| n | PDBid | N   | $F_{\text{max}}$ [e/Å] | $L_{\text{max}}$ [Å] | $\lambda$ | CATH | SCOP   |
|---|------|-----|-----------------|------------------|------|-------|-------|
| 82 | 2duk | 138 | 3.8             | 241.2            | 0.43 |       | b.60.1.1 |
| 83 | 1hep | 149 | 3.8             | 197.7            | 0.32 | 2.40.128.20 | b.60.1.1 |
| 84 | 1cuu | 197 | 3.8             | 421.4            | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 85 | 1afk | 124 | 3.8             | 175.4            | 0.33 | 3.10.130.10 | d.5.1.1  |
| 86 | 2o5w | 147 | 3.8             | 214.8            | 0.33 |       |       |
| 87 | 1xc | 197  | 3.8             | 422.9            | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 88 | 1qoz | 206 | 3.8             | 238.7            | 0.29 | 3.40.50.1820 | c.69.1.30 |
| 89 | 3pcf | 200 | 3.8             | 421.4            | 0.55 |       |       |
| 90 | 1odi | 234 | 3.8             | 458.8            | 0.51 | 3.40.50.1580 | c.56.2.1 |
| 91 | 1y2x | 142 | 3.8             | 38.1             | 0.01 | 2.60.270.20 | b.97.1.2 |
| 92 | 1mbq | 220 | 3.8             | 106.8            | 0.09 | 2.40.10.10 | b.47.1.2 |
| 93 | 1bj7 | 150 | 3.8             | 195.1            | 0.31 | 2.40.128.20 | b.60.1.1 |
| 94 | 1odl | 234 | 3.8             | 458.8            | 0.51 | 3.40.50.1580 | c.56.2.1 |
| 95 | 1cxu | 196 | 3.8             | 416.5            | 0.54 | 3.40.50.1820 | c.69.1.30 |
| 96 | 3pch | 200 | 3.8             | 252.3            | 0.31 | 2.60.130.10 | b.3.6.1  |
| 97 | 1oxm | 196 | 3.8             | 418.8            | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 98 | 1h2p | 125 | 3.8             | 129.7            | 0.14 | 2.10.70.10 | g.18.1.1 |
| 99 | 1gwy | 175 | 3.8             | 143.2            | 0.18 | 2.60.270.20 | b.97.1.1 |
| 100 | 1cud | 197 | 3.8             | 420.1            | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 101 | 1vvd | 118 | 3.8             | 112.1            | 0.14 | 2.10.70.10 | g.18.1.1 |
| 102 | 1hfh | 120 | 3.8             | 107.3            | 0.15 | 2.10.70.10 | g.18.1.1 |
| 103 | 1vwc | 118 | 3.8             | 112.9            | 0.14 | 2.10.70.10 | g.18.1.1 |
| 104 | 1cuv | 197 | 3.8             | 420.3            | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 105 | 1c77 | 130 | 3.8             | 109.5            | 0.18 | 3.10.20.130 | d.15.5.1 |
| 106 | 1xuk | 223 | 3.8             | 115.0            | 0.10 | 2.40.10.10 | b.47.1.2 |
| 107 | 1c2k | 223 | 3.8             | 114.4            | 0.10 | 2.40.10.10 | b.47.1.2 |
| 108 | 2stb | 222 | 3.8             | 113.1            | 0.09 | 2.40.10.10 | b.47.1.2 |
| 109 | 3tgj | 223 | 3.8             | 110.5            | 0.10 | 2.40.10.10 | b.47.1.2 |
| 110 | 3byr | 88  | 3.8             | 196.8            | 0.57 |       |       |
| 111 | 1a0j | 223 | 3.8             | 111.6            | 0.10 | 2.40.10.10 | b.47.1.2 |
| 112 | 2pcd | 200 | 3.7             | 251.3            | 0.31 | 2.60.130.10 | b.3.6.1  |
| 113 | 1vve | 118 | 3.7             | 104.3            | 0.11 | 2.10.70.10 | g.18.1.1 |
| 114 | 2pf6 | 231 | 3.7             | 488.0            | 0.51 |       |       |
| 115 | 3pcl | 200 | 3.7             | 252.5            | 0.31 | 2.60.130.10 | b.3.6.1  |
| 116 | 1afl | 124 | 3.7             | 175.3            | 0.33 | 3.10.130.10 | d.5.1.1  |
| 117 | 1bs9 | 207 | 3.7             | 241.4            | 0.29 | 3.40.50.1820 | c.69.1.30 |
| 118 | 1tpa | 223 | 3.7             | 113.4            | 0.10 | 2.40.10.10 | b.47.1.2 |
| 119 | 3rn3 | 124 | 3.7             | 168.5            | 0.31 | 3.10.130.10 | d.5.1.1  |
| 120 | 2grk | 228 | 3.7             | 135.6            | 0.12 | 2.60.240.10 |       |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 122 | 1xzh | 197 | 3.7 | 421.1 | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 123 | 1xui | 223 | 3.7 | 113.7 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 124 | 1rpg | 124 | 3.7 | 204.4 | 0.40 | 3.10.130.10 | d.5.1.1 |
| 125 | 1xuj | 223 | 3.7 | 115.3 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 126 | 1bra | 223 | 3.7 | 112.1 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 127 | 1rtb | 124 | 3.7 | 202.9 | 0.39 | 3.10.130.10 | d.5.1.1 |
| 128 | 1c1o | 123 | 3.7 | 113.8 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 129 | 1gkg | 136 | 3.7 | 142.9 | 0.21 | 2.10.70.10 | g.18.1.1 |
| 130 | 1c5v | 223 | 3.7 | 115.0 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 131 | 1tnk | 223 | 3.7 | 113.5 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 132 | 1tzh | 94  | 3.7 | 0.10  | 2.40.10.10 | b.47.1.2 |
| 133 | 1c1k | 126 | 3.7 | 127.3 | 0.16 | 2.10.70.10 | g.18.1.1 |
| 134 | 2fwu | 157 | 3.7 | 0.10  | 2.40.10.10 | b.47.1.2 |
| 135 | 1aqp | 124 | 3.7 | 204.7 | 0.40 | 3.10.130.10 | d.5.1.1 |
| 136 | 2g4x | 124 | 3.7 | 205.1 | 0.40 | 3.10.130.10 | d.5.1.1 |
| 137 | 2sta | 222 | 3.7 | 114.3 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 138 | 1h03 | 125 | 3.7 | 128.9 | 0.14 | 2.10.70.10 | g.18.1.1 |
| 139 | 1mrvv | 223 | 3.7 | 112.2 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 140 | 1co7 | 223 | 3.7 | 110.7 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 141 | 2olc | 147 | 3.7 | 215.3 | 0.33 | 2.40.10.10 | b.47.1.2 |
| 142 | 1anc | 223 | 3.7 | 110.7 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 143 | 1utl | 222 | 3.7 | 113.1 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 144 | 1tbp | 223 | 3.7 | 113.2 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 145 | 1xuh | 223 | 3.7 | 115.4 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 146 | 1f72 | 175 | 3.7 | 142.9 | 0.18 | 2.60.270.20 | b.97.1.1 |
| 147 | 2ofc | 141 | 3.7 | 37.7  | 0.01 | 2.60.270.20 | b.97.1.1 |
| 148 | 6rsa | 124 | 3.7 | 203.7 | 0.39 | 3.10.130.10 | d.5.1.1 |
| 149 | 2ofe | 141 | 3.7 | 37.8  | 0.01 | 2.60.270.20 | b.47.1.2 |
| 150 | 2ofd | 141 | 3.7 | 37.9  | 0.01 | 2.60.270.20 | b.47.1.2 |
| 151 | 2dsb | 206 | 3.7 | 470.0 | 0.58 | 2.40.10.10 | b.47.1.2 |
| 152 | 1y3y | 223 | 3.7 | 111.9 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 153 | 1xi0 | 143 | 3.7 | 41.1  | 0.01 | 2.60.270.20 | b.47.1.2 |
| 154 | 1h0i | 223 | 3.7 | 110.4 | 0.09 | 2.40.10.10 | b.47.1.2 |
| 155 | 2dsc | 195 | 3.7 | 429.0 | 0.56 | 2.40.10.10 | d.5.1.1 |
| 156 | 1w4o | 124 | 3.7 | 203.3 | 0.39 | 3.10.130.10 | d.5.1.1 |
| 157 | 1lqe | 223 | 3.7 | 114.8 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 158 | 1tgn | 222 | 3.7 | 112.6 | 0.09 | 2.40.10.10 | b.47.1.2 |
| 159 | 1tnl | 223 | 3.7 | 114.3 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 160 | 1otx | 236 | 3.6 | 463.5 | 0.50 | 3.40.50.1580 | c.56.2.1 |
| 161 | 1ffe | 197 | 3.6 | 420.9 | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 162 | 1bju | 223 | 3.6 | 113.8 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 163 | 1anb | 223 | 3.6 | 111.5 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 164 | 1ssa | 113 | 3.6 | 163.2 | 0.36 | 3.10.130.10 | d.5.1.1 |
| 165 | 1c9p | 222 | 3.6 | 114.1 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 166 | 1tx6 | 223 | 3.6 | 111.7 | 0.10 | 2.40.10.10 | b.47.1.2 |
| 167 | 2fws | 139 | 3.6 | 91.9  | 0.12 |          | b.1.27.1  |
| 168 | 1j16 | 223 | 3.6 | 111.5 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 169 | 2g4w | 124 | 3.6 | 204.0 | 0.40 | 3.10.130.10 | d.5.1.1   |
| 170 | 3pca | 200 | 3.6 | 251.3 | 0.31 | 2.60.130.10 | b.3.6.1   |
| 171 | 3pce | 200 | 3.6 | 251.8 | 0.31 | 2.60.130.10 | b.3.6.1   |
| 172 | 1fy8 | 215 | 3.6 | 112.8 | 0.09 | 2.40.10.10 | b.47.1.2  |
| 173 | 3pci | 200 | 3.6 | 251.5 | 0.31 | 2.60.130.10 | b.3.6.1   |
| 174 | 1vc8 | 126 | 3.6 | 199.1 | 0.37 |          | d.113.1.1  |
| 175 | 2a2g | 158 | 3.6 | 208.4 | 0.32 | 2.40.128.20 | b.60.1.1  |
| 176 | 2p78 | 171 | 3.6 | 168.7 | 0.23 | 3.40.50.1240 |          |
| 177 | 1c78 | 130 | 3.6 | 109.8 | 0.18 | 3.10.20.130 | d.15.5.1  |
| 178 | 1xzg | 197 | 3.6 | 421.8 | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 179 | 2boc | 219 | 3.6 | 228.3 | 0.23 | 2.60.40.10 | f.14.1.1  |
| 180 | 1cuy | 197 | 3.6 | 420.3 | 0.55 | 3.40.50.1820 | c.69.1.30 |
| 181 | 2d3j | 157 | 3.6 | 99.8  | 0.07 |          |          |
| 182 | 2pqx | 245 | 3.6 | 147.4 | 0.12 |          |          |
| 183 | 1ql9 | 223 | 3.6 | 110.7 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 184 | 1ntp | 223 | 3.6 | 114.0 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 185 | 1fmq | 223 | 3.6 | 115.1 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 186 | 1sxt | 224 | 3.6 | 415.9 | 0.48 | 2.40.50.110 | b.40.2.2  |
| 187 | 1c2d | 223 | 3.6 | 133.6 | 0.12 | 2.40.10.10 | b.47.1.2  |
| 188 | 1ppe | 223 | 3.6 | 113.9 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 189 | 1ane | 223 | 3.6 | 113.3 | 0.10 | 2.40.10.10 | b.47.1.2  |
| 190 | 1xzb | 197 | 3.6 | 421.2 | 0.55 | 3.40.50.1820 | c.69.1.30 |

Table 1S. Continuation of Table 1 of the main text.