

## Analysis output: all-atom contacts and geometry for Model\_rH.pdb

## **Summary statistics**

| All-Atom<br>Contacts | Clashscore, all atoms:  | 15.66       |        | 47 <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   | 6           | 6.00%  | Goal: <1%  |
|                      | Ramachandran outliers   | 0           | 0.00%  | Goal: <0.05%   |
|                      | Ramachandran<br>favored   | 99          | 93.40% | Goal: >98%   |
|                      | MolProbity score <sup>^</sup>   | 2.72        |        | 35 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)       |
|                      | Cβ deviations >0.25Å  | 1           | 0.96%  | Goal: 0  |
|                      | Bad backbone bonds:   | 0 / 894     | 0.00%  | Goal: 0%   |
|                      | Bad backbone angles:  | 4 /<br>1206 | 0.33%  | Goal: <0.1%  |

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

## **Multi-criterion visualizations**



View (110 Kb)

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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.

## Single-criterion visualizations

- Clash list (1.1 Kb): View
- Ramachandran plot kinemage (411 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (16 Kb): View in KiNG | Download



About MolProbity | Website for the Richardson Lab | Using ecloud x-H | Internal reference 4.1-537

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