



# Analysis output: all-atom contacts and geometry for MYO6\_771-913H.pdb

## Summary statistics

|                      |   |           |   |                                |
|----------------------|---|-----------|---|--------------------------------|
| All-Atom<br>Contacts | Clashscore, all atoms:  | 41.44     | 7 <sup>th</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   | 2         | 1.49%   | Goal: <0.3%                    |
|                      | Favored rotamers  | 128       | 95.52%  | Goal: >98%                     |
|                      | Ramachandran outliers   | 2         | 1.42%   | Goal: <0.05%                   |
|                      | Ramachandran favored  | 138       | 97.87%  | Goal: >98%                     |
|                      | MolProbity score^   | 2.26      | 61 <sup>st</sup> percentile* (N=27675, 0Å - 99Å)      |                                |
|                      | Cβ deviations >0.25Å  | 3         | 2.14%   | Goal: 0                        |
|                      | Bad bonds:  | 10 / 1188 | 0.84%   | Goal: 0%                       |
|                      | Bad angles:   | 17 / 1587 | 1.07%   | Goal: <0.1%                    |
| Peptide Omegas       | Cis Prolines:   | 0 / 3     | 0.00%   | Expected: ≤1 per chain, or ≤5% |
|                      | Twisted Peptides:   | 1 / 142   | 0.70%   | 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 0.41 points.

## Multi-criterion visualizations



[View](#) (163 Kb)

## Single-criterion visualizations

- **Clash list** (4.4 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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