Analysis output: all-atom contacts and geometry for MET_42-741_FFX1H.pdb

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	4.94		94th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	25	3.97%	Goal: <0.3%
	Favored rotamers	517	82.19%	Goal: >98%
	Ramachandran outliers	35	5.01%	Goal: <0.05%
	Ramachandran favored	555	79.51%	Goal: >98%
	MolProbity score^	2.46		50th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	6	0.91%	Goal: 0
	Bad bonds:	8 / 5646	0.14%	Goal: 0%
	Bad angles:	79 / 7658	1.03%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 34	5.88%	Expected: ≤1 per chain, or ≤5%
	Cis nonProlines:	2 / 665	0.30%	Goal: <0.05%
	Twisted Peptides:	4 / 699	0.57%	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.

Multi-criterion visualizations

View (743 Kb)

Single-criterion visualizations

- **Clash list** (2.4 Kb): View
- **Ramachandran plot kinemage** (449 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (49 Kb): View in KiNG | Download

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