

Analysis output: all-atom contacts and geometry for COL2A1_1271-1487H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	18.2		37 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.54%	Goal: <0.3%
	Favored rotamers	180	96.77%	Goal: >98%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	211	98.14%	Goal: >98%
	MolProbity score [^]	1.76		87 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	10 / 1751	0.57%	Goal: 0%
	Bad angles:	7 / 2373	0.29%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 12	16.67%	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 1.49 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 (235 Kb)

Single-criterion visualizations

- Clash list (1.8 Kb): View
- Ramachandran plot kinemage (417 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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