

Analysis output: all-atom contacts and geometry for RDX_1-325.pdb_29_1H.pdb

Summary statistics

Contacts	Clashscore, all atoms:	1.28		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	0	0.00%	Goal: <1%
	Ramachandran outliers	5	1.55%	Goal: <0.05%
	Ramachandran favored	296	91.64%	Goal: >98%
	MolProbity score [^]	1.35		98 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	2.24%	Goal: 0
	Bad backbone bonds:	0 / 2785	0.00%	Goal: 0%
	Bad backbone angles:	30 / 3753	0.80%	Goal: <0.1%

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

Multi-criterion visualizations



View (311 Kb)

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^{* 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 (427 bytes): View
- Ramachandran plot kinemage (424 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (30 Kb): View in KiNG | Download



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