |
|  | a - aL | 0.001577557 | 0.058 | Yes |
|  | a - e | 0.002764081 | 0.005 | Yes |
|  | a - Contig. | 0.002569522 | 0.008 | Yes |
|  | aL - e | 0.00292343 | 0.053 | Yes |
|  | aL – Contig. | 0.002740208 | 0.05 | Yes |
|  | e – Contig. | 0.003558117 | 0.003 | **No** |
| Gln | b - a | 0.000938276 | 0.074 | Yes |
|  | b - aL | 0.002172634 | 0.119 | Yes |
|  | b - Contig. | 0.001999037 | 0.068 | Yes |
|  | a - aL | 0.002272473 | 0.045 | Yes |
|  | a - Contig. | 0.002107118 | 0.006 | Yes |
|  | aL – Contig. | 0.002877485 | 0.051 | Yes |
| Arg:NE | b - a | 0.001146713 | 0.076 | Yes |
|  | b - aL | 0.002422498 | 0.138 | Yes |
|  | b - Contig. | 0.002058295 | 0.083 | Yes |
|  | a - aL | 0.00260021 | 0.062 | Yes |
|  | a - Contig. | 0.002264768 | 0.007 | Yes |
|  | aL – Contig. | 0.003111707 | 0.055 | Yes |
| Arg:NH | b - a | 0.001041185 | 0.068 | Yes |
|  | b - aL | 0.002672573 | 0.116 | Yes |
|  | b - Contig. | 0.002129416 | 0.07 | Yes |
|  | a - aL | 0.002788307 | 0.048 | Yes |
|  | a - Contig. | 0.002272976 | 0.002 | **No** |
|  | aL – Contig. | 0.003350373 | 0.046 | Yes |
| Asp:H | b - a | 0.000959992 | 0.081 | Yes |
|  | b - aL | 0.001501309 | 0.148 | Yes |
|  | b - e | 0.003154958 | 0.102 | Yes |
|  | b - Contig. | 0.002283595 | 0.087 | Yes |
|  | a - aL | 0.001631757 | 0.067 | Yes |
|  | a - e | 0.003219077 | 0.021 | Yes |
|  | a - Contig. | 0.002371393 | 0.006 | Yes |
|  | aL - e | 0.003419767 | 0.046 | Yes |
|  | aL – Contig. | 0.002637395 | 0.061 | Yes |
|  | e – Contig. | 0.003828274 | 0.015 | Yes |
| Glu:H | b - a | 0.001007304 | 0.076 | Yes |
|  | b - aL | 0.002327409 | 0.132 | Yes |
|  | b - Contig. | 0.00215152 | 0.077 | Yes |
|  | a - aL | 0.002449656 | 0.056 | Yes |
|  | a - Contig. | 0.002283203 | 0.001 | **No** |
|  | aL – Contig. | 0.003100837 | 0.055 | Yes |
| LysN | b - a | 0.001166088 | 0.079 | Yes |
|  | b - aL | 0.002069079 | 0.129 | Yes |
|  | b - e | 0.005856529 | 0.081 | Yes |
|  | b - Contig. | 0.002223292 | 0.086 | Yes |
|  | a - aL | 0.002261637 | 0.05 | Yes |
|  | a - e | 0.005927296 | 0.002 | **No** |
|  | a - Contig. | 0.002403527 | 0.007 | Yes |
|  | aL - e | 0.006168806 | 0.048 | Yes |
|  | aL – Contig. | 0.002949283 | 0.043 | Yes |
|  | e – Contig. | 0.006222227 | 0.005 | **No** |
| Arg | b - a | 0.001085224 | 0.066 | Yes |
|  | b - aL | 0.003378922 | 0.113 | Yes |
|  | b - Contig. | 0.002167941 | 0.071 | Yes |
|  | a - aL | 0.003488757 | 0.047 | Yes |
|  | a - Contig. | 0.002335441 | 0.005 | Yes |
|  | aL – Contig. | 0.003961525 | 0.042 | Yes |
| His+ | b - a | 0.001162914 | 0.017 | Yes |
|  | b - aL | 0.001497396 | 0.072 | Yes |
|  | b - Contig. | 0.00156755 | 0.041 | Yes |
|  | a - aL | 0.001705415 | 0.055 | Yes |
|  | a - Contig. | 0.001767331 | 0.024 | Yes |
|  | aL – Contig. | 0.002003319 | 0.031 | Yes |
| Lys | b - a | 0.001005969 | 0.071 | Yes |
|  | b - aL | 0.002952453 | 0.13 | Yes |
|  | b - Contig. | 0.00201047 | 0.079 | Yes |
|  | a - aL | 0.003053282 | 0.059 | Yes |
|  | a - Contig. | 0.002155815 | 0.008 | Yes |
|  | aL – Contig. | 0.003514619 | 0.051 | Yes |
| Asp | b - a | 0.001021235 | 0.089 | Yes |
|  | b - aL | 0.002688775 | 0.138 | Yes |
|  | b - e | 0.004677139 | 0.11 | Yes |
|  | b - Contig. | 0.002189037 | 0.081 | Yes |
|  | a - aL | 0.002808743 | 0.049 | Yes |
|  | a - e | 0.004747121 | 0.021 | Yes |
|  | a - Contig. | 0.002334826 | 0.008 | Yes |
|  | aL - e | 0.005359267 | 0.028 | Yes |
|  | aL – Contig. | 0.003411451 | 0.057 | Yes |
|  | e – Contig. | 0.005126804 | 0.029 | Yes |
| Glu | b - a | 0.001066592 | 0.086 | Yes |
|  | b - aL | 0.003653569 | 0.154 | Yes |
|  | b - Contig. | 0.002317664 | 0.09 | Yes |
|  | a - aL | 0.003758952 | 0.068 | Yes |
|  | a - Contig. | 0.002480468 | 0.004 | Yes |
|  | aL – Contig. | 0.004285285 | 0.064 | Yes |
| Cys- | b - a | 0.000797736 | 0.102 | Yes |
|  | b - Contig. | 0.0031464 | 0.062 | Yes |
|  | a - Contig. | 0.003203372 | 0.04 | Yes |
| Tyr- | b - a | 0.001222602 | 0.065 | Yes |
|  | b - aL | 0.002881165 | 0.139 | Yes |
|  | b - Contig. | 0.002111575 | 0.069 | Yes |
|  | a - aL | 0.00306702 | 0.074 | Yes |
|  | a - Contig. | 0.002358866 | 0.004 | Yes |
|  | aL – Contig. | 0.003517187 | 0.07 | Yes |
| Cys-Cys | b - a | 0.00108985 | 0.095 | Yes |
|  | b - aL | 0.001963734 | 0.053 | Yes |
|  | b - Contig. | 0.001952613 | 0.06 | Yes |
|  | a - aL | 0.002145397 | 0.042 | Yes |
|  | a - Contig. | 0.002135222 | 0.035 | Yes |
|  | aL – Contig. | 0.002688429 | 0.007 | Yes |
| Pro:cis | b - a | 0.00062579 | 0.104 | Yes |
|  | b - Contig. | 0.00421518 | 0.058 | Yes |
|  | a - Contig. | 0.00424193 | 0.046 | Yes |
| Pro:trans | b - a | 0.001351201 | 0.137 | Yes |
|  | b - Contig. | 0.001138559 | 0.088 | Yes |
|  | a - Contig. | 0.001731027 | 0.049 | Yes |

**Table S40.** Scheffe’s pairwise comparison of the solvent accessible surface area (SASA) for the side chain Xaa residue of Ac-Ala-Xaa-Ala-NH2 as a function of b, a, aL, e, and contiguous regions of f,y dihedral space assigned by density clustering and demonstrated in Figure S2.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Ac-Ala-Xaa-Ala-NH2 | Pairwise Interaction | Calculated Value | Critical Value | Statistically Significant |
| Ala | b - a | 0.000791832 | 0.04 | Yes |
|  | b - aL | 0.002937557 | 0.027 | Yes |
|  | b - e | 0.00284451 | 0.081 | Yes |
|  | b - Contig. | 0.001520141 | 0.027 | Yes |
|  | a - aL | 0.003003871 | 0.067 | Yes |
|  | a - e | 0.002912943 | 0.121 | Yes |
|  | a - Contig. | 0.001644637 | 0.067 | Yes |
|  | aL - e | 0.004060478 | 0.054 | Yes |
|  | aL – Contig. | 0.003272167 | 0 | **No** |
|  | e – Contig. | 0.003188898 | 0.054 | Yes |
| Val | b - a | 0.001903644 | 0.074 | Yes |
|  | b - aL | 0.004652487 | 0.062 | Yes |
|  | b - Contig. | 0.003717885 | 0.002 | **No** |
|  | a - aL | 0.004978567 | 0.136 | Yes |
|  | a - Contig. | 0.004118636 | 0.072 | Yes |
|  | aL – Contig. | 0.005914807 | 0.064 | Yes |
| Leu | b - a | 0.001303287 | 0.053 | Yes |
|  | b - aL | 0.004375424 | 0.009 | Yes |
|  | b - Contig. | 0.002878736 | 0.03 | Yes |
|  | a - aL | 0.00448222 | 0.062 | Yes |
|  | a - Contig. | 0.003038599 | 0.083 | Yes |
|  | aL – Contig. | 0.005165158 | 0.021 | Yes |
| Ile | b - a | 0.001839968 | 0.091 | Yes |
|  | b - aL | 0.005390784 | 0.057 | Yes |
|  | b - Contig. | 0.00414951 | 0.013 | Yes |
|  | a - aL | 0.005642349 | 0.148 | Yes |
|  | a - Contig. | 0.004471463 | 0.078 | Yes |
|  | aL – Contig. | 0.006757888 | 0.07 | Yes |
| Met | b - a | 0.001823279 | 0.056 | Yes |
|  | b - aL | 0.004534184 | 0.016 | Yes |
|  | b - Contig. | 0.003526669 | 0.027 | Yes |
|  | a - aL | 0.004739391 | 0.04 | Yes |
|  | a - Contig. | 0.003786872 | 0.083 | Yes |
|  | aL – Contig. | 0.005619153 | 0.043 | Yes |
| His:ND1 | b - a | 0.001736585 | 0.073 | Yes |
|  | b - aL | 0.00262039 | 0.015 | Yes |
|  | b - e | 0.011061674 | 0.051 | Yes |
|  | b - Contig. | 0.003106359 | 0.022 | Yes |
|  | a - aL | 0.002948465 | 0.058 | Yes |
|  | a - e | 0.01114395 | 0.124 | Yes |
|  | a - Contig. | 0.003387693 | 0.095 | Yes |
|  | aL - e | 0.011315403 | 0.066 | Yes |
|  | aL – Contig. | 0.003914995 | 0.037 | Yes |
|  | e – Contig. | 0.011437717 | 0.029 | Yes |
| His:NE2 | b - a | 0.001870769 | 0.049 | Yes |
|  | b - aL | 0.002046495 | 0.014 | Yes |
|  | b - e | 0.003664757 | 0.053 | Yes |
|  | b - Contig. | 0.003702862 | 0.017 | Yes |
|  | a - aL | 0.002526315 | 0.035 | Yes |
|  | a - e | 0.003952793 | 0.102 | Yes |
|  | a - Contig. | 0.003988147 | 0.066 | Yes |
|  | aL - e | 0.004038928 | 0.067 | Yes |
|  | aL – Contig. | 0.004073534 | 0.031 | Yes |
|  | e – Contig. | 0.005082911 | 0.036 | Yes |
| Phe | b - a | 0.002099685 | 0.077 | Yes |
|  | b - aL | 0.004171805 | 0.027 | Yes |
|  | b - e | 0.006775832 | 0.041 | Yes |
|  | b - Contig. | 0.003353148 | 0.014 | Yes |
|  | a - aL | 0.004557222 | 0.05 | Yes |
|  | a - e | 0.007019702 | 0.118 | Yes |
|  | a - Contig. | 0.00382203 | 0.091 | Yes |
|  | aL - e | 0.007891229 | 0.068 | Yes |
|  | aL – Contig. | 0.005253874 | 0.041 | Yes |
|  | e – Contig. | 0.007490737 | 0.027 | Yes |
| Tyr | b - a | 0.001868058 | 0.088 | Yes |
|  | b - aL | 0.00411138 | 0.032 | Yes |
|  | b - e | 0.008018848 | 0.035 | Yes |
|  | b - Contig. | 0.003413755 | 0.004 | Yes |
|  | a - aL | 0.004394354 | 0.056 | Yes |
|  | a - e | 0.008167547 | 0.123 | Yes |
|  | a - Contig. | 0.00374975 | 0.092 | Yes |
|  | aL - e | 0.008951124 | 0.067 | Yes |
|  | aL – Contig. | 0.005241606 | 0.036 | Yes |
|  | e – Contig. | 0.008652913 | 0.031 | Yes |
| Trp | b - a | 0.001940511 | 0.131 | Yes |
|  | b - aL | 0.008387895 | 0.038 | Yes |
|  | b - Contig. | 0.003582465 | 0.024 | Yes |
|  | a - aL | 0.008554775 | 0.169 | Yes |
|  | a - Contig. | 0.003957453 | 0.107 | Yes |
|  | aL – Contig. | 0.009069324 | 0.062 | Yes |
| Ser | b - a | 0.001086287 | 0.055 | Yes |
|  | b - aL | 0.002142357 | 0.006 | Yes |
|  | b - e | 0.00261489 | 0.053 | Yes |
|  | b - Contig. | 0.001682699 | 0.025 | Yes |
|  | a - aL | 0.002322725 | 0.061 | Yes |
|  | a - e | 0.002764599 | 0.108 | Yes |
|  | a - Contig. | 0.001907049 | 0.08 | Yes |
|  | aL - e | 0.003324557 | 0.047 | Yes |
|  | aL – Contig. | 0.002654526 | 0.019 | Yes |
|  | e – Contig. | 0.003048682 | 0.028 | Yes |
| Thr | b - a | 0.001542484 | 0.072 | Yes |
|  | b - aL | 0.005001884 | 0.057 | Yes |
|  | b - Contig. | 0.002963928 | 0.022 | Yes |
|  | a - aL | 0.005177292 | 0.129 | Yes |
|  | a - Contig. | 0.003251212 | 0.094 | Yes |
|  | aL – Contig. | 0.005762809 | 0.035 | Yes |
| Cys | b - a | 0.001274571 | 0.053 | Yes |
|  | b - aL | 0.002113813 | 0.02 | Yes |
|  | b - Contig. | 0.002219167 | 0.035 | Yes |
|  | a - aL | 0.002368566 | 0.073 | Yes |
|  | a - Contig. | 0.002463048 | 0.088 | Yes |
|  | aL – Contig. | 0.002985009 | 0.015 | Yes |
| Asn | b - a | 0.001216299 | 0.039 | Yes |
|  | b - aL | 0.001656339 | 0.017 | Yes |
|  | b - e | 0.00315096 | 0.07 | Yes |
|  | b - Contig. | 0.002912249 | 0.023 | Yes |
|  | a - aL | 0.0018631 | 0.056 | Yes |
|  | a - e | 0.003264389 | 0.109 | Yes |
|  | a - Contig. | 0.003034614 | 0.062 | Yes |
|  | aL - e | 0.00345258 | 0.053 | Yes |
|  | aL – Contig. | 0.003236194 | 0.006 | Yes |
|  | e – Contig. | 0.004202148 | 0.047 | Yes |
| Gln | b - a | 0.001535768 | 0.043 | Yes |
|  | b - aL | 0.003556161 | 0.016 | Yes |
|  | b - Contig. | 0.003272019 | 0.027 | Yes |
|  | a - aL | 0.003719579 | 0.027 | Yes |
|  | a - Contig. | 0.003448925 | 0.07 | Yes |
|  | aL – Contig. | 0.004709861 | 0.043 | Yes |
| Arg:NE | b - a | 0.002295596 | 0.055 | Yes |
|  | b - aL | 0.004849579 | 0.022 | Yes |
|  | b - Contig. | 0.004120484 | 0.026 | Yes |
|  | a - aL | 0.005205339 | 0.033 | Yes |
|  | a - Contig. | 0.004533819 | 0.081 | Yes |
|  | aL – Contig. | 0.0062293 | 0.048 | Yes |
| Arg:NH | b - a | 0.001999595 | 0.047 | Yes |
|  | b - aL | 0.005132672 | 0.014 | Yes |
|  | b - Contig. | 0.00408954 | 0.029 | Yes |
|  | a - aL | 0.005354938 | 0.033 | Yes |
|  | a - Contig. | 0.004365247 | 0.076 | Yes |
|  | aL – Contig. | 0.006434386 | 0.043 | Yes |
| Asp:H | b - a | 0.001191092 | 0.034 | Yes |
|  | b - aL | 0.001862721 | 0.02 | Yes |
|  | b - e | 0.003914455 | 0.081 | Yes |
|  | b - Contig. | 0.002833327 | 0.025 | Yes |
|  | a - aL | 0.002024571 | 0.054 | Yes |
|  | a - e | 0.00399401 | 0.115 | Yes |
|  | a - Contig. | 0.002942261 | 0.059 | Yes |
|  | aL - e | 0.004243011 | 0.061 | Yes |
|  | aL – Contig. | 0.003272298 | 0.005 | Yes |
|  | e – Contig. | 0.004749859 | 0.056 | Yes |
| Glu:H | b - a | 0.001340267 | 0.027 | Yes |
|  | b - aL | 0.003096731 | 0.027 | Yes |
|  | b - Contig. | 0.002862701 | 0.042 | Yes |
|  | a - aL | 0.003259387 | 0.054 | Yes |
|  | a - Contig. | 0.003037913 | 0.069 | Yes |
|  | aL – Contig. | 0.004125814 | 0.015 | Yes |
| LysN | b - a | 0.001979318 | 0.038 | Yes |
|  | b - aL | 0.003512055 | 0 | **No** |
|  | b - e | 0.009940873 | 0.061 | Yes |
|  | b - Contig. | 0.003773817 | 0.035 | Yes |
|  | a - aL | 0.003838903 | 0.038 | Yes |
|  | a - e | 0.010060994 | 0.099 | Yes |
|  | a - Contig. | 0.004079748 | 0.073 | Yes |
|  | aL - e | 0.010470932 | 0.061 | Yes |
|  | aL – Contig. | 0.005006113 | 0.035 | Yes |
|  | e – Contig. | 0.010561609 | 0.026 | Yes |
| Arg | b - a | 0.002291963 | 0.051 | Yes |
|  | b - aL | 0.00713619 | 0 | **No** |
|  | b - Contig. | 0.004578633 | 0.032 | Yes |
|  | a - aL | 0.007368159 | 0.051 | Yes |
|  | a - Contig. | 0.004932387 | 0.083 | Yes |
|  | aL – Contig. | 0.008366633 | 0.032 | Yes |
| His+ | b - a | 0.001973867 | 0.066 | Yes |
|  | b - aL | 0.002541598 | 0.068 | Yes |
|  | b - Contig. | 0.002660675 | 0.015 | Yes |
|  | a - aL | 0.002894679 | 0.002 | **No** |
|  | a - Contig. | 0.002999772 | 0.081 | Yes |
|  | aL – Contig. | 0.003400324 | 0.083 | Yes |
| Lys | b - a | 0.001770198 | 0.047 | Yes |
|  | b - aL | 0.005195414 | 0.001 | **No** |
|  | b - Contig. | 0.003537812 | 0.035 | Yes |
|  | a - aL | 0.005372841 | 0.046 | Yes |
|  | a - Contig. | 0.003793575 | 0.082 | Yes |
|  | aL – Contig. | 0.006184653 | 0.036 | Yes |
| Asp | b - a | 0.001122258 | 0.03 | Yes |
|  | b - aL | 0.002954756 | 0.018 | Yes |
|  | b - e | 0.005139815 | 0.089 | Yes |
|  | b - Contig. | 0.002405583 | 0.034 | Yes |
|  | a - aL | 0.003086591 | 0.048 | Yes |
|  | a - e | 0.005216719 | 0.119 | Yes |
|  | a - Contig. | 0.002565793 | 0.064 | Yes |
|  | aL - e | 0.005889421 | 0.071 | Yes |
|  | aL – Contig. | 0.003748921 | 0.016 | Yes |
|  | e – Contig. | 0.005633962 | 0.055 | Yes |
| Glu | b - a | 0.001331344 | 0.032 | Yes |
|  | b - aL | 0.004560467 | 0.029 | Yes |
|  | b - Contig. | 0.00289296 | 0.035 | Yes |
|  | a - aL | 0.004692008 | 0.061 | Yes |
|  | a - Contig. | 0.003096175 | 0.067 | Yes |
|  | aL – Contig. | 0.005348989 | 0.006 | Yes |
| Cys- | b - a | 0.000915404 | 0.018 | Yes |
|  | b - Contig. | 0.003610503 | 0.032 | Yes |
|  | a - Contig. | 0.003675878 | 0.05 | Yes |
| Tyr- | b - a | 0.002133753 | 0.074 | Yes |
|  | b - aL | 0.005028367 | 0.037 | Yes |
|  | b - Contig. | 0.003685236 | 0.004 | Yes |
|  | a - aL | 0.005352731 | 0.037 | Yes |
|  | a - Contig. | 0.004116822 | 0.07 | Yes |
|  | aL – Contig. | 0.006138387 | 0.033 | Yes |
| Cys-Cys | b - a | 0.001739682 | 0.034 | Yes |
|  | b - aL | 0.003134628 | 0.03 | Yes |
|  | b - Contig. | 0.003116876 | 0.034 | Yes |
|  | a - aL | 0.003424608 | 0.064 | Yes |
|  | a - Contig. | 0.003408367 | 0 | **No** |
|  | aL – Contig. | 0.004291429 | 0.064 | Yes |
| Pro:cis | b - a | 0.00056256 | 0.032 | Yes |
|  | b - Contig. | 0.003789278 | 0.037 | Yes |
|  | a - Contig. | 0.003813325 | 0.005 | Yes |
| Pro:trans | b - a | 0.001384589 | 0.012 | Yes |
|  | b - Contig. | 0.001166693 | 0.007 | Yes |
|  | a - Contig. | 0.0017738 | 0.005 | Yes |