

## Analysis output: all-atom contacts and geometry for TECTA\_587-690H.pdb

## **Summary statistics**

	Clashscore, all atoms:	62.89		1 <sup>st</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
	Poor rotamers	5	5.43%	Goal: <0.3%
	Favored rotamers	82	89.13%	Goal: >98%
	Ramachandran outliers	5	4.90%	Goal: <0.05%
	Ramachandran favored	84	82.35%	Goal: >98%
	MolProbity score <sup>^</sup>	3.53		8 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	23	23.96%	Goal: 0
Peptide Omegas	Cis Prolines:	0/4	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.

## **Multi-criterion visualizations**



View (105 Kb)

## Single-criterion visualizations

- Clash list (1.8 Kb): View
- Ramachandran plot kinemage (411 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- **C**β **deviation scatter plot** (16 Kb): View in KiNG | Download

<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.