

## Analysis output: all-atom contacts and geometry for COL4A4\_1465-1688H.pdb

## **Summary statistics**

All-Atom Contacts	Clashscore, all atoms:	16.48		43 <sup>rd</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	1.07%	Goal: <0.3%
	Favored rotamers	180	96.26%	Goal: >98%
	Ramachandran outliers	5	2.25%	Goal: <0.05%
	Ramachandran favored	204	91.89%	Goal: >98%
	MolProbity score <sup>^</sup>	2.23		63 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.48%	Goal: 0
	Bad bonds:	16 / 1795	0.89%	Goal: 0%
	Bad angles:	4 / 2448	0.16%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 17	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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* fix 1 bad rotamers and improve your clashscore by 2.06 points.

## **Multi-criterion visualizations**

<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.



**View** (242 Kb)

## Single-criterion visualizations

- Clash list (2.5 Kb): View
- Ramachandran plot kinemage (418 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (23 Kb): View in KiNG | Download

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