



# Viewing crb1\_sm\_148-184H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	20.53		31 <sup>st</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	3.33%	Goal: <1%
	Ramachandran outliers	1	2.86%	Goal: <0.05%
	Ramachandran favored	28	80.00%	Goal: >98%
	MolProbity score^	2.94		25 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	2 / 277	0.72%	Goal: 0%
	Bad backbone angles:	2 / 375	0.53%	Goal: <0.1%

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.

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 52.70	Clashscore: 20.53	Outliers: 1 of 35	Poor rotamers: 1 of 30	Outliers: 0 of 32	Outliers: 2 of 37	Outliers: 2 of 37
A 148	ASP	50	-	-	0.1% chi angles: 242.8,70.1	0.046Å	-	-
A 149	HIS	50	-	OUTLIER (0.02%) General / -174.4,66.7	20.5% ( <i>t</i> -160) chi angles: 185.5,204	0.038Å	OUTLIER(S) worst is CG--ND1: 4.681 σ	-
A 150	ASP	50	-	Favored (2.11%) General / -129.3,-31.0	13% ( <i>m</i> -20) chi angles: 300,273.5	0.047Å	-	-
A 151	GLU	50	0.428Å HB3 with A 170 TYR CD1	Favored (52.1%) General / -52.5,-34.9	20.7% ( <i>mm</i> -40) chi angles: 292.5,289.7,17.9	0.084Å	-	-

A 152	CYS	50	-	Allowed (0.92%) General / -90.3,38.1	48.9% ( <i>t</i> ) chi angles: 186.6	0.049Å	-	-
A 153	ALA	50	-	Favored (26.21%) General / -86.2,-24.1	-	0.047Å	-	-
A 154	SER	50	-	Favored (4.66%) General / -131.6,27.7	84.6% ( <i>p</i> ) chi angles: 68.4	0.028Å	-	-
A 155	SER	50	-	Favored (4.01%) Pre-proline / 50.4,67.8	89.4% ( <i>p</i> ) chi angles: 65.7	0.05Å	-	-
A 156	PRO	50	0.452Å O with A 182 HIS HD2	Favored (8.98%) Trans-proline / -68.2,-2.5	74.9% ( <i>Cg_endo</i> ) chi angles: 33.3	0.033Å	-	-
A 157	CYS	50	0.795Å HB3 with A 161 ALA HB3	Favored (14.47%) General / -98.6,160.1	43% ( <i>m</i> ) chi angles: 307.3	0.157Å	-	-
A 158	GLN	50	-	Favored (23.29%) General / -124.5,162.8	24.1% ( <i>mt-30</i> ) chi angles: 297.7,167.6,208.6	0.062Å	-	-
A 159	ASN	50	0.636Å HB3 with A 178 TYR CD2	Favored (16.46%) General / 60.7,40.2	80% ( <i>m-20</i> ) chi angles: 295.2,306.1	0.055Å	-	-
A 160	GLY	50	-	Favored (50.81%) Glycine / 53.8,34.2	-	-	-	-
A 161	ALA	50	0.924Å HB2 with A 183 CYS SG	Favored (35.65%) General / -69.2,158.1	-	0.248Å	-	OUTLIER(S) worst is C-CA- CB: 6.03 $\sigma$
A 162	VAL	50	0.681Å HB with A 173 PHE HB2	Favored (4.33%) Isoleucine or valine / -71.8,162.3	46.9% ( <i>t</i> ) chi angles: 183.3	0.079Å	-	-
A 163	CYS	50	-	Favored (5.05%) General /	26.4% ( <i>p</i> ) chi angles: 58.8	0.122Å	-	-

A 164	GLN	50	0.411Å O with A 170 TYR HB2	-132.3,100.6 Favored (16.95%) General / -96.4,155.0	52.4% ( <i>tt0</i> ) chi angles: 185.4,179.8,61.8	0.043Å	-	-
A 165	ASP	50	-	Favored (21.36%) General / -114.6,111.5	10.8% ( <i>t70</i> ) chi angles: 195.8,276.8	0.095Å	-	-
A 166	GLY	50	-	Favored (37.97%) Glycine / -93.6,-167.4	-	-	-	-
A 167	ILE	50	-	Favored (7.29%) Isoleucine or valine / -87.2,-21.3	45.7% ( <i>pt</i> ) chi angles: 63.2,169.4	0.085Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 52.70	Clashscore: 20.53	Outliers: 1 of 35	Poor rotamers: 1 of 30	Outliers: 0 of 32	Outliers: 2 of 37	Outliers: 2 of 37
A 168	ASP	50	-	Favored (13.58%) General / -102.7,-25.3	63.5% ( <i>m-20</i> ) chi angles: 295.5,303.2	0.025Å	-	-
A 169	GLY	50	-	Allowed (0.17%) Glycine / -177.0,-104.0	-	-	-	-
A 170	TYR	50	0.428Å CD1 with A 151 GLU HB3	Allowed (0.82%) General / -174.0,142.0	38.3% ( <i>p90</i> ) chi angles: 56.2,276.3	0.057Å	-	-
A 171	SER	50	-	Favored (15.12%) General / -126.1,111.8	25.7% ( <i>t</i> ) chi angles: 185.8	0.009Å	-	-
A 172	CYS	50	0.515Å HB2 with A 181 ARG O	Favored (47.78%) General / -72.8,143.7	68.8% ( <i>m</i> ) chi angles: 301.8	0.052Å	-	-
A 173	PHE	50	0.681Å HB2 with A 162 VAL HB	Allowed (1.64%) General / -110.6,82.7	43.1% ( <i>m-85</i> ) chi angles: 287.4,74.4	0.01Å	-	-
				Favored				

A 174	CYS	50	-	(3.03%) General / -58.7,163.9	28.7% ( <i>m</i> ) chi angles: 310.4	0.1Å	-	-
A 175	VAL	50	0.434Å HB with A 176 PRO HD2	Favored (12.23%) Pre-proline / -82.0,171.3	26.9% ( <i>m</i> ) chi angles: 296.3	0.13Å	-	-
A 176	PRO	50	0.434Å HD2 with A 175 VAL HB	Favored (25.62%) Trans-proline / -53.2,-24.3	81.3% ( <i>Cg_exo</i> ) chi angles: 330.4	0.077Å	-	-
A 177	GLY	50	-	Favored (95.05%) Glycine / -65.7,-39.0	-	-	-	-
A 178	TYR	99.99	0.636Å CD2 with A 159 ASN HB3	Allowed (1.54%) General / -118.9,-168.3	98.7% ( <i>m-85</i> ) chi angles: 296.6,273.7	0.044Å	-	-
A 179	GLN	50	-	Allowed (0.91%) General / -174.1,143.3	65.3% ( <i>tt0</i> ) chi angles: 186.1,178.6,0.4	0.073Å	-	-
A 180	GLY	50	-	Favored (12%) Glycine / 124.5,164.7	-	-	-	-
A 181	ARG	50	0.515Å O with A 172 CYS HB2	Favored (48.06%) General / -55.0,-27.9	2.3% ( <i>tpt180</i> ) chi angles: 197.4,93.8,161.1,253.9	0.115Å	-	-
A 182	HIS	50	0.452Å HD2 with A 156 PRO O	Favored (4.03%) General / -133.3,17.6	79% ( <i>m80</i> ) chi angles: 297.7,88.5	0.059Å	OUTLIER(S) worst is CD2-- NE2: 4.224 σ	OUTLIER(S) worst is CB- CG-CD2: 4.145 σ
A 183	CYS	50	0.924Å SG with A 161 ALA HB2	Favored (7.66%) General / 58.2,21.0	4% ( <i>m</i> ) chi angles: 319.8	0.067Å	-	-
A 184	ASP	99.99	-	-	36.2% ( <i>t70</i> ) chi angles: 185,67.6	0.091Å	-	-

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