Analysis output: all-atom contacts and geometry for KITLG_33-507H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	31.9		13th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	21	4.93%	Goal: <0.3%
	Favored rotamers	367	86.15%	Goal: >98%
	Ramachandran outliers	24	5.07%	Goal: <0.05%
	Ramachandran favored	380	80.34%	Goal: >98%
	MolProbity score^	3.24		15th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	22 / 3863	0.57%	Goal: 0%
	Bad angles:	11 / 5255	0.21%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	3 / 25	12.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 474	0.21%	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 2 bad rotamers and improve your clashscore by 0.94 points.

Multi-criterion visualizations

View (526 Kb)

Single-criterion visualizations

- **Clash list** (10 Kb): View
- **Ramachandran plot kinemage** (435 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (36 Kb): View in KiNG | Download

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