

Analysis output: all-atom contacts and geometry for TECTA_587-690_FFX1H.pdb

Summary statistics

| All-Atom Contacts | Clashscore, all atoms: | 0 | | 100 th percentile* (N=1784, all resolutions) |
|----------------------|---|-------------|--------|---|
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 6 | 6.52% | Goal: <0.3% |
| | Favored rotamers | 75 | 81.52% | Goal: >98% |
| | Ramachandran outliers | 9 | 8.82% | Goal: <0.05% |
| | Ramachandran favored | 85 | 83.33% | Goal: >98% |
| | MolProbity score [^] | 1.81 | | 85 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 0 | 0.00% | Goal: 0 |
| | Bad bonds: | 0 / 790 | 0.00% | Goal: 0% |
| | Bad angles: | 6 / 1076 | 0.56% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 4 | 0.00% | Expected: ≤1 per chain, or ≤5% |

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

Multi-criterion visualizations



View (111 Kb)

Single-criterion visualizations

^{* 100&}lt;sup>th</sup> 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.

- Clash list (175 bytes): View
- Ramachandran plot kinemage (411 Kb): View in KiNG | Download
 Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (17 Kb): View in KiNG | Download

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