Viewing crb1_sm_1145-1250_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0		100th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	3.30%	Goal: <1%
	Ramachandran outliers	6	5.77%	Goal: <0.05%
	Ramachandran favored	86	82.69%	Goal: >98%
	MolProbity score^	1.59		93rd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 815	0.00%	Goal: 0%
	Bad backbone angles:	12 / 1106	1.08%	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: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1145		SER	50	-	-	45.1% (*t*) chi angles: 180.7	0.079Å	-	-
A1146		ASN	50	-	Favored (94.38%) Pre-proline / -67.1,137.3	53.6% (*t-20*) chi angles: 192.5,350	0.095Å	-	-
A1147		PRO	50	-	Favored (10.21%) Trans-proline / -83.0,-10.7	62.5% (*Cg_endo*) chi angles: 34.3	0.047Å	-	-
A1148		CYS	50	-	Favored (16.97%) General / -94.0,155.8	3.7% (*m*) chi angles: 321.1	0.08Å	-	-

A1149	LEU	50	-	Favored (6.35%) General / -112.7,173.5	50% (*mt*) chi angles: 307,183.3	0.04Å	-	-
A1150	HIS	50	-	Favored (11.63%) General / 57.0,26.3	70.6% (*m80*) chi angles: 300.7,94.2	0.097Å	-	-
A1151	GLY	50	-	Favored (80.18%) Glycine / 85.6,8.6	-	-	-	-
A1152	GLY	50	-	Favored (34.86%) Glycine / -58.9,150.9	-	-	-	-
A1153	ASN	50	-	Favored (36.08%) General / -80.6,135.4	60.8% (*t30*) chi angles: 186.8,29.2	0.066Å	-	-
A1154	CYS	50	-	Favored (10.76%) General / -94.5,98.3	40.6% (*t*) chi angles: 177.6	0.034Å	-	-
A1155	GLU	50	-	Favored (3.54%) General / -124.6,91.9	24.2% (*tt0*) chi angles: 201.3,181,262.2	0.198Å	-	-
A1156	ASP	50	-	Favored (5.06%) General / -101.0,177.0	2.5% (*t0*) chi angles: 215.5,316.8	0.152Å	-	OUTLIER(S) worst is C-N-CA: 6.878 σ
A1157	ILE	50	-	OUTLIER (0.01%) Isoleucine or valine / -150.0,-132.5	15% (*pt*) chi angles: 48.3,175.9	0.186Å	-	-
A1158	TYR	50	-	Favored (7.49%) General / -85.7,84.8	70.5% (*t80*) chi angles: 184.1,85.3	0.05Å	-	-
A1159	SER	50	-	Favored (22.65%) General / 57.9,42.6	29.2% (*t*) chi angles: 185.1	0.082Å	-	-
A1160	SER	50	-	Allowed (0.78%) General / -152.9,62.1	7.8% (*t*) chi angles: 195.7	0.059Å	-	-
A1161	TYR	50	-	Favored (12.25%)	27.8% (*p90*)	0.064Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					General / -52.5,123.9	chi angles: 67.2,103.1			
A1162		HIS	50	-	Favored (15.67%) General / -95.7,157.9	0.1% chi angles: 19.4,108.3	0.106Å	-	OUTLIER(S) worst is CA-CB-CG: 5.086 σ
A1163		CYS	50	-	Favored (14.38%) General / -132.7,114.6	64.5% (*m*) chi angles: 302.5	0.054Å	-	-
A1164		SER	50	-	Favored (11.23%) General / -86.9,98.5	1.3% (*m*) chi angles: 323.6	0.063Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1165		CYS	50	-	Favored (87.8%) Pre-proline / -63.4,125.7	80.4% (*m*) chi angles: 299.6	0.053Å	-	-
A1166		PRO	50	-	Favored (4.33%) Trans-proline / -90.6,158.6	27.1% (*Cg_endo*) chi angles: 37.7	0.052Å	-	-
A1167		LEU	99.99	-	Favored (8.38%) General / -47.9,138.8	45.9% (*mt*) chi angles: 305.9,185.2	0.052Å	-	-
A1168		GLY	50	-	Favored (56.69%) Glycine / 93.6,-18.4	-	-	-	-
A1169		TRP	99.99	-	Favored (50.37%) General / -129.2,151.0	15.5% (*m95*) chi angles: 316,90.4	0.049Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.914 σ
A1170		SER	50	-	Allowed (1.17%) General / -145.6,-160.7	10.2% (*t*) chi angles: 192.2	0.134Å	-	-
A1171		GLY	50	-	Favored (46.42%) Glycine / 85.2,-171.6	-	-	-	-
					Favored				

A1172	LYS	50	-	(47.51%) General / -78.8,-21.5	17.7% (*tptp*) chi angles: 173.9,60.2,202.2,68.3	0.141Å	-	-
A1173	HIS	50	-	Favored (9.27%) General / -124.0,15.2	46.4% (*m80*) chi angles: 305.1,76.6	0.049Å	-	-
A1174	CYS	50	-	Favored (15.67%) General / 62.8,32.8	2.7% (*m*) chi angles: 325.3	0.094Å	-	-
A1175	GLU	50	-	Favored (8.91%) General / -100.9,-36.8	2.9% (*pm0*) chi angles: 71.3,286.1,55.6	0.108Å	-	-
A1176	LEU	50	-	Favored (48.09%) General / -69.6,149.5	69.8% (*mt*) chi angles: 304.5,180.5	0.042Å	-	-
A1177	ASN	50	-	Favored (33.04%) General / -92.9,136.7	2% (*t30*) chi angles: 195.2,99.1	0.129Å	-	-
A1178	ILE	50	-	Favored (12.43%) Isoleucine or valine / -100.5,101.7	2.4% (*tp*) chi angles: 215.7,76	0.169Å	-	-
A1179	ASP	50	-	Favored (9.9%) General / -69.9,116.1	19% (*t0*) chi angles: 175.3,29.7	0.034Å	-	-
A1180	GLU	50	-	Favored (23.26%) General / -85.8,7.6	67.5% (*mt-10*) chi angles: 295.4,161.5,15.5	0.143Å	-	-
A1181	CYS	50	-	Favored (21.29%) General / -93.7,-19.3	46.9% (*m*) chi angles: 283.3	0.094Å	-	-
A1182	PHE	50	-	Favored (71.34%) General / -64.4,-30.3	77.6% (*t80*) chi angles: 182.5,84.2	0.132Å	-	-
A1183	SER	50	-	Favored (60.4%) General / -75.5,-14.2	78.3% (*p*) chi angles: 59.1	0.089Å	-	-
A1184	ASN	50	-	Allowed (0.34%) Pre-proline /	3.3% (*m120*) chi angles: 314.9,152.9	0.085Å	-	OUTLIER(S) worst is CA-CB-CG: 6 σ

67.3,45.0

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1185		PRO	50	-	Allowed (0.4%) Trans-proline / -76.5,31.4	0.4% chi angles: 43.3	0.044Å	-	-
A1186		CYS	50	-	Favored (24.86%) General / -128.9,119.7	52.8% (*m*) chi angles: 284	0.085Å	-	-
A1187		ILE	99.99	-	Favored (5.92%) Isoleucine or valine / -86.6,-28.1	24.9% (*mm*) chi angles: 310.6,307.8	0.107Å	-	-
A1188		HIS	99.99	-	Allowed (1.28%) General / -152.7,87.0	11.9% (*m80*) chi angles: 316,79.7	0.059Å	-	OUTLIER(S) worst is CA-CB-CG: 6.307 σ
A1189		GLY	99.99	-	Favored (32.25%) Glycine / 153.5,-173.7	-	-	-	-
A1190		ASN	50	-	Favored (31.61%) General / -107.0,146.0	7.9% (*t-20*) chi angles: 163.1,251.7	0.098Å	-	-
A1191		CYS	50	-	Favored (16.9%) General / -109.2,159.5	15.6% (*t*) chi angles: 193	0.034Å	-	-
A1192		SER	50	-	Favored (52.46%) General / -126.5,140.4	47.9% (*t*) chi angles: 179.8	0.07Å	-	-
A1193		ASP	50	-	Favored (10.95%) General / -56.0,152.0	49.7% (*t0*) chi angles: 188.8,16.2	0.077Å	-	-
A1194		ARG	50	-	Allowed (0.13%) General / -142.2,-101.0	4.2% (*mmp_?*) chi angles: 285.1,293.8,90.7,169.5	0.143Å	-	OUTLIER(S) worst is C-N-CA: 4.401 σ
A1195		VAL	50	-	OUTLIER (0%) Isoleucine or valine / 153.4,70.4	9.3% (*p*) chi angles: 60.5	0.224Å	-	OUTLIER(S) worst is C-N-CA: 5.246 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1196		ALA	50	-	OUTLIER (0%) General / 107.7,6.9	-	0.205Å	-	-
A1197		ALA	50	-	Allowed (0.05%) General / 179.9,117.6	-	0.083Å	-	-
A1198		TYR	50	-	Favored (37.56%) General / -57.0,143.5	21.4% (p90) chi angles: 51.9,77.8	0.03Å	-	-
A1199		HIS	50	-	Favored (6.88%) General / -102.8,96.5	60.3% (t-80) chi angles: 184.1,278.5	0.065Å	-	-
A1200		CYS	50	-	Favored (57.7%) General / -61.9,135.8	57% (m) chi angles: 305.8	0.08Å	-	-
A1201		THR	50	-	Favored (2.56%) General / -130.3,87.8	1.5% (m) chi angles: 324.8	0.053Å	-	-
A1202		CYS	50	-	Favored (33.02%) General / -54.6,141.0	60.6% (m) chi angles: 304.1	0.087Å	-	-
A1203		GLU	50	-	Favored (92.43%) Pre-proline / -61.0,133.0	5.5% (tp10) chi angles: 161.7,39.7,46.7	0.079Å	-	-
A1204		PRO	50	-	OUTLIER (0.02%) Trans-proline / -50.0,71.2	0.1% chi angles: 318.1	0.02Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1205		GLY	50	-	Allowed (0.11%) Glycine / 159.2,-4.1	-	-	-	-
A1206		TYR	50	-	Favored (32.04%) General / -118.5,154.7	96.5% (m-85) chi angles: 297.8,269.4	0.037Å	-	-
					Allowed				

A1207	THR	50	-	(1.15%) General / -140.5,-161.1	11.2% (*t*) chi angles: 192.1	0.198Å	-	-
A1208	GLY	50	-	Favored (24.51%) Glycine / 95.1,-163.9	-	-	-	-
A1209	VAL	50	-	Favored (11.07%) Isoleucine or valine / -81.4,-19.9	69.7% (*t*) chi angles: 173.6	0.137Å	-	-
A1210	ASN	50	-	Allowed (1.06%) General / -145.5,34.4	17.9% (*m120*) chi angles: 295.6,89.1	0.022Å	-	-
A1211	CYS	50	-	Favored (19.97%) General / 48.5,47.9	14.2% (*p*) chi angles: 53.2	0.216Å	-	OUTLIER(S) worst is C-N-CA: 5.115 σ
A1212	GLU	50	-	Favored (7.72%) General / -103.5,-37.1	11.4% (*pm0*) chi angles: 76.7,291.5,24.8	0.07Å	-	OUTLIER(S) worst is CB-CG-CD: 4.445 σ
A1213	VAL	50	-	Favored (36.22%) Isoleucine or valine / -75.5,130.4	90.6% (*t*) chi angles: 177.1	0.053Å	-	-
A1214	ASP	50	-	Favored (32.11%) General / -80.0,127.3	23.6% (*t0*) chi angles: 199.7,29.4	0.032Å	-	-
A1215	ILE	50	-	Favored (18.55%) Isoleucine or valine / -57.8,138.6	44.3% (*pt*) chi angles: 59.9,169.1	0.176Å	-	-
A1216	ASP	50	-	Favored (23.16%) General / -95.4,147.8	29.4% (*t70*) chi angles: 176.6,62	0.026Å	-	-
A1217	ASN	50	-	Favored (4.79%) General / -129.4,-5.4	5.5% (*m120*) chi angles: 314.5,141.3	0.041Å	-	OUTLIER(S) worst is CA-CB-CG: 5.552 σ
A1218	CYS	50	-	Favored (80.73%) General / -68.6,-38.5	98.1% (*m*) chi angles: 294.3	0.075Å	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1219		GLN	50	-	(53.06%) General / -77.3,-21.8	7.1% (*tp-100*) chi angles: 193.2,63.3,261.7	0.099Å	-	-
A1220		SER	50	-	Favored (72.3%) General / -71.0,-36.3	3.2% (*p*) chi angles: 90.5	0.147Å	-	-
A1221		HIS	50	-	Allowed (0.1%) General / 75.3,47.4	64% (*m80*) chi angles: 303.4,83.5	0.159Å	-	-
A1222		GLN	99.99	-	Favored (70.23%) General / -59.2,-32.8	21.9% (*mm-40*) chi angles: 298.8,295.6,266.1	0.109Å	-	-
A1223		CYS	50	-	Favored (10.34%) General / -88.7,95.6	56.8% (*m*) chi angles: 306	0.045Å	-	-
A1224		ALA	50	-	Favored (8.83%) General / -55.6,152.7	-	0.049Å	-	-
#	**Alt**	**Res**	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1225		ASN	99.99	-	Favored (4.11%) General / 73.5,15.7	24.2% (*m-80*) chi angles: 314,295.4	0.102Å	-	-
A1226		GLY	50	-	Favored (78.43%) Glycine / 89.0,2.2	-	-	-	-
A1227		ALA	50	-	Favored (50.93%) General / -59.3,142.9	-	0.046Å	-	-
A1228		THR	50	-	Favored (47.21%) General / -72.5,138.9	24.9% (*m*) chi angles: 308.9	0.036Å	-	-
A1229		CYS	50	-	Favored (43.2%) General / -113.1,144.1	48.5% (*t*) chi angles: 182.5	0.096Å	-	-
A1230		ILE	50	-	Allowed (1.58%) Isoleucine or valine	4.5% (*mp*) chi angles: 305,95.8	0.032Å	-	-

				/ -138.6,100.5				
A1231	SER	50	-	Favored (12.95%) General / -55.6,150.1	57.7% (*m*) chi angles: 299.4	0.077Å	-	-
A1232	HIS	50	-	Favored (27.56%) General / -159.3,168.0	24.8% (*m80*) chi angles: 312.5,88.1	0.119Å	-	-
A1233	THR	50	-	OUTLIER (0.03%) General / -41.9,103.8	10.4% (*m*) chi angles: 313.1	0.061Å	-	-
A1234	ASN	50	-	Favored (12.9%) General / 47.6,41.0	11.2% (*t-20*) chi angles: 210.8,349.2	0.094Å	-	-
A1235	GLY	50	-	OUTLIER (0.05%) Glycine / 173.5,81.5	-	-	-	-
A1236	TYR	99.99	-	Favored (47.63%) General / -62.1,147.4	37% (*p90*) chi angles: 67.6,279.4	0.049Å	-	-
A1237	SER	50	-	Favored (11.16%) General / -103.8,165.2	68.1% (*p*) chi angles: 57.3	0.081Å	-	-
A1238	CYS	50	-	Favored (38.19%) General / -124.4,155.8	32.3% (*m*) chi angles: 309.7	0.095Å	-	-
A1239	LEU	50	-	Favored (4.76%) General / -129.1,97.9	2.9% (*tt*) chi angles: 206.5,173.9	0.031Å	-	-
A1240	CYS	50	-	Favored (9.66%) General / -65.7,118.5	83.9% (*m*) chi angles: 300.1	0.062Å	-	-
A1241	PHE	99.99	-	Favored (39.33%) General / -68.4,155.7	55.5% (*t80*) chi angles: 188.9,85.7	0.034Å	-	-
A1242	GLY	50	-	Favored (31.43%) Glycine /	-	-	-	OUTLIER(S) worst is C-N-CA: 5.49 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A1243		ASN	50	-	-58.3,122.9 Favored (2.21%) General / -126.9,48.2	78.1% (*m-20*) chi angles: 297.3,344.8	0.048Å	-	-
A1244		PHE	50	-	Favored (26.78%) General / -79.9,158.2	42.1% (*m-85*) chi angles: 308.6,295	0.027Å	-	-

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			Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 3 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 12 of 106
A1245		THR	50	-	Favored (40.23%) General / -153.3,163.2	12.2% (*t*) chi angles: 191.4	0.114Å	-	OUTLIER(S) worst is C-N-CA: 4.279 σ
A1246		GLY	50	-	Favored (2.14%) Glycine / -123.1,-23.8	-	-	-	-
A1247		LYS	50	-	Favored (3.19%) General / -126.9,-26.4	26.5% (*tptp*) chi angles: 194.9,66.7,177.4,64.4	0.079Å	-	-
A1248		PHE	99.99	-	Favored (17.17%) General / -108.5,-4.5	87.9% (*m-85*) chi angles: 302.9,97.1	0.056Å	-	-
A1249		CYS	50	-	Favored (16.94%) General / 61.9,34.6	36.6% (*m*) chi angles: 308.3	0.143Å	-	-
A1250		ARG	99.99	-	-	43% (*tpt85*) chi angles: 185.5,63.1,195.3,78.9	0.047Å	-	-

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