

## Analysis output: all-atom contacts and geometry for COL9A2\_22-60\_FFX1H.pdb

## **Summary statistics**

All-Atom Contacts	Clashscore, all atoms:	40.57		8 <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	16.00%	Goal: <0.3%
	Favored rotamers	16	64.00%	Goal: >98%
	Ramachandran outliers	4	10.81%	Goal: <0.05%
	Ramachandran favored	22	59.46%	Goal: >98%
	MolProbity score <sup>^</sup>	3.92		3 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	5	18.52%	Goal: 0
	Bad bonds:	17 / 264	6.44%	Goal: 0%
	Bad angles:	26 / 363	7.16%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 11	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	1/27	3.70%	Goal: <0.05%
	Twisted Peptides:	4/38	10.53%	Goal: 0

In the two column results, the left column gives the raw count, right column gives the percentage.

## **Multi-criterion visualizations**



View (48 Kb)

## Single-criterion visualizations

• Clash list (1 Kb): View

<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.

- Ramachandran plot kinemage (407 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (12 Kb): View in KiNG | Download

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