



Analysis output: all-atom contacts and geometry for PEX6_466-971_FFX1H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.39		99 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	17	4.13%	Goal: <0.3%
	Favored rotamers	344	83.50%	Goal: >98%
	Ramachandran outliers	13	2.58%	Goal: <0.05%
	Ramachandran favored	432	85.71%	Goal: >98%
	MolProbity score [^]	1.75		87 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	13	2.78%	Goal: 0
	Bad bonds:	0 / 3851	0.00%	Goal: 0%
	Bad angles:	31 / 5228	0.59%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 29	6.90%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	2 / 476	0.42%	Goal: <0.05%
	Twisted Peptides:	3 / 505	0.59%	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.

Multi-criterion visualizations



Multi-criterion
chart

[View \(529 Kb\)](#)

Single-criterion visualizations

- **Clash list** (301 bytes): [View](#)
- **Ramachandran plot kinemage** (435 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (39 Kb): [View in KiNG](#) | [Download](#)

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