

Analysis output: all-atom contacts and geometry for AIFM1_127-610_FFX1H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.67		99 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	13	3.27%	Goal: <0.3%
	Favored rotamers	358	90.18%	Goal: >98%
	Ramachandran outliers	7	1.45%	Goal: <0.05%
	Ramachandran favored	438	90.87%	Goal: >98%
	MolProbity score [^]	1.63		91 st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	0.68%	Goal: 0
	Bad bonds:	0/3796	0.00%	Goal: 0%
	Bad angles:	25 / 5137	0.49%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0/26	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 483	0.21%	Goal: 0

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

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 0.14 points.

Multi-criterion visualizations

^{* 100&}lt;sup>th</sup> 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.



View (501 Kb)

Single-criterion visualizations

- Clash list (385 bytes): View
- Ramachandran plot kinemage (433 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (38 Kb): View in KiNG | Download

Continue >

About MolProbity | Website for the Richardson Lab | Using ecloud x-H | Internal reference 4.3