



Viewing crb1_sm_148-260_FFX1H-multi.table

When finished, you should [close this window](#).

Hint: Use File | Save As... to save a copy of this page.

All-Atom Contacts	Clashscore, all atoms:	0		100 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	4.26%	Goal: <1%
	Ramachandran outliers	9	8.11%	Goal: <0.05%
	Ramachandran favored	75	67.57%	Goal: >98%
	MolProbity score [^]	1.84		84 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	2.94%	Goal: 0
	Bad backbone bonds:	0 / 859	0.00%	Goal: 0%
	Bad backbone angles:	15 / 1169	1.28%	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	C β deviation	Bond lengths	Bond angles
		Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 148	ASP	50	-	-	0.9% chi angles: 302.6,34.6	0.065Å	-	-
A 149	HIS	99.99	-	OUTLIER (0.01%) General / 170.2,120.5	10.2% (<i>p</i> 80) chi angles: 44.2,80.6	0.079Å	-	-
A 150	ASP	99.99	-	Favored (56.73%) General / -66.0,144.4	6.7% (<i>p</i> -10) chi angles: 46.9,313.6	0.066Å	-	OUTLIER(S) worst is CA-CB-CG: 5.443 σ
A 151	GLU	99.99	-	Favored (32.01%) General / -121.6,119.5	73.3% (<i>mm</i> -40) chi angles: 289,304,323.5	0.097Å	-	OUTLIER(S) worst is C-N-CA: 7.737 σ

A 152	CYS	50	-	OUTLIER (0.01%) General / 96.7,-40.6	57.1% (<i>m</i>) chi angles: 305.8	0.363Å	-	OUTLIER(S) worst is N-CA- CB: 4.087 σ
A 153	ALA	50	-	Allowed (0.32%) General / -148.5,-16.7	-	0.063Å	-	-
A 154	SER	50	-	Allowed (0.47%) General / -154.1,28.2	22.9% (<i>t</i>) chi angles: 187.7	0.051Å	-	-
A 155	SER	50	-	Favored (40.98%) Pre-proline / -66.6,117.1	7.8% (<i>t</i>) chi angles: 195.7	0.05Å	-	-
A 156	PRO	50	-	Allowed (0.93%) Trans-proline / -89.5,47.0	0.1% chi angles: 46.6	0.134Å	-	OUTLIER(S) worst is N-CA- CB: 4.529 σ
A 157	CYS	50	-	Favored (26.16%) General / -92.9,-15.7	79.3% (<i>m</i>) chi angles: 299.4	0.167Å	-	-
A 158	GLN	50	-	Allowed (0.27%) General / 56.4,-105.5	10.2% (<i>tp-100</i>) chi angles: 181.8,48,238.3	0.224Å	-	OUTLIER(S) worst is C-CA- CB: 4.435 σ
A 159	ASN	50	-	Favored (4.58%) General / -132.1,25.3	51.5% (<i>m-80</i>) chi angles: 283.9,276.8	0.079Å	-	-
A 160	GLY	50	-	Allowed (0.4%) Glycine / 177.8,114.3	-	-	-	-
A 161	ALA	50	-	OUTLIER (0.03%) General / 167.8,149.8	-	0.082Å	-	-
A 162	VAL	50	-	Favored (38.15%) Isoleucine or valine / -99.2,114.8	86.5% (<i>t</i>) chi angles: 175	0.064Å	-	-
A 163	CYS	50	-	Favored (10.32%) General / -83.7,72.5	4.7% (<i>p</i>) chi angles: 46.3	0.094Å	-	-
				Favored				

A 164	GLN	50	-	(8.61%) General / -75.5,108.8	13.8% (<i>tp60</i>) chi angles: 170.4,58.3,91.9	0.048Å	-	-
A 165	ASP	50	-	Favored (9.83%) General / -55.7,152.2	40.1% (<i>t0</i>) chi angles: 196.1,9.2	0.03Å	-	-
A 166	GLY	50	-	Favored (10.84%) Glycine / -137.1,-166.6	-	-	-	-
A 167	ILE	50	-	Favored (5.12%) Isoleucine or valine / -70.5,112.2	20.6% (<i>tt</i>) chi angles: 188.1,166	0.151Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 168	ASP	50	-	OUTLIER (0.03%) General / 62.1,-89.2	48.4% (<i>t0</i>) chi angles: 180.9,15.6	0.182Å	-	-
A 169	GLY	50	-	Favored (53.49%) Glycine / -69.3,157.4	-	-	-	-
A 170	TYR	50	-	Favored (31.99%) General / -71.5,160.8	1.4% (<i>p90</i>) chi angles: 45,241.6	0.094Å	-	-
A 171	SER	50	-	Allowed (0.7%) General / -109.6,53.1	32.3% (<i>t</i>) chi angles: 175.1	0.031Å	-	-
A 172	CYS	50	-	Favored (10.52%) General / -53.9,148.5	49.1% (<i>t</i>) chi angles: 185.9	0.03Å	-	-
A 173	PHE	50	-	Favored (25.46%) General / -133.5,123.5	45.3% (<i>m-85</i>) chi angles: 305.5,298.1	0.072Å	-	-
A 174	CYS	50	-	Favored (10.48%) General / -86.7,172.0	27.6% (<i>p</i>) chi angles: 60.2	0.055Å	-	-
				Favored				

A 175	VAL	50	-	(32.52%) Pre-proline / -77.4,167.9	17.3% (<i>m</i>) chi angles: 291.4	0.129Å	-	-
A 176	PRO	50	-	Allowed (0.96%) Trans-proline / -53.8,-59.4	84.1% (<i>Cg_exo</i>) chi angles: 331.8	0.158Å	-	-
A 177	GLY	50	-	Favored (4.13%) Glycine / -86.3,63.7	-	-	-	-
A 178	TYR	50	-	Favored (3.37%) General / -135.0,-173.6	2.1% (<i>m-85</i>) chi angles: 264.1,42.2	0.067Å	-	-
A 179	GLN	50	-	Allowed (0.2%) General / -143.5,-147.0	29.5% (<i>pt20</i>) chi angles: 63.5,177.5,328.4	0.141Å	-	-
A 180	GLY	50	-	Favored (15.98%) Glycine / 123.8,-168.1	-	-	-	-
A 181	ARG	50	-	Favored (24.87%) General / -93.0,-16.6	0.2% chi angles: 61.1,240.3,169.6,263.2	0.099Å	-	-
A 182	HIS	50	-	Allowed (0.64%) General / -152.2,17.3	77.7% (<i>t60</i>) chi angles: 185.5,76.6	0.069Å	-	OUTLIER(S) worst is CA-CB- CG: 4.413 σ
A 183	CYS	50	-	OUTLIER (0.04%) General / 77.1,65.3	57.7% (<i>m</i>) chi angles: 305.6	0.131Å	-	-
A 184	ASP	99.99	-	Allowed (0.07%) General / -164.6,28.4	52% (<i>p-10</i>) chi angles: 58.7,357	0.084Å	-	-
A 185	LEU	50	-	Favored (42.46%) General / -143.0,159.3	61% (<i>mt</i>) chi angles: 290.8,181.6	0.091Å	-	-
A 186	GLU	50	-	Favored (21.87%) General / -83.2,160.3	1.6% (<i>pm0</i>) chi angles: 55.5,280.6,253.4	0.055Å	-	-
A 187	VAL	50	-	Favored (25.63%) Isoleucine or valine	3.6% (<i>p</i>) chi angles: 79.2	0.087Å	-	-

/ -140.1,161.3

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 188	ASP	50	-	Favored (23.23%) General / -95.5,111.3	55.3% (<i>t0</i>) chi angles: 177.4,350.6	0.048Å	-	-
A 189	GLU	50	-	Favored (21.2%) General / -88.8,-27.4	36% (<i>mt-10</i>) chi angles: 301.8,168,288.7	0.062Å	-	-
A 190	CYS	50	-	Favored (48.21%) General / -78.4,-22.2	5.3% (<i>p</i>) chi angles: 47	0.205Å	-	-
A 191	ALA	50	-	Favored (69.11%) General / -70.9,-32.3	-	0.074Å	-	-
A 192	SER	50	-	Favored (10.04%) General / -92.5,-41.8	95.7% (<i>p</i>) chi angles: 63.7	0.101Å	-	-
A 193	ASP	50	-	Favored (12.02%) Pre-proline / -121.3,62.7	2.2% (<i>m-20</i>) chi angles: 301.7,203	0.055Å	-	OUTLIER(S) worst is CA-CB-CG: 4.971 σ
A 194	PRO	50	-	Favored (6.35%) Trans-proline / -88.7,-4.5	15.9% (<i>Cg_endo</i>) chi angles: 39.2	0.024Å	-	-
A 195	CYS	50	-	Favored (2.32%) General / 51.7,63.2	68.7% (<i>m</i>) chi angles: 288.1	0.156Å	-	-
A 196	LYS	99.99	-	OUTLIER (0.02%) General / 80.5,-155.6	52.5% (<i>mtpt</i>) chi angles: 293.2,162,57.2,182.7	0.256Å	-	-
A 197	ASN	50	-	Favored (3.4%) General / -133.5,35.7	11.2% (<i>m120</i>) chi angles: 297.9,155.9	0.02Å	-	OUTLIER(S) worst is CA-CB-CG: 7.484 σ
A 198	GLU	99.99	-	Allowed (1.58%) General / -135.3,64.4	2% (<i>tp10</i>) chi angles: 172.6,40.9,125.1	0.087Å	-	-

A 199	ALA	50	-	Allowed (0.48%) General / -175.9,141.6	-	0.094Å	-	-
A 200	THR	50	-	Favored (6.97%) General / -83.4,88.2	82.2% (<i>p</i>) chi angles: 60.5	0.071Å	-	-
A 201	CYS	50	-	Favored (51.85%) General / -69.5,136.8	31.9% (<i>p</i>) chi angles: 64.4	0.041Å	-	-
A 202	LEU	50	-	Favored (28.89%) General / -142.8,136.5	66.8% (<i>mt</i>) chi angles: 303.7,173.5	0.087Å	-	-
A 203	ASN	50	-	Favored (30.66%) General / -105.2,145.4	1.8% (<i>t-20</i>) chi angles: 156.1,247	0.116Å	-	OUTLIER(S) worst is CA-CB- CG: 4.513 σ
A 204	GLU	50	-	Allowed (0.36%) General / -143.4,-151.4	0.1% chi angles: 203.4,236.2,242	0.179Å	-	-
A 205	ILE	50	-	Allowed (0.98%) Isoleucine or valine / -84.8,74.0	72% (<i>mt</i>) chi angles: 299.8,164.5	0.115Å	-	-
A 206	GLY	50	-	Favored (61.59%) Glycine / 71.3,39.8	-	-	-	-
A 207	ARG	50	-	Allowed (0.7%) General / -171.8,131.8	32.5% (<i>ptt180</i>) chi angles: 55.3,185.2,190.5,168.9	0.034Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 208	TYR	50	-	Favored (4.35%) General / -124.1,-179.2	41.9% (<i>p90</i>) chi angles: 70.3,270.5	0.071Å	-	-
A 209	THR	50	-	Favored (40.63%) General / -155.7,161.8	11.4% (<i>t</i>) chi angles: 184.8	0.111Å	-	-
				Favored				

A 210	CYS	50	-	(2.01%) General / -144.6,89.6	14.2% (<i>p</i>) chi angles: 53.2	0.057Å	-	-
A 211	ILE	50	-	Favored (4.59%) Isoleucine or valine / -83.5,97.3	45.8% (<i>mm</i>) chi angles: 305,299.4	0.045Å	-	-
A 212	CYS	50	-	Favored (86.11%) Pre-proline / -72.9,159.1	32% (<i>p</i>) chi angles: 64.4	0.041Å	-	-
A 213	PRO	50	-	Favored (2.16%) Trans-proline / -81.3,83.5	65.7% (<i>Cg_endo</i>) chi angles: 33.9	0.036Å	-	-
A 214	HIS	50	-	OUTLIER (0.02%) General / -63.0,83.1	57% (<i>t-80</i>) chi angles: 192,292.5	0.064Å	-	-
A 215	ASN	50	-	Favored (6.95%) General / -91.8,-48.1	9.5% (<i>t30</i>) chi angles: 178.6,85.8	0.024Å	-	-
A 216	TYR	50	-	Favored (49.09%) General / -70.5,147.7	92.8% (<i>m-85</i>) chi angles: 291.7,89.6	0.1Å	-	OUTLIER(S) worst is C-N-CA: 4.138 σ
A 217	SER	50	-	Allowed (0.28%) General / -135.8,-148.0	1.1% (<i>t</i>) chi angles: 209.7	0.132Å	-	-
A 218	GLY	50	-	Favored (35.43%) Glycine / 72.1,-179.4	-	-	-	-
A 219	VAL	50	-	Favored (46.44%) Isoleucine or valine / -59.3,-31.5	31.8% (<i>m</i>) chi angles: 297	0.214Å	-	-
A 220	ASN	50	-	Allowed (1.85%) General / -140.7,39.4	34.2% (<i>m120</i>) chi angles: 302.1,110.3	0.041Å	-	-
A 221	CYS	50	-	Favored (2.13%) General / 65.5,47.9	33.4% (<i>m</i>) chi angles: 309.5	0.101Å	-	-
				Allowed	29.5% (<i>tp10</i>)			OUTLIER(S)

A 222	GLU	50	-	(0.85%) General / -141.1,-16.5	chi angles: 174.8,51.2,208.5	0.059Å	-	worst is CB-CG- CD: 5.329 σ	
A 223	LEU	50	-	Favored (8.19%) General / -114.6,100.3	4.8% (<i>mt</i>) chi angles: 325.9,170	0.056Å	-	-	
A 224	GLU	50	-	Favored (25.37%) General / -70.0,163.8	12% (<i>pt-20</i>) chi angles: 56,190.9,111.2	0.221Å	-	-	
A 225	ILE	50	-	OUTLIER (0.02%) Isoleucine or valine / 48.8,-137.7	12.2% (<i>pt</i>) chi angles: 61.4,155.3	0.362Å	-	OUTLIER(S) worst is C-CA- CB: 4.308 σ	
A 226	ASP	50	-	Favored (30.53%) General / -160.8,159.8	52.2% (<i>t0</i>) chi angles: 188,13.2	0.055Å	-	-	
A 227	GLU	50	-	Allowed (0.07%) General / -162.6,13.7	16.4% (<i>tp10</i>) chi angles: 174.1,42.5,25.5	0.123Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 228	CYS	50	-	Favored (75.33%) General / -61.2,-34.6	30.1% (<i>p</i>) chi angles: 65.8	0.11Å	-	-	
A 229	TRP	50	-	Favored (19.77%) General / -50.3,-33.5	4.6% (<i>p-90</i>) chi angles: 75.3,297.4	0.126Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.165 σ	
A 230	SER	50	-	Favored (71.5%) General / -67.5,-31.4	58.3% (<i>m</i>) chi angles: 291	0.098Å	-	-	
A 231	GLN	99.99	-	Favored (19.48%) Pre-proline / -118.3,83.0	8.6% (<i>tp-100</i>) chi angles: 187.8,52.4,259.3	0.057Å	-	-	
A 232	PRO	50	-	Favored (10.66%) Trans-proline / -83.4,-8.2	79.5% (<i>Cg_endo</i>) chi angles: 33.2	0.054Å	-	-	

A 233	CYS	50	-	Allowed (0.21%) General / 67.6,-66.5	8.3% (<i>m</i>) chi angles: 316	0.205Å	-	-
A 234	LEU	50	-	Allowed (0.21%) General / 77.4,159.9	20% (<i>tp</i>) chi angles: 194.8,61.9	0.099Å	-	-
A 235	ASN	50	-	Allowed (0.08%) General / 75.1,-74.9	61.8% (<i>t30</i>) chi angles: 191.7,46.8	0.19Å	-	-
A 236	GLY	50	-	Allowed (0.18%) Glycine / -163.0,22.4	-	-	-	-
A 237	ALA	50	-	Favored (21.72%) General / -113.5,157.7	-	0.07Å	-	-
A 238	THR	50	-	Favored (41.97%) General / -135.0,136.2	16.9% (<i>p</i>) chi angles: 46.8	0.086Å	-	-
A 239	CYS	50	-	Favored (15.7%) General / -74.3,170.4	31.4% (<i>p</i>) chi angles: 64	0.063Å	-	-
A 240	GLN	50	-	Favored (5.94%) General / -149.7,116.6	12.9% (<i>tp60</i>) chi angles: 167.7,64.2,92.1	0.081Å	-	-
A 241	ASP	50	-	Favored (5.77%) General / -52.4,149.3	54.8% (<i>t0</i>) chi angles: 185.8,11.3	0.055Å	-	-
A 242	ALA	50	-	Allowed (0.07%) General / 179.1,129.5	-	0.052Å	-	-
A 243	LEU	50	-	Allowed (0.16%) General / -56.2,105.0	49.9% (<i>mt</i>) chi angles: 288.8,162.9	0.051Å	-	-
A 244	GLY	50	-	Favored (45.05%) Glycine / 106.1,-12.9	-	-	-	-

A 245	ALA	50	-	OUTLIER (0.03%) General / 176.8,122.3	-	0.094Å	-	-
A 246	TYR	99.99	-	Favored (28.66%) General / -65.9,158.2	3% (<i>p90</i>) chi angles: 42.1,68.5	0.057Å	-	-
A 247	PHE	50	-	Favored (7.43%) General / -107.3,171.3	53.9% (<i>t80</i>) chi angles: 174.9,63.7	0.121Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 53.98	Clashscore: 0	Outliers: 9 of 111	Poor rotamers: 4 of 94	Outliers: 3 of 102	Outliers: 0 of 113	Outliers: 15 of 113
A 248	CYS	50	-	Favored (5.92%) General / -162.1,134.8	7.5% (<i>t</i>) chi angles: 166.4	0.084Å	-	-
A 249	ASP	50	-	Favored (14.26%) General / -151.5,173.7	4% (<i>t0</i>) chi angles: 214.9,325	0.041Å	-	-
A 250	CYS	50	-	Favored (41.07%) General / -75.4,133.8	48.6% (<i>t</i>) chi angles: 185.6	0.028Å	-	-
A 251	ALA	50	-	Favored (9.28%) Pre-proline / -115.9,81.0	-	0.046Å	-	-
A 252	PRO	50	-	Favored (13.77%) Trans-proline / -73.5,-3.5	87.2% (<i>Cg_endo</i>) chi angles: 30.1	0.064Å	-	-
A 253	GLY	50	-	Favored (74.66%) Glycine / -68.1,-25.0	-	-	-	-
A 254	PHE	50	-	Favored (6.99%) General / -105.1,-37.3	13.2% (<i>m-30</i>) chi angles: 310.8,312.2	0.069Å	-	-
A 255	LEU	50	-	Favored (7.16%) General /	22.2% (<i>tp</i>) chi angles: 188.1,72.8	0.046Å	-	-

A 256	GLY	50	-	-90.2,73.4 Favored (4.32%) Glycine / -80.6,62.7	-	-	-	-
A 257	ASP	50	-	Allowed (0.08%) General / -144.1,-128.4	36.4% (<i>t</i> 70) chi angles: 185,67.1	0.196Å	-	OUTLIER(S) worst is C-CA- CB: 4.293 σ
A 258	HIS	50	-	Favored (57.25%) General / -89.0,-6.4	31% (<i>p</i> -80) chi angles: 77.6,282.1	0.161Å	-	-
A 259	CYS	50	-	Allowed (0.17%) General / 81.5,28.3	3.4% (<i>t</i>) chi angles: 206	0.158Å	-	-
A 260	GLU	99.99	-	-	6.2% (<i>tm</i> -20) chi angles: 167.7,281,343	0.142Å	-	OUTLIER(S) worst is CB-CG- CD: 5.305 σ

About [MolProbity](#) | [Website for the Richardson Lab](#) | Using [ecloud x-H](#) | Internal reference 4.1-537