

Analysis output: all-atom contacts and geometry for POU4F3_186-332H.pdb

Summary statistics

| Contacts | Clashscore, all atoms: | 171.95 | | O th percentile* (N=1784, all resolutions) |
|---------------------|---|--------------|--------|---|
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 5 | 4.03% | Goal: <1% |
| | Ramachandran outliers | 4 | 2.76% | Goal: <0.05% |
| | Ramachandran favored | 133 | 91.72% | Goal: >98% |
| | MolProbity score [^] | 3.65 | | 6 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 14 | 9.86% | Goal: 0 |
| | Bad backbone bonds: | 35 / 1194 | 2.93% | Goal: 0% |
| | Bad backbone angles: | 96 / 1601 | 6.00% | Goal: <0.1% |

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* fix 1 bad rotamers and improve your clashscore by 0.41 points.

Multi-criterion visualizations

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^{* 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.



View (154 Kb)

Single-criterion visualizations

- Clash list (4 Kb): View
- Ramachandran plot kinemage (413 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (19 Kb): View in KiNG | Download

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