

Analysis output: all-atom contacts and geometry for COL4A3_1445-1668H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	26.54		19 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	1.05%	Goal: <0.3%
	Favored rotamers	185	96.86%	Goal: >98%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	217	97.75%	Goal: >98%
	MolProbity score [^]	1.98		77 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	17 / 1789	0.95%	Goal: 0%
	Bad angles:	9 / 2435	0.37%	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* improve your clashscore by 0.88 points.

Multi-criterion visualizations

^{* 100&}lt;sup>th</sup> percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

[^] 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 (4 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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