



# Analysis output: all-atom contacts and geometry for Tmprss3\_108-449H.pdb

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	91.23		0 <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	2	0.70%	Goal: <0.3%
	Favored rotamers	277	97.19%	Goal: >98%
	Ramachandran outliers	11	3.24%	Goal: <0.05%
	Ramachandran favored	306	90.00%	Goal: >98%
	MolProbity score^	2.98		24 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	6	1.95%	Goal: 0
	Bad bonds:	45 / 2694	1.67%	Goal: 0%
	Bad angles:	80 / 3674	2.18%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 17	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	1 / 324	0.31%	Goal: <0.05%
	Twisted Peptides:	2 / 341	0.59%	Goal: 0

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

\* 100<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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 1.77 points.

## Multi-criterion visualizations



[View \(386 Kb\)](#)

# Single-criterion visualizations

- **Clash list** (20 Kb): [View](#)
- **Ramachandran plot kinemage** (425 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (29 Kb): [View in KiNG](#) | [Download](#)

[Continue >](#)