

## Analysis output: all-atom contacts and geometry for MYO3A\_323-996H.pdb

## **Summary statistics**

Contacts	Clashscore, all atoms:	71.37		1 <sup>st</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	0.17%	Goal: <1%
	Ramachandran outliers	16	2.38%	Goal: <0.05%
	Ramachandran favored	623	92.71%	Goal: >98%
	MolProbity score <sup>^</sup>	2.78		32 <sup>nd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	10	1.56%	Goal: 0
	Bad backbone bonds:	49 / 5519	0.89%	Goal: 0%
	Bad backbone angles:	100 / 7457	1.34%	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 0.56 points.

## Multi-criterion visualizations

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<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 (682 Kb)

## Single-criterion visualizations

- Clash list (14 Kb): View
- Ramachandran plot kinemage (445 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (47 Kb): View in KiNG | Download

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