



# Viewing crb1\_sm\_383-482\_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	2.14	99 <sup>th</sup> percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	4.60%	Goal: <1%
	Ramachandran outliers	8	8.16%	Goal: <0.05%
	Ramachandran favored	67	68.37%	Goal: >98%
	MolProbity score <sup>^</sup>	2.35		56 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	1.15%	Goal: 0
	Bad backbone bonds:	0 / 763	0.00%	Goal: 0%
	Bad backbone angles:	17 / 1036	1.64%	Goal: <0.1%

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

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

<sup>^</sup> 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: 66.00	Clashscore: 2.14	Outliers: 8 of 98	Poor rotamers: 4 of 87	Outliers: 1 of 87	Outliers: 0 of 100	Outliers: 16 of 100
A 383	CYS	50	0.691Å N with A 394 CYS HG	-	36.2% (t) chi angles: 188.4	0.217Å	-	OUTLIER(S) worst is C-CA-CB: 4.231 σ
A 384	ILE	50	-	Favored (55.68%) Isoleucine or valine /-102.2,123.7	32.8% (pt) chi angles: 55.2,167.6	0.074Å	-	-
A 385	CYS	50	-	Favored (58.9%) General / -63.6,140.7	71.3% (m) chi angles: 297.7	0.044Å	-	-
A 386	GLN	50	-	Favored (10.48%) Pre-proline / -110.5,166.6	39.8% (mt-30) chi angles: 295.5,174.8,101.7	0.064Å	-	-
				Favored (2.67%)	92.7% (Cg_endo)			

A 387	PRO	50	-	Trans-proline / -76.8,81.0	chi angles: 30.3	0.04Å	-	-
A 388	GLY	50	-	Favored (4.9%) Glycine / 133.7,-7.3	-	-	-	-
A 389	PHE	50	-	Favored (17.93%) General / -135.2,119.6	13.3% ( <i>m</i> -85) chi angles: 307.9,73.4	0.076Å	-	-
A 390	THR	50	-	Allowed (0.16%) General / -138.8,-142.7	11.5% ( <i>p</i> ) chi angles: 76.9	0.245Å	-	-
A 391	GLY	50	-	Favored (14.22%) Glycine / 63.3,-171.2	-	-	-	-
A 392	ILE	50	-	Favored (82.05%) Isoleucine or valine / -61.9,-39.0	45.8% ( <i>pt</i> ) chi angles: 60.5,173.8	0.234Å	-	-
A 393	HIS	50	-	Favored (38.01%) General / -81.3,-23.2	45.7% ( <i>m</i> 170) chi angles: 289.8,180.9	0.126Å	-	-
A 394	CYS	50	0.691Å HG with A 383 CYS N	Allowed (0.3%) General / 70.6,53.8	86.2% ( <i>m</i> ) chi angles: 300.5	0.288Å	-	OUTLIER(S) worst is C-N- CA: 5.169 $\sigma$
A 395	GLU	99.99	-	Favored (3.27%) General / -138.6,-172.3	27.9% ( <i>tt</i> 0) chi angles: 196.4,177.2,58.8	0.246Å	-	OUTLIER(S) worst is N-CA- CB: 4.48 $\sigma$
A 396	GLU	99.99	-	Favored (19.87%) General / -109.1,0.4	2.9% ( <i>pm</i> 0) chi angles: 58.2,274.4,69.6	0.077Å	-	-
A 397	ASP	99.99	-	Allowed (0.45%) General / -104.4,-87.0	25.8% ( <i>t</i> 70) chi angles: 184,81.6	0.18Å	-	-
A 398	VAL	99.99	-	Allowed (0.8%) Isoleucine or valine / -74.3,94.6	7.9% ( <i>p</i> ) chi angles: 68.9	0.244Å	-	OUTLIER(S) worst is C-N- CA: 4.301 $\sigma$
A 399	ASN	99.99	-	OUTLIER (0.01%) General / 85.3,50.3	0.1% chi angles: 339,119	0.212Å	-	OUTLIER(S) worst is CA- CB-CG: 6.851 $\sigma$
				Allowed	5.9% ( <i>mp</i> 0)			OUTLIER(S)

A 400	GLU	99.99	-	(0.05%) General / 68.4,147.2	chi angles: 296.5,85.4,61	0.114Å	-	worst is C-N- CA: 6.316 σ
A 401	CYS	50	-	OUTLIER (0.04%) General / 51.9,-169.3	56.4% ( <i>m</i> ) chi angles: 306.1	0.214Å	-	-
A 402	SER	50	-	Allowed (1.12%) General / -149.9,72.4	92.6% ( <i>p</i> ) chi angles: 65.1	0.06Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 66.00	Clashscore: 2.14	Outliers: 8 of 98	Poor rotamers: 4 of 87	Outliers: 1 of 87	Outliers: 0 of 100	Outliers: 16 of 100
A 403	SER	99.99	-	Favored (10.34%) General / -74.0,173.2	29.5% ( <i>p</i> ) chi angles: 52	0.053Å	-	-
A 404	ASN	99.99	-	Favored (13.19%) Pre-proline / -74.9,111.4	47.2% ( <i>t30</i> ) chi angles: 181.6,37.2	0.048Å	-	-
A 405	PRO	99.99	-	Favored (8.63%) Trans-proline / -81.0,67.4	13.8% ( <i>Cg_endo</i> ) chi angles: 39.5	0.032Å	-	-
A 406	CYS	99.99	-	Favored (5.13%) General / -167.5,147.2	8.8% ( <i>t</i> ) chi angles: 197.1	0.123Å	-	OUTLIER(S) worst is C-N- CA: 4.789 σ
A 407	GLN	50	-	Favored (11.44%) General / -96.4,-34.7	15.7% ( <i>tt0</i> ) chi angles: 184.2,193.6,111	0.028Å	-	-
A 408	ASN	50	-	Favored (3.05%) General / -130.9,91.4	35.7% ( <i>m-80</i> ) chi angles: 281.6,271.3	0.05Å	-	-
A 409	GLY	50	-	Allowed (1.01%) Glycine / -66.2,-161.5	-	-	-	-
A 410	GLY	99.99	-	Favored (27.75%) Glycine / -68.4,176.2	-	-	-	OUTLIER(S) worst is C-N- CA: 4.121 σ
A 411	THR	99.99	-	Allowed (1.07%) General /	72.7% ( <i>p</i> ) chi angles: 57.9	0.032Å	-	-

				-147.3,53.6				
A 412	CYS	99.99	-	Favored (22.01%) General / -97.8,149.7	50% ( <i>t</i> ) chi angles: 182.1	0.078Å	-	-
A 413	GLU	99.99	-	Favored (37.61%) General / -92.6,126.3	5.5% ( <i>tm-20</i> ) chi angles: 202.9,300,334.2	0.093Å	-	-
A 414	ASN	99.99	-	Allowed (1.04%) General / -145.8,35.7	0.3% chi angles: 206.2,115.7	0.072Å	-	OUTLIER(S) worst is C-N- CA: 5.191 σ
A 415	LEU	99.99	-	OUTLIER (0.03%) Pre-proline / 98.8,162.2	92.6% ( <i>mt</i> ) chi angles: 296.2,171.9	0.167Å	-	-
A 416	PRO	99.99	-	OUTLIER (0.04%) Trans-proline / -53.9,91.8	0.1% chi angles: 316.9	0.018Å	-	-
A 417	GLY	99.99	-	Favored (25.24%) Glycine / -175.3,158.1	-	-	-	-
A 418	ASN	99.99	-	Favored (3.67%) General / -98.8,87.1	6.6% ( <i>t30</i> ) chi angles: 179.5,90.3	0.031Å	-	-
A 419	TYR	99.99	-	Favored (33.1%) General / -81.7,141.9	84.5% ( <i>m-85</i> ) chi angles: 289.2,91.7	0.035Å	-	-
A 420	THR	99.99	-	Favored (27.39%) General / -74.9,-47.9	11.8% ( <i>p</i> ) chi angles: 45	0.033Å	-	-
A 421	CYS	50	0.436Å HB2 with A 426 ASP OD2	Allowed (0.86%) General / -159.1,-160.6	31.1% ( <i>p</i> ) chi angles: 65.4	0.116Å	-	-
A 422	HIS	50	-	Allowed (0.12%) General / -158.1,5.2	2.2% ( <i>t-80</i> ) chi angles: 220.4,293.5	0.138Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:		Poor rotamers:	Outliers:	Outliers:	Outliers:
			66.00	2.14	Outliers: 8 of 98	4 of 87	1 of 87	0 of 100	16 of 100

A 423	CYS	50	-	Favored (54.06%) Pre-proline / -125.2,160.6	78.5% ( <i>m</i> ) chi angles: 301	0.061Å	-	-
A 424	PRO	50	-	Favored (32.58%) Trans-proline / -61.2,130.5	9.4% ( <i>Cg_exo</i> ) chi angles: 322.7	0.097Å	-	-
A 425	PHE	50	-	Allowed (1.28%) General / 78.1,16.9	24.7% ( <i>m-85</i> ) chi angles: 313.4,297.9	0.185Å	-	-
A 426	ASP	50	0.436Å OD2 with A 421 CYS HB2	Allowed (0.16%) General / -60.3,179.2	35.5% ( <i>m-20</i> ) chi angles: 300.1,356.7	0.051Å	-	-
A 427	ASN	50	-	OUTLIER (0.02%) General / -174.1,64.4	16.6% ( <i>t-20</i> ) chi angles: 180.4,240.3	0.025Å	-	-
A 428	LEU	50	-	Favored (44.46%) General / -67.5,130.9	20.9% ( <i>mt</i> ) chi angles: 305.5,191.9	0.059Å	-	-
A 429	SER	50	-	Favored (6.82%) General / -75.4,106.2	52% ( <i>p</i> ) chi angles: 54.7	0.043Å	-	-
A 430	ARG	50	-	Favored (6.68%) General / -53.8,151.2	19.3% ( <i>ttm180</i> ) chi angles: 198.2,152.4,295.4,161.8	0.078Å	-	-
A 431	THR	50	-	Favored (13.4%) General / -51.6,125.0	11.1% ( <i>m</i> ) chi angles: 312.9	0.029Å	-	-
A 432	PHE	50	-	Allowed (1.63%) General / 75.7,21.8	57.7% ( <i>m-85</i> ) chi angles: 302.2,296.1	0.176Å	-	-
A 433	TYR	50	-	Favored (51.17%) General / -132.7,153.4	74.8% ( <i>m-85</i> ) chi angles: 287.8,84.5	0.076Å	-	-
A 434	GLY	50	-	Favored (11.38%) Glycine / -145.7,-165.5	-	-	-	-
A 435	GLY	50	-	Favored (25.96%) Glycine / 79.8,162.8	-	-	-	-

A 436	ARG	50	-	Favored (14.25%) General / -81.9,7.0	15.6% ( <i>tpt180</i> ) chi angles: 178.2,55.4,196.6,195	0.169Å	-	-	
A 437	ASP	50	-	Favored (13.23%) General / -116.2,2.1	25.1% ( <i>p-10</i> ) chi angles: 67.7,335.2	0.05Å	-	-	
A 438	CYS	50	-	Favored (3.11%) General / 40.7,53.7	86.8% ( <i>m</i> ) chi angles: 289.5	0.153Å	-	-	
A 439	SER	50	-	Favored (7.79%) General / -123.9,-8.6	1.6% ( <i>p</i> ) chi angles: 93.2	0.106Å	-	-	
A 440	ASP	50	-	Favored (2.67%) General / -75.7,81.4	79.8% ( <i>m-20</i> ) chi angles: 297,344.2	0.07Å	-	OUTLIER(S) worst is CA- CB-CG: 4.16 σ	
A 441	ILE	50	-	Favored (19.26%) Isoleucine or valine / -56.1,135.8	29.4% ( <i>pt</i> ) chi angles: 54.6,166.7	0.088Å	-	-	
A 442	LEU	50	-	Favored (18.08%) General / -114.2,16.4	14.5% ( <i>mt</i> ) chi angles: 317.4,175.5	0.043Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 66.00	Clashscore: 2.14	Outliers: 8 of 98	Poor rotamers: 4 of 87	Outliers: 1 of 87	Outliers: 0 of 100	Outliers: 16 of 100
A 443	LEU	99.99	-	Favored (10.16%) General / -152.0,127.7	3.4% ( <i>tt</i> ) chi angles: 200.5,143.4	0.079Å	-	-	
A 444	GLY	99.99	-	Favored (19.04%) Glycine / -112.2,-9.8	-	-	-	-	
A 445	CYS	99.99	-	Favored (59.36%) General / -57.8,-24.9	5.6% ( <i>t</i> ) chi angles: 201.1	0.154Å	-	OUTLIER(S) worst is C-N- CA: 4.578 σ	
A 446	THR	50	-	OUTLIER (0.02%) General / -44.8,-13.9	1.7% ( <i>m</i> ) chi angles: 323.9	0.048Å	-	-	
A 447	HIS	50	-	Favored (3.31%) General / -134.7,4.2	5.4% ( <i>m-70</i> ) chi angles: 326.3,301.3	0.043Å	-	-	

A 448	GLN	50	-	Favored (25.86%) General / 53.3,46.7	38.1% ( <i>mt-30</i> ) chi angles: 293.9,181.3,244.1	0.095Å	-	-
A 449	GLN	99.99	-	Favored (86.73%) General / -60.8,-38.8	34.1% ( <i>mt-30</i> ) chi angles: 286.8,183.7,235.1	0.124Å	-	-
A 450	CYS	50	-	Favored (6.58%) General / -78.2,100.2	0.4% chi angles: 222	0.061Å	-	-
A 451	LEU	50	-	Favored (17.6%) General / -78.7,169.8	14.9% ( <i>mt</i> ) chi angles: 315.7,186.1	0.047Å	-	-
A 452	ASN	50	-	Favored (20.45%) General / 51.5,37.8	76.3% ( <i>m-20</i> ) chi angles: 301.1,328.4	0.083Å	-	-
A 453	ASN	50	-	Allowed (1.46%) General / 76.9,19.2	20.8% ( <i>m-80</i> ) chi angles: 311.4,280.8	0.12Å	-	-
A 454	GLY	50	-	Favored (54.77%) Glycine / -73.0,162.4	-	-	-	-
A 455	THR	50	-	Favored (11.73%) General / -80.3,105.7	19.6% ( <i>m</i> ) chi angles: 310.5	0.08Å	-	-
A 456	CYS	50	-	Allowed (1.56%) General / -68.1,103.6	47.7% ( <i>t</i> ) chi angles: 182.6	0.033Å	-	-
A 457	ILE	99.99	-	Allowed (0.24%) Pre-proline / -94.7,-22.3	41.5% ( <i>mm</i> ) chi angles: 298.1,295.5	0.153Å	-	OUTLIER(S) worst is CA-C- N: 4.926 $\sigma$
A 458	PRO	99.99	0.4Å HA with A 461 GLN O	Favored (2.93%) Trans-proline / -75.8,109.6	93.6% ( <i>Cg_endo</i> ) chi angles: 30.3	0.079Å	-	OUTLIER(S) worst is C-N- CA: 4.257 $\sigma$
A 459	HIS	99.99	-	OUTLIER (0.01%) General / 177.3,88.8	2.3% ( <i>p80</i> ) chi angles: 36.3,63	0.044Å	-	OUTLIER(S) worst is C-N- CA: 4.391 $\sigma$
A 460	PHE	99.99	-	OUTLIER (0.03%) General / 88.0,-61.4	67.9% ( <i>t80</i> ) chi angles: 170.1,81.3	0.208Å	-	-
A			0.4Å	Favored (57%)	22.9% ( <i>mt-30</i> )			OUTLIER(S)

461	GLN	99.99	O with A 458 PRO HA	General / -58.2,135.0	chi angles: 287.7,199.9,247.3	0.08Å	-	worst is C-N- CA: 4.888 σ	
A 462	ASP	50	-	Allowed (1.15%) General / -124.0,72.2	49.5% ( <i>m</i> -20) chi angles: 295.8,295.5	0.073Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 66.00	Clashscore: 2.14	Outliers: 8 of 98	Poor rotamers: 4 of 87	Outliers: 1 of 87	Outliers: 0 of 100	Outliers: 16 of 100
A 463	GLY	50	-	Favored (46.35%) Glycine / 63.2,-152.9	-	-	-	-	
A 464	GLN	50	-	Allowed (0.73%) General / -68.3,97.3	5.9% ( <i>pt</i> 20) chi angles: 59.7,196,142.3	0.093Å	-	-	
A 465	HIS	50	-	Allowed (0.53%) General / 85.2,-15.3	80.8% ( <i>m</i> -70) chi angles: 308.3,281.4	0.18Å	-	-	
A 466	GLY	50	-	Favored (50.25%) Glycine / -74.7,157.1	-	-	-	-	
A 467	PHE	99.99	-	Favored (40.82%) General / -155.2,163.0	51.4% ( <i>p</i> 90) chi angles: 64.6,273.7	0.067Å	-	-	
A 468	SER	50	-	Favored (46.47%) General / -134.9,142.2	74% ( <i>m</i> ) chi angles: 295.1	0.097Å	-	-	
A 469	CYS	50	-	Favored (6.5%) General / -135.9,106.5	85.6% ( <i>m</i> ) chi angles: 289.4	0.099Å	-	-	
A 470	LEU	50	-	Favored (17.41%) General / -83.7,109.3	14.4% ( <i>mt</i> ) chi angles: 317.1,183.1	0.128Å	-	-	
A 471	CYS	50	-	Favored (18.61%) Pre-proline / -49.5,134.8	51.5% ( <i>m</i> ) chi angles: 306.8	0.09Å	-	-	
A	PRO	50	-	Favored (25.91%)	85.4% ( <i>Cg_exo</i> )	0.052Å	-	-	



472				Trans-proline / -70.8,167.4	chi angles: 331.7			
A 473	SER	50	-	Allowed (0.29%) General / -65.6,97.1	71.4% ( <i>p</i> ) chi angles: 57.8	0.022Å	-	-
A 474	GLY	50	-	Favored (5.77%) Glycine / 130.7,-4.0	-	-	-	-
A 475	TYR	50	-	Favored (16.5%) General / -114.7,162.7	93.3% ( <i>m-85</i> ) chi angles: 293.3,266.3	0.069Å	-	OUTLIER(S) worst is C-N- CA: 4.173 $\sigma$
A 476	THR	50	-	Allowed (0.16%) General / -134.9,-133.0	21% ( <i>p</i> ) chi angles: 73	0.207Å	-	-
A 477	GLY	50	-	Favored (25.94%) Glycine / 64.8,-169.4	-	-	-	-
A 478	SER	50	-	Favored (9.26%) General / -105.3,-31.0	9.4% ( <i>p</i> ) chi angles: 84.3	0.139Å	-	-
A 479	LEU	50	-	Favored (37.93%) General / -102.3,11.6	7.6% ( <i>mp</i> ) chi angles: 278.2,76.5	0.053Å	-	-
A 480	CYS	50	-	Allowed (1.76%) General / 68.7,40.7	27.7% ( <i>m</i> ) chi angles: 310.6	0.175Å	-	-
A 481	GLU	50	-	Favored (15.44%) General / -104.7,-14.8	4.5% ( <i>pt-20</i> ) chi angles: 69.8,212.3,313.5	0.077Å	-	-
A 482	ILE	99.99	-	-	12.3% ( <i>mt</i> ) chi angles: 314.1,183.6	0.064Å	-	-

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