

Analysis output: all-atom contacts and geometry for LOXL3_187-536H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	159.91		0 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	8	2.92%	Goal: <0.3%
	Favored rotamers	259	94.53%	Goal: >98%
	Ramachandran outliers	14	4.02%	Goal: <0.05%
	Ramachandran favored	310	89.08%	Goal: >98%
	MolProbity score [^]	3.59		7 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	16	5.26%	Goal: 0
	Bad bonds:	87 / 2688	3.24%	Goal: 0%
	Bad angles:	130 / 3640	3.57%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 12	0.00%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	2/337	0.59%	Goal: <0.05%
	Twisted Peptides:	7 / 349	2.01%	Goal: 0

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

By adding H to this model and allowing Asn/Gln/His flips, we could *automatically* improve your clashscore by 1.19 points.

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 (403 Kb)

Single-criterion visualizations

- Clash list (35 Kb): View
- Ramachandran plot kinemage (426 Kb): View in KiNG | Download
- Ramachandran plot PDF (1.7 Mb): View
- Cβ deviation scatter plot (28 Kb): View in KiNG | Download

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