



Analysis output: all-atom contacts and geometry for S1PR2_225-301H.pdb

Summary statistics

| | | | | |
|----------------------|---|---------|--|--|
| All-Atom Contacts | Clashscore, all atoms: | 22.73 | 25 th percentile* (N=1784, all resolutions) | |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 0 | 0.00% | Goal: <0.3% |
| | Favored rotamers | 66 | 94.29% | Goal: >98% |
| | Ramachandran outliers | 1 | 1.33% | Goal: <0.05% |
| | Ramachandran favored | 71 | 94.67% | Goal: >98% |
| | MolProbity score [^] | 2.21 | | 64 th percentile* (N=27675, 0Å - 99Å) |
| | Cβ deviations >0.25Å | 0 | 0.00% | Goal: 0 |
| | Bad bonds: | 4 / 643 | 0.62% | Goal: 0% |
| | Bad angles: | 0 / 883 | 0.00% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 5 | 0.00% | Expected: ≤1 per chain, or ≤5% |

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.

Multi-criterion visualizations



[View](#) (87 Kb)

Single-criterion visualizations

- **Clash list** (1.4 Kb): [View](#)
- **Ramachandran plot kinemage** (409 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (15 Kb): [View in KiNG](#) | [Download](#)

