



Analysis output: all-atom contacts and geometry for cnga3_sm_407-599H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	65.92		1 st percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	12	1.78%	Goal: <1%
	Ramachandran outliers	16	2.09%	Goal: <0.05%
	Ramachandran favored	652	85.34%	Goal: >98%
	MolProbity score^	3.13		18 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	0.55%	Goal: 0
	Bad backbone bonds:	20 / 6252	0.32%	Goal: 0%
	Bad backbone angles:	92 / 8404	1.09%	Goal: <0.1%

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

* 100th 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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 2.48 points.

Multi-criterion visualizations



[View](#) (782 Kb)

Single-criterion visualizations

- **Clash list** (19 Kb): [View](#)
- **Ramachandran plot kinemage** (455 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (54 Kb): [View in KiNG](#) | [Download](#)

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