



Analysis output: all-atom contacts and geometry for SIX5_86-259H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	42.19	7 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.71%	Goal: <0.3%
	Favored rotamers	139	98.58%	Goal: >98%
	Ramachandran outliers	5	2.91%	Goal: <0.05%
	Ramachandran favored	165	95.93%	Goal: >98%
	MolProbity score [^]	2.38		54 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	5	3.07%	Goal: 0
	Bad bonds:	16 / 1450	1.10%	Goal: 0%
	Bad angles:	34 / 1954	1.74%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 10	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	2 / 173	1.16%	Goal: 0

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.

Multi-criterion visualizations



[View](#) (193 Kb)

Single-criterion visualizations

- **Clash list** (5.2 Kb): [View](#)
- **Ramachandran plot kinemage** (415 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (20 Kb): [View in KiNG](#) | [Download](#)

