Viewing crb1_sm_1268-1335H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	14.95		50th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	1	0.96%	Goal: <0.05%
	Ramachandran favored	97	93.27%	Goal: >98%
	MolProbity score^	2.12		69th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	14 / 815	1.72%	Goal: 0%
	Bad backbone angles:	2 / 1106	0.18%	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: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1145		SER	50	-	-	37.3% (*t*) chi angles: 182.2	0.039Å	-	-
A1146		ASN	50	-	Favored (29.7%) Pre-proline / -76.1,113.6	48.9% (*t30*) chi angles: 184.5,19.5	0.048Å	-	-
A1147		PRO	50	-	Favored (69.7%) Trans-proline / -62.8,-19.9	79.4% (*Cg_endo*) chi angles: 29.8	0.069Å	-	-
A1148		CYS	50	-	Favored (22.87%) General / -87.6,113.0	49.4% (*m*) chi angles: 306.9	0.043Å	-	-
				0.506Å	Favored	96.5% (*mt*)			

A1149	LEU	50	~~0.508Å~~ HD12 with A1175 GLU HB3	~~Favored~~ (38.48%) General / -70.6,157.1	~~98.5% (mt)~~ chi angles: 295.8,177.1	0.015Å	-	-
A1150	HIS	50	0.501Å CE1 with A1169 TRP CZ3	Favored (13.94%) General / 60.8,42.0	66.3% (*m80*) chi angles: 300.6,99.2	0.068Å	OUTLIER(S) worst is CG--ND1: 4.448 σ	OUTLIER(S) worst is CB-CG-CD2: 4.545 σ
A1151	GLY	50	-	Favored (65.88%) Glycine / 58.2,31.5		-	-	-
A1152	GLY	50	-	Favored (39.34%) Glycine / -69.8,144.1		-	-	-
A1153	ASN	50	-	Favored (37.24%) General / -76.7,130.1	24.6% (*t-20*) chi angles: 187.7,297.9	0.046Å	-	-
A1154	CYS	50	-	Favored (39.98%) General / -94.8,126.3	48.7% (*t*) chi angles: 185.7	0.042Å	-	-
A1155	GLU	50	-	Favored (25.4%) General / -118.2,115.8	10.8% (*pt-20*) chi angles: 56.9,176.6,72	0.046Å	-	-
A1156	ASP	50	-	Favored (43.52%) General / -73.8,135.1	40.9% (*t0*) chi angles: 190,327.8	0.052Å	-	-
A1157	ILE	50	0.635Å HD11 with A1160 SER HB3	Favored (14.69%) Isoleucine or valine / -122.2,168.4	31.3% (*pt*) chi angles: 67.9,168.2	0.065Å	-	-
A1158	TYR	50	-	Favored (14.84%) General / -84.4,104.9	1.9% (*m-30*) chi angles: 291.8,31.4	0.084Å	-	-
A1159	SER	50	-	OUTLIER (0.01%) General / 111.6,-28.7	43.6% (*t*) chi angles: 178.2	0.104Å	-	-
A1160	SER	50	0.635Å HB3 with A1157 ILE HD11	Allowed (0.15%) General / -145.8,-144.3	32.8% (*t*) chi angles: 184	0.128Å	-	-

~~Favored~~

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1161		TYR	50	-	Favored (17.37%) General / -164.5,157.7	54.6% (*p90*) chi angles: 63.3,89.8	0.043Å	-	-
A1162		HIS	50	-	Favored (42.72%) General / -127.5,156.1	53.2% (*m170*) chi angles: 298.1,158.6	0.016Å	OUTLIER(S) worst is CG--ND1: 4.468 σ	-
A1163		CYS	50	-	Favored (56.55%) General / -114.5,131.7	93.1% (*m*) chi angles: 291.4	0.04Å	-	-
A1164		SER	50	-	Favored (5.58%) General / -100.4,93.3	38.7% (*t*) chi angles: 181.8	0.04Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1165		CYS	50	-	Favored (92%) Pre-proline / -70.0,143.8	60.2% (*m*) chi angles: 304.4	0.033Å	-	-
A1166		PRO	50	-	Favored (51.51%) Trans-proline / -70.5,159.8	96.4% (*Cg_endo*) chi angles: 30.7	0.022Å	-	-
A1167		LEU	99.99	0.507Å C with A1196 ALA HB2	Favored (3.54%) General / -57.6,116.7	96.1% (*mt*) chi angles: 296.3,174.7	0.027Å	-	-
A1168		GLY	50	0.709Å O with A1178 ILE HG22	Favored (27.82%) Glycine / 111.5,-1.1	-	-	-	-
A1169		TRP	99.99	0.576Å CZ3 with A1177 ASN HB2	Favored (52.73%) General / -127.9,139.2	93.8% (*m95*) chi angles: 297.3,93.6	0.022Å	-	-
A1170		SER	50	-	Favored (21.57%) General / -134.4,167.0	26.4% (*t*) chi angles: 185.7	0.024Å	-	-
A1171		GLY	50	-	Favored (14.19%) Glycine / 113.6,161.1	-	-	-	-

Favored

32.7% (*mmmt*)

A1172	LYS	50	-	(66.26%) General / -59.1,-28.1	52.7% (mmmt) chi angles: 294,295.6,293.8,181	0.019Å	-	-
A1173	HIS	50	-	Favored (12.07%) General / -120.6,17.1	56.5% (m170) chi angles: 297.2,159.3	0.007Å	OUTLIER(S) worst is CD2--NE2: 4.671 σ	-
A1174	CYS	50	-	Favored (25.5%) General / 57.7,35.4	18.1% (m) chi angles: 312.6	0.015Å	-	-
A1175	GLU	50	0.506Å HB3 with A1149 LEU HD12	Favored (58.5%) General / -85.8,-7.8	1.5% (pm0) chi angles: 59.9,273,80.2	0.126Å	-	-
A1176	LEU	50	-	Favored (32.55%) General / -103.3,116.5	95.7% (mt) chi angles: 294.1,175	0.035Å	-	-
A1177	ASN	50	0.576Å HB2 with A1169 TRP CZ3	Favored (7.63%) General / -81.6,96.9	57.3% (t30) chi angles: 186.9,52	0.072Å	-	-
A1178	ILE	50	0.709Å HG22 with A1168 GLY O	Favored (5.03%) Isoleucine or valine / -50.4,126.4	8% (tp) chi angles: 182.4,67.8	0.103Å	-	-
A1179	ASP	50	-	Favored (11.4%) General / -88.0,98.2	49.8% (t0) chi angles: 188.4,334.7	0.054Å	-	-
A1180	GLU	50	0.572Å OE2 with A1178 ILE HG23	Favored (23.2%) General / -71.4,-3.8	49.7% (mp0) chi angles: 288.3,76.7,18.2	0.079Å	-	-
A1181	CYS	50	-	Favored (27.24%) General / -107.2,5.0	86.6% (m) chi angles: 292.2	0.07Å	-	-
A1182	PHE	50	-	Favored (71.35%) General / -65.8,-30.7	79.9% (t80) chi angles: 183.7,80.4	0.033Å	-	-
A1183	SER	50	-	Favored (31.14%) General / -96.0,12.2	76.4% (p) chi angles: 58.4	0.026Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1184		ASN	50	-	Favored (3.48%) Pre-proline / 49.1,68.5	26.9% (*m120*) chi angles: 299.3,132.1	0.049Å	-	-
			Avg: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1185		PRO	50	-	Favored (13.05%) Trans-proline / -72.2,-30.6	91.9% (*Cg_endo*) chi angles: 32.1	0.059Å	-	-
A1186		CYS	50	-	Favored (25.45%) General / -78.8,121.9	62.1% (*m*) chi angles: 303.4	0.028Å	-	-
A1187		ILE	99.99	-	Favored (7.77%) Isoleucine or valine / -75.2,-56.8	46.6% (*mm*) chi angles: 305.7,302.3	0.081Å	-	-
A1188		HIS	99.99	-	Favored (3.08%) General / -119.2,89.2	75.4% (*m80*) chi angles: 299.1,90.2	0.034Å	OUTLIER(S) worst is CG--ND1: 4.713 σ	OUTLIER(S) worst is CB-CG-CD2: 4.143 σ
A1189		GLY	99.99	-	Favored (18.27%) Glycine / 123.7,-160.0	-	-	-	-
A1190		ASN	50	-	Favored (29.41%) General / -87.0,140.6	14.5% (*t-20*) chi angles: 195.5,293.5	0.116Å	-	-
A1191		CYS	50	-	Favored (47.93%) General / -108.7,136.6	22.9% (*t*) chi angles: 191	0.07Å	-	-
A1192		SER	50	-	Favored (17.85%) General / -110.4,108.0	69.2% (*m*) chi angles: 297.9	0.043Å	-	-
A1193		ASP	50	-	Favored (2%) General / -72.2,97.7	41.3% (*t0*) chi angles: 188.9,25.5	0.042Å	-	-
A1194		ARG	50	-	Favored (7.27%) General / -109.2,171.7	56.5% (*mmm-85*) chi angles: 297,295.9,293.2,278.5	0.048Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1195		VAL	50	-	Allowed (0.87%) Isoleucine or valine / -69.3,103.7	10.8% (*p*) chi angles: 61.3	0.11Å	-	-
A1196		ALA	50	0.507Å HB2 with A1167 LEU C	Favored (6.81%) General / 70.1,19.4	-	0.054Å	-	-
A1197		ALA	50	-	Favored (9.37%) General / -168.7,158.7	-	0.025Å	-	-
A1198		TYR	50	-	Favored (47.7%) General / -124.7,148.9	55.5% (*p90*) chi angles: 62.4,89.7	0.057Å	-	-
A1199		HIS	50	-	Favored (50.99%) General / -128.6,142.6	55.2% (*m170*) chi angles: 296.3,157.9	0.007Å	OUTLIER(S) worst is CG--ND1: 4.417 σ	-
A1200		CYS	50	-	Favored (54.86%) General / -107.4,130.1	77.5% (*m*) chi angles: 299.1	0.046Å	-	-
A1201		THR	50	-	Favored (10.56%) General / -101.7,100.2	99.5% (*m*) chi angles: 298.6	0.032Å	-	-
A1202		CYS	50	-	Favored (57.86%) General / -66.8,140.9	60% (*m*) chi angles: 304.5	0.014Å	-	-
A1203		GLU	50	0.415Å CD with A1204 PRO HD2	Favored (88.37%) Pre-proline / -69.7,138.5	43.9% (*tp10*) chi angles: 189.3,57.5,16.1	0.067Å	-	-
A1204		PRO	50	0.415Å HD2 with A1203 GLU CD	Favored (10.62%) Trans-proline / -45.8,127.9	53.2% (*Cg_exo*) chi angles: 326.8	0.069Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1205		GLY	50	0.579Å O with A1215 ILE HG12	Favored (33.89%) Glycine / -100.0,-15.0	-	-	-	-

				HG12	109.0,-15.0				
A1206	TYR	50	-		Favored (42.7%) General / -119.4,148.9	99.4% (*m-85*) chi angles: 296.9,276.6	0.025Å	-	-
A1207	THR	50	-		Favored (23.64%) General / -143.3,166.8	55.6% (*p*) chi angles: 56.2	0.022Å	-	-
A1208	GLY	50	-		Favored (15.94%) Glycine / 116.8,171.6	-	-	-	-
A1209	VAL	50	-		Favored (73.95%) Isoleucine or valine / -64.7,-35.1	59.1% (*t*) chi angles: 181.7	0.045Å	-	-
A1210	ASN	50	-		Favored (22.53%) General / -110.8,10.0	93.7% (*m-20*) chi angles: 293.7,339.1	0.02Å	-	-
A1211	CYS	50	-		Favored (28.71%) General / 56.7,37.3	54.3% (*m*) chi angles: 306.6	0.022Å	-	-
A1212	GLU	50	-		Favored (35.29%) General / -82.2,-23.8	16.6% (*pm0*) chi angles: 69.3,286.6,356.8	0.097Å	-	-
A1213	VAL	50	-		Favored (42.45%) Isoleucine or valine / -90.9,122.6	44.3% (*t*) chi angles: 183.9	0.039Å	-	-
A1214	ASP	50	-		Favored (12.15%) General / -83.8,102.2	47% (*t0*) chi angles: 187.7,331.2	0.045Å	-	-
A1215	ILE	50	0.579Å HG12 with A1205 GLY O		Allowed (1.47%) Isoleucine or valine / -45.2,127.3	37.5% (*pt*) chi angles: 66.3,173.7	0.038Å	-	-
A1216	ASP	50	0.443Å O with A1219 GLN HG2		Favored (10.83%) General / -87.7,97.3	37.2% (*t0*) chi angles: 183.9,26.7	0.054Å	-	-
					Favored	33.4% (*m120*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1217		ASN	50	-	(63.72%) General / -64.8,-16.9	55.1% (m-120) chi angles: 293.1,115.7	0.04Å	-	-
A1218		CYS	50	-	Favored (59.51%) General / -81.9,-9.7	71.7% (m) chi angles: 297.8	0.012Å	-	-
A1219		GLN	50	0.443Å HG2 with A1216 ASP O	Favored (84%) General / -63.2,-36.5	17.9% (pt20) chi angles: 67.3,182.7,55.2	0.04Å	-	-
A1220		SER	50	-	Favored (55.76%) General / -83.5,-2.3	28.5% (p) chi angles: 51.9	0.021Å	-	-
A1221		HIS	50	-	Allowed (0.63%) General / 55.5,70.5	17.7% (t-160) chi angles: 178.8,207.3	0.078Å	OUTLIER(S) worst is CG--ND1: 4.453 σ	-
A1222		GLN	99.99	-	Favored (68.79%) General / -71.7,-33.3	95% (mm-40) chi angles: 293.5,297.8,320.8	0.031Å	-	-
A1223		CYS	50	0.823Å HB3 with A1227 ALA HB3	Favored (7%) General / -74.2,108.4	36.2% (m) chi angles: 308.3	0.054Å	-	-
A1224		ALA	50	-	Favored (36.21%) General / -68.9,157.7	-	0.027Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1225		ASN	99.99	0.587Å ND2 with A1244 PHE CE1	Favored (19.95%) General / 61.0,32.6	84.9% (m-20) chi angles: 297,334.5	0.05Å	-	-
A1226		GLY	50	-	Favored (8.59%) Glycine / 55.5,60.6	-	-	-	-
A1227		ALA	50	0.823Å HB3 with A1223 CYS HB3	Favored (23.46%) General / -96.7,147.9	-	0.057Å	-	-
A1228		THR	50	0.656Å OG1 with	Favored (46.1%)	64.3% (p)	0.027Å		

A1228	THR	50	A1239 LEU HB3	General / -70.3,132.7	chi angles: 62.9	0.027Å	-	-
A1229	CYS	50	-	Favored (55.46%) General / -113.3,132.7	52.4% (*t*) chi angles: 181.4	0.079Å	-	-
A1230	ILE	50	0.526Å CG1 with A1237 SER HB3	Favored (65.1%) Isoleucine or valine / -121.1,121.5	20.7% (*pt*) chi angles: 72.5,172.8	0.145Å	-	-
A1231	SER	50	-	Favored (46.1%) General / -72.4,136.5	27.4% (*t*) chi angles: 185.5	0.055Å	-	-
A1232	HIS	50		Allowed (0.58%) General / -124.3,-153.8	60.3% (*m170*) chi angles: 296.8,161.2	0.046Å	OUTLIER(S) worst is CG-- ND1: 4.655 σ	-
A1233	THR	50	-	Favored (28.14%) General / -104.3,114.1	96.9% (*m*) chi angles: 299.4	0.026Å	-	-
A1234	ASN	50	-	Favored (16.21%) General / 51.6,36.0	62.4% (*t30*) chi angles: 197.3,28	0.053Å	-	-
A1235	GLY	50	-	Favored (18.67%) Glycine / -169.3,151.9	-	-	-	-
A1236	TYR	99.99	0.498Å CE2 with A1247 LYS NZ	Favored (36.49%) General / -125.9,157.9	54.6% (*p90*) chi angles: 61.4,270.3	0.019Å	-	-
A1237	SER	50	0.526Å HB3 with A1230 ILE CG1	Favored (10.06%) General / -129.8,108.3	17.8% (*t*) chi angles: 169.3	0.099Å	-	-
A1238	CYS	50	-	Favored (31.55%) General / -84.3,124.7	86.1% (*m*) chi angles: 292.2	0.026Å	-	-
A1239	LEU	50	0.656Å HB3 with A1228 THR OG1	Favored (5.02%) General / -105.3,94.1	6.2% (*tt*) chi angles: 179.3,163.7	0.11Å	-	-
A1240	CYS	50		Favored (55.54%)	60.1% (*m*)	0.027Å		

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1240		CYS	50	-	(33.34%) General / -66.6,145.5	80.1% (m) chi angles: 304.4	0.007Å	-	-
A1241		PHE	99.99	0.413Å CG with A1242 GLY N	Favored (14.6%) General / -74.7,171.0	79.5% (t80) chi angles: 184.6,77.3	0.055Å	-	-
A1242		GLY	50	0.425Å HA2 with A1243 ASN HA	Favored (5.49%) Glycine / -77.5,120.2	-	-	-	-
A1243		ASN	50	0.425Å HA with A1242 GLY HA2	Favored (3.87%) General / -124.3,93.3	27.2% (t-20) chi angles: 187.6,300.2	0.048Å	-	-
A1244		PHE	50	0.587Å CE1 with A1225 ASN ND2	Favored (24.31%) General / -127.0,163.2	98.8% (m-85) chi angles: 296.1,276	0.016Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 14.95	Outliers: 1 of 104	Poor rotamers: 0 of 91	Outliers: 0 of 95	Outliers: 7 of 106	Outliers: 2 of 106
A1245		THR	50	-	Favored (9.81%) General / -164.3,148.9	12.6% (t) chi angles: 185.7	0.059Å	-	-
A1246		GLY	50	-	Allowed (0.12%) Glycine / -138.4,-38.7	-	-	-	-
A1247		LYS	50	0.498Å NZ with A1236 TYR CE2	Favored (10.28%) General / -96.8,-37.4	28.1% (tptp) chi angles: 185.4,61.5,181.1,66.9	0.03Å	-	-
A1248		PHE	99.99	0.401Å CZ with A1236 TYR OH	Favored (12.18%) General / -115.7,-4.3	97.5% (m-85) chi angles: 294.4,94.5	0.027Å	-	-
A1249		CYS	50	-	Favored (20.74%) General / 60.2,37.4	31.9% (m) chi angles: 309.8	0.024Å	-	-
A1250		ARG	99.99	-	-	30.6% (ptt-85) chi angles: 62.9,174,180.2,280.4	0.046Å	-	-

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