Analysis output: all-atom contacts and geometry for CIB2_13-185H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	51.37		3rd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.64%	Goal: <0.3%
	Favored rotamers	152	96.82%	Goal: >98%
	Ramachandran outliers	4	2.34%	Goal: <0.05%
	Ramachandran favored	160	93.57%	Goal: >98%
	MolProbity score^	2.61		41st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.60%	Goal: 0
	Bad bonds:	13 / 1434	0.91%	Goal: 0%
	Bad angles:	26 / 1938	1.34%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 8	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	2 / 172	1.16%	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 0.72 points.

Multi-criterion visualizations

View (197 Kb)

Single-criterion visualizations

- **Clash list** (6.1 Kb): View

- **Ramachandran plot kinemage** (415 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (20 Kb): View in KiNG | Download

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