



Viewing crb1_sm_36-148_FFX1H-multi.table

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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	3	3.03%	Goal: <1%
	Ramachandran outliers	3	2.70%	Goal: <0.05%
	Ramachandran favored	82	73.87%	Goal: >98%
	MolProbity score^	1.67		90 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.94%	Goal: 0
	Bad backbone bonds:	0 / 841	0.00%	Goal: 0%
	Bad backbone angles:	9 / 1139	0.79%	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: 56.19	Clashscore: 0	Outliers: 3 of 111	Poor rotamers: 3 of 99	Outliers: 2 of 103	Outliers: 0 of 113	Outliers: 9 of 113
A 36	SER	50	-	-	48.4% (t) chi angles: 179.5	0.078Å	-	-
A 37	ASN	50	-	Favored (57.36%) General / -60.3,134.8	4.6% (t30) chi angles: 193.1,92.4	0.128Å	-	-
A 38	SER	50	-	Favored (21.35%) General / -73.2,-50.7	89.9% (p) chi angles: 62.5	0.103Å	-	-
A 39	CYS	50	-	Favored (52.09%) General / -56.0,136.3	1.9% (m) chi angles: 327.8	0.124Å	-	-

A 40	GLN	99.99	-	Favored (5.65%) General / -89.1,-178.4	21% (<i>mm-40</i>) chi angles: 303.7,301.9,267.9	0.046Å	-	-
A 41	ASN	50	-	Favored (28.56%) General / 56.5,37.1	75.9% (<i>m-20</i>) chi angles: 300.3,332.6	0.095Å	-	-
A 42	ASN	50	-	Favored (2.13%) General / 70.9,-3.0	6.2% (<i>m-80</i>) chi angles: 318.3,279.9	0.145Å	-	-
A 43	SER	50	-	Favored (54.08%) General / -66.0,135.0	71.9% (<i>m</i>) chi angles: 293.5	0.067Å	-	-
A 44	THR	50	-	Favored (33.19%) General / -84.0,138.3	90.1% (<i>m</i>) chi angles: 297.8	0.064Å	-	-
A 45	CYS	50	-	Favored (19.37%) General / -100.2,107.5	42.2% (<i>t</i>) chi angles: 175.9	0.088Å	-	-
A 46	LYS	50	-	Favored (23.73%) General / -84.0,118.0	16.7% (<i>tptp</i>) chi angles: 173.6,70.1,201.5,80.4	0.042Å	-	-
A 47	ASP	50	-	Favored (56.36%) General / -57.1,135.7	5.8% (<i>p-10</i>) chi angles: 49.5,295.7	0.044Å	-	-
A 48	PHE	50	-	Favored (43.35%) General / -152.2,160.5	22.9% (<i>m-85</i>) chi angles: 282.8,125.6	0.072Å	-	-
A 49	SER	50	-	Favored (10.54%) General / -85.8,72.4	89.9% (<i>p</i>) chi angles: 65.3	0.075Å	-	OUTLIER(S) worst is C-N- CA: 4.08 σ
A 50	LYS	50	-	OUTLIER (0.01%) General / 150.8,-37.3	13.6% (<i>tptp</i>) chi angles: 166.2,57.5,204,62.8	0.225Å	-	-
A 51	ASP	99.99	-	Favored (5.91%) General / -146.0,-178.0	51.2% (<i>m-20</i>) chi angles: 294.4,297	0.053Å	-	-
A 52	ASN	99.99	-	Favored (41.36%) General / -142.1,159.9	76% (<i>m-20</i>) chi angles: 300.8,302.7	0.13Å	-	-

A 53	ASP	50	-	Favored (36.43%) General / -91.8,125.2	2.3% (<i>m-20</i>) chi angles: 318.6,156.4	0.101Å	-	-	
A 54	CYS	50	-	Favored (6.32%) General / -89.8,85.1	61.8% (<i>m</i>) chi angles: 303.5	0.055Å	-	-	
A 55	SER	50	-	Favored (2.09%) General / -74.6,85.2	47.6% (<i>t</i>) chi angles: 180	0.03Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.19	Clashscore: 0	Outliers: 3 of 111	Poor rotamers: 3 of 99	Outliers: 2 of 103	Outliers: 0 of 113	Outliers: 9 of 113
A 56	CYS	50	-	Favored (30.95%) General / -51.8,131.6	71.7% (<i>m</i>) chi angles: 297.3	0.081Å	-	-	
A 57	SER	50	-	Favored (13.62%) General / -65.9,165.1	70.9% (<i>m</i>) chi angles: 297.4	0.067Å	-	-	
A 58	ASP	50	-	Favored (30.83%) General / -62.8,127.3	63.8% (<i>t0</i>) chi angles: 187.6,359.1	0.05Å	-	-	
A 59	THR	50	-	Favored (2.02%) General / 75.2,20.8	3.3% (<i>m</i>) chi angles: 319.4	0.184Å	-	-	
A 60	ALA	50	-	Favored (46.13%) General / -120.5,146.6	-	0.057Å	-	-	
A 61	ASN	50	-	Favored (33.87%) General / -148.5,150.7	42.4% (<i>t30</i>) chi angles: 179.1,53.1	0.111Å	-	-	
A 62	ASN	99.99	-	Favored (5.68%) General / -114.8,175.0	22.4% (<i>p-10</i>) chi angles: 69.8,321.8	0.066Å	-	-	
A 63	LEU	99.99	-	Allowed (0.09%) General / -147.2,-100.7	5.2% (<i>tt</i>) chi angles: 200.8,165.3	0.182Å	-	OUTLIER(S) worst is C-CA-CB: 4.343 σ	
A 64	ASP	99.99	-	Allowed (1.07%) General / -89.3,42.2	22.5% (<i>p-10</i>) chi angles: 60.4,326.1	0.085Å	-	-	

A 65	LYS	99.99	-	Favored (2.61%) General / -148.2,-166.7	44.6% (<i>mmtm</i>) chi angles: 303.4,295.7,171.9,296.9	0.062Å	-	OUTLIER(S) worst is C-N- CA: 8.663 σ
A 66	ASP	50	-	OUTLIER (0.01%) General / 105.3,6.7	87.5% (<i>m-20</i>) chi angles: 285.4,173.1	0.363Å	-	-
A 67	CYS	50	-	Favored (15.41%) General / 63.4,28.3	83.7% (<i>m</i>) chi angles: 300.7	0.129Å	-	-
A 68	ASP	99.99	-	Favored (78.07%) General / -60.5,-36.3	0.6% chi angles: 312.8,18.3	0.088Å	-	OUTLIER(S) worst is CA- CB-CG: 4.959 σ
A 69	ASN	50	-	Favored (2.65%) General / -74.6,94.2	2.1% (<i>t-20</i>) chi angles: 174,207.6	0.032Å	-	OUTLIER(S) worst is CA- CB-CG: 5.942 σ
A 70	MET	50	-	Favored (24.83%) General / -65.8,125.3	26.4% (<i>ttt</i>) chi angles: 186.8,181.4,181.4	0.044Å	-	-
A 71	LYS	50	-	Favored (38.71%) General / -71.7,157.0	44.9% (<i>tttm</i>) chi angles: 187.8,186.4,164.5,295.3	0.051Å	-	-
A 72	ASP	50	-	Favored (22.17%) Pre-proline / -114.1,135.9	18.8% (<i>t0</i>) chi angles: 178.5,41.3	0.05Å	-	-
A 73	PRO	50	-	Allowed (0.87%) Trans-proline / -94.6,-13.3	12.3% (<i>Cg_endo</i>) chi angles: 39.8	0.023Å	-	-
A 74	CYS	50	-	Favored (70.92%) General / -58.9,-33.8	69% (<i>m</i>) chi angles: 301.7	0.14Å	-	-
A 75	PHE	50	-	Favored (4.13%) General / -47.3,-31.7	89.3% (<i>t80</i>) chi angles: 180.7,76.6	0.075Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 56.19	Clashscore: 0	Outliers: 3 of 111	Poor rotamers: 3 of 99	Outliers: 2 of 103	Outliers: 0 of 113	Outliers: 9 of 113
A 76	SER	50	-	Favored (28.69%) General / -75.0,-2.8	53.2% (<i>p</i>) chi angles: 74.5	0.119Å	-	-

A 77	ASN	50	-	Allowed (0.56%) Pre-proline / 63.2,44.5	3.6% (<i>m</i> -80) chi angles: 286.7,246.8	0.123Å	-	-
A 78	PRO	50	-	Allowed (0.49%) Trans-proline / -79.3,28.8	0.5% chi angles: 42.9	0.044Å	-	-
A 79	CYS	50	-	Allowed (1.22%) General / -93.4,46.8	77% (<i>m</i>) chi angles: 296.3	0.054Å	-	-
A 80	GLN	50	-	Favored (51.68%) General / -63.2,132.4	34.7% (<i>mt</i> -30) chi angles: 286.1,184.3,108.8	0.033Å	-	-
A 81	GLY	50	-	Favored (64.3%) Glycine / 68.8,12.2	-	-	-	-
A 82	SER	50	-	Allowed (0.08%) General / 86.2,20.9	13.4% (<i>t</i>) chi angles: 190.6	0.174Å	-	-
A 83	ALA	50	-	Favored (46.27%) General / -54.5,134.6	-	0.059Å	-	-
A 84	THR	50	-	Favored (9.09%) General / -88.0,92.3	27.8% (<i>m</i>) chi angles: 307.8	0.053Å	-	-
A 85	CYS	50	-	Allowed (0.1%) General / -64.0,-174.2	4.9% (<i>t</i>) chi angles: 202.3	0.119Å	-	-
A 86	VAL	50	-	Allowed (0.14%) Isoleucine or valine / -178.1,141.7	7.4% (<i>p</i>) chi angles: 69.3	0.076Å	-	-
A 87	ASN	50	-	Favored (52.29%) General / -66.1,148.1	37.7% (<i>t</i> -20) chi angles: 196.8,355.5	0.029Å	-	-
A 88	THR	50	-	Favored (24.76%) Pre-proline / -139.9,166.3	4.3% (<i>p</i>) chi angles: 41.2	0.045Å	-	-
A 89	PRO	99.99	-	Favored (7.06%) Trans-proline / -82.5,70.1 Allowed	68.6% (<i>Cg_endo</i>) chi angles: 33.6	0.032Å	-	-

A 90	GLY	99.99	-	(0.85%) Glycine / 157.7,125.6	-	-	-	-
A 91	GLU	99.99	-	Favored (31.68%) General / -80.5,-37.4	52.7% (<i>tp10</i>) chi angles: 177.8,64.6,17.3	0.025Å	-	OUTLIER(S) worst is C-N- CA: 4.048 σ
A 92	ARG	99.99	-	Allowed (1.01%) General / -44.6,-31.0	10.6% (<i>ptt-85</i>) chi angles: 55.6,165.1,209.1,283.2	0.056Å	-	-
A 93	SER	99.99	-	Allowed (0.76%) General / -163.0,92.5	96.6% (<i>p</i>) chi angles: 63.9	0.04Å	-	-
A 94	PHE	50	-	Favored (34.29%) General / -110.6,147.4	9.3% (<i>p90</i>) chi angles: 41.9,266.9	0.053Å	-	-
A 95	LEU	50	-	Favored (7.75%) General / -86.6,82.9	7.3% (<i>mp</i>) chi angles: 264.3,65	0.152Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 56.19</div> <div>Clashscore: 0</div> <div>Outliers: 3 of 111</div> <div>Poor rotamers: 3 of 99</div> <div>Outliers: 2 of 103</div> <div>Outliers: 0 of 113</div> <div>Outliers: 9 of 113</div> </div>								
A 96	CYS	50	-	Allowed (1.74%) General / -73.9,86.5	92.8% (<i>m</i>) chi angles: 295	0.057Å	-	-
A 97	LYS	50	-	Favored (13.37%) General / -75.1,114.2	30.1% (<i>mtmm</i>) chi angles: 292.7,164.7,293.7,299.9	0.044Å	-	-
A 98	CYS	50	-	Favored (10.53%) Pre-proline / -47.6,134.0	37.8% (<i>m</i>) chi angles: 308	0.056Å	-	-
A 99	PRO	50	-	Favored (5.21%) Trans-proline / -89.0,169.8	5.2% (<i>Cg_endo</i>) chi angles: 41.2	0.09Å	-	-
A 100	PRO	50	-	Allowed (0.73%) Trans-proline / -68.1,74.4	33.5% (<i>Cg_exo</i>) chi angles: 341	0.055Å	-	-
A				Allowed (1.28%)				

101	GLY	50	-	Glycine / 147.3,-9.7	-	-	-	-
A 102	TYR	50	-	Favored (45.7%) General / -128.7,155.0	3.5% (<i>m-85</i>) chi angles: 300.6,243.6	0.063Å	-	-
A 103	SER	50	-	Allowed (0.82%) General / -147.6,-157.6	96% (<i>p</i>) chi angles: 63.7	0.085Å	-	-
A 104	GLY	50	-	Favored (16.86%) Glycine / 107.4,-150.7	-	-	-	-
A 105	THR	50	-	Favored (15.96%) General / -80.2,-46.6	35.2% (<i>m</i>) chi angles: 306.3	0.098Å	-	-
A 106	ILE	50	-	Allowed (1.65%) Isoleucine or valine / -129.1,29.6	10.6% (<i>mt</i>) chi angles: 316.4,180.9	0.118Å	-	-
A 107	CYS	50	-	Allowed (1.55%) General / 69.7,39.1	64.7% (<i>m</i>) chi angles: 302.5	0.175Å	-	-
A 108	GLU	50	-	Favored (7.37%) General / -100.5,-40.6	0% chi angles: 69.2,301.1,265.7	0.12Å	-	-
A 109	THR	50	-	Favored (4.94%) General / -70.1,110.0	70% (<i>p</i>) chi angles: 59.2	0.05Å	-	-
A 110	THR	50	-	Favored (48.3%) General / -56.6,131.3	11.2% (<i>p</i>) chi angles: 44.7	0.061Å	-	-
A 111	ILE	50	-	Favored (16.02%) Isoleucine or valine / -59.3,141.6	32.1% (<i>pt</i>) chi angles: 64.1,178.4	0.147Å	-	-
A 112	GLY	50	-	Allowed (1.7%) Glycine / -75.5,72.6	-	-	-	-
A 113	SER	50	-	Favored (71.22%) General / -60.6,-32.0	3.5% (<i>t</i>) chi angles: 202.3	0.124Å	-	-
A 114	CYS	50	-	Favored (50.32%) General /	38.4% (<i>m</i>) chi angles: 307.9	0.119Å	-	-

A 115	GLY	50	-	-80.3,-18.0 Favored (79.74%) Glycine / -73.2,-13.2	-	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.19	Clashscore: 0	Outliers: 3 of 111	Poor rotamers: 3 of 99	Outliers: 2 of 103	Outliers: 0 of 113	Outliers: 9 of 113
A 116	LYS	50	-	-	Favored (57.58%) General / -76.1,-20.6	21.6% (<i>pttm</i>) chi angles: 54.4,179,172.3,289.9	0.162Å	-	-
A 117	ASN	50	-	-	Favored (11.78%) General / 59.0,47.8	61.9% (<i>t30</i>) chi angles: 193.6,24.3	0.099Å	-	-
A 118	SER	50	-	-	Favored (8.84%) General / -83.9,65.9	81.2% (<i>p</i>) chi angles: 60.5	0.038Å	-	-
A 119	CYS	50	-	-	Allowed (0.84%) General / -148.8,38.6	78.6% (<i>m</i>) chi angles: 299.3	0.097Å	-	-
A 120	GLN	50	-	-	Favored (2.99%) General / -46.5,142.6	33.7% (<i>mt-30</i>) chi angles: 289.1,165.6,236	0.096Å	-	-
A 121	HIS	50	-	-	Allowed (1.35%) General / 75.3,-9.7	13.6% (<i>m80</i>) chi angles: 319,97.2	0.184Å	-	-
A 122	GLY	50	-	-	Allowed (1.21%) Glycine / 126.1,26.6	-	-	-	-
A 123	GLY	50	-	-	Favored (49.17%) Glycine / -86.5,178.9	-	-	-	-
A 124	ILE	50	-	-	Favored (9.92%) Isoleucine or valine / -118.1,168.5	48% (<i>pt</i>) chi angles: 60.3,171.7	0.113Å	-	-
A 125	CYS	50	-	-	Favored (51.78%) General / -134.9,154.1	42% (<i>t</i>) chi angles: 183.7	0.055Å	-	-
A 126	HIS	50	-	-	Favored (51.8%) General / -121.6,128.3	21.2% (<i>t-80</i>) chi angles: 169.2,273.7	0.086Å	-	-

A 127	GLN	50	-	Favored (51.73%) General / -68.4,135.4	33.9% (<i>tt0</i>) chi angles: 184.1,198.6,74.7	0.064Å	-	-
A 128	ASP	50	-	Favored (45.02%) Pre-proline / -146.0,159.9	40.4% (<i>m-20</i>) chi angles: 294.1,291.7	0.08Å	-	-
A 129	PRO	50	-	Favored (4.52%) Trans-proline / -72.4,115.9	88.8% (<i>Cg_endo</i>) chi angles: 30.1	0.017Å	-	-
A 130	ILE	50	-	Allowed (0.35%) Isoleucine or valine / 47.9,41.4	14.3% (<i>pt</i>) chi angles: 57.2,157.5	0.269Å	-	-
A 131	TYR	50	-	Favored (9.38%) Pre-proline / -158.1,139.0	64% (<i>t80</i>) chi angles: 175.5,66.6	0.081Å	-	-
A 132	PRO	50	-	OUTLIER (0.05%) Trans-proline / -108.0,136.4	23.9% (<i>Cg_endo</i>) chi angles: 38.1	0.101Å	-	-
A 133	VAL	50	-	Favored (65.86%) Isoleucine or valine / -109.3,127.7	14.3% (<i>p</i>) chi angles: 63.2	0.122Å	-	-
A 134	CYS	50	-	Favored (37.13%) General / -118.2,151.7	23% (<i>m</i>) chi angles: 311.4	0.029Å	-	-
A 135	ILE	50	-	Favored (59.06%) Isoleucine or valine / -119.0,118.8	46.4% (<i>mm</i>) chi angles: 305.3,302.9	0.037Å	-	-

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			Avg: 56.19	Clashscore: 0	Outliers: 3 of 111	Poor rotamers: 3 of 99	Outliers: 2 of 103	Outliers: 0 of 113	Outliers: 9 of 113

A 136	CYS	50	-	Favored (66.09%) Pre-proline / -83.3,153.8	3.3% (<i>m</i>) chi angles: 322.7	0.04Å	-	-
A 137	PRO	50	-	Allowed (1.07%) Trans-proline / -81.9,91.2	60.2% (<i>Cg_endo</i>) chi angles: 34.5	0.041Å	-	-

A Favored (7.39%) OUTLIER(S)

138	ALA	50	-	General / -45.0,130.2	-	0.059Å	-	worst is C-N- CA: 4.067 σ
A 139	GLY	50	-	Favored (85.64%) Glycine / -87.3,0.4	-	-	-	-
A 140	TYR	50	-	Favored (20.88%) General / -58.0,150.4	42.4% (<i>m-85</i>) chi angles: 281.2,104.9	0.057Å	-	-
A 141	ALA	50	-	Favored (8.6%) General / -140.1,176.6	-	0.078Å	-	OUTLIER(S) worst is C-N- CA: 4.696 σ
A 142	GLY	50	-	Allowed (1.67%) Glycine / -133.6,-11.7	-	-	-	-
A 143	ARG	50	-	Favored (2.49%) General / -122.2,-40.6	13.3% (<i>ttm-85</i>) chi angles: 169.6,145.3,291.7,288	0.089Å	-	-
A 144	PHE	50	-	Favored (7.02%) General / -126.7,9.4	22.7% (<i>m-85</i>) chi angles: 306.3,308.5	0.033Å	-	-
A 145	CYS	50	-	Allowed (1.98%) General / 71.2,33.6	1.8% (<i>m</i>) chi angles: 328.3	0.112Å	-	-
A 146	GLU	50	-	Favored (34.72%) General / -82.2,-24.8	1% chi angles: 52.3,280.5,84.7	0.234Å	-	-
A 147	ILE	50	-	Favored (3.28%) Isoleucine or valine / -72.2,164.7	41.9% (<i>pt</i>) chi angles: 64.6,169.5	0.114Å	-	OUTLIER(S) worst is C-N- CA: 5.825 σ
A 148	ASP	99.99	-	-	12.7% (<i>m-20</i>) chi angles: 279.3,296.9	0.038Å	-	-

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