



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

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	20.23	32 nd percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	0.38%	Goal: <0.3%
	Favored rotamers	755	96.79%	Goal: >98%
	Ramachandran outliers	8	0.89%	Goal: <0.05%
	Ramachandran favored	868	96.66%	Goal: >98%
	MolProbity score [^]	2.01		75 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	0.24%	Goal: 0
	Bad bonds:	33 / 7280	0.45%	Goal: 0%
	Bad angles:	15 / 9794	0.15%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 34	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	2 / 900	0.22%	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.

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 0.07 points.

Multi-criterion visualizations



Multi-criterion chart

[View](#) (963 Kb)

Single-criterion visualizations

- **Clash list** (12 Kb): [View](#)
- **Ramachandran plot kinemage** (463 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C β deviation scatter plot** (57 Kb): [View in KiNG](#) | [Download](#)

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