



# Analysis output: all-atom contacts and geometry for HSD17B4\_323-606H.pdb

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	18.93		35 <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	16	3.48%	Goal: <0.3%
	Favored rotamers	427	92.83%	Goal: >98%
	Ramachandran outliers	21	3.76%	Goal: <0.05%
	Ramachandran favored	494	88.53%	Goal: >98%
	MolProbity score^	2.77		33 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	0.39%	Goal: 0
	Bad bonds:	18 / 4426	0.41%	Goal: 0%
	Bad angles:	13 / 5991	0.22%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 30	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	3 / 530	0.57%	Goal: <0.05%

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* fix 1 bad rotamers and improve your clashscore by 0.58 points.

## Multi-criterion visualizations



## Multi-criterion chart

[View](#) (604 Kb)

## Single-criterion visualizations

- **Clash list** (7.1 Kb): [View](#)
- **Ramachandran plot kinemage** (443 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (40 Kb): [View in KiNG](#) | [Download](#)

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