

Analysis output: all-atom contacts and geometry for CDH23_2231-2340H.pdb

Summary statistics

Contacts	Clashscore, all atoms:	31.06		14 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	4.17%	Goal: <1%
	Ramachandran outliers	6	5.56%	Goal: <0.05%
	Ramachandran favored	96	88.89%	Goal: >98%
	MolProbity score [^]	3.03		22 nd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	3.85%	Goal: 0
	Bad backbone bonds:	0 / 845	0.00%	Goal: 0%
	Bad backbone angles:	11 / 1160	0.95%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* fix 1 bad rotamers and improve your clashscore by 2.39 points.

Multi-criterion visualizations

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^{* 100&}lt;sup>th</sup> 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.



View (112 Kb)

Single-criterion visualizations

- Clash list (1.6 Kb): View
- Ramachandran plot kinemage (411 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (17 Kb): View in KiNG | Download



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