



Analysis output: all-atom contacts and geometry for MET_1024-1352H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	12.42	61 st percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	1.70%	Goal: <0.3%
	Favored rotamers	285	96.94%	Goal: >98%
	Ramachandran outliers	5	1.53%	Goal: <0.05%
	Ramachandran favored	308	94.19%	Goal: >98%
	MolProbity score^	2.17		66 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	0.65%	Goal: 0
	Bad bonds:	36 / 2678	1.34%	Goal: 0%
	Bad angles:	17 / 3635	0.47%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 18	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 328	0.30%	Goal: 0

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

* 100th 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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* fix 1 bad rotamers and improve your clashscore by 0.95 points.

Multi-criterion visualizations



[View \(356 Kb\)](#)

Single-criterion visualizations

- **Clash list** (2.9 Kb): [View](#)
- **Ramachandran plot kinemage** (424 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (28 Kb): [View in KiNG](#) | [Download](#)

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