

Analysis output: all-atom contacts and geometry for TIMM8A_29-84H.pdb

Summary statistics

| | Clashscore, all atoms: | 31.52 | | 14 th percentile* (N=1784, all resolutions) |
|----------------|---|---------|--------|--|
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| | Poor rotamers | 1 | 1.89% | Goal: <0.3% |
| | Favored rotamers | 49 | 92.45% | Goal: >98% |
| | Ramachandran outliers | 0 | 0.00% | Goal: <0.05% |
| | Ramachandran favored | 50 | 92.59% | Goal: >98% |
| | MolProbity score [^] | 2.66 | | 39 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 0 | 0.00% | Goal: 0 |
| | Bad bonds: | 2 / 476 | 0.42% | Goal: 0% |
| | Bad angles: | 2 / 640 | 0.31% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 2 | 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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 2.17 points.

Multi-criterion visualizations



View (65 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 (1.4 Kb): View
- Ramachandran plot kinemage (408 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (14 Kb): View in KiNG | Download

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