



# Analysis output: all-atom contacts and geometry for MSRB3\_49-166H.pdb

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	21.17		30 <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	0	0.00%	Goal: <1%
	Ramachandran outliers	2	1.72%	Goal: <0.05%
	Ramachandran favored	111	95.69%	Goal: >98%
	MolProbity score^	2.12		69 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	16 / 957	1.67%	Goal: 0%
	Bad backbone angles:	7 / 1294	0.54%	Goal: <0.1%

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 2.23 points.

## Multi-criterion visualizations



[View](#) (119 Kb)

## Single-criterion visualizations

- **Clash list** (1.1 Kb): [View](#)
- **Ramachandran plot kinemage** (411 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (17 Kb): [View in KiNG](#) | [Download](#)

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