

## Analysis output: all-atom contacts and geometry for CDH23\_1358-1567.pdb\_18\_1H.pdb

## **Summary statistics**

Contacts	Clashscore, all atoms:	1.59		99 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.56%	Goal: <1%
	Ramachandran outliers	12	5.77%	Goal: <0.05%
	Ramachandran favored	163	78.37%	Goal: >98%
	MolProbity score <sup>^</sup>	1.66		90 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	2.07%	Goal: 0
	Bad backbone bonds:	0 / 1620	0.00%	Goal: 0%
	Bad backbone angles:	37 / 2214	1.67%	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* improve your clashscore by 0.32 points.

## Multi-criterion visualizations

1 of 2 6/13/14, 1:52 PM

<sup>\* 100&</sup>lt;sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

<sup>^</sup> 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 (203 Kb)

## Single-criterion visualizations

- Clash list (343 bytes): View
- Ramachandran plot kinemage (418 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (24 Kb): View in KiNG | Download



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2 of 2