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## **Supporting Material**

## Driving Forces for Transmembrane *a*-helix Oligomerization

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|   | ALA   | ARG  | ASN  | ASP  | CYS   |
|---|---|--|--|--|---|
| ALA   | 95.7  | 9  | 27.5   | 18.3   | 17.5  |
| ARG   | 9   | 1.5  | 1  | 3.7  | 1   |
| ASN   | 27.5  | 1  | 5  | 5.5  | 4   |
| ASP   | 18.3  | 3.7  | 5.5  | 0  | 0   |
| CYS   | 17.5  | 1  | 4  | 0  | 0   |
| GLU   | 14.5  | 3  | 6.5  | 2.5  | 2   |
| GLN   | 16  | 3  | 3  | 1  | 6   |
| GLY   | 201.7   | 6.7  | 17   | 12   | 15.3  |
| HIS   | 10  | 2  | 1  | 3  | 1   |
| ILE   | 131.3   | 5  | 23.2   | 13.5   | 17.2  |
| LEU   | 233   | 14.5   | 15.5   | 10.5   | 18.8  |
| LYS   | 3   | 0  | 3  | 1  | 0   |
| MET   | 55.2  | 8  | 1.5  | 4.5  | 11  |
| PHE   | 95.7  | 8.3  | 14   | 8  | 9.5   |
| PRO   | 32.2  | 3  | 10   | 6  | 4   |
| SER   | 83.2  | 3  | 15   | 9  | 8   |
| THR   | 100.8   | 7  | 15   | 12   | 6.2   |
| TRP   | 36.7  | 1  | 5  | 3  | 4   |
| TYR   | 41  | 8.3  | 6.5  | 2  | 4   |
| VAL   | 175.1   | 7  | 13.7   | 10   | 15.3  |
| LIP   | 1000.8  | 28.2   | 108  | 52.7   | 110.2   |
| SURFACE   | 803.3   | 281.3  | 203.5  | 109.2  | 73.5  |
|   |   |  |  |  |   |
|   |   | <u></u>  | <u> </u>   |  |   |
| A.L. A.   | GLU   | GLN  | GLY  | HIS  | ILE   |
| ALA   | GLU<br>14.5   | GLN<br>16  | GLY 201.7  | HIS<br>10  | ILE<br>131.3  |
| ALA<br>ARG  | GLU<br>14.5<br>3  | GLN 16<br>3  | GLY 201.7<br>6.7   | HIS 10<br>2  | ILE<br>131.3<br>5   |
| ALA<br>ARG<br>ASN   | GLU<br>14.5<br>3<br>6.5   | GLN<br>16<br>3<br>3  | GLY<br>201.7<br>6.7<br>17  | HIS<br>10<br>2<br>1  | ILE<br>131.3<br>5<br>23.2   |
| ALA<br>ARG<br>ASN<br>ASP  | GLU<br>14.5<br>3<br>6.5<br>2.5  | GLN 16<br>3<br>3<br>1  | GLY<br>201.7<br>6.7<br>17<br>12  | HIS<br>10<br>2<br>1<br>3   | ILE<br>131.3<br>5<br>23.2<br>13.5   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2   | GLN<br>16<br>3<br>3<br>1<br>6  | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11  | HIS<br>10<br>2<br>1<br>3<br>1  | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU  | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1  | GLN<br>16<br>3<br>3<br>1<br>6<br>2   | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22 5  | HIS<br>10<br>2<br>1<br>3<br>1<br>1   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>2<br>1  | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>2  | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>96  | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>2<br>1<br>2<br>11   | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1  | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11 3  | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>11.3<br>2  | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>IJ F   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>2<br>1<br>1<br>2<br>11<br>2<br>11   | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7   | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>11.3<br>2<br>8  | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>ILE   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17 7   | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7   | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7  | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>11.3<br>2<br>8<br>4   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103 7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3  | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7<br>11   | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4 5   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>11.3<br>2<br>8<br>4   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5 4  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MFT  | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3   | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5 5   | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>11.3<br>2<br>8<br>4<br>1<br>3   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHF  | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>2<br>1<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6  | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7  | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>11.3<br>2<br>8<br>4<br>1<br>3<br>8   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO   | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3 5                                   | GLN<br>16<br>3<br>1<br>6<br>2<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3                                       | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>2<br>8<br>4<br>1<br>3<br>8<br>0   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER                                    | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3.5<br>6<br>3                              | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5                                    | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>3<br>2<br>8<br>4<br>1<br>3<br>8<br>0<br>3   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64 5  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR                             | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3.5<br>6.3<br>9                       | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5<br>4                               | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96<br>61.7                                 | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>3<br>2<br>8<br>4<br>1<br>3<br>8<br>0<br>3<br>6<br>5   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64.5<br>68 2                                    |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP                      | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3.5<br>6.3<br>9<br>2                  | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5<br>4<br>2                          | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96<br>61.7<br>31                           | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>3<br>2<br>8<br>4<br>1<br>3<br>8<br>4<br>1<br>3<br>8<br>0<br>3<br>6.5<br>1.5                   | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64.5<br>68.2<br>14 5                            |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR               | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3.5<br>6.3<br>9<br>2<br>3             | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5<br>4<br>2<br>4<br>2<br>4<br>2<br>4 | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96<br>61.7<br>31<br>29 7                   | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>1<br>2<br>8<br>4<br>1<br>1<br>3<br>8<br>4<br>1<br>3<br>8<br>0<br>3<br>6.5<br>1.5<br>4         | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64.5<br>68.2<br>14.5<br>14.7                    |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL        | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>1<br>2<br>11<br>1<br>1<br>3<br>17.7<br>3<br>3<br>6<br>3.5<br>6.3<br>9<br>2<br>3<br>10.5     | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5<br>4<br>2<br>4<br>2<br>4<br>10     | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96<br>61.7<br>31<br>29.7<br>137.4          | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>2<br>8<br>4<br>1<br>1<br>1.3<br>2<br>8<br>4<br>1<br>3<br>8<br>0<br>3<br>6.5<br>1.5<br>4<br>8  | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64.5<br>68.2<br>14.5<br>14.7<br>109.2           |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL<br>LIP | GLU<br>14.5<br>3<br>6.5<br>2.5<br>2<br>1<br>2<br>11<br>1<br>1<br>13<br>17.7<br>3<br>3<br>6<br>3.5<br>6.3<br>9<br>2<br>3<br>10.5<br>52.7 | GLN<br>16<br>3<br>1<br>6<br>2<br>22.5<br>1<br>7<br>11<br>0<br>5.5<br>7<br>3<br>12.5<br>4<br>2<br>4<br>10<br>83.8       | GLY<br>201.7<br>6.7<br>17<br>12<br>15.3<br>11<br>22.5<br>86<br>11.3<br>106.8<br>154.7<br>4.5<br>31.2<br>90.8<br>48<br>96<br>61.7<br>31<br>29.7<br>137.4<br>691.6 | HIS<br>10<br>2<br>1<br>3<br>1<br>1<br>1<br>1<br>1<br>3<br>2<br>8<br>4<br>1<br>3<br>8<br>4<br>1<br>3<br>8<br>0<br>3<br>6.5<br>1.5<br>4<br>8<br>50.5 | ILE<br>131.3<br>5<br>23.2<br>13.5<br>17.2<br>13<br>7<br>106.8<br>8<br>64.7<br>103.7<br>5.4<br>27.7<br>70.4<br>23.2<br>64.5<br>68.2<br>14.5<br>14.7<br>109.2<br>1148.7 |

|   | LEU  | LYS  | MET  | PHE  | PRO  |
|---|--|--|--|--|--|
| ALA   | 233  | 3  | 55.2   | 95.7   | 32.2   |
| ARG   | 14.5   | 0  | 8  | 8.3  | 3  |
| ASN   | 15.5   | 3  | 1.5  | 14   | 10   |
| ASP   | 10.5   | 1  | 4.5  | 8  | 6  |
| CYS   | 18.8   | 0  | 11   | 9.5  | 4  |
| GLU   | 17 7   | 3  |  | 6  | 3.5  |
| GLN   | 11   | 0  | 55   | 7  | 3  |
| GLY   | 154 7  | 4 5  | 31.2   | ,<br>90 8  | 48   |
| HIS   | 4  | 1.0  | 3  | 8  | 0  |
| IIF   | 103 7  | 5 4  | 5<br>7 7   | 70.4   | 23.2   |
|   | 114 5  | 6.2  | 54.3   | 114 5  | 23.2   |
|   | 6.2  | 0.2  | 1 F  | 114.5  | 20   |
| MET   | 5/ 3   | 15   | 1.J<br>8 5   | 35   | J.7<br>7 5   |
|   | 111 E  | 1.5  | 25   | 30   | 1.5  |
|   | 114.0  | ן<br>ד כ   | 30<br>7 E  | 20   | 10.2   |
| PRU   | 28   | 3.7<br>2 E   | 7.5  | 10.2   | 4.3  |
| SER   | 00 F   | 3.5  | 21.3   | 38   | 15.5   |
|   | 80.5   | 2  | 28.5   | 43.2   | 20.3   |
|   | 33.7   | 0  | 8  | 11.5   | 9  |
| IYR   | 35.7   | 1  | 15.7   | 14   | 10   |
| VAL   | 153.9  | 8.7  | 41.2   | 46.8   | 25.6   |
| LIP   | 1936.8   | 51.5   | 325.6  | 847.5  | 182.8  |
| SURFACE   | 1340.4   | 181.8  | 330  | 732  | 251.4  |
|   |  |  |  |  |  |
|   | SER  | тнр  | TRP  | TVR  | νΔι  |
| ΔΙΔ   | SER  | THR<br>100.8   | TRP  | TYR  | VAL 175 1  |
| ALA   | SER<br>83.2  | THR<br>100.8<br>7  | TRP<br>36.7  | TYR 41   | VAL<br>175.1<br>7  |
| ALA<br>ARG<br>ASN   | SER<br>83.2<br>3   | THR<br>100.8<br>7<br>15  | TRP<br>36.7<br>1   | TYR<br>41<br>8.3<br>6.5  | VAL<br>175.1<br>7<br>13.7  |
| ALA<br>ARG<br>ASN<br>ASP  | SER<br>83.2<br>3<br>15   | THR<br>100.8<br>7<br>15<br>12  | TRP<br>36.7<br>1<br>5  | TYR<br>41<br>8.3<br>6.5<br>2   | VAL<br>175.1<br>7<br>13.7<br>10  |
| ALA<br>ARG<br>ASN<br>ASP  | SER<br>83.2<br>3<br>15<br>9  | THR<br>100.8<br>7<br>15<br>12<br>6 2   | TRP<br>36.7<br>1<br>5<br>3   | TYR<br>41<br>8.3<br>6.5<br>2   | VAL<br>175.1<br>7<br>13.7<br>10  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS   | SER<br>83.2<br>3<br>15<br>9<br>8<br>6 2  | THR<br>100.8<br>7<br>15<br>12<br>6.2   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2   | TYR<br>41<br>8.3<br>6.5<br>2<br>4  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU  | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9  | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2   | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3   | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN   | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>20.7  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY  | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS   | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3   | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5  | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5   | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4   | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE  | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5   | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2  | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>2<br>31<br>1.5<br>14.5  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7   | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU   | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59   | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5  | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7   | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS  | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0   | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET   | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8   | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE  | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO                                    | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3   | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER                             | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2                                     | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10                                  | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19                                      | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8                                     |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR                             | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5<br>18.5<br>40.2                        | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2<br>9.5                              | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10<br>14                       | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19<br>17.7                              | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8<br>67                               |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP                      | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5<br>18.5<br>40.2<br>10                  | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2<br>9.5<br>14                        | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10<br>14<br>2                       | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19<br>17.7<br>7.3                       | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8<br>67                               |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR               | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5<br>40.2<br>10<br>19 | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2<br>9.5<br>14<br>17.7                | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10<br>14<br>2<br>7.3                | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19<br>17.7<br>7.3<br>5                  | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8<br>67<br>17<br>35.2                 |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL        | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5<br>40.2<br>10<br>19<br>67.8            | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2<br>9.5<br>14<br>17.7<br>67          | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10<br>14<br>2<br>7.3<br>17          | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19<br>17.7<br>7.3<br>5<br>35.2          | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8<br>67<br>17<br>35.2<br>57           |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL<br>LIP | SER<br>83.2<br>3<br>15<br>9<br>8<br>6.3<br>12.5<br>96<br>3<br>64.5<br>59<br>3.5<br>21.3<br>38<br>15.5<br>18.5<br>40.2<br>10<br>19<br>67.8<br>318     | THR<br>100.8<br>7<br>15<br>12<br>6.2<br>9<br>4<br>61.7<br>6.5<br>68.2<br>80.5<br>2<br>28.5<br>43.2<br>20.3<br>40.2<br>9.5<br>14<br>17.7<br>67<br>449.6 | TRP<br>36.7<br>1<br>5<br>3<br>4<br>2<br>2<br>31<br>1.5<br>14.5<br>33.7<br>0<br>8<br>11.5<br>9<br>10<br>14<br>2<br>7.3<br>17<br>273.2 | TYR<br>41<br>8.3<br>6.5<br>2<br>4<br>3<br>4<br>29.7<br>4<br>14.7<br>35.7<br>1<br>15.7<br>14<br>10<br>19<br>17.7<br>7.3<br>5<br>35.2<br>249.2 | VAL<br>175.1<br>7<br>13.7<br>10<br>15.3<br>10.5<br>10<br>137.4<br>8<br>109.2<br>153.9<br>8.7<br>41.2<br>46.8<br>25.6<br>67.8<br>67<br>17<br>35.2<br>57<br>1094.2 |

Table S1: The native contact distribution for the 20 amino acids, lipid, and surface contacts.

|   | ALA   | ARG   | ASN   | ASP  | CYS   |
|---|---|---|---|--|---|
| ALA   | 92.6  | 10.2  | 26.2  | 12.4   | 14.2  |
| ARG   | 10.2  | 1.5   | 1.9   | 1.4  | 0.8   |
| ASN   | 26.2  | 1.9   | 3.7   | 2.8  | 2.6   |
| ASP   | 12.4  | 1.4   | 2.8   | 0.1  | 1.9   |
| CYS   | 14.2  | 0.8   | 2.6   | 1.9  | 0.7   |
| GLU   | 11.1  | 1.7   | 2.5   | 1.4  | 1.3   |
| GLN   | 16.3  | 1   | 3.6   | 0.9  | 2   |
| GLY   | 158.3   | 11.3  | 20  | 9.6  | 15  |
| HIS   | 10.2  | 1.1   | 0.8   | 0.5  | 0.8   |
| ILE   | 136.9   | 8.1   | 21.6  | 9.7  | 14  |
| LEU   | 239.2   | 16.2  | 27.8  | 15.5   | 15.4  |
| LYS   | 6.5   | 1.4   | 1.9   | 0.8  | 0.5   |
| MET   | 48.2  | 3.2   | 6   | 4.5  | 5   |
| PHE   | 99.9  | 6.6   | 13.7  | 8  | 9.4   |
| PRO   | 38.3  | 2.5   | 4.9   | 2.8  | 4.2   |
| SER   | 68  | 3.5   | 11.3  | 5.7  | 8.3   |
| THR   | 76.3  | 4.9   | 10.8  | 8  | 6.1   |
| TRP   | 36.6  | 2.6   | 4   | 2.1  | 3.1   |
| TYR   | 40.9  | 4.9   | 4.8   | 3.6  | 2.8   |
| VAL   | 150.7   | 8.2   | 19.7  | 11.4   | 14.9  |
| LIP   | 1078.7  | 47.4  | 121.2   | 82.2   | 127.7   |
| SURFACE   | 846.5   | 263.9   | 202   | 100  | 79.3  |
|   |   |   |   |  |   |
|   | 0111  |   |   | 1110   |   |
|   | GLU   | GLN   | GLY   | HIS 10.2   | ILE   |
| ALA   | GLU<br>11.1   | GLN<br>16.3   | GLY<br>158.3  | HIS<br>10.2  | ILE<br>136.9  |
| ALA<br>ARG  | GLU<br>11.1<br>1.7  | GLN 16.3  | GLY<br>158.3<br>11.3  | HIS<br>10.2<br>1.1   | ILE<br>136.9<br>8.1   |
| ALA<br>ARG<br>ASN   | GLU<br>11.1<br>1.7<br>2.5   | GLN<br>16.3<br>1<br>3.6   | GLY<br>158.3<br>11.3<br>20  | HIS<br>10.2<br>1.1<br>0.8  | ILE<br>136.9<br>8.1<br>21.6   |
| ALA<br>ARG<br>ASN<br>ASP  | GLU<br>11.1<br>1.7<br>2.5<br>1.4  | GLN<br>16.3<br>1<br>3.6<br>0.9  | GLY<br>158.3<br>11.3<br>20<br>9.6   | HIS<br>10.2<br>1.1<br>0.8<br>0.5   | ILE<br>136.9<br>8.1<br>21.6<br>9.7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3   | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU  | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.8  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4   | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>1.4  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>60 5   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY  | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9   | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>1.4<br>12.4  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2<br>9   | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9  | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2<br>9<br>0.6<br>5 5   | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>644 2   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE  | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.2  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2<br>9<br>0.6<br>5.5   | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>145.2   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU  | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7   | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199  | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>2.7  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2  | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>42.6   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41 9  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6 5   | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>228  | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41.8<br>880   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE  | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>2.0   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>20.0   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5   | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>21.0   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLV<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO   | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.2   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>41.2   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8  | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER                                    | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>4.2   | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2   | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>2.5   | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>50.7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR                             | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2  | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>6.8<br>2.4                           | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2<br>66<br>24.0                                 | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>3.5<br>2.4                                    | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>59.7<br>20.1  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP                      | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2<br>2.6                                 | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>6.8<br>2.6<br>4.2                    | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2<br>66<br>26.9<br>31.2                         | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>3.5<br>2.6<br>2.2                             | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>59.7<br>29.1                                     |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR               | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2<br>2.6<br>3.5                          | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>6.8<br>2.6<br>4.2<br>10.2            | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2<br>66<br>26.9<br>31.2<br>125                  | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>3.5<br>2.6<br>2.9<br>7.2                      | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>59.7<br>29.1<br>32.4<br>122.4                                     |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL        | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2<br>2.6<br>3.5<br>10.2<br>70.2          | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>6.8<br>2.6<br>4.2<br>10.8<br>10.0           | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2<br>66<br>26.9<br>31.2<br>125<br>774.2         | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>3.5<br>2.6<br>2.9<br>7.8<br>4.5               | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>59.7<br>29.1<br>32.4<br>122.6<br>1028.2                           |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL<br>LIP | GLU<br>11.1<br>1.7<br>2.5<br>1.4<br>1.3<br>0.5<br>1.4<br>10.9<br>0.8<br>11.1<br>14.9<br>1.7<br>3.7<br>6.5<br>2.6<br>4.9<br>5.2<br>2.6<br>3.5<br>10.2<br>79.3<br>111 5 | GLN<br>16.3<br>1<br>3.6<br>0.9<br>2<br>1.4<br>12.4<br>0.2<br>11.8<br>18.3<br>0.7<br>5.2<br>7.9<br>3.9<br>8.3<br>6.8<br>2.6<br>4.2<br>10.8<br>100.1<br>146.1 | GLY<br>158.3<br>11.3<br>20<br>9.6<br>15<br>10.9<br>12.4<br>69.5<br>9<br>110.7<br>199<br>5.5<br>43.6<br>82.8<br>30.9<br>61.2<br>66<br>26.9<br>31.2<br>125<br>774.9<br>60.2 | HIS<br>10.2<br>1.1<br>0.8<br>0.5<br>0.8<br>0.2<br>9<br>0.6<br>5.5<br>8.4<br>0.4<br>1.6<br>4.5<br>1.5<br>2.8<br>3.5<br>2.6<br>2.9<br>7.8<br>65.5<br>25 \u03e9 | ILE<br>136.9<br>8.1<br>21.6<br>9.7<br>14<br>11.1<br>11.8<br>110.7<br>5.5<br>64.3<br>165.3<br>64.3<br>165.3<br>6.8<br>41.8<br>88.9<br>31.8<br>58.6<br>59.7<br>29.1<br>32.4<br>122.6<br>1038.8<br>008.2 |

|   | LEU   | LYS   | MET  | PHE   | PRO  |
|---|---|---|--|---|--|
| ALA   | 239.2   | 6.5   | 48.2   | 99.9  | 38.3   |
| ARG   | 16.2  | 1.4   | 3.2  | 6.6   | 2.5  |
| ASN   | 27.8  | 1.9   | 6  | 13.7  | 4.9  |
| ASP   | 15.5  | 0.8   | 4.5  | 8   | 2.8  |
| CYS   | 15.4  | 0.5   | 5  | 9.4   | 4.2  |
| GLU   | 14.9  | 1.7   | 3.7  | 6.5   | 2.6  |
| GLN   | 18.3  | 0.7   | 5.2  | 7.9   | 3.9  |
| GLY   | 199   | 5.5   | 43.6   | 82.8  | 30.9   |
| HIS   | 8.4   | 0.4   | 1.6  | 4.5   | 1.5  |
| ILE   | 165.3   | 6.8   | 41.8   | 88.9  | 31.8   |
| LEU   | 160.7   | 11.5  | 62.6   | 123.8   | 42.9   |
| LYS   | 11.5  | 0.4   | 2.4  | 5.4   | 2.1  |
| MET   | 62.6  | 2.4   | 7.8  | 31.4  | 9  |
| PHE   | 123.8   | 5.4   | 31.4   | 29.8  | 18.7   |
| PRO   | 42.9  | 2.1   | 9  | 18.7  | 3.3  |
| SER   | 75.2  | 3   | 19.6   | 43.6  | 15.6   |
| THR   | 89.5  | 4.6   | 23.3   | 44  | 18.1   |
| TRP   | 48  | 1.4   | 12.5   | 22  | 10.3   |
| TYR   | 49.6  | 2.4   | 10.7   | 22.7  | 8.6  |
| VAL   | 199.7   | 7   | 39.7   | 82.7  | 28.5   |
| LIP   | 1616.1  | 51.3  | 326.5  | 778.7   | 172.8  |
| SURFACE   | 1348.2  | 164.7   | 325.8  | 716.8   | 261.9  |
|   |   |   |  |   |  |
|   | SER   | THR   | TRP  | TYR   | VΔI  |
| ΔΙΔ   | SER   | THR<br>76-3   | TRP<br>36.6  | TYR<br>40.9   | VAL 150.7  |
| ALA   | SER<br>68<br>3 5  | THR<br>76.3<br>4 9  | TRP<br>36.6<br>2.6   | TYR<br>40.9<br>4 9  | VAL<br>150.7<br>8 2  |
| ALA<br>ARG<br>ASN   | SER<br>68<br>3.5<br>11.3  | THR<br>76.3<br>4.9<br>10.8  | TRP<br>36.6<br>2.6<br>4  | TYR<br>40.9<br>4.9<br>4.8   | VAL<br>150.7<br>8.2<br>19.7  |
| ALA<br>ARG<br>ASN<br>ASP  | SER<br>68<br>3.5<br>11.3<br>5.7   | THR<br>76.3<br>4.9<br>10.8<br>8   | TRP<br>36.6<br>2.6<br>4<br>2.1   | TYR<br>40.9<br>4.9<br>4.8<br>3.6  | VAL<br>150.7<br>8.2<br>19.7<br>11.4  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU  | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9   | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2   | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6   | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY  | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>2.6<br>26.9   | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8   | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5   | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>2.6<br>26.9<br>2.6  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE  | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6   | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7   | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1   | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2   | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5   | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48   | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7  |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS  | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4   | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>2.6<br>29.1<br>48<br>1.4<br>12.5  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE  | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7   | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO   | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER                                    | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9   |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR                             | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9<br>27.9                                  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9<br>15.7                                  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4<br>17.8                                | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1<br>18.2                                | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9<br>66.5                                 |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP                      | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9<br>27.9<br>15.4                          | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9<br>15.7<br>17.8                          | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4<br>17.8<br>5.5                         | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1<br>18.2<br>8.9                         | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9<br>66.5<br>31.6                         |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR               | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9<br>27.9<br>15.4<br>17.1                  | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9<br>15.7<br>17.8<br>18.2                  | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4<br>17.8<br>5.5<br>8.9                  | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1<br>18.2<br>8.9<br>7.9                  | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9<br>66.5<br>31.6<br>30.8                 |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL        | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9<br>27.9<br>15.4<br>17.1<br>61.9          | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9<br>15.7<br>17.8<br>18.2<br>66.5          | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4<br>17.8<br>5.5<br>8.9<br>31.6          | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1<br>18.2<br>8.9<br>7.9<br>30.8          | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9<br>66.5<br>31.6<br>30.8<br>64           |
| ALA<br>ARG<br>ASN<br>ASP<br>CYS<br>GLU<br>GLN<br>GLY<br>HIS<br>ILE<br>LEU<br>LYS<br>MET<br>PHE<br>PRO<br>SER<br>THR<br>TRP<br>TYR<br>VAL<br>LIP | SER<br>68<br>3.5<br>11.3<br>5.7<br>8.3<br>4.9<br>8.3<br>61.2<br>2.8<br>58.6<br>75.2<br>3<br>19.6<br>43.6<br>15.6<br>13.9<br>27.9<br>15.4<br>17.1<br>61.9<br>392.7 | THR<br>76.3<br>4.9<br>10.8<br>8<br>6.1<br>5.2<br>6.8<br>66<br>3.5<br>59.7<br>89.5<br>4.6<br>23.3<br>44<br>18.1<br>27.9<br>15.7<br>17.8<br>18.2<br>66.5<br>458.6 | TRP<br>36.6<br>2.6<br>4<br>2.1<br>3.1<br>2.6<br>2.6<br>26.9<br>2.6<br>29.1<br>48<br>1.4<br>12.5<br>22<br>10.3<br>15.4<br>17.8<br>5.5<br>8.9<br>31.6<br>254.9 | TYR<br>40.9<br>4.9<br>4.8<br>3.6<br>2.8<br>3.5<br>4.2<br>31.2<br>2.9<br>32.4<br>49.6<br>2.4<br>10.7<br>22.7<br>8.6<br>17.1<br>18.2<br>8.9<br>7.9<br>30.8<br>267.7 | VAL<br>150.7<br>8.2<br>19.7<br>11.4<br>14.9<br>10.2<br>10.8<br>125<br>7.8<br>122.6<br>199.7<br>7<br>39.7<br>82.7<br>28.5<br>61.9<br>66.5<br>31.6<br>30.8<br>64<br>1020.4 |

Table S2: The neutral contact distribution for the 20 amino acids, lipid, and surface contacts.



Figure S1. Register odds of the B/V/N/L breakdown, part 1. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S2. Register odds of the B/V/N/L breakdown, part 2. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S3. Register odds of the B/V/N/L breakdown, part 3. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S4. Register odds of the B/V/N/L breakdown, part 4. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S5. Register odds of the B/V/N/L breakdown, part 1. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S6. Register odds of the B/V/N/L breakdown, part 2. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S7. Register odds of the B/V/N/L breakdown, part 3. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S8. Register odds of the B/V/N/L breakdown, part 4. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S9. Register odds of the S/MS/ML/L breakdown, part 1. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S10. Register odds of the S/MS/ML/L breakdown, part 2. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S11. Register odds of the S/MS/ML/L breakdown, part 3. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S12. Register odds of the S/MS/ML/L breakdown, part 4. Ile/Val/Gly are included. Error bars show 95% confidence intervals.



Figure S13. Register odds of the S/MS/ML/L breakdown, part 1. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S14. Register odds of the S/MS/ML/L breakdown, part 2. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S15. Register odds of the S/MS/ML/L breakdown, part 3. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S16. Register odds of the S/MS/ML/L breakdown, part 4. Ile/Val/Gly are not included. Error bars show 95% confidence intervals.



Figure S17. Shown above is an example of two interacting helices, with potential contacts within 7.75 Angstroms shown. Alpha carbons are shown in licorice and allatoms are shown in lines. The contacts labeled 6.98 and 7.56 are discarded based on an angle criterion described in the main text. The contact labeled 6.98 has angles 112.4 and -19.5, while the contact labeled 7.56 has angles -19.5 and -86.5. An angle of 112.4 is outside the 100 degree per-angle cutoff, while -19.5 and -86.5 sum to be greater than 100 degrees. The illustration was created with VMD (Humphrey, W., Dalke, A. and

Schulten, K., "VMD - Visual Molecular Dynamics", *J. Molec. Graphics*, 1996, **14** 33-38). See inset for an example of the angle computation.

Inset:

Inset is an example of the angle computation (angle section shown in blue). The circles represent helices looking down the bilayer normal, with alpha-carbons on the circle. Residues R1 and R2 are contacts based on the angle cutoff (they have opposite signs) whereas R1/R3 would not be a contact (they have the same sign, and so add to be greater than 100 degrees).