

Analysis output: all-atom contacts and geometry for CEACAM16_21-223 FFX1H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.32		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	7	4.14%	Goal: <0.3%
	Favored rotamers	144	85.21%	Goal: >98%
	Ramachandran outliers	8	3.98%	Goal: <0.05%
	Ramachandran favored	155	77.11%	Goal: >98%
	MolProbity score [^]	1.86		83 rd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.09%	Goal: 0
	Bad bonds:	0 / 1592	0.00%	Goal: 0%
	Bad angles:	18 / 2179	0.83%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	1 / 15	6.67%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	1 / 187	0.53%	Goal: <0.05%
	Twisted Peptides:	2 / 202	0.99%	Goal: 0

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

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.

Single-criterion visualizations

- Clash list (217 bytes): View
- Ramachandran plot kinemage (417 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (22 Kb): View in KiNG | Download

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