

## Analysis output: all-atom contacts and geometry for DCDC2\_132-226H.pdb

## **Summary statistics**

All-Atom	Clashscore, all atoms:	10.28		70 <sup>th</sup> percentile* (N=1784, all resolutions)
Contacts	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <0.3%
	Favored rotamers	79	94.05%	Goal: >98%
	Ramachandran outliers	2	2.15%	Goal: <0.05%
	Ramachandran favored	82	88.17%	Goal: >98%
	MolProbity score <sup>^</sup>	2.13		69 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	4 / 781	0.51%	Goal: 0%
	Bad angles:	0 / 1056	0.00%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0/5	0.00%	Expected: ≤1 per chain, or ≤5%

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

## **Multi-criterion visualizations**



View (104 Kb)

## Single-criterion visualizations

- Clash list (848 bytes): View
- Ramachandran plot kinemage (410 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (16 Kb): View in KiNG | Download

<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.

