Analysis output: all-atom contacts and geometry for ATP6V1B1_43-498H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	17.28		41st percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	1.03%	Goal: <0.3%
	Favored rotamers	376	97.16%	Goal: >98%
	Ramachandran outliers	12	2.64%	Goal: <0.05%
	Ramachandran favored	417	91.85%	Goal: >98%
	MolProbity score^	2.24		62nd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.24%	Goal: 0
	Bad bonds:	19 / 3632	0.52%	Goal: 0%
	Bad angles:	23 / 4922	0.47%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	1 / 25	4.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	1 / 430	0.23%	Goal: <0.05%

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 0.56 points.

Multi-criterion visualizations

View (486 Kb)

Single-criterion visualizations

- **Clash list** (5.3 Kb): View
- **Ramachandran plot kinemage** (432 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (35 Kb): View in KiNG | Download

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