



# Viewing crb1\_mb\_1143-1176\_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0	100 <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	1	3.33%	Goal: <1%
	Ramachandran outliers	1	3.12%	Goal: <0.05%
	Ramachandran favored	24	75.00%	Goal: >98%
	MolProbity score <sup>^</sup>	1.69		89 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 264	0.00%	Goal: 0%
	Bad backbone angles:	2 / 358	0.56%	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	Cβ deviation	Bond lengths	Bond angles
		Avg: 71.90	Clashscore: 0	Outliers: 1 of 32	Poor rotamers: 1 of 30	Outliers: 0 of 30	Outliers: 0 of 34	Outliers: 2 of 34
1143	CYS	30.63	-	-	32.8% (m) chi angles: 309.6	0.116Å	-	-
1144	ASN	76.37	-	Favored (13.53%) General / -47.5,130.1	1.4% (t30) chi angles: 204.1,100.7	0.054Å	-	-
1145	SER	101.47	-	Allowed (1.37%) General / 75.8,-9.8	39.8% (m) chi angles: 303.1	0.17Å	-	-
1146	ASN	77.38	-	Allowed (0.8%) Pre-proline / 51.4,40.5	23.8% (m-20) chi angles: 301.9,358.5	0.038Å	-	-
1147	PRO	84.18	-	Allowed (0.54%)	0.1%	0.121Å	-	OUTLIER(S) worst is N-CA-

			Trans-proline / -86.4,37.5	chi angles: 47.6	CB: 4.73 $\sigma$			
1148	CYS	79.05	-	Favored (35%) General / -118.3,152.9	83.6% ( <i>m</i> ) chi angles: 295.7	0.081Å	-	-
1149	LEU	115.67	-	Favored (11.64%) General / -125.2,170.0	4.6% ( <i>mp</i> ) chi angles: 303.6,90.3	0.042Å	-	-
1150	HIS	74.48	-	Allowed (0.97%) General / 62.4,3.0	75.3% ( <i>m80</i> ) chi angles: 298.3,92.8	0.138Å	-	-
1151	GLY	23.8	-	Favored (57.94%) Glycine / 97.1,6.3	-	-	-	-
1152	GLY	20.3	-	Favored (49.16%) Glycine / -68.0,148.4	-	-	-	-
1153	ASN	33.21	-	Favored (16.14%) General / -99.4,157.8	24.7% ( <i>t-20</i> ) chi angles: 201.5,349.9	0.045Å	-	-
1154	CYS	42.88	-	Favored (51.18%) General / -122.9,129.1	1.5% ( <i>t</i> ) chi angles: 159.1	0.077Å	-	-
1155	GLU	53.11	-	Favored (25.72%) General / -121.8,159.9	1.1% ( <i>pm0</i> ) chi angles: 96.9,302.5,20.7	0.139Å	-	-
1156	ASP	48.54	-	Favored (7.86%) General / -124.8,103.1	26.1% ( <i>m-20</i> ) chi angles: 308.6,329.8	0.037Å	-	-
1157	ILE	101.26	-	Favored (7.19%) Isoleucine or valine / -102.3,148.9	1.7% ( <i>mp</i> ) chi angles: 283.2,60.6	0.08Å	-	-
1158	TYR	176.1	-	Favored (34.72%) General / -53.5,138.0	77.6% ( <i>t80</i> ) chi angles: 176,70.6	0.031Å	-	-
1159	SER	150.74	-	Favored (2.01%) General / 72.6,-4.7	5% ( <i>t</i> ) chi angles: 199.8	0.198Å	-	-
1160	SER	104.47	-	OUTLIER (0.04%) General / 174.6,134.0	32.4% ( <i>t</i> ) chi angles: 184.2	0.122Å	-	-

1161	TYR	148.55	-	Favored (14.68%) General / -68.6,167.6	9.4% ( <i>p</i> 90) chi angles: 82.7,273.7	0.052Å	-	-
1162	HIS	57.62	-	Favored (8.85%) General / -134.7,176.2	8.6% ( <i>m</i> -70) chi angles: 322,305.5	0.074Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 71.90	Clashscore: 0	Outliers: 1 of 32	Poor rotamers: 1 of 30	Outliers: 0 of 30	Outliers: 0 of 34	Outliers: 2 of 34
1163	CYS	100.49	-	Favored (49.68%) General / -131.3,139.9	28.4% ( <i>t</i> ) chi angles: 190.1	0.09Å	-	-
1164	SER	90.14	-	Allowed (1.97%) General / -99.0,73.6	79.3% ( <i>p</i> ) chi angles: 70	0.056Å	-	-
1165	CYS	46.25	-	Favored (50.42%) Pre-proline / -60.6,120.2	79.6% ( <i>m</i> ) chi angles: 299.5	0.032Å	-	-
1166	PRO	61.4	-	Favored (64.6%) Trans-proline / -70.7,153.2	78.3% ( <i>Cg_exo</i> ) chi angles: 333.5	0.065Å	-	-
1167	LEU	41.07	-	Favored (13.4%) General / -48.1,128.1	57% ( <i>tp</i> ) chi angles: 182.4,63.6	0.062Å	-	-
1168	GLY	21.04	-	Favored (37.78%) Glycine / 107.8,-14.9	-	-	-	-
1169	TRP	49.32	-	Favored (15.24%) General / -127.2,168.1	4.1% ( <i>m</i> 95) chi angles: 325.6,96.5	0.034Å	-	-
1170	SER	75.67	-	Allowed (0.55%) General / -149.4,-154.4	8.8% ( <i>t</i> ) chi angles: 193.4	0.147Å	-	-
1171	GLY	21.21	-	Favored (52.09%) Glycine / 72.4,-156.4	-	-	-	-
1172	LYS	56.89	-	Favored (29.24%)	41% ( <i>tttt</i> ) chi angles:	0.065Å	-	-

				General / -107.7,8.8 Allowed (0.46%) General / -146.9,-9.8	210,192.8,180.7,194.1			
1173	HIS	94.62	-		11.4% ( <i>m80</i> ) chi angles: 315.3,76.7	0.085Å	-	OUTLIER(S) worst is CA- CB-CG: 4.694 σ
1174	CYS	72.07	-	Favored (6.4%) General / 64.7,39.4	6.4% ( <i>m</i> ) chi angles: 317.1	0.172Å	-	-
1175	GLU	83.27	-	Favored (77.31%) General / -67.9,-34.8	4.1% ( <i>pm0</i> ) chi angles: 55.8,280.6,57.6	0.172Å	-	-
1176	LEU	31.34	-	-	88.9% ( <i>mt</i> ) chi angles: 301.2,177.3	0.055Å	-	-

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