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

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	75.5		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	2.43%	Goal: <0.3%
	Favored rotamers	379	91.99%	Goal: >98%
	Ramachandran outliers	28	5.56%	Goal: <0.05%
	Ramachandran favored	408	80.95%	Goal: >98%
	MolProbity score^	3.36		12th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	1.50%	Goal: 0
	Bad bonds:	24 / 3851	0.62%	Goal: 0%
	Bad angles:	71 / 5228	1.36%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 29	6.90%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	5 / 476	1.05%	Goal: <0.05%
	Twisted Peptides:	6 / 505	1.19%	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* fix 1 bad rotamers and improve your clashscore by 0.92 points.

Multi-criterion visualizations

View (575 Kb)

Single-criterion visualizations

- **Clash list** (24 Kb): View
- **Ramachandran plot kinemage** (437 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (37 Kb): View in KiNG | Download

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