



Analysis output: all-atom contact and geometry for MARVELD2_441-548.pdb_12_1H.p

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	1.08	99 th 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	0	0.00%	Goal: <0.05%
	Ramachandran favored	104	98.11%	Goal: >98%
	MolProbity score^	0.81	100 th percentile* (N=27675, 0Å - 99Å)	
	Cβ deviations >0.25Å	4	3.70%	Goal: 0
	Bad backbone bonds:	0 / 952	0.00%	Goal: 0%
	Bad backbone angles:	5 / 1272	0.39%	Goal: <0.1%

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 on the same scale as X-ray resolution.

Multi-criterion visualizations



[View](#) (106 Kb)

Single-criterion visualizations

- **Clash list** (259 bytes): [View](#)
- **Ramachandran plot kinemage** (411 Kb): [View in KiNG](#) | [Download](#)

- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (18 Kb): [View in KiNG](#) | [Download](#)

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