

## Analysis output: all-atom contacts and geometry for COL4A6\_1466-1689H.pdb

## **Summary statistics**

All-Atom Contacts	Clashscore, all atoms:	11.69		64 <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	4	2.07%	Goal: <0.3%
	Favored rotamers	185	95.85%	Goal: >98%
	Ramachandran outliers	3	1.35%	Goal: <0.05%
	Ramachandran favored	201	90.54%	Goal: >98%
	MolProbity score <sup>^</sup>	2.36		55 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	14 / 1803	0.78%	Goal: 0%
	Bad angles:	8 / 2456	0.33%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 15	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 0.59 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 (1.9 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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