



# Analysis output: all-atom contacts and geometry for FGF3\_36-183H.pdb

## Summary statistics

|                      |   |           |        |   |
|----------------------|---|-----------|--------|---|
| All-Atom<br>Contacts | Clashscore, all atoms:  | 68.69     |        | 1 <sup>st</sup> percentile* (N=1784, all resolutions) |
|                      | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. |           |        |   |
| Protein<br>Geometry  | Poor rotamers   | 7         | 5.65%  | Goal: <0.3%   |
|                      | Favored rotamers  | 111       | 89.52% | Goal: >98%  |
|                      | Ramachandran outliers   | 5         | 3.42%  | Goal: <0.05%  |
|                      | Ramachandran favored  | 121       | 82.88% | Goal: >98%  |
|                      | MolProbity score^   | 3.57      |        | 7 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)       |
|                      | Cβ deviations >0.25Å  | 10        | 7.41%  | Goal: 0   |
|                      | Bad bonds:  | 20 / 1224 | 1.63%  | Goal: 0%  |
|                      | Bad angles:   | 43 / 1648 | 2.61%  | Goal: <0.1%   |
| Peptide Omegas       | Cis Prolines:   | 0 / 6     | 0.00%  | Expected: ≤1 per chain, or ≤5%                        |
|                      | Cis nonProlines:  | 1 / 141   | 0.71%  | Goal: <0.05%  |
|                      | Twisted Peptides:   | 1 / 147   | 0.68%  | Goal: 0   |

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

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

<sup>^</sup> MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 2.08 points.

## Multi-criterion visualizations



[View \(172 Kb\)](#)

## Single-criterion visualizations

- **Clash list** (7.1 Kb): [View](#)
- **Ramachandran plot kinemage** (413 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (18 Kb): [View in KiNG](#) | [Download](#)

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