|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **All-Atom**  **Contacts** | Clashscore, all atoms: | 0.16 | | 99th percentile\* (N=1784, all resolutions) |
| Clashscore is the number of serious steric overlaps (>0.4 Å) per 1000 atoms. | | | |
| **Protein Geometry** | Poor rotamers | 3 | 0.89% | Goal: <0.3% |
| Favored rotamers | 323 | 96.13% | Goal: >98% |
| Ramachandran outliers | 2 | 0.51% | Goal: <0.05% |
| Ramachandran favored | 373 | 94.91% | Goal: >98% |
| Molprobity score | 0.91 | | 100th percentile\* (N=27675, 0 Å - 99 Å) |
| Cβ deviations >0.25 Å | 4 | 1.11% | Goal: 0 |
| Bad bonds: | 0/3131 | 0.00% | Goal: 0% |
| Bad angles: | 17/4257 | 0.40% | Goal: <0.1% |
| **Peptide Omegas** | Cis Prolines: | 0/28 | 0.00% | Expected: ≤1 per chain, or ≤5% |
| Twisted Peptides: | 1/394 | 0.25% | Goal: 0 |

In the two column results, the left column gives the raw count, right column gives the percentage.

\*100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for Molprobity score in 2006

Molprobity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution