

Analysis output: all-atom contacts and geometry for LARS2_78-901_FFX1H.pdb

Summary statistics

All-Atom Contacts	,	5.15		97 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	24	3.39%	Goal: <0.3%
	Favored rotamers	601	84.89%	Goal: >98%
	Ramachandran outliers	22	2.68%	Goal: <0.05%
	Ramachandran favored	711	86.50%	Goal: >98%
	MolProbity score [^]	2.14		68 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	22	2.83%	Goal: 0
	Bad bonds:	12 / 6702	0.18%	Goal: 0%
	Bad angles:	69 / 9114	0.76%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 50	4.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	6 / 773	0.78%	Goal: <0.05%
	Twisted Peptides:	1 / 823	0.12%	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.

View (867 Kb)

Single-criterion visualizations

- Clash list (1.9 Kb): View
- Ramachandran plot kinemage (454 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (58 Kb): View in KiNG | Download

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