Analysis output: all-atom contacts and geometry for RDX_3-583H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	36.45		9th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	0.97%	Goal: <0.3%
	Favored rotamers	501	97.09%	Goal: >98%
	Ramachandran outliers	11	1.90%	Goal: <0.05%
	Ramachandran favored	548	94.65%	Goal: >98%
	MolProbity score^	2.41		52nd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	1.24%	Goal: 0
	Bad bonds:	26 / 4892	0.53%	Goal: 0%
	Bad angles:	86 / 6568	1.31%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	1 / 24	4.17%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	2 / 556	0.36%	Goal: <0.05%
	Twisted Peptides:	2 / 580	0.34%	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* fix 1 bad rotamers and improve your clashscore by 0.52 points.

Multi-criterion visualizations

View (642 Kb)

Single-criterion visualizations

- **Clash list** (15 Kb): View
- **Ramachandran plot kinemage** (439 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (40 Kb): View in KiNG | Download

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