

## Analysis output: all-atom contacts and geometry for DIAPH1\_92-452.pdb\_31\_1H.pdb

## **Summary statistics**

Contacts	Clashscore, all atoms:	2.05		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	1	0.30%	Goal: <1%
	Ramachandran outliers	3	0.84%	Goal: <0.05%
	Ramachandran favored	339	94.43%	Goal: >98%
	MolProbity score <sup>^</sup>	1.35		98 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	21	6.05%	Goal: 0
	Bad backbone bonds:	1 / 2946	0.03%	Goal: 0%
	Bad backbone angles:	32 / 3966	0.81%	Goal: <0.1%

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

## **Multi-criterion visualizations**



View (345 Kb)

1 of 2 6/13/14, 1:04 PM

<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 be on the same scale as X-ray resolution.

## Single-criterion visualizations

- Clash list (553 bytes): View
- Ramachandran plot kinemage (426 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (34 Kb): View in KiNG | Download



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http://molprobity.biochem.duke.edu/index.php?MolProbSID=be...

2 of 2 6/13/14, 1:04 PM