



# Viewing crb1\_sm\_113-222\_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.3		99 <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	3	3.26%	Goal: <1%
	Ramachandran outliers	7	6.48%	Goal: <0.05%
	Ramachandran favored	72	66.67%	Goal: >98%
	MolProbity score^	2.11		69 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	3.06%	Goal: 0
	Bad backbone bonds:	0 / 833	0.00%	Goal: 0%
	Bad backbone angles:	13 / 1131	1.15%	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: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 113	SER	50	0.573Å N with A 125 CYS HG	-	54.2% ( <i>p</i> ) chi angles: 55.1	0.199Å	-	-
A 114	CYS	50	-	Allowed (1.17%) General / -96.1,-164.6	58.6% ( <i>m</i> ) chi angles: 305.1	0.102Å	-	-
A 115	GLY	50	-	Favored (93.99%) Glycine / -57.6,-44.0	-	-	-	-
A 116	LYS	50	-	Favored (6.03%) General / -75.4,104.6	25.4% ( <i>tptp</i> ) chi angles: 169.4,58.8,168.9,75.6	0.057Å	-	-

A 117	ASN	50	-	Favored (8.74%) General / -68.1,116.5	58.9% ( <i>t30</i> ) chi angles: 186.4,42.1	0.051Å	-	-
A 118	SER	50	-	Favored (71.92%) General / -57.2,-37.2	45.3% ( <i>m</i> ) chi angles: 302.4	0.097Å	-	-
A 119	CYS	50	-	Favored (41.81%) General / -97.6,-2.3	29% ( <i>p</i> ) chi angles: 66.2	0.049Å	-	-
A 120	GLN	50	-	OUTLIER (0.03%) General / 50.8,-94.5	29.3% ( <i>mt-30</i> ) chi angles: 290.2,160.9,231.3	0.169Å	-	-
A 121	HIS	50	-	Favored (73.45%) General / -66.9,-32.3	28.4% ( <i>p-80</i> ) chi angles: 55.7,267.6	0.133Å	-	-
A 122	GLY	50	-	Favored (9%) Glycine / 162.2,157.5	-	-	-	-
A 123	GLY	50	-	Favored (20.37%) Glycine / 132.2,-174.3	-	-	-	-
A 124	ILE	50	-	Allowed (1.93%) Isoleucine or valine / -85.2,82.5	51.6% ( <i>mm</i> ) chi angles: 302.1,302.4	0.073Å	-	-
A 125	CYS	50	0.573Å HG with A 113 SER N	Favored (4.41%) General / -73.7,103.9	21.1% ( <i>p</i> ) chi angles: 55.3	0.063Å	-	-
A 126	HIS	50	-	Favored (8.99%) General / -115.4,169.7	23.8% ( <i>t-80</i> ) chi angles: 170.4,274.5	0.161Å	-	OUTLIER(S) worst is CA- CB-CG: 6.597 σ
A 127	GLN	50	-	Favored (52.67%) General / -127.6,137.9	39.3% ( <i>tp60</i> ) chi angles: 182.5,61.7,79.8	0.087Å	-	-
A 128	ASP	50	-	Allowed (0.12%) Pre-proline / -132.2,-166.9	5.5% ( <i>m-20</i> ) chi angles: 303,81.6	0.115Å	-	-
A	PRO	50	-	Allowed (0.27%)	21.9% ( <i>Cg_exo</i> )	0.032Å	-	-

129				Trans-proline / -65.1,96.8 Allowed (0.13%)	chi angles: 324.3			
A 130	ILE	50	-	Isoleucine or valine / 80.1,-67.6	49.3% ( <i>mm</i> ) chi angles: 301,297.6	0.191Å	-	-
A 131	TYR	50	-	Favored (74.98%) Pre-proline / -58.2,125.4	81.3% ( <i>m-85</i> ) chi angles: 304,277.9	0.072Å	-	-
A 132	PRO	50	-	Allowed (0.12%) Trans-proline / -95.8,78.7	10.3% ( <i>Cg_endo</i> ) chi angles: 40.2	0.087Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 133	VAL	50	-	Favored (13.75%) Isoleucine or valine / -74.9,143.1	85% ( <i>t</i> ) chi angles: 179	0.066Å	-	-
A 134	CYS	50	-	Favored (13.02%) General / -85.0,170.4	92.5% ( <i>m</i> ) chi angles: 293.6	0.096Å	-	-
A 135	ILE	50	-	Favored (46.67%) Isoleucine or valine / -101.6,117.3	37.6% ( <i>mm</i> ) chi angles: 305.9,306.1	0.048Å	-	-
A 136	CYS	50	-	Favored (75.33%) Pre-proline / -56.2,131.6	0.7% chi angles: 28.5	0.092Å	-	-
A 137	PRO	50	-	Favored (4.76%) Trans-proline / -83.7,129.0	67.1% ( <i>Cg_endo</i> ) chi angles: 33.8	0.052Å	-	-
A 138	ALA	50	-	Allowed (1.26%) General / 45.6,-126.6	-	0.221Å	-	OUTLIER(S) worst is C-CA- CB: 5.145 σ
A 139	GLY	50	-	Favored (52.53%) Glycine / -86.2,14.9 Favored	-	-	-	-

A 140	TYR	50	-	(6.42%) General / -55.1,120.1	21.9% ( <i>t80</i> ) chi angles: 197.7,95.6	0.055Å	-	-
A 141	ALA	50	-	Allowed (0.07%) General / -155.4,-83.0	-	0.098Å	-	-
A 142	GLY	50	-	Allowed (1.37%) Glycine / 75.2,-75.2	-	-	-	-
A 143	ARG	50	-	Allowed (1.66%) General / -131.2,-31.4	44.3% ( <i>tpt85</i> ) chi angles: 185.8,64.1,192.5,77	0.073Å	-	-
A 144	PHE	50	-	Allowed (0.12%) General / -161.6,24.4	27.1% ( <i>m-85</i> ) chi angles: 280.2,299.9	0.045Å	-	-
A 145	CYS	50	-	Allowed (0.36%) General / 72.8,44.5	33.3% ( <i>m</i> ) chi angles: 309.5	0.209Å	-	-
A 146	GLU	50	-	Favored (2.48%) General / -133.3,-15.9	16.3% ( <i>pt-20</i> ) chi angles: 68.6,177.5,324.6	0.068Å	-	-
A 147	ILE	50	-	Favored (28.27%) Isoleucine or valine / -136.2,147.0	8.9% ( <i>mm</i> ) chi angles: 285.5,284.3	0.093Å	-	-
A 148	ASP	50	-	Favored (2.69%) General / -52.7,154.5	3.9% ( <i>m-20</i> ) chi angles: 304.2,192.6	0.054Å	-	OUTLIER(S) worst is CA- CB-CG: 4.343 σ
A 149	HIS	50	-	Favored (2.69%) General / -145.5,95.6	41.8% ( <i>t-80</i> ) chi angles: 173.5,257.4	0.096Å	-	-
A 150	ASP	50	-	Favored (17.76%) General / -52.4,142.3	11.1% ( <i>t70</i> ) chi angles: 170.7,49	0.11Å	-	-
A 151	GLU	50	-	Favored (13.95%) General / -105.8,-18.8	68.3% ( <i>mm-40</i> ) chi angles: 299.7,304,342.5	0.082Å	-	-
				Favored				

A 152	CYS	50	-	(81.33%) General / -67.1,-36.1	0.6% chi angles: 91.7	0.247Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 153	ALA	50	-	Favored (43.84%) General / -79.1,-23.9	-	0.094Å	-	-
A 154	SER	50	-	Favored (45.75%) General / -79.2,-21.8	29.8% ( <i>m</i> ) chi angles: 286.4	0.16Å	-	-
A 155	SER	50	-	Favored (4.62%) Pre-proline / -146.7,58.7	32.3% ( <i>t</i> ) chi angles: 175.1	0.07Å	-	-
A 156	PRO	50	-	Favored (19.92%) Trans-proline / -75.8,-12.9	23.6% ( <i>Cg_endo</i> ) chi angles: 38.1	0.034Å	-	-
A 157	CYS	50	-	Allowed (0.57%) General / 64.6,67.1	93% ( <i>m</i> ) chi angles: 293.6	0.138Å	-	-
A 158	GLN	50	-	Allowed (1.18%) General / 57.8,-119.6	5.3% ( <i>tt0</i> ) chi angles: 201.8,202.6,128.3	0.192Å	-	OUTLIER(S) worst is C-CA- CB: 4.099 σ
A 159	ASN	50	-	Favored (4.07%) General / -133.2,9.4	4.3% ( <i>p30</i> ) chi angles: 60.6,100.2	0.074Å	-	-
A 160	GLY	50	-	Favored (6.97%) Glycine / -86.8,26.0	-	-	-	-
A 161	ALA	50	-	Favored (15.13%) General / -163.9,154.2	-	0.114Å	-	-
A 162	VAL	50	-	Favored (13.43%) Isoleucine or valine / -93.3,102.2	16.8% ( <i>m</i> ) chi angles: 291	0.127Å	-	-
				Favored				

A 163	CYS	50	-	(26.5%) General / -82.3,151.9	17.8% ( <i>p</i> ) chi angles: 71.6	0.107Å	-	-
A 164	GLN	50	-	Favored (10.47%) General / -157.2,134.5	28.4% ( <i>tp60</i> ) chi angles: 178.2,66.5,87.3	0.139Å	-	-
A 165	ASP	50	-	Allowed (1.39%) General / -126.0,-165.1	2.6% ( <i>t70</i> ) chi angles: 209.7,101.6	0.09Å	-	OUTLIER(S) worst is C-N- CA: 4.063 $\sigma$
A 166	GLY	50	-	Allowed (0.4%) Glycine / 156.5,-16.3	-	-	-	-
A 167	ILE	50	-	Allowed (0.72%) Isoleucine or valine / -137.7,23.8	1.6% ( <i>pp</i> ) chi angles: 46.5,58.2	0.166Å	-	-
A 168	ASP	99.99	-	Allowed (0.61%) General / 71.0,44.1	2% ( <i>m-20</i> ) chi angles: 319.8,92.2	0.156Å	-	-
A 169	GLY	50	-	Allowed (1.47%) Glycine / -179.5,130.2	-	-	-	-
A 170	TYR	50	-	Favored (6.53%) General / -120.7,174.5	4.9% ( <i>p90</i> ) chi angles: 82.7,290.8	0.066Å	-	-
A 171	SER	50	-	Favored (13.08%) General / -139.5,172.2	10.5% ( <i>t</i> ) chi angles: 191.9	0.04Å	-	-
A 172	CYS	50	-	Favored (3.8%) General / -152.9,112.0	16.5% ( <i>p</i> ) chi angles: 72.8	0.122Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 173	PHE	50	-	Favored (14.18%) General / -86.7,102.4	6.9% ( <i>m-30</i> ) chi angles: 315.5,314.1	0.046Å	-	-
A 174	CYS	50	-	Favored (19.98%) General /	7.5% ( <i>p</i> ) chi angles: 49.7	0.031Å	-	-

A 175	VAL	50	-	-64.4,160.0 Favored (91.66%) Pre-proline / -60.4,141.0	5.7% ( <i>p</i> ) chi angles: 75.3	0.096Å	-	-
A 176	PRO	50	-	Allowed (1.28%) Trans-proline / -75.7,88.6	74.1% ( <i>Cg_endo</i> ) chi angles: 28.7	0.053Å	-	-
A 177	GLY	50	-	Allowed (1.12%) Glycine / 149.9,-19.9	-	-	-	-
A 178	TYR	50	-	Favored (8.81%) General / -131.6,107.4	88.8% ( <i>m-85</i> ) chi angles: 298.3,84.6	0.035Å	-	-
A 179	GLN	50	-	Allowed (0.29%) General / -134.1,-147.5	1.7% ( <i>pp0?</i> ) chi angles: 61,103.4,0.7	0.222Å	-	-
A 180	GLY	50	-	Favored (16.68%) Glycine / 91.2,-143.6	-	-	-	-
A 181	ARG	50	-	Favored (5.6%) General / -124.7,31.8	6% ( <i>mmp_?</i> ) chi angles: 284.1,293.9,81.7,187	0.172Å	-	-
A 182	HIS	50	-	Favored (2.98%) General / -134.2,-0.7	0% chi angles: 7.6,289.5	0.243Å	-	OUTLIER(S) worst is CA- CB-CG: 4.644 σ
A 183	CYS	50	-	Favored (13.66%) General / 57.1,49.4	71.8% ( <i>m</i> ) chi angles: 297.8	0.254Å	-	OUTLIER(S) worst is C-N- CA: 4.265 σ
A 184	ASP	50	-	Allowed (0.38%) General / -150.6,-1.8	11.8% ( <i>p30</i> ) chi angles: 46.4,10.3	0.039Å	-	-
A 185	LEU	99.99	-	Favored (23.3%) General / -88.1,113.0	18.8% ( <i>mt</i> ) chi angles: 310.8,189.4	0.047Å	-	-
A 186	GLU	50	-	Favored (31.91%) General / -64.3,127.5	29.8% ( <i>tt0</i> ) chi angles: 196.3,173.8,265.4	0.058Å	-	-

A 187	VAL	50	-	OUTLIER (0.02%) Isoleucine or valine / 42.8,-137.7	27.4% ( <i>m</i> ) chi angles: 295.9	0.333Å	-	OUTLIER(S) worst is C-CA- CB: 4.261 σ	
A 188	ASP	50	-	Favored (29.02%) General / -140.8,164.9	2.7% ( <i>t0</i> ) chi angles: 211.4,302.9	0.051Å	-	-	
A 189	GLU	50	-	Allowed (1.04%) General / -139.9,-14.6	17.1% ( <i>tt0</i> ) chi angles: 198.7,199,209.7	0.098Å	-	-	
A 190	CYS	50	-	Favored (58.68%) General / -77.4,-16.8	16% ( <i>p</i> ) chi angles: 73.3	0.136Å	-	-	
A 191	ALA	50	-	Favored (2.42%) General / -51.0,-22.7	-	0.122Å	-	-	
A 192	SER	50	-	Favored (58.8%) General / -80.2,-14.0	14.5% ( <i>p</i> ) chi angles: 48.7	0.125Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 193	ASP	99.99	-	Favored (23.66%) Pre-proline / -116.1,131.7	49.5% ( <i>t0</i> ) chi angles: 176.7,8	0.092Å	-	OUTLIER(S) worst is CA- CB-CG: 5.612 σ	
A 194	PRO	50	-	Allowed (0.83%) Trans-proline / -88.8,22.6	1.8% ( <i>Cg_endo</i> ) chi angles: 42.1	0.035Å	-	-	
A 195	CYS	50	-	Allowed (0.31%) General / 78.7,-42.1	67.8% ( <i>m</i> ) chi angles: 287.8	0.232Å	-	-	
A 196	LYS	50	-	Allowed (1.26%) General / 65.9,52.2	7% ( <i>tptp</i> ) chi angles: 154.7,59.6,207.8,75.4	0.303Å	-	OUTLIER(S) worst is C-CA- CB: 4.759 σ	
A 197	ASN	50	-	OUTLIER (0%) General / 121.7,-156.0	9.1% ( <i>m-20</i> ) chi angles: 289.4,21.1	0.223Å	-	-	
				Favored					



A 198	GLU	99.99	-	(60.51%) General / -67.8,-12.4	3.8% ( <i>mp0</i> ) chi angles: 306.5,94.6,302.7	0.057Å	-	-
A 199	ALA	50	-	Allowed (0.12%) General / -44.3,154.3	-	0.11Å	-	-
A 200	THR	50	-	Favored (39.31%) General / -129.7,126.9	22.7% ( <i>p</i> ) chi angles: 49.4	0.092Å	-	-
A 201	CYS	50	-	Favored (6.97%) General / -82.5,85.4	21.3% ( <i>p</i> ) chi angles: 55.4	0.077Å	-	-
A 202	LEU	50	-	Favored (6.52%) General / -72.0,110.5	64.6% ( <i>tp</i> ) chi angles: 179.1,63.4	0.031Å	-	-
A 203	ASN	99.99	-	Favored (11.84%) General / -48.0,136.1	40.7% ( <i>t30</i> ) chi angles: 180.1,22.4	0.062Å	-	-
A 204	GLU	50	-	Favored (3.75%) General / -148.9,-170.9	1.9% ( <i>mm-40</i> ) chi angles: 251,314.8,333	0.07Å	-	-
A 205	ILE	50	-	OUTLIER (0.05%) Isoleucine or valine / -70.3,61.5	44.6% ( <i>pt</i> ) chi angles: 57.2,172	0.139Å	-	-
A 206	GLY	50	-	Favored (34.63%) Glycine / 72.7,45.5	-	-	-	-
A 207	ARG	50	0.411Å HH12 with A 209 THR HG22	OUTLIER (0%) General / 170.7,52.2	3% ( <i>ptm-85</i> ) chi angles: 48.1,162.5,304.1,302.2	0.099Å	-	-
A 208	TYR	99.99	-	Favored (22.2%) General / -50.7,136.2	40.6% ( <i>p90</i> ) chi angles: 64.2,83	0.089Å	-	-
A 209	THR	50	0.411Å HG22 with A 207 ARG HH12	Favored (4.64%) General / -95.8,87.5	16.2% ( <i>p</i> ) chi angles: 75.3	0.132Å	-	-
A	CYS	50	-	Allowed (1.2%) General /	43.3% ( <i>t</i> )	0.055Å	-	-

210				-65.7,105.2	chi angles: 176.2				
A 211	ILE	50	-	Favored (42.58%) Isoleucine or valine / -132.7,142.4	32.6% ( <i>pt</i> ) chi angles: 57.4,177.8	0.052Å	-	-	
A 212	CYS	50	-	Favored (17.97%) Pre-proline / -119.5,75.6	10.6% ( <i>t</i> ) chi angles: 195.7	0.035Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 1.3	Outliers: 7 of 108	Poor rotamers: 3 of 92	Outliers: 3 of 98	Outliers: 0 of 110	Outliers: 12 of 110
A 213	PRO	50	-	Favored (3.68%) Trans-proline / -91.1,166.9	9% ( <i>Cg_endo</i> ) chi angles: 40.5	0.101Å	-	-	
A 214	HIS	50	-	Favored (3.14%) General / -76.4,75.2	7.5% ( <i>t60</i> ) chi angles: 204.2,91.1	0.048Å	-		OUTLIER(S) worst is CA- CB-CG: 4.381 σ
A 215	ASN	50	-	Favored (39.11%) General / -76.8,-42.7	13.7% ( <i>p30</i> ) chi angles: 46.4,16.4	0.111Å	-	-	
A 216	TYR	50	-	OUTLIER (0.03%) General / -168.1,14.4	9.2% ( <i>p90</i> ) chi angles: 45.7,255	0.041Å	-	-	
A 217	SER	99.99	-	Favored (12.95%) General / -83.8,171.6	96.9% ( <i>p</i> ) chi angles: 63.9	0.073Å	-	-	
A 218	GLY	50	-	Favored (4.67%) Glycine / -98.1,-36.5	-	-	-	-	
A 219	VAL	50	-	Favored (2.75%) Isoleucine or valine / -63.1,160.1	1.7% ( <i>p</i> ) chi angles: 83.7	0.103Å	-	-	
A 220	ASN	50	-	Favored (2.21%) General / -73.6,-60.5	10.1% ( <i>t30</i> ) chi angles: 168.6,75.4	0.124Å	-		OUTLIER(S) worst is C-N- CA: 4.104 σ
A				OUTLIER					

221	CYS	50	-	(0.02%) General / -169.8,38.4	94.4% ( <i>m</i> ) chi angles: 293.8	0.079Å	-	-
A 222	GLU	99.99	-	-	19% ( <i>mp0</i> ) chi angles: 302.1,70.4,43.8	0.082Å	-	-

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