Analysis output: all-atom contacts and geometry for KCNQ1_250-357H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	74.85		0th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	2.30%	Goal: <0.3%
	Favored rotamers	78	89.66%	Goal: >98%
	Ramachandran outliers	1	0.94%	Goal: <0.05%
	Ramachandran favored	99	93.40%	Goal: >98%
	MolProbity score^	3.05		21st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	7.29%	Goal: 0
	Bad bonds:	12 / 860	1.40%	Goal: 0%
	Bad angles:	41 / 1171	3.50%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 2	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 107	0.93%	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 1.20 points.

Multi-criterion visualizations

View (127 Kb)

Single-criterion visualizations

- **Clash list** (5.4 Kb): View
- **Ramachandran plot kinemage** (411 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (16 Kb): View in KiNG | Download

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