

## Analysis output: all-atom contact and geometry for DFNB31\_WT\_132-226.pdb\_5\_1H.pd

## **Summary statistics**

7 7	Clashscore, all atoms:	0.7		99 <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	3	3.23%	Goal: <0.05%
	Ramachandran favored	75	80.65%	Goal: >98%
	MolProbity score <sup>^</sup>	1.45		96 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 707	0.00%	Goal: 0%
	Bad backbone angles:	0 / 948	0.00%	Goal: <0.1%

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

## **Multi-criterion visualizations**



View (90 Kb)

## Single-criterion visualizations

• Clash list (217 bytes): View

• Ramachandran plot kinemage (410 Kb): View in KiNG | Download

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<sup>\* 100&</sup>lt;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 on the same scale as X-ray resolution.

- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (16 Kb): View in KiNG | Download



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