



# Analysis output: all-atom contacts and geometry for MYH14\_47- 921\_FFX1H.pdb

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	11.91	63 <sup>rd</sup> percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	11	1.47%	Goal: <0.3%
	Favored rotamers	629	84.20%	Goal: >98%
	Ramachandran outliers	18	2.06%	Goal: <0.05%
	Ramachandran favored	763	87.40%	Goal: >98%
	MolProbity score^	2.33	57 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)	
	Cβ deviations >0.25Å	16	1.95%	Goal: 0
	Bad bonds:	18 / 7183	0.25%	Goal: 0%
	Bad angles:	96 / 9692	0.99%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 38	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	1 / 836	0.12%	Goal: <0.05%
	Twisted Peptides:	5 / 874	0.57%	Goal: 0

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

\* 100<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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 0.21 points.

## Multi-criterion visualizations



## Multi-criterion chart

[View](#) (927 Kb)

## Single-criterion visualizations

- **Clash list** (7.2 Kb): [View](#)
- **Ramachandran plot kinemage** (457 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (61 Kb): [View in KiNG](#) | [Download](#)

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