Viewing crb1_sm_113-222H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	42.85		6th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	10	10.87%	Goal: <1%
	Ramachandran outliers	13	12.04%	Goal: <0.05%
	Ramachandran favored	69	63.89%	Goal: >98%
	MolProbity score^	3.79		4th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	2.04%	Goal: 0
	Bad backbone bonds:	10 / 833	1.20%	Goal: 0%
	Bad backbone angles:	5 / 1131	0.44%	Goal: <0.1%

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

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ 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: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 113		SER	50	-	-	8.7% (*t*) chi angles: 193.5	0.017Å	-	-
A 114		CYS	50	-	OUTLIER (0.01%) General / -70.3,-92.9	71.9% (*m*) chi angles: 297.8	0.052Å	-	-
A 115		GLY	50	-	Allowed (1.06%) Glycine / -150.4,20.7	-	-	-	-
A 116		LYS	50	-	Favored (2.78%) General / -127.2,88.3	28.4% (*tptp*) chi angles: 185.6,64.1,181.8,65.5	0.044Å	-	-

A 117	ASN	50	-	Favored (5.13%) General / -110.2,94.7	0.9% chi angles: 205.7,103.8	0.037Å	-	-
A 118	SER	50	0.677Å O with A 120 GLN HG3	Favored (74.02%) General / -69.6,-34.4	30.3% (*p*) chi angles: 52.2	0.106Å	-	-
A 119	CYS	50	-	Allowed (1.58%) General / -50.2,-22.0	20.2% (*m*) chi angles: 312.1	0.104Å	-	-
A 120	GLN	50	0.677Å HG3 with A 118 SER O	Allowed (0.05%) General / 70.2,-105.7	97.9% (*mt-30*) chi angles: 295.9,176.2,331.3	0.051Å	-	-
A 121	HIS	50	-	Favored (3.52%) General / -129.6,40.9	11.4% (*m-70*) chi angles: 283.7,230.1	0.059Å	OUTLIER(S) worst is CG-- ND1: 4.687 σ	-
A 122	GLY	50	0.609Å C with A 137 PRO HG3	OUTLIER (0.09%) Glycine / 173.3,94.5	-	-	-	-
A 123	GLY	50	0.417Å HA2 with A 137 PRO HD3	Favored (33.57%) Glycine / 163.8,174.4	-	-	-	-
A 124	ILE	50	0.736Å HB with A 135 ILE HB	Favored (48.47%) Isoleucine or valine / -106.4,134.3	51.3% (*mm*) chi angles: 302,301.8	0.055Å	-	-
A 125	CYS	50	-	Favored (38.69%) General / -116.1,120.3	0.5% chi angles: 94.5	0.021Å	-	-
A 126	HIS	50	0.704Å HB3 with A 133 VAL HG13	Favored (23.63%) General / -123.8,162.2	14.2% (*t-160*) chi angles: 181.1,213.4	0.12Å	OUTLIER(S) worst is CD2-- NE2: 4.512 σ	-
A 127	GLN	50	0.515Å H with A 126 HIS CD2	Favored (44.05%) General / -101.6,134.8	52.9% (*tt0*) chi angles: 185.3,179.5,59.8	0.103Å	-	-
A 128	ASP	50	0.567Å HB3 with A 131 TYR O	Favored (68.01%) Pre-proline /	20% (*t70*) chi angles: 175.1,82.1	0.158Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-124.1,153.3				
A 129		PRO	50	-	Favored (11.8%) Trans-proline / -55.9,122.5	60.6% (*Cg_exo*) chi angles: 327.2	0.086Å	-	-
A 130		ILE	50	0.715Å HG22 with A 131 TYR CE1	Allowed (0.15%) Isoleucine or valine / 83.6,-56.4	37.2% (*mm*) chi angles: 308.5,299.2	0.162Å	-	-
A 131		TYR	50	0.715Å CE1 with A 130 ILE HG22	Favored (59.53%) Pre-proline / -122.1,152.1	2.4% (*m-85*) chi angles: 287.1,36.1	0.043Å	-	-
A 132		PRO	50	-	Favored (10.74%) Trans-proline / -85.3,152.6	62.4% (*Cg_endo*) chi angles: 34.3	0.019Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 133		VAL	50	0.704Å HG13 with A 126 HIS HB3	Favored (41.41%) Isoleucine or valine / -115.4,139.5	6.9% (*p*) chi angles: 55.8	0.101Å	-	-
A 134		CYS	50	0.437Å HA with A 124 ILE O	Favored (39.33%) General / -132.8,130.1	3.6% (*t*) chi angles: 163.2	0.028Å	-	-
A 135		ILE	50	0.736Å HB with A 124 ILE HB	Favored (5.44%) Isoleucine or valine / -76.8,157.7	46% (*mm*) chi angles: 305.8,302.7	0.075Å	-	-
A 136		CYS	50	0.478Å HB2 with A 140 TYR HB2	Favored (19.81%) Pre-proline / -101.5,135.5	1% chi angles: 35.1	0.096Å	-	-
A 137		PRO	50	0.619Å HD2 with A 140 TYR CG	Allowed (1.37%) Trans-proline / -89.7,125.3	40.2% (*Cg_endo*) chi angles: 36.5	0.045Å	-	-
A 138		ALA	50	0.6Å HB3 with A 168 ASP CG	OUTLIER (0.01%) General / 41.1,-86.4	-	0.273Å	-	-

A 139	GLY	50	0.848A H with A 168 ASP HB2	Allowed (0.33%) Glycine / -121.2,75.2	-	-	-	-
A 140	TYR	50	0.644Å CZ with A 148 ASP HB2	Favored (20.01%) General / -104.0,154.2	2.3% (m-85) chi angles: 264.1,46.5	0.024Å	-	-
A 141	ALA	50	0.58Å HB2 with A 149 HIS HB2	Allowed (0.12%) General / -94.6,-127.0	-	0.118Å	-	-
A 142	GLY	50	0.493Å N with A 147 ILE HB	Favored (26.89%) Glycine / 83.7,158.5	-	-	-	-
A 143	ARG	50	0.412Å HG3 with A 144 PHE CD1	Favored (96.63%) General / -64.5,-41.3	21.9% (ptt-85) chi angles: 54.2,169.4,188.1,286.8	0.127Å	-	-
A 144	PHE	50	0.43Å HB2 with A 146 GLU OE1	Favored (15.89%) General / -116.2,14.3	1.5% (m-30) chi angles: 294.7,28.6	0.019Å	-	-
A 145	CYS	50	0.55Å HA with A 141 ALA O	Allowed (0.12%) General / 73.6,70.3	0.1% chi angles: 225.4	0.051Å	-	-
A 146	GLU	50	0.43Å OE1 with A 144 PHE HB2	Allowed (0.54%) General / -152.1,10.8	16.3% (pm0) chi angles: 62.9,259.4,31.9	0.039Å	-	-
A 147	ILE	50	0.493Å HB with A 142 GLY N	Favored (25.26%) Isoleucine or valine / -121.9,148.8	46.5% (mm) chi angles: 301.5,304	0.068Å	-	-
A 148	ASP	50	0.644Å HB2 with A 140 TYR CZ	Favored (42.24%) General / -96.6,127.1	10% (t0) chi angles: 179.5,312.9	0.062Å	-	-
A 149	HIS	50	0.58Å HB2 with A 141 ALA HB2	Favored (17.55%) General / -101.2,156.2	18% (t-160) chi angles: 187.9,206.6	0.058Å	OUTLIER(S) worst is CD2-- NE2: 4.576 σ	-
A 150	ASP	50	0.485Å H with A 149 HIS CD2	Favored (8.21%) General /	48.5% (t0) chi angles: 190.6,337.8	0.085Å	-	-

-92.7,92.9

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 151		GLU	50	0.878Å HG3 with A 170 TYR HD1	Favored (57.8%) General / -67.3,-11.5	4.5% (*pm0*) chi angles: 39.9,257.8,33.6	0.068Å	-	-
A 152		CYS	50	-	Favored (35.41%) General / -68.8,-7.6	0.1% chi angles: 109.5	0.051Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 153		ALA	50	-	Favored (21.68%) General / -88.6,-26.9	-	0.009Å	-	-
A 154		SER	50	-	Favored (14.42%) General / -110.3,-12.5	32% (*m*) chi angles: 286.8	0.055Å	-	-
A 155		SER	50	0.492Å HB2 with A 170 TYR CZ	Favored (16.77%) Pre-proline / -136.3,57.3	21.6% (*m*) chi angles: 305.3	0.068Å	-	-
A 156		PRO	50	-	Allowed (1.87%) Trans-proline / -71.2,6.3	88.4% (*Cg_endo*) chi angles: 32.9	0.029Å	-	-
A 157		CYS	50	0.495Å HB3 with A 161 ALA HB3	Favored (17.46%) General / 62.2,29.2	0.5% chi angles: 251.4	0.093Å	-	-
A 158		GLN	50	-	OUTLIER (0.01%) General / 80.1,-141.2	3% (*tt0*) chi angles: 198.4,204.8,163	0.102Å	-	-
A 159		ASN	50	-	Favored (3.61%) General / -113.8,36.6	11.6% (*p30*) chi angles: 64.4,83.1	0.054Å	-	-
A 160		GLY	50	-	Allowed (1.45%) Glycine / -146.2,33.8	-	-	-	-
A 161		ALA	50	0.496Å HB1 with A	Allowed (0.46%) General /		0.030Å		

161	ALA	50	HB1 with A 172 CYS HB2	General / -173.4,132.0	-	0.039A	-	-
A 162	VAL	50	0.701Å HG22 with A 173 PHE HB2	Favored (2.04%) Isoleucine or valine / -72.0,105.4	25.9% (*m*) chi angles: 301.9	0.104Å	-	-
A 163	CYS	50	-	Favored (58.41%) General / -63.1,138.0	0.5% chi angles: 101.6	0.051Å	-	-
A 164	GLN	50	0.52Å OE1 with A 173 PHE CE1	Favored (2.75%) General / -136.9,92.6	87.8% (*mt-30*) chi angles: 296.5,179.7,301.3	0.018Å	-	-
A 165	ASP	50	-	Favored (13.93%) General / -63.1,121.6	33.7% (*t0*) chi angles: 185.5,30	0.08Å	-	-
A 166	GLY	50	-	Favored (15.49%) Glycine / -120.2,-175.1	-	-	-	-
A 167	ILE	50	-	Allowed (0.16%) Isoleucine or valine / -61.1,102.1	1.1% (*pp*) chi angles: 31,59.7	0.019Å	-	-
A 168	ASP	99.99	0.848Å HB2 with A 139 GLY H	Allowed (1.62%) General / 52.2,21.5	4% (*p30*) chi angles: 69,45.5	0.122Å	-	OUTLIER(S) worst is CA-CB-CG: 6.896 σ
A 169	GLY	50	-	Favored (20.95%) Glycine / -164.0,151.6	-	-	-	-
A 170	TYR	50	0.878Å HD1 with A 151 GLU HG3	Favored (48.32%) General / -137.2,156.4	51.1% (*p90*) chi angles: 62.6,274.7	0.034Å	-	-
A 171	SER	50	-	Favored (43.61%) General / -134.8,137.7	59.7% (*p*) chi angles: 56	0.035Å	-	-
A 172	CYS	50	0.496Å HB2 with A 161 ALA HB1	Favored (32.87%) General / 118.7,118.9	1% chi angles: 34.9	0.081Å	-	-

-118.7,118.9

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 173		PHE	50	0.701Å HB2 with A 162 VAL HG22	Favored (25.43%) General / -95.8,113.8	1.4% (*m-30*) chi angles: 299.4,18.7	0.086Å	-	-
A 174		CYS	50	-	Favored (5.88%) General / -113.5,174.5	7.3% (*p*) chi angles: 49.5	0.124Å	-	-
A 175		VAL	50	-	Favored (94.24%) Pre-proline / -62.0,144.3	11.8% (*p*) chi angles: 66.3	0.118Å	-	-
A 176		PRO	50	-	Allowed (0.87%) Trans-proline / -70.6,49.3	96.2% (*Cg_endo*) chi angles: 32.3	0.049Å	-	-
A 177		GLY	50	-	OUTLIER (0.07%) Glycine / -142.8,-40.7	-	-	-	-
A 178		TYR	50	0.517Å CE2 with A 186 GLU HB3	Favored (10.9%) General / -114.1,167.2	42.5% (*m-85*) chi angles: 281.8,78.4	0.048Å	-	-
A 179		GLN	50	0.614Å HG2 with A 180 GLY H	Favored (12.97%) General / -160.8,175.1	49.5% (*tt0*) chi angles: 189.8,184,56.1	0.065Å	-	-
A 180		GLY	50	0.614Å H with A 179 GLN HG2	Favored (17.77%) Glycine / 124.5,-164.8	-	-	-	-
A 181		ARG	50	-	Favored (67.46%) General / -71.1,-31.2	63.1% (*ttm-85*) chi angles: 184.1,179.6,293.3,276.6	0.04Å	-	-
A 182		HIS	50	-	Favored (19.46%) General / -109.4,0.7	0.4% chi angles: 340.4,261	0.078Å	OUTLIER(S) worst is CD2--NE2: 4.466 σ	OUTLIER(S) worst is CB-CG-CD2: 4.963 σ
A 183		CYS	50	-	Favored (3.1%) General / 43.8,40.5	89.7% (*m*) chi angles: 289.7	0.004Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			43.8,40.5				
A 184	ASP 50	-	Favored (12.23%) General / -117.8,4.4	36.6% (*t0*) chi angles: 193.5,328.4	0.005Å	-	-
A 185	LEU 99.99	0.869Å HD23 with A 205 ILE HG23	Favored (18.69%) General / -100.2,107.0	37.3% (*mt*) chi angles: 301.5,165.3	0.116Å	-	-
A 186	GLU 50	0.517Å HB3 with A 178 TYR CE2	OUTLIER (0.02%) General / -61.4,88.0	9.5% (*pt-20*) chi angles: 53.6,175.6,72.5	0.047Å	-	-
A 187	VAL 50	-	OUTLIER (0%) Isoleucine or valine / 51.9,174.9	26.3% (*m*) chi angles: 301.8	0.156Å	-	-
A 188	ASP 50	-	Favored (17.48%) General / -96.0,154.0	7% (*t0*) chi angles: 208.2,326.5	0.071Å	-	-
A 189	GLU 50	-	Allowed (1.92%) General / -142.4,24.5	1.3% (*pm0*) chi angles: 48.8,282.2,276.3	0.038Å	-	-
A 190	CYS 50	-	Favored (40.67%) General / -98.9,10.8	0.5% chi angles: 98.9	0.075Å	-	-
A 191	ALA 50	-	Favored (62.82%) General / -61.7,-19.8	-	0.057Å	-	-
A 192	SER 50	-	Favored (8.36%) General / -101.3,25.4	67.5% (*m*) chi angles: 298.2	0.026Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 193	ASP 99.99	0.485Å OD1 with A 195 CYS SG	Allowed (0.64%) Pre-proline / -168.6,88.8	47.5% (*t0*) chi angles: 191.6,339.4	0.013Å	-	-
A 194	PRO 50		Favored (3.48%) Trans-proline /	87.3% (*Cg_endo*) chi angles: 30.1	0.042Å		

194	PRO	50	-	trans-proline / -71.2,-40.1	chi angles: 30.1	0.043Å	-	-
A 195	CYS	50	0.531Å HB3 with A 199 ALA CB	Allowed (0.24%) General / 68.1,-34.1	34.6% (*m*) chi angles: 308.9	0.071Å	-	OUTLIER(S) worst is CA-CB-SG: 4.523 σ
A 196	LYS	50	-	Allowed (0.13%) General / 62.2,170.5	27.4% (*tptp*) chi angles: 185.7,61.9,184.1,66.6	0.085Å	-	-
A 197	ASN	50	0.432Å HB3 with A 198 GLU OE1	OUTLIER (0.04%) General / 71.0,-104.4	34.1% (*m120*) chi angles: 293.7,113.9	0.057Å	-	-
A 198	GLU	99.99	0.784Å HG2 with A 217 SER HB3	Favored (9.13%) General / -111.0,-26.7	59.7% (*mp0*) chi angles: 296.2,83.2,6.1	0.091Å	-	-
A 199	ALA	50	0.531Å CB with A 195 CYS HB3	Allowed (0.58%) General / -53.4,110.6	-	0.287Å	-	OUTLIER(S) worst is C-CA-CB: 6.331 σ
A 200	THR	50	0.491Å HG23 with A 198 GLU O	Favored (33.51%) General / -106.7,117.2	17.4% (*p*) chi angles: 47.1	0.071Å	-	-
A 201	CYS	50	-	Favored (40.85%) General / -76.5,142.8	18.2% (*p*) chi angles: 71.3	0.103Å	-	-
A 202	LEU	50	-	Favored (52.79%) General / -107.8,126.6	2.1% (*tp*) chi angles: 228.4,64.3	0.056Å	-	-
A 203	ASN	99.99	-	Favored (4.38%) General / -75.6,99.7	50.8% (*t-20*) chi angles: 184.6,7	0.072Å	-	-
A 204	GLU	50	0.465Å HB2 with A 207 ARG O	Favored (32.28%) General / -110.7,148.4	63.1% (*mm-40*) chi angles: 292.4,292,356.5	0.054Å	-	-
A 205	ILE	50	0.869Å HG23 with A 185 LEU HD23	OUTLIER (0.1%) Isoleucine or valine / -74.5,61.3	26.3% (*pt*) chi angles: 52.4,170.6	0.046Å	-	-
A				Allowed (0.15%)				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 206		GLY	50	-	(0.13 %) Glycine / 173.9,-43.8	-	-	-	-
A 207		ARG	50	0.87Å HG2 with A 208 TYR H	Allowed (1.38%) General / -164.7,-168.0	54.1% (*ttm-85*) chi angles: 188.6,186.2,285.3,280.9	0.088Å	-	-
A 208		TYR	99.99	0.87Å H with A 207 ARG HG2	Favored (39.28%) General / -114.4,147.4	54.7% (*p90*) chi angles: 63.1,89.2	0.102Å	-	-
A 209		THR	50	0.561Å HG22 with A 211 ILE HG23	Favored (7.15%) General / -117.9,99.8	69.5% (*m*) chi angles: 303.3	0.036Å	-	-
A 210		CYS	50	-	Allowed (1.01%) General / -70.9,93.8	44.9% (*t*) chi angles: 178.7	0.056Å	-	-
A 211		ILE	50	0.561Å HG23 with A 209 THR HG22	Allowed (1.11%) Isoleucine or valine / -101.0,173.5	44.4% (*pt*) chi angles: 61.3,167.8	0.042Å	-	-
A 212		CYS	50	-	Favored (50.59%) Pre-proline / -115.2,106.8	35.9% (*t*) chi angles: 188.5	0.057Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.64	Clashscore: 42.85	Outliers: 13 of 108	Poor rotamers: 10 of 92	Outliers: 2 of 98	Outliers: 5 of 110	Outliers: 4 of 110
A 213		PRO	50	0.443Å HG2 with A 198 GLU HB3	OUTLIER (0.05%) Trans-proline / -65.5,-161.4	62% (*Cg_endo*) chi angles: 34.3	0.022Å	-	-
A 214		HIS	50	0.475Å HA with A 217 SER OG	OUTLIER (0.01%) General / -174.9,-36.8	19.9% (*t-160*) chi angles: 183.4,205.4	0.011Å	OUTLIER(S) worst is CG--ND1: 4.833 σ	-
A 215		ASN	50	-	Favored (27.04%) General / -51.7,-31.6	22.8% (*t-20*) chi angles: 186.7,295.4	0.041Å	-	-
A 216		TYR	50	-	Allowed (0.75%) General / -90.8,-69.0	23% (*m-30*) chi angles: 297.8,329.9	0.045Å	-	-

				90.8, 89.8				
A 217	SER	99.99	0.784Å HB3 with A 198 GLU HG2	Favored (6.9%) General / -46.2,136.5	22.7% (*p*) chi angles: 50.7	0.107Å	-	-
A 218	GLY	50	-	Favored (5.56%) Glycine / -117.9,31.8	-	-	-	-
A 219	VAL	50	0.696Å HG13 with A 220 ASN H	Allowed (0.2%) Isoleucine or valine / -104.6,-84.7	7.4% (*p*) chi angles: 56.2	0.196Å	-	-
A 220	ASN	50	0.696Å H with A 219 VAL HG13	OUTLIER (0.02%) General / -172.2,-42.1	33.8% (*m120*) chi angles: 293.3,110.9	0.053Å	-	-
A 221	CYS	50	-	OUTLIER (0.03%) General / 57.8,94.7	0.8% chi angles: 156.4	0.034Å	-	-
A 222	GLU	99.99	-	-	4.7% (*pm0*) chi angles: 67,298.1,336.1	0.183Å	-	-

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