

## Analysis output: all-atom contacts and geometry for SLC26A5\_505-718H.pdb

## **Summary statistics**

| Contacts            | Clashscore, all atoms:  | 38.99        |        | 8 <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   | 3            | 1.67%  | Goal: <1%   |
|                     | Ramachandran outliers   | 6            | 2.83%  | Goal: <0.05%  |
|                     | Ramachandran<br>favored   | 199          | 93.87% | Goal: >98%  |
|                     | MolProbity score <sup>^</sup>   | 2.65         |        | 39 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)      |
|                     | Cβ deviations >0.25Å  | 5            | 2.50%  | Goal: 0   |
|                     | Bad backbone bonds:   | 8 / 1710     | 0.47%  | Goal: 0%  |
|                     | Bad backbone angles:  | 37 /<br>2322 | 1.59%  | 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 0.9 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 (214 Kb)

## Single-criterion visualizations

- Clash list (3.3 Kb): View
- Ramachandran plot kinemage (417 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (22 Kb): View in KiNG | Download

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