

Analysis output: all-atom contacts and geometry for HARS2_55-505_FFX1H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.21		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	22	2.82%	Goal: <0.3%
	Favored rotamers	680	87.18%	Goal: >98%
	Ramachandran outliers	3	0.33%	Goal: <0.05%
	Ramachandran favored	829	92.32%	Goal: >98%
	MolProbity score [^]	1.40		97 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	12	1.45%	Goal: 0
	Bad bonds:	0 / 7280	0.00%	Goal: 0%
	Bad angles:	63 / 9794	0.64%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0/34	0.00%	Expected: ≤1 per chain, or ≤5%

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

Multi-criterion visualizations



View (937 Kb)

Single-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.

- Clash list (301 bytes): View
- Ramachandran plot kinemage (462 Kb): View in KiNG | Download
 Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (61 Kb): View in KiNG | Download

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