# Analysis output: all-atom contacts and geometry for DFNB31_43-236H.pdb

## Summary statistics

| | | | | |
|---|---|---|---|---|
| All-Atom Contacts | Clashscore, all atoms: | 55.52 | | 3rd percentile* (N=1784, all resolutions) |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 3 | 1.89% | Goal: <0.3% |
| | Favored rotamers | 153 | 96.23% | Goal: >98% |
| | Ramachandran outliers | 5 | 2.60% | Goal: <0.05% |
| | Ramachandran favored | 179 | 93.23% | Goal: >98% |
| | MolProbity score^ | 2.87 | | 28th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 4 | 2.27% | Goal: 0 |
| | Bad bonds: | 24 / 1547 | 1.55% | Goal: 0% |
| | Bad angles: | 30 / 2097 | 1.43% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 10 | 0.00% | Expected: ≤1 per chain, or ≤5% |
| | Cis nonProlines: | 1 / 183 | 0.55% | Goal: <0.05% |
| | Twisted Peptides: | 1 / 193 | 0.52% | Goal: 0 |

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

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ 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 0.98 points.

## Multi-criterion visualizations


View (221 Kb)

# Single-criterion visualizations

- **Clash list** (7.3 Kb): View
- **Ramachandran plot kinemage** (416 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (21 Kb): View in KiNG | Download

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