Analysis output: all-atom contacts and geometry for PNPT1_49-752H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	162.28		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	22	1.22%	Goal: <0.3%
	Favored rotamers	1717	95.23%	Goal: >98%
	Ramachandran outliers	204	9.69%	Goal: <0.05%
	Ramachandran favored	1604	76.16%	Goal: >98%
	MolProbity score^	3.52		8th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	34	1.73%	Goal: 0
	Bad bonds:	181 / 16569	1.09%	Goal: 0%
	Bad angles:	227 / 22428	1.01%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 102	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	36 / 2007	1.79%	Goal: <0.05%
	Twisted Peptides:	10 / 2109	0.47%	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* improve your clashscore by 1.10 points.

Multi-criterion visualizations

View (2.1 Mb)

Single-criterion visualizations

- **Clash list** (225 Kb): View
- **Ramachandran plot kinemage** (562 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.8 Mb): View
- **Cβ deviation scatter plot** (119 Kb): View in KiNG | Download

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