

Supplementary Table 2. PDB codes, R factors, and rms deviations of bond lengths for groups of 25 structures each, refined with CNS, REFMAC, TNT, or SHELXL, respectively. The numbers following program names are the total number of such structures at resolution 1.95 to 2.05 Å, available in PDB in February 2007. Entries “NR” denote those structures that are not providing information on rms deviation of bond lengths.

| CNS: 1639 | | | REFMAC: 1176 | | | TNT: 195 | | | SHELX: 97 | | |
|-----------|----------|-----------|--------------|----------|-----------|----------|----------|-----------|-----------|----------|-----------|
| PDB ID | R-factor | rms bonds | PDB ID | R-factor | rms bonds | PDB ID | R-factor | rms bonds | PDB ID | R-factor | rms bonds |
| 2O36 | 0.202 | 0.005 | 2NY4 | 0.204 | 0.005 | 1P7T | 0.197 | 0.020 | 1ZPA | 0.197 | 0.006 |
| 2O71 | 0.231 | NR | 2O1F | 0.187 | 0.022 | 1P6C | 0.185 | 0.012 | 1ZP8 | 0.197 | 0.012 |
| 2O7F | 0.172 | 0.005 | 2OLT | 0.205 | 0.018 | 1Q4S | 0.183 | 0.013 | 2B4W | 0.135 | 0.008 |
| 2OD2 | 0.114 | 0.007 | 2OO3 | 0.166 | 0.016 | 1PQK | 0.180 | 0.012 | 1YUN | 0.171 | 0.006 |
| 2OGS | 0.204 | 0.006 | 2FYO | 0.182 | 0.010 | 1RSR | 0.202 | 0.020 | 2G73 | 0.213 | 0.029 |
| 2OQH | 0.205 | 0.006 | 2CCL | 0.183 | 0.007 | 1NZK | 0.196 | 0.008 | 2G74 | 0.201 | 0.021 |
| 2OTF | 0.188 | 0.006 | 2DYV | 0.175 | 0.009 | 1OV7 | 0.189 | 0.017 | 1ZSF | 0.222 | 0.004 |
| 2TOD | 0.212 | NR | 2ISY | 0.178 | 0.011 | 1OVH | 0.185 | 0.017 | 2F4A | 0.160 | 0.007 |
| 3CBS | 0.200 | 0.006 | 2J6Z | 0.233 | 0.023 | 1T6O | 0.232 | 0.005 | 2F56 | 0.162 | 0.008 |
| 3HAD | 0.218 | 0.008 | 2J7O | 0.204 | 0.021 | 1XT4 | 0.169 | 0.011 | 2F5M | 0.178 | 0.007 |
| 4PAH | 0.169 | 0.023 | 2JAJ | 0.213 | 0.017 | 1YBQ | 0.185 | 0.012 | 2F5W | 0.186 | 0.007 |
| 5LVE | 0.186 | 0.005 | 2JC1 | 0.193 | 0.013 | 2A48 | 0.181 | NR | 1ZVJ | 0.188 | 0.005 |
| 6ATJ | 0.166 | 0.009 | 2JDS | 0.211 | 0.013 | 2AQO | 0.180 | NR | 1ZVK | 0.189 | 0.009 |
| 2IAS | 0.185 | NR | 2O4X | 0.234 | NR | 2AQV | 0.185 | NR | 2B2K | 0.215 | 0.005 |
| 2IAV | 0.209 | NR | 2O63 | 0.194 | 0.010 | 2AHA | 0.204 | 0.013 | 2H5J | 0.202 | 0.006 |
| 2IB6 | 0.198 | 0.006 | 2OAF | 0.168 | 0.014 | 2H8Q | 0.230 | 0.019 | 2I1X | 0.239 | 0.015 |
| 2IFR | 0.204 | 0.012 | 2ODT | 0.181 | 0.019 | 2NU0 | 0.145 | 0.010 | 2EY5 | 0.194 | 0.006 |
| 2IH8 | 0.183 | 0.011 | 2OGQ | 0.162 | 0.025 | 2E3D | 0.202 | 0.014 | 2F0E | 0.203 | 0.006 |
| 2IH9 | 0.263 | 0.013 | 2C2J | 0.179 | 0.018 | 2IHQ | 0.209 | 0.005 | 2F0M | 0.193 | 0.005 |
| 2IIO | 0.218 | 0.006 | 2CA3 | 0.163 | 0.012 | 1M9H | 0.214 | 0.008 | 1YWR | 0.221 | 0.006 |
| 2IKF | 0.228 | 0.014 | 2G4O | 0.210 | 0.020 | 1L0K | 0.157 | NR | 1YW2 | 0.207 | NR |
| 2IM8 | 0.236 | 0.006 | 2G4X | 0.176 | 0.027 | 1NS2 | 0.166 | 0.012 | 1RL8 | 0.226 | 0.014 |
| 2IOM | 0.209 | 0.011 | 2G4Y | 0.195 | 0.026 | 1GQ3 | 0.195 | 0.008 | 1U7T | 0.215 | 0.005 |
| 2IOO | 0.210 | 0.006 | 2G4Z | 0.191 | 0.025 | 1M0Q | 0.194 | 0.026 | 1PR9 | 0.178 | 0.006 |
| 2ISG | 0.241 | 0.006 | 2OIW | 0.178 | 0.014 | 1GWG | 0.167 | 0.017 | 1OW2 | 0.228 | 0.008 |
| Average | 0.202 | 0.0085 | Average | 0.190 | 0.0165 | Average | 0.189 | 0.013 | Average | 0.197 | 0.009 |