



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

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All-Atom Contacts	Clashscore, all atoms:	53.01	3 <sup>rd</sup> percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	2.30%	Goal: <1%
	Ramachandran outliers	4	4.08%	Goal: <0.05%
	Ramachandran favored	84	85.71%	Goal: >98%
	MolProbity score^	3.12		19 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	4.60%	Goal: 0
	Bad backbone bonds:	11 / 763	1.44%	Goal: 0%
	Bad backbone angles:	33 / 1036	3.19%	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: 53.01	Outliers: 4 of 98	Poor rotamers: 2 of 87	Outliers: 4 of 87	Outliers: 6 of 100	Outliers: 19 of 100
A 383	CYS	50	-	-	34.7% (t) chi angles: 189	0.024Å	-	-
A 384	ILE	50	-	Favored (33%) Isoleucine or valine / -84.1,131.8	48% (pt) chi angles: 62.1,173.6	0.068Å	-	-
A 385	CYS	50	-	Favored (32.16%) General / -89.2,137.6	62.3% (m) chi angles: 303.3	0.032Å	-	-
A 386	GLN	50	-	Favored (89.04%) Pre-proline / -60.4,143.9	36.9% (tt0) chi angles: 189.8,172.3,84	0.171Å	-	-

A 387	PRO	50	-	Favored (12.83%) Trans-proline / -57.1,123.0	66.5% ( <i>Cg_endo</i> ) chi angles: 27.9	0.035Å	-	-
A 388	GLY	50	-	Favored (25.46%) Glycine / 111.6,-17.6	-	-	-	-
A 389	PHE	50	-	Favored (28.15%) General / -111.0,151.3	1.7% ( <i>m-30</i> ) chi angles: 292.8,31.2	0.062Å	-	-
A 390	THR	50	-	Favored (12.04%) General / -149.2,174.7	62.7% ( <i>p</i> ) chi angles: 62.3	0.044Å	-	-
A 391	GLY	50	-	Favored (22.38%) Glycine / 106.8,164.0	-	-	-	-
A 392	ILE	50	0.414Å HG13 with A 393 HIS CD2	Favored (46.49%) Isoleucine or valine / -57.5,-34.3	48.2% ( <i>pt</i> ) chi angles: 59.9,172.2	0.046Å	-	-
A 393	HIS	50	0.414Å CD2 with A 392 ILE HG13	Favored (23.62%) General / -110.1,7.9	96.6% ( <i>m-70</i> ) chi angles: 293.1,287.4	0.01Å	OUTLIER(S) worst is CG-- ND1: 4.487 σ	OUTLIER(S) worst is CB- CG-CD2: 4.361 σ
A 394	CYS	50	-	Favored (27.22%) General / 55.4,36.5	78.3% ( <i>m</i> ) chi angles: 296.2	0.011Å	-	-
A 395	GLU	99.99	0.713Å HG2 with A 397 ASP H	Favored (37.67%) General / -106.3,141.4	44% ( <i>tt0</i> ) chi angles: 178.1,180.8,68.7	0.083Å	-	-
A 396	GLU	99.99	0.885Å HA with A 401 CYS H	Favored (66.92%) General / -64.5,-22.3	10.7% ( <i>pm0</i> ) chi angles: 66.9,290.9,350.4	0.123Å	-	-
A 397	ASP	99.99	0.713Å H with A 395 GLU HG2	Favored (73.09%) General / -62.1,-32.5	25.6% ( <i>t70</i> ) chi angles: 178.7,80.8	0.037Å	-	-
A	VAL	99.99	-	Favored (46.44%) Isoleucine or	7.3% ( <i>p</i> )	0.044Å	-	-

398				valine / -99.3,118.8	chi angles: 57.6			
A 399	ASN	99.99	0.537Å O with A 400 GLU HB2	Favored (9.33%) General / 45.3,44.8	29.2% ( <i>t30</i> ) chi angles: 175.5,33.9	0.06Å	-	-
A 400	GLU	99.99	0.861Å OE2 with A 420 THR HB	Allowed (0.12%) General / 60.8,-174.1	36.6% ( <i>mp0</i> ) chi angles: 293.8,95.9,10.6	0.278Å	-	OUTLIER(S) worst is O-C- N: 6.561 σ
A 401	CYS	50	0.885Å H with A 396 GLU HA	OUTLIER (0%) General / 35.6,156.5	25.6% ( <i>p</i> ) chi angles: 67.3	0.351Å	-	OUTLIER(S) worst is C-CA- CB: 5.174 σ
A 402	SER	50	-	Favored (32.6%) General / -107.4,116.8	45% ( <i>t</i> ) chi angles: 180.7	0.045Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 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: 66.00</div> <div>Clashscore: 53.01</div> <div>Outliers: 4 of 98</div> <div>Poor rotamers: 2 of 87</div> <div>Outliers: 4 of 87</div> <div>Outliers: 6 of 100</div> <div>Outliers: 19 of 100</div> </div>								
A 403	SER	99.99	0.526Å HB3 with A 421 CYS HB3	Favored (22.43%) General / -105.5,152.9	79.8% ( <i>p</i> ) chi angles: 59.9	0.037Å	-	-
A 404	ASN	99.99	-	Favored (23.62%) Pre-proline / -59.7,117.5	54.7% ( <i>t30</i> ) chi angles: 184.5,27.5	0.04Å	-	-
A 405	PRO	99.99	-	Favored (7.72%) Trans-proline / -60.1,167.3	71.9% ( <i>Cg_endo</i> ) chi angles: 29.4	0.063Å	-	-
A 406	CYS	99.99	0.462Å HA with A 407 GLN HB2	Allowed (0.11%) General / 57.0,82.9	44.8% ( <i>t</i> ) chi angles: 178.7	0.044Å	-	-
A 407	GLN	50	0.462Å HB2 with A 406 CYS HA	OUTLIER (0.02%) General / -170.7,-70.9	53.2% ( <i>tt0</i> ) chi angles: 186.2,177.1,52.3	0.113Å	-	-
A 408	ASN	50	0.78Å HB2 with A 433 TYR HD2	Favored (4.58%) General / -113.7,93.9	11.6% ( <i>m-80</i> ) chi angles: 313.6,275.4	0.118Å	-	OUTLIER(S) worst is CA- CB-CG: 6.804 σ
A			0.806Å	Favored				OUTLIER(S)

409	GLY	50	O with A 430 ARG HG3	(32.79%) Glycine / -73.7,143.6	-	-	-	worst is C-N- CA: 8.397 $\sigma$
A 410	GLY	99.99	0.63Å HA2 with A 429 SER C	Allowed (0.85%) Glycine / -38.2,137.3	-	-	-	OUTLIER(S) worst is O-C- N: 6.331 $\sigma$
A 411	THR	99.99	0.49Å HG23 with A 430 ARG CG	Favored (34.49%) General / -111.4,118.0	39.9% ( <i>p</i> ) chi angles: 53.5	0.053Å	-	-
A 412	CYS	99.99	-	Favored (39.79%) General / -111.3,144.9	43.1% ( <i>t</i> ) chi angles: 183.3	0.06Å	-	-
A 413	GLU	99.99	0.471Å HA with A 417 GLY O	Favored (15.15%) General / -116.1,107.6	80.7% ( <i>tt0</i> ) chi angles: 178.7,178.9,14.3	0.062Å	-	-
A 414	ASN	99.99	0.767Å HB3 with A 419 TYR CE1	Favored (53.37%) General / -124.3,133.8	13.3% ( <i>t30</i> ) chi angles: 167.8,29.4	0.138Å	-	-
A 415	LEU	99.99	0.459Å C with A 414 ASN O	Allowed (0.33%) Pre-proline / 41.7,79.2	90.1% ( <i>mt</i> ) chi angles: 300.4,178.1	0.01Å	-	-
A 416	PRO	99.99	-	OUTLIER (0%) Trans-proline / 9.4,37.9	0.1% chi angles: 318.3	0.122Å	-	-
A 417	GLY	99.99	0.471Å O with A 413 GLU HA	Favored (14.44%) Glycine / -126.3,143.5	-	-	-	-
A 418	ASN	99.99	-	Favored (38.96%) General / -77.0,134.2	40.3% ( <i>t30</i> ) chi angles: 180.3,16.9	0.045Å	-	-
A 419	TYR	99.99	0.767Å CE1 with A 414 ASN HB3	Favored (34.64%) General / -128.6,124.0	95.6% ( <i>m-85</i> ) chi angles: 297.9,87.5	0.098Å	-	OUTLIER(S) worst is CD1- CE1-CZ: 4.508 $\sigma$
A 420	THR	99.99	0.861Å HB with A 400 GLU OE2	Allowed (0.1%) General / -89.8,-99.8	11.8% ( <i>m</i> ) chi angles: 312.6	0.119Å	-	-
A			0.759Å	Favored (33.3%)	2.9% ( <i>p</i> )			OUTLIER(S)

421	CYS	50	SG with A 400 GLU HB3	General / -62.2,152.4	chi angles: 83.4	0.199Å	-	worst is N-CA- CB: 4.068 $\sigma$
A 422	HIS	50	-	Favored (6.18%) General / -112.2,-33.6	62.3% ( <i>t</i> -80) chi angles: 186.6,274.6	0.064Å	OUTLIER(S) worst is CG-- ND1: 4.522 $\sigma$	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 66.00	Clashscore: 53.01	Outliers: 4 of 98	Poor rotamers: 2 of 87	Outliers: 4 of 87	Outliers: 6 of 100	Outliers: 19 of 100
A 423	CYS	50	-	Favored (52.96%) Pre-proline / -119.0,154.0	75.9% ( <i>m</i> ) chi angles: 298.8	0.078Å	-	-
A 424	PRO	50	-	Favored (79.97%) Trans-proline / -55.0,140.6	71.9% ( <i>Cg_exo</i> ) chi angles: 328	0.134Å	-	-
A 425	PHE	50	-	Favored (4.98%) General / 71.3,20.4	1.2% ( <i>m</i> -30) chi angles: 295.3,31.3	0.05Å	-	-
A 426	ASP	50	0.419Å HB2 with A 421 CYS HB2	Favored (21.39%) General / -97.2,150.0	83.5% ( <i>m</i> -20) chi angles: 296.5,339.1	0.014Å	-	-
A 427	ASN	50	0.664Å OD1 with A 438 CYS SG	Allowed (1.4%) General / -137.3,71.4	24.7% ( <i>t</i> -20) chi angles: 191.8,301.4	0.107Å	-	OUTLIER(S) worst is OD1- CG-ND2: 5.904 $\sigma$
A 428	LEU	50	0.611Å O with A 410 GLY N	Favored (36.08%) General / -79.6,131.8	32.4% ( <i>mt</i> ) chi angles: 311.2,175.4	0.276Å	OUTLIER(S) worst is C--N: 4.733 $\sigma$	OUTLIER(S) worst is CA-C- O: 10.251 $\sigma$
A 429	SER	50	0.63Å C with A 410 GLY HA2	Favored (31.82%) General / -82.1,126.2	24.6% ( <i>m</i> ) chi angles: 304.7	0.3Å	-	OUTLIER(S) worst is C-CA- CB: 7.628 $\sigma$
A 430	ARG	50	0.806Å HG3 with A 409 GLY O	Favored (6.1%) General / -62.0,164.8	2.1% ( <i>mtp</i> 85) chi angles: 265.7,154.4,104.9,87.9	0.163Å	-	OUTLIER(S) worst is CG- CD-NE: 7.246 $\sigma$
A 431	THR	50	-	Favored (48.78%) General / -55.0,133.6	87.1% ( <i>m</i> ) chi angles: 301.2	0.084Å	-	-

A 432	PHE	50	0.468Å C with A 433 TYR HD1	Favored (3.18%) General / 75.6,12.0	20.7% ( <i>m-30</i> ) chi angles: 294.3,328.6	0.153Å	-	-
A 433	TYR	50	0.78Å HD2 with A 408 ASN HB2	Favored (54.2%) General / -121.0,131.3	1.2% ( <i>m-30</i> ) chi angles: 294.6,33.9	0.035Å	-	OUTLIER(S) worst is CB- CG-CD1: 5.311 σ
A 434	GLY	50	-	Favored (17.64%) Glycine / -125.8,171.2	-	-	-	-
A 435	GLY	50	-	Favored (29.3%) Glycine / 98.9,157.3	-	-	-	-
A 436	ARG	50	-	Favored (67.23%) General / -61.6,-25.2	31.8% ( <i>ptt-85</i> ) chi angles: 60.8,176.9,179.5,278.9	0.041Å	-	-
A 437	ASP	50	-	Favored (25.14%) General / -103.0,-4.0	57.8% ( <i>m-20</i> ) chi angles: 296.9,299.1	0.029Å	-	-
A 438	CYS	50	0.664Å SG with A 427 ASN OD1	Favored (18.04%) General / 59.1,43.0	85.2% ( <i>m</i> ) chi angles: 300.6	0.048Å	-	-
A 439	SER	50	-	Favored (14.22%) General / -113.8,-0.5	71.4% ( <i>p</i> ) chi angles: 57.8	0.016Å	-	-
A 440	ASP	50	0.89Å HA with A 465 HIS NE2	Favored (26.6%) General / -96.9,114.9	32.1% ( <i>m-20</i> ) chi angles: 302.3,288.5	0.129Å	-	-
A 441	ILE	50	0.458Å HG12 with A 465 HIS ND1	Favored (35.36%) Isoleucine or valine / -71.9,128.9	50.6% ( <i>pt</i> ) chi angles: 62.3,172.7	0.064Å	-	-
A 442	LEU	50	-	Favored (24.14%) General / -101.0,-6.7	80.5% ( <i>mt</i> ) chi angles: 302.9,176.5	0.02Å	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:		Clashscore:	Outliers: 4 of	Poor rotamers: 2 of	Outliers:	Outliers: 6	Outliers: 19	

	66.00	53.01	98	87	4 of 87	of 100	of 100
A 443	LEU 99.99	0.882Å HD21 with A 445 CYS HB3	Favored (24.69%) General / -129.2,119.8	5.7% ( <i>tt</i> ) chi angles: 180.2,166	0.118Å	-	OUTLIER(S) worst is CD1- CG-CD2: 4.304 σ
A 444	GLY 99.99	0.433Å H with A 458 PRO HB2	Favored (53.99%) Glycine / -101.6,18.1	-	-	-	-
A 445	CYS 99.99	0.882Å HB3 with A 443 LEU HD21	Favored (55.03%) General / -75.0,-7.9	42.2% ( <i>t</i> ) chi angles: 183.9	0.03Å	-	-
A 446	THR 50	-	Favored (74.3%) General / -59.8,-35.2	88.1% ( <i>m</i> ) chi angles: 301	0.092Å	-	-
A 447	HIS 50	-	Favored (6.49%) General / -114.0,-31.1	97.7% ( <i>m-70</i> ) chi angles: 296.2,279.9	0.067Å	OUTLIER(S) worst is CG-- ND1: 4.463 σ	OUTLIER(S) worst is CB- CG-CD2: 4.261 σ
A 448	GLN 50	-	Allowed (0.64%) General / 51.8,69.6	5.5% ( <i>mt-30</i> ) chi angles: 302.9,140.1,265	0.071Å	-	-
A 449	GLN 99.99	0.611Å NE2 with A 467 PHE CE1	Favored (27.14%) General / -83.6,-30.1	67.9% ( <i>mt-30</i> ) chi angles: 290.1,187,62.9	0.068Å	-	-
A 450	CYS 50	-	Favored (4.07%) General / -69.3,109.3	53.6% ( <i>m</i> ) chi angles: 306.6	0.011Å	-	-
A 451	LEU 50	-	Favored (18.33%) General / -84.3,165.4	77.8% ( <i>mt</i> ) chi angles: 301.3,173.3	0.049Å	-	-
A 452	ASN 50	0.423Å O with A 453 ASN HB3	Favored (23.14%) General / 59.5,37.0	76.3% ( <i>m-20</i> ) chi angles: 293.7,301.7	0.043Å	-	-
A 453	ASN 50	0.423Å HB3 with A 452 ASN O	Favored (2.22%) General / 75.7,18.0	21.1% ( <i>t-20</i> ) chi angles: 184.5,293.3	0.061Å	-	OUTLIER(S) worst is CA- CB-CG: 4.205 σ
A			Favored (47.74%)				

454	GLY	50	-	Glycine / -66.0,158.3	-	-	-	-
A 455	THR	50	-	Favored (51.83%) General / -107.6,133.6	97.5% ( <i>m</i> ) chi angles: 299.2	0.038Å	-	-
A 456	CYS	50	0.519Å SG with A 458 PRO HD3	Favored (30.6%) General / -98.4,142.0	4.7% ( <i>t</i> ) chi angles: 202.8	0.103Å	-	-
A 457	ILE	99.99	0.97Å HG22 with A 461 GLN H	Allowed (0.23%) Pre-proline / -117.0,37.4	36.8% ( <i>mm</i> ) chi angles: 308.3,298.2	0.163Å	-	OUTLIER(S) worst is O-C- N: 4.652 $\sigma$
A 458	PRO	99.99	0.751Å HA with A 461 GLN O	Favored (97.95%) Trans-proline / -58.7,-35.9	48.6% ( <i>Cg_endo</i> ) chi angles: 35.3	0.08Å	-	-
A 459	HIS	99.99	-	Favored (94.7%) General / -62.7,-39.7	35% ( <i>p80</i> ) chi angles: 64.9,81.5	0.025Å	OUTLIER(S) worst is CD2-- NE2: 4.236 $\sigma$	-
A 460	PHE	99.99	0.807Å O with A 462 ASP HA	Allowed (0.86%) General / -103.2,-67.9	79.1% ( <i>t80</i> ) chi angles: 178.3,85.7	0.046Å	-	-
A 461	GLN	99.99	0.985Å O with A 467 PHE HA	Allowed (0.07%) General / -64.9,89.6	98.1% ( <i>mt-30</i> ) chi angles: 293.1,175.1,321.2	0.122Å	-	OUTLIER(S) worst is CA- CB-CG: 4.269 $\sigma$
A 462	ASP	50	0.807Å HA with A 460 PHE O	OUTLIER (0.01%) General / -173.6,7.3	0.9% chi angles: 222.6,305.2	0.139Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 66.00	Clashscore: 53.01	Outliers: 4 of 98	Poor rotamers: 2 of 87	Outliers: 4 of 87	Outliers: 6 of 100	Outliers: 19 of 100
A 463	GLY	50	-	Favored (27.92%) Glycine / 144.8,-160.1	-	-	-	-
A 464	GLN	50	0.793Å HB2 with A 440 ASP HB3	Favored (7.71%) General / -70.5,113.5	20.1% ( <i>pt20</i> ) chi angles: 60.8,179.3,66	0.056Å	-	-



A 465	HIS	50	0.89Å NE2 with A 440 ASP HA	Favored (15.54%) General / 61.8,25.7	98.8% ( <i>m-70</i> ) chi angles: 296.6,282.9	0.05Å	OUTLIER(S) worst is CG-- ND1: 5.159 σ	OUTLIER(S) worst is CB- CG-CD2: 6.182 σ
A 466	GLY	50	-	Favored (16.12%) Glycine / -123.1,145.4	-	-	-	-
A 467	PHE	99.99	0.985Å HA with A 461 GLN O	Favored (20.35%) General / -151.7,170.2	44.1% ( <i>p90</i> ) chi angles: 68.2,275.3	0.234Å	-	-
A 468	SER	50	0.583Å HB2 with A 461 GLN OE1	Favored (29.28%) General / -146.0,143.2	5.3% ( <i>m</i> ) chi angles: 314.3	0.081Å	-	-
A 469	CYS	50	-	Favored (42.21%) General / -108.9,140.6	90.6% ( <i>m</i> ) chi angles: 295.2	0.064Å	-	-
A 470	LEU	50	-	Favored (20%) General / -111.0,109.8	95.9% ( <i>mt</i> ) chi angles: 295.3,176.1	0.019Å	-	-
A 471	CYS	50	-	Favored (29.91%) Pre-proline / -88.7,141.2	58.9% ( <i>m</i> ) chi angles: 305	0.025Å	-	-
A 472	PRO	50	-	Favored (9.2%) Trans-proline / -63.7,170.0	50.9% ( <i>Cg_exo</i> ) chi angles: 335.3	0.082Å	-	-
A 473	SER	50	-	Favored (13.68%) General / -62.4,121.6	49.2% ( <i>m</i> ) chi angles: 300.7	0.072Å	-	-
A 474	GLY	50	-	Favored (34.91%) Glycine / 107.4,-4.0	-	-	-	-
A 475	TYR	50	-	Favored (49.04%) General / -125.1,147.3	77.1% ( <i>m-85</i> ) chi angles: 304.4,280.4	0.007Å	-	-
A 476	THR	50	0.429Å OG1 with A 482 ILE HB	Favored (12.9%) General / -146.7,172.9	69.1% ( <i>p</i> ) chi angles: 62	0.027Å	-	-
A				Favored (28.59%)				

477	GLY	50	-	Glycine / 100.3,164.6	-	-	-	-
A 478	SER	50	-	Favored (68.08%) General / -61.5,-26.7	78.2% ( <i>p</i> ) chi angles: 59.1	0.06Å	-	-
A 479	LEU	50	-	Favored (12.05%) General / -120.0,20.8	10.6% ( <i>mp</i> ) chi angles: 279.4,65.3	0.007Å	-	-
A 480	CYS	50	-	Favored (22.06%) General / 57.2,32.6	34.7% ( <i>m</i> ) chi angles: 308.9	0.033Å	-	-
A 481	GLU	50	-	Favored (30.9%) General / -83.6,-25.4	1.1% ( <i>pm0</i> ) chi angles: 59.9,271,88.2	0.123Å	-	-
A 482	ILE	99.99	0.429Å HB with A 476 THR OG1	-	67.4% ( <i>mt</i> ) chi angles: 303.4,167.8	0.098Å	-	-

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