

Analysis output: all-atom contacts and geometry for MYO6_2-825H.pdb

Summary statistics

Contacts	Clashscore, all atoms:	6.2		90 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	32	4.38%	Goal: <1%
	Ramachandran outliers	5	0.61%	Goal: <0.05%
	Ramachandran favored	778	94.65%	Goal: >98%
	MolProbity score [^]	2.20		65 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.13%	Goal: 0
	Bad backbone bonds:	45 / 6754	0.67%	Goal: 0%
	Bad backbone angles:	11 / 9092	0.12%	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 2 bad rotamers and improve your clashscore by 0.37 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 (159 Kb)

Single-criterion visualizations

- Clash list (2.6 Kb): View
- Ramachandran plot kinemage (453 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (52 Kb): View in KiNG | Download

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