



# Analysis output: all-atom contacts and geometry for S1PR2\_6-218H.pdb

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	36.36	9 <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	2	1.11%	Goal: <0.3%
	Favored rotamers	174	96.67%	Goal: >98%
	Ramachandran outliers	3	1.42%	Goal: <0.05%
	Ramachandran favored	201	95.26%	Goal: >98%
	MolProbity score^	2.41	53 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)	
	Cβ deviations >0.25Å	1	0.49%	Goal: 0
	Bad bonds:	16 / 1670	0.96%	Goal: 0%
	Bad angles:	19 / 2278	0.83%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 4	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 212	0.47%	Goal: 0

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

\* 100<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.

## Multi-criterion visualizations



[View](#) (237 Kb)

## Single-criterion visualizations

- **Clash list** (5.3 Kb): [View](#)
- **Ramachandran plot kinemage** (417 Kb): [View in KiNG](#) | [Download](#)
- **Ramachandran plot PDF** (1.7 Mb): [View](#)
- **C $\beta$  deviation scatter plot** (22 Kb): [View in KiNG](#) | [Download](#)

