Analysis output: all-atom contacts and geometry for POU3F4H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	128.08		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	10	7.52%	Goal: <1%
	Ramachandran outliers	4	2.70%	Goal: <0.05%
	Ramachandran favored	132	89.19%	Goal: >98%
	MolProbity score^	3.81		4th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	14	9.86%	Goal: 0
	Bad backbone bonds:	50 / 1215	4.12%	Goal: 0%
	Bad backbone angles:	83 / 1628	5.10%	Goal: <0.1%

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* fix 1 bad rotamers.

Multi-criterion visualizations

View (156 Kb)

Single-criterion visualizations

- **Clash list** (3.1 Kb): View
- **Ramachandran plot kinemage** (413 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (18 Kb): View in KiNG | Download

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