

## Analysis output: all-atom contacts and geometry for MYO3A\_16-287H.pdb

## **Summary statistics**

| Contacts | Clashscore, all atoms:  | 33.82        |        | 12 <sup>th</sup> percentile* (N=1784, all resolutions) |
|----------|---|--------------|--------|--|
|          | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. |              |        |  |
| Geometry | Poor rotamers   | 0            | 0.00%  | Goal: <1%  |
|          | Ramachandran<br>outliers  | 5            | 1.85%  | Goal: <0.05%   |
|          | Ramachandran<br>favored   | 250          | 92.59% | Goal: >98%   |
|          | MolProbity score <sup>^</sup>   | 2.48         |        | 48 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)       |
|          | Cβ deviations >0.25Å  | 4            | 1.58%  | Goal: 0  |
|          | Bad backbone bonds:   | 19 /<br>2218 | 0.86%  | Goal: 0%   |
|          | Bad backbone angles:  | 16 /<br>3006 | 0.53%  | 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* improve your clashscore by 1.15 points.

## Multi-criterion visualizations

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<sup>\* 100&</sup>lt;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.



View (272 Kb)

## Single-criterion visualizations

- Clash list (4.2 Kb): View
- Ramachandran plot kinemage (421 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (25 Kb): View in KiNG | Download

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