

## Analysis output: all-atom contacts and geometry for USH2A\_3729-4051\_FFX1H.pdb

## **Summary statistics**

All-Atom Contacts	Clashscore, all atoms:	4.81		94 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	7	2.48%	Goal: <0.3%
	Favored rotamers	259	91.84%	Goal: >98%
	Ramachandran outliers	13	4.05%	Goal: <0.05%
	Ramachandran favored	275	85.67%	Goal: >98%
	MolProbity score <sup>^</sup>	2.20		65 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	0.66%	Goal: 0
	Bad bonds:	0 / 2618	0.00%	Goal: 0%
	Bad angles:	38 / 3586	1.06%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	1/30	3.33%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	3 / 292	1.03%	Goal: <0.05%
	Twisted Peptides:	5/322	1.55%	Goal: 0

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

## **Multi-criterion visualizations**



View (348 Kb)

<sup>\* 100&</sup>lt;sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

<sup>^</sup> 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 (1.1 Kb): View
- Ramachandran plot kinemage (425 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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