

## Analysis output: all-atom contacts and geometry for COL2A1\_27-97H.pdb

## **Summary statistics**

All-Atom Contacts	Clashscore, all atoms:	13.75		55 <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	8	12.50%	Goal: <0.3%
	Favored rotamers	43	67.19%	Goal: >98%
	Ramachandran outliers	2	2.90%	Goal: <0.05%
	Ramachandran favored	53	76.81%	Goal: >98%
	MolProbity score <sup>^</sup>	3.25		15 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 546	0.00%	Goal: 0%
	Bad angles:	0 / 749	0.00%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0/6	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* improve your clashscore by 1.96 points.

## **Multi-criterion visualizations**



Single-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.

- Clash list (722 bytes): View
- Ramachandran plot kinemage (409 Kb): View in KiNG | Download
  Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (14 Kb): View in KiNG | Download

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