

## Analysis output: all-atom contacts and geometry for CLDN14\_4181H.pdb

## **Summary statistics**

	Clashscore, all atoms:	34.34		11 <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	7	4.83%	Goal: <0.3%
	Favored rotamers	135	93.10%	Goal: >98%
	Ramachandran outliers	2	1.14%	Goal: <0.05%
	Ramachandran favored	168	95.45%	Goal: >98%
	MolProbity score <sup>^</sup>	2.85		29 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	1.86%	Goal: 0
	Bad bonds:	6 / 1365	0.44%	Goal: 0%
	Bad angles:	9 / 1859	0.48%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0/5	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	3 / 172	1.74%	Goal: <0.05%

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

## **Multi-criterion visualizations**



View (197 Kb)

## Single-criterion visualizations

- Clash list (4.1 Kb): View
- Ramachandran plot kinemage (415 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.

- Ramachandran plot PDF (1.7 Mb): View
  Cβ deviation scatter plot (20 Kb): View in KiNG | Download

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