



Analysis output: all-atom contacts and geometry for PEX1_13-179H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	10.97		67 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.69%	Goal: <0.3%
	Favored rotamers	140	97.22%	Goal: >98%
	Ramachandran outliers	1	0.61%	Goal: <0.05%
	Ramachandran favored	158	95.76%	Goal: >98%
	MolProbity score [^]	1.85		83 rd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	15 / 1357	1.11%	Goal: 0%
	Bad angles:	5 / 1852	0.27%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	1 / 8	12.50%	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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 1.89 points.

Multi-criterion visualizations



[View \(181 Kb\)](#)

Single-criterion visualizations

- **Clash list** (1.4 Kb): [View](#)
- **Ramachandran plot kinemage** (414 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (19 Kb): [View in KiNG](#) | [Download](#)

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