

## Viewing crb1\_sm\_186-299\_FFX1Hmulti.table

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All-Atom	Clashscore, all atoms:	0		100 <sup>th</sup> percentile* (N=1784, all resolutions)			
Contacts	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.						
	Poor rotamers	3	3.16%	Goal: <1%			
	Ramachandran outliers	4	3.57%	Goal: <0.05%			
II I	Ramachandran favored	88 78.57%		Goal: >98%			
Protein Geometry	MolProbity score <sup>^</sup>	1.63		91 <sup>st</sup> percentile* (N=27675, 0Å - 99Å)			
	Cβ deviations >0.25Å	0	0.00%	Goal: 0			
	Bad backbone bonds:	0 / 858	0.00%	Goal: 0%			
	Bad backbone angles:	10 / 1167	0.86%	Goal: <0.1%			

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

<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	<b>Bond angles</b>
			0			Poor rotamers: 3 of			
			54.82	0	112	95	0 of 102	0 of 114	of 114
A 186	1	GLU	50	-	-	3.5% ( <i>mp0</i> ) chi angles: 306.4,85.8,302.6	0.04Å	-	OUTLIER(S) worst is C-N-CA: $4.674 \sigma$
A 187		VAL	50	-	Allowed (1.05%) Isoleucine or valine /-168.7,153.9	1% chi angles: 140.9	0.071Å	-	-
A 188		ASP	50	-	Favored (3.38%) General / -148.7,103.4	19% ( <i>t0</i> ) chi angles: 196.6,318.9	0.026Å	-	-
A 189		GLU	50	-	Favored (33.32%) General / -83.4,-20.9	1.4% ( <i>mp0</i> ) chi angles: 326.3,86.9,294.5	0.122Å	-	-
					Favored				

<sup>\* 100&</sup>lt;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.

A 190	CYS 50	-	(68.82%) General / -66.4,-28.7	59.2% ( <i>m</i> ) chi angles: 304.8	0.118Å	-	-
A 191	ALA 50	-	Favored (6.59%) General / -70.7,0.7	-	0.058Å	-	-
A 192	SER 99.99	-	Allowed (0.57%) General / -107.0,-80.0	20.7% ( <i>t</i> ) chi angles: 188.5	0.089Å	-	-
A 193	ASP 99.99	-	Favored (75.6%) Pre-proline / -137.3,155.9	4.4% ( <i>m</i> -20) chi angles: 290.5,81.2	0.066Å	-	-
A 194	PRO 99.99	-	Favored (6.59%) Trans-proline / -88.4,152.9	20.7% ( <i>Cg_endo</i> ) chi angles: 38.5	0.068Å	-	-
A 195	CYS 99.99	-	Favored (15.59%) General / -86.0,166.9	6.6% ( <i>t</i> ) chi angles: 199.8	0.059Å	-	-
A 196	LYS 99.99	-	Favored (25.6%) General / -81.1,156.8	18.8% ( <i>pttp</i> ) chi angles: 72.4,174,188.4,76.5	0.091Å	-	-
A 197	ASN 50	-	Allowed (0.94%) General / 78.2,20.2	26.3% ( <i>m120</i> ) chi angles: 306.2,121.4	0.132Å	-	-
A 198	GLU 50	-	Favored (29.87%) General / 55.4,38.1	44.6% ( <i>mt-10</i> ) chi angles: 294.4,189.8,47.4	0.106Å	-	-
A 199	ALA 50	-	Favored (27.89%) General / -81.0,152.7	-	0.044Å	-	-
A 200	THR 50	-	Favored (7.81%) General / -81.0,98.1	37.1% ( <i>m</i> ) chi angles: 306.1	0.083Å	-	-
A 201	CYS 50	-	Favored (26.38%) General / -60.7,126.2	92.2% ( <i>m</i> ) chi angles: 295	0.083Å	-	-
A 202	LEU 50	-	Favored (23.82%) General / -135.2,124.0	90.8% ( <i>mt</i> ) chi angles: 299.6,178.6	0.061Å	-	-
A 203	ASN 50	-	Favored (29.51%) General / -91.1,140.8	53.2% ( <i>t</i> 30) chi angles: 186.2,20.7	0.019Å	-	-

A 204	GLU	50	-	Allowed (0.53%) General / -97.0,-156.4	60.7% ( <i>mt-10</i> ) chi angles: 298.9,163.1,20.9	0.073Å	-	-
A 205	ILE	50	-	OUTLIER (0.07%) Isoleucine or valine / -86.5,32.9	45.6% ( <i>pt</i> ) chi angles: 60.7,169.4	0.178Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
		Avg:	Clashscore:	Outliers: 4 of	Poor rotamers: 3 of	Outliers:	Outliers:	Outliers: 10
		54.82	0	112	95	0 of 102	0 of 114	of 114
A 206	GLY	50	-	Allowed (0.17%) Glycine / 155.2,-1.2	-	-	-	-
A 207	ARG	50	-	Favored (4.19%) General / -171.2,154.9	5.5% ( <i>ptm-85</i> ) chi angles: 54.7,153.3,292.1,278.9	0.063Å	-	-
A 208	TYR	50	-	Favored (17.66%) General / -107.0,157.6	3.1% ( <i>p</i> 90) chi angles: 89.6,103.7	0.065Å	-	OUTLIER(S) worst is C-N-CA: $4.125 \sigma$
A 209	THR	50	-	Favored (39.21%) General / -119.0,150.9	91.2% ( <i>m</i> ) chi angles: 300.6	0.088Å	-	-
A 210	CYS	50	-	Favored (45.99%) General / -99.8,130.6	59.1% ( <i>m</i> ) chi angles: 285.7	0.101Å	-	-
A 211	ILE	50	-	Favored (3.17%) Isoleucine or valine /-84.7,92.3	35% ( <i>mm</i> ) chi angles: 305.8,307.2	0.059Å	-	-
A 212	CYS	50	-	Favored (52.67%) Pre-proline / -54.7,142.6	61.4% ( <i>m</i> ) chi angles: 303.7	0.085Å	-	-
A 213	PRO	50	-	Favored (7.47%) Trans-proline / -87.8,157.4	23.7% ( <i>Cg_endo</i> ) chi angles: 38.1	0.052Å	-	-
A 214	HIS	50	-	Allowed (1.51%) General / -65.5,106.8	24.4% ( <i>t-80</i> ) chi angles: 169.6,270.9	0.027Å	-	OUTLIER(S) worst is C-N- CA: 4.323 σ
A 215	ASN	50	-	OUTLIER (0%) General / 146.4,-22.3	26.3% ( <i>p-10</i> ) chi angles: 51.7,358.7	0.187Å	-	-

A 216	TYR	50	-	Favored (46.75%) General / -129.6,154.8	13.3% ( <i>m-85</i> ) chi angles: 317.3,284.7	0.048Å	-	-
A 217	SER	50	-	Favored (5.24%) General / -135.2,-178.8	20% (t) chi angles: 188.7	0.083Å	-	-
A 218	GLY	50	-	Favored (18.74%) Glycine / 100.8,-165.1	-	-	-	-
A 219	VAL	50	-	Favored (7.45%) Isoleucine or valine /-89.3,-19.5	8.4% (p) chi angles: 73.5	0.192Å	-	-
A 220	ASN	50	-	Allowed (1.46%) General / -144.1,27.1	13.6% ( <i>m120</i> ) chi angles: 286.6,86.9	0.032Å	-	-
A 221	CYS	50	-	Favored (19.54%) General / 60.5,37.9	85.1% ( <i>m</i> ) chi angles: 300.3	0.146Å	-	-
A 222	GLU	50	-	Favored (54.05%) General / -80.5,-16.5	19.6% ( <i>pm0</i> ) chi angles: 69.3,284.8,25.1	0.136Å	-	OUTLIER(S) worst is CB- CG-CD: 4.097 σ
A 223	LEU	50	-	Favored (4.56%) General / -106.8,93.4	15.4% ( <i>mt</i> ) chi angles: 317,175.2	0.049Å	-	-
A 224	GLU	50	-	Favored (57.91%) General / -59.4,136.2	3% ( <i>mp0</i> ) chi angles: 267.7,55.5,19	0.051Å	-	OUTLIER(S) worst is CB- CG-CD: 4.216 σ
A 225	ILE	50	-	Favored (20.04%) Isoleucine or valine / -118.0,153.1	45.5% ( <i>mm</i> ) chi angles: 299.4,303.3	0.103Å	-	OUTLIER(S) worst is C-N- CA: 4.023 σ
# Al	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
		Avg: 54.82	Clashscore: 0	Outliers: 4 of 112	Poor rotamers: 3 of 95		Outliers: 0 of 114	Outliers: 10 of 114
A 226	ASP	50	-	Favored (36.77%) General / -126.1,122.8	13.8% ( <i>t0</i> ) chi angles: 166.9,10	0.106Å	-	-
A 227	GLU	50	-	Favored (15.72%) General /	44.6% ( <i>mt-10</i> ) chi angles: 296.4,193.6,304.7	0.12Å	-	-

				-104.1,-14.9				
A 228	CYS	50	-	Favored (69.14%) General / -64.7,-27.8	74.9% ( <i>m</i> ) chi angles: 288.8	0.15Å	-	-
A 229	TRP	50	-	Favored (2.61%) General / -45.8,-32.6	25.1% ( <i>t-105</i> ) chi angles: 193.3,278.3	0.042Å	-	-
A 230	SER	50	-	Favored (2.09%) General / -77.6,11.4	10.4% ( <i>t</i> ) chi angles: 192	0.101Å	-	-
A 231	GLN	50	-	Favored (5.1%) Pre-proline / 59.2,55.6	2.7% ( <i>tp60</i> ) chi angles: 184.7,40.3,99.4	0.166Å	-	-
A 232	PRO	50	-	Favored (15.79%) Trans-proline / -78.3,-12.0	20.6% ( <i>Cg_endo</i> ) chi angles: 38.5	0.027Å	-	-
A 233	CYS	50	-	Favored (11.45%) General / -92.4,98.4	92.9% ( <i>m</i> ) chi angles: 291.5	0.025Å	-	-
A 234	LEU	50	-	Favored (21.62%) General / -88.0,153.0	46.7% ( <i>mt</i> ) chi angles: 309.3,178.5	0.034Å	-	-
A 235	ASN	50	-	Favored (8.82%)	48% ( <i>m</i> -20) chi angles: 302.3,346.9	0.069Å	-	_
A 236	GLY	50	-	Favored (63.58%) Glycine / 93.5,5.1	-	-	-	-
A 237	ALA	50	-	Favored (15.28%) General / -59.0,154.5	-	0.028Å	-	-
A 238	THR	50	-	Favored (31.1%) General / -102.5,144.3	91.5% ( <i>m</i> ) chi angles: 302.5	0.052Å	-	-
A 239	CYS	50	-	Favored (32.38%) General / -82.0,142.4	93.1% ( <i>m</i> ) chi angles: 290	0.117Å	-	-
A 240	GLN	50	-	Favored (2.15%) General / -152.8,96.9	8% ( <i>tp60</i> ) chi angles: 175.5,59.7,100.1	0.026Å	-	-
A 241	ASP	50	-	Favored (11.31%) General /	1.4% ( <i>t0</i> ) chi angles: 220.1,315.2	0.093Å	-	-

A 242	ALA	50	-	-70.9,171.1 Favored (17.95%) General / -162.0,153.1	-	0.076Å	-	-
A 243	LEU	50	-	Allowed (0.77%) General / -70.8,89.7	41.1% ( <i>mt</i> ) chi angles: 308.7,183.5	0.071Å	-	-
A 244	GLY	50	-	Favored (2.58%) Glycine / 141.4,-21.2	-	-	-	-
A 245	ALA	50	-	Allowed (0.1%) General / 175.2,150.2	-	0.092Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
		Avg: 54.82	Clashscore: 0	Outliers: 4 of 112	Poor rotamers: 3 of 95	Outliers: 0 of 102		Outliers: 10 of 114
A 246	TYR	50	-	Favored (45.37%) General / -66.8,152.6	41.6% ( <i>p90</i> ) chi angles: 70.6,91.2	0.061Å	-	-
A 247	PHE	50	-	Favored (13.53%) General / -133.3,171.8	88.4% ( <i>m-85</i> ) chi angles: 292.8,83.8	0.03Å	-	-
A 248	CYS	50	-	Favored (21.01%) General / -143.9,168.0	56.7% (m) chi angles: 306	0.088Å	-	-
A 249	ASP	50	-	Favored (47.58%) General / -119.8,143.9	48.5% ( <i>t0</i> ) chi angles: 192.4,4.1	0.017Å	-	-
A 250	CYS	50	-	Favored (36.15%) General / -78.0,145.0	97.1% ( <i>m</i> ) chi angles: 290.9	0.056Å	-	-
A 251	ALA	50	-	Favored (92.8%) Pre-proline / -61.9,130.8	-	0.061Å	-	-
A 252	PRO	50	-	Allowed (0.11%) Trans-proline / -62.9,80.3	4.2% ( <i>Cg_exo</i> ) chi angles: 321.9	0.027Å	-	-
A	GLY	50	-	Favored (2.08%)	-	-	-	-

253				Glycine / 141.1,-2.4				
A 254	РНЕ	50	-	Favored (37.76%) General / -120.7,152.8	94.1% ( <i>m-85</i> ) chi angles: 294.3,86.5	0.054Å	-	-
A 255	LEU	50	-	Allowed (1.82%) General / -147.5,-163.7	10.9% ( <i>tp</i> ) chi angles: 200.5,47.8	0.118Å	-	-
A 256	GLY	50	-	Favored (17.02%) Glycine / 110.2,-144.7	-	-	-	-
A 257	ASP	50	-	Favored (22.71%) General / -84.2,-36.5	22.1% ( <i>t70</i> ) chi angles: 192.5,250.4	0.062Å	-	-
A 258	HIS	50	-	Allowed (1.9%) General / -143.2,18.3	57.9% ( <i>m80</i> ) chi angles: 285.1,73.9	0.037Å	-	-
A 259	CYS	50	-	Allowed (0.09%) General / 85.8,20.6	58.6% ( <i>m</i> ) chi angles: 305.2	0.247Å	-	-
A 260	GLU	50	-	Favored (83.26%) General / -67.4,-37.5	4.4% ( <i>pm0</i> ) chi angles: 68.4,298.5,334.3	0.141Å	-	-
A 261	LEU	50	-	Favored (28.15%) General / -76.3,124.8	3.7% ( <i>tt</i> ) chi angles: 179.2,133.9	0.032Å	-	-
A 262	ASN	50	-	Favored (34.33%) General / -81.8,140.3	1.1% ( <i>t30</i> ) chi angles: 200.3,103.4	0.087Å	-	-
A 263	THR	50	-	Favored (24.17%) General / -55.1,144.3	97.4% ( <i>m</i> ) chi angles: 299.3	0.035Å	-	-
A 264	ASP	50	-	Favored (22.03%) General / -103.7,110.1	21.2% ( <i>t0</i> ) chi angles: 176.9,30.2	0.074Å	-	-
A 265	GLU	50	-	Favored (56.41%) General / -78.6,-17.2	5.3% ( <i>mp0</i> ) chi angles: 316.3,92.6,138.2	0.103Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>
			Avg: 54.82	Clashscore:	Outliers: 4 of 112	Poor rotamers: 3 of 95		•	Outliers: 10 of 114
A 266	,	CYS	50	-	Favored (97.31%) General / -63.9,-42.6	83.2% ( <i>m</i> ) chi angles: 300.7	0.114Å	-	-
A 267		ALA	50	-	Favored (18.4%) General / -53.1,-27.0	-	0.076Å	-	-
A 268		SER	50	-	Favored (60.46%) General / -74.1,-12.0	27.3% (p) chi angles: 77.9	0.12Å	-	-
A 269	,	GLN	50	-	Allowed (0.87%) Pre-proline / 61.5,45.5	11.4% ( <i>tt0</i> ) chi angles: 200.8,182.7,123.1	0.1Å	-	-
A 270	ı	PRO	50	-	Favored (13.02%) Trans-proline / -79.7,-3.7	0.3% chi angles: 43.7	0.02Å	-	-
A 271		CYS	50	-	Allowed (1.03%) General / -112.8,77.3	84.2% ( <i>m</i> ) chi angles: 292.5	0.069Å	-	-
A 272		LEU	50	-	Favored (3.71%) General / -58.4,162.5	9.4% ( <i>mp</i> ) chi angles: 279.5,55.7	0.048Å	-	-
A 273		HIS	50	-	Favored (2.53%) General / 69.2,-0.3	71.8% ( <i>m80</i> ) chi angles: 299.4,95.1	0.144Å	-	-
A 274		GLY	50	-	Favored (11.43%) Glycine / 104.5,19.4	-	-	-	-
A 275		GLY	50	-	Favored (52.59%) Glycine / -70.5,164.9	-	-	-	-
A 276	,	LEU	50	-	Favored (20.68%) General / -91.1,152.2	51.6% ( <i>tp</i> ) chi angles: 182.2,66	0.057Å	-	-
A 277		CYS	50	-	Favored (23.33%) General /	11.6% ( <i>t</i> ) chi angles: 195	0.041Å	-	-

				-115.8,158.2				
A 278	VAL	50	-	Favored (31.97%) Isoleucine or valine / -139.9,142.5	12.2% ( <i>p</i> ) chi angles: 62.2	0.071Å	-	OUTLIER(S) worst is C-N- CA: 4.972 σ
A 279	ASP	50	-	Favored (8.62%) General / -61.0,161.2	4.8% ( <i>p-10</i> ) chi angles: 44.4,315.2	0.041Å	-	OUTLIER(S) worst is CA-CB-CG: $5.968 \sigma$
A 280	GLY	50	-	Favored (12.13%) Glycine / -165.8,-159.7	-	-	-	-
A 281	GLU	50	-	Favored (2.88%) General / -95.7,68.4	19.1% ( <i>pt-20</i> ) chi angles: 66.9,196,171.3	0.172Å	-	-
A 282	ASN	50	-	Favored (4.91%) General / 62.5,47.7	39.8% ( <i>t-20</i> ) chi angles: 195.5,5.6	0.093Å	-	-
A 283	ARG	50	-	OUTLIER (0.02%) General / 179.0,97.6	23.1% ( <i>ttp-105</i> ) chi angles: 180.8,175,67.9,271.5	0.073Å	-	-
A 284	TYR	99.99	-	Allowed (0.26%) General /	44.3% ( <i>p90</i> ) chi angles: 61.7,277.3	0.096Å	-	-
				-49.1,159.6				
A 285	SER	50	-	-49.1,159.6 Favored (53.65%) General / -119.1,137.3	14.7% ( <i>t</i> ) chi angles: 190.1	0.053Å	-	-
285	SER Alt Res	50 <b>High B</b>	- Clash > 0.4Å	Favored (53.65%) General /		0.053Å Cβ deviation	- Bond lengths	- Bond angles
285		High B		Favored (53.65%) General / -119.1,137.3	chi angles: 190.1	Cβ deviation	<b>lengths</b> Outliers:	
285	Alt Res	High B Avg:	<b>0.4Å</b> Clashscore:	Favored (53.65%) General / -119.1,137.3  Ramachandran Outliers: 4 of	chi angles: 190.1  Rotamer  Poor rotamers: 3 of	<b>C</b> β <b>deviation</b> Outliers:	<b>lengths</b> Outliers:	Outliers: 10
285 # A	Alt Res	<b>High B</b> Avg: 54.82	<b>0.4Å</b> Clashscore:	Favored (53.65%) General / -119.1,137.3  Ramachandran  Outliers: 4 of 112 Favored (41.87%) General /	chi angles: 190.1  Rotamer  Poor rotamers: 3 of 95  59.7% (m)	<b>C</b> β <b>deviation</b> Outliers: 0 of 102	<b>lengths</b> Outliers:	Outliers: 10
285 # A 286	Alt Res	High B Avg: 54.82	<b>0.4Å</b> Clashscore:	Favored (53.65%) General / -119.1,137.3  Ramachandran  Outliers: 4 of 112 Favored (41.87%) General / -74.8,132.9 Allowed (1.11%) General /	chi angles: 190.1 <b>Rotamer</b> Poor rotamers: 3 of 95  59.7% ( <i>m</i> ) chi angles: 285.8  11.1% ( <i>m-80</i> )	Cβ deviation Outliers: 0 of 102 0.067Å	<b>lengths</b> Outliers:	Outliers: 10

A 290	GLY 99.99	-	-59.0,140.6 Favored (54.24%) Glycine / -72.6,160.9	-	-	-	-
A 291	SER 99.99	-	Favored (12.76%) General / 63.9,33.2	11.5% ( <i>t</i> ) chi angles: 191.4	0.12Å	-	OUTLIER(S) worst is C-N- CA: 5.89 σ
A 292	GLY 50	-	Allowed (0.78%) Glycine / 166.7,125.6	-	-	-	-
A 293	PHE 50	-	Favored (39.75%) General / -140.3,160.5	92.2% ( <i>m-85</i> ) chi angles: 300.3,280.4	0.087Å	-	-
A 294	THR 50	-	Allowed (0.16%) General / -177.8,132.1	4.1% ( <i>t</i> ) chi angles: 174.3	0.053Å	-	OUTLIER(S) worst is C-N-CA: $4.199 \sigma$
A 295	GLY 50	-	OUTLIER (0.05%) Glycine / -168.0,8.9	-	-	-	-
A 296	THR 50	-	Favored (25.15%) General / -86.7,-24.5	1.5% (p) chi angles: 36.7	0.123Å	-	-
A 297	HIS 99.99	-	Allowed (0.62%) General / -151.0,31.6	35.5% ( <i>m-70</i> ) chi angles: 274.9,292.8	0.043Å	-	-
A 298	CYS 50	-	Favored (12.38%) General / 46.4,50.6	5.3% ( <i>m</i> ) chi angles: 317.9	0.122Å	-	-
A 299	GLU 99.99	-	-	0.7% chi angles: 58.8,281.3,263.8	0.087Å	-	-

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