

All Atom Contacts	Clashscore, all atom:	15.12	49 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (>0.4Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	31	2.81%	Goal: < 0.3%
	Favored rotamers	1006	91.29%	Goal: > 98%
	Ramachandran outliers	3	0.25%	Goal: < 0.05%
	Ramachandran favored	1163	96.20%	Goal: > 98%
	Rama distribution Z-score	-2.35 ± 0.21		Goal: abs (Z score) < 2
	MolProbity score [^]	2.28		60 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0/10212	0.00%	Goal: 0%
	Bad angles:	3/13740	0.02%	Goal: < 0.1%
Peptide Omegas	Cis Prolines:	2/43	4.65%	Expected: ≤1 per chain, or ≤5%
Low-resolution Criteria	CaBLAM outliers	15	1.3%	Goal: < 1.0%
	CA Geometry outliers	3	0.25%	Goal: < 0.5%
Additional Validations	Chiral volume outliers	0/1542		
	Waters with clashes	4/100	4.00%	

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.

Table 2. Molprobity validation score summary for retromer heterotrimer structure.