



# Analysis output: all-atom contacts and geometry for KCNJ10\_27-338\_FFX1H.pdb

## Summary statistics

|                      |   |             |        |  |
|----------------------|---|-------------|--------|--|
| All-Atom<br>Contacts | Clashscore, all atoms:  | 0.45        |        | 99 <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   | 38          | 3.47%  | Goal: <0.3%  |
|                      | Favored rotamers  | 945         | 86.22% | Goal: >98%   |
|                      | Ramachandran outliers   | 21          | 1.69%  | Goal: <0.05%   |
|                      | Ramachandran favored  | 1082        | 87.26% | Goal: >98%   |
|                      | MolProbity score^   | 1.68        |        | 90 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)       |
|                      | Cβ deviations >0.25Å  | 37          | 3.14%  | Goal: 0  |
|                      | Bad bonds:  | 0 / 10140   | 0.00%  | Goal: 0%   |
|                      | Bad angles:   | 116 / 13792 | 0.84%  | Goal: <0.1%  |
| Peptide<br>Omegas    | Cis Prolines:   | 0 / 48      | 0.00%  | Expected: ≤1 per chain, or ≤5%                         |
|                      | Cis nonProlines:  | 6 / 1196    | 0.50%  | Goal: <0.05%   |
|                      | Twisted Peptides:   | 2 / 1244    | 0.16%  | 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.

## Multi-criterion visualizations



[View \(1.3 Mb\)](#)

# Single-criterion visualizations

- **Clash list** (553 bytes): [View](#)
- **Ramachandran plot kinemage** (486 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (84 Kb): [View in KiNG](#) | [Download](#)

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