



# Viewing crb1\_sm\_307-424H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	37.9		9 <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	1	0.96%	Goal: <1%
	Ramachandran outliers	3	2.59%	Goal: <0.05%
	Ramachandran favored	106	91.38%	Goal: >98%
	MolProbity score^	2.57		43 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	1.87%	Goal: 0
	Bad backbone bonds:	11 / 906	1.21%	Goal: 0%
	Bad backbone angles:	15 / 1235	1.21%	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: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118
A 307	SER	50	-	-	41.2% (t) chi angles: 181.3	0.044Å	-	-
A 308	LYS	99.99	-	Favored (33.67%) Pre-proline / -74.8,114.4	99.1% (mttt) chi angles: 296,180.4,179.3,180	0.016Å	-	-
A 309	PRO	50	-	Favored (71.06%) Trans-proline / -63.4,-20.9	71.8% (Cg_endo) chi angles: 29.4	0.067Å	-	-
A 310	CYS	50	0.718Å HB3 with A 314 ALA HB3	Favored (23.29%) General / -87.3,113.8	58% (m) chi angles: 305.4	0.081Å	-	-

A 311	HIS	50	-	Favored (35.24%) General / -72.5,158.7	59.7% ( <i>m170</i> ) chi angles: 297.7,161.8	0.023Å	OUTLIER(S) worst is CG-- ND1: 4.661 $\sigma$	-
A 312	ASN	50	-	Favored (10.36%) General / 61.0,44.4	33.1% ( <i>m120</i> ) chi angles: 292.6,115.9	0.06Å	-	-
A 313	ASN	50	-	Favored (6.01%) General / 62.6,13.2	22% ( <i>t-20</i> ) chi angles: 186.1,283.6	0.036Å	-	-
A 314	ALA	50	0.718Å HB3 with A 310 CYS HB3	Favored (46.7%) General / -61.6,147.1	-	0.089Å	-	-
A 315	THR	50	0.644Å OG1 with A 326 HIS HB3	Favored (37.16%) General / -78.3,131.7	73% ( <i>p</i> ) chi angles: 63.6	0.029Å	-	-
A 316	CYS	50	-	Favored (42.34%) General / -96.3,127.4	43.1% ( <i>t</i> ) chi angles: 184.6	0.052Å	-	-
A 317	GLU	50	-	Favored (33.35%) General / -118.2,119.0	11% ( <i>pt-20</i> ) chi angles: 56.6,178.1,70.3	0.047Å	-	-
A 318	ASP	50	0.701Å HA with A 323 TYR CD1	Favored (45.48%) General / -67.3,131.3	60.8% ( <i>t0</i> ) chi angles: 187.1,343.2	0.017Å	-	-
A 319	SER	50	-	Favored (30.69%) General / -122.4,158.0	33.1% ( <i>t</i> ) chi angles: 183.8	0.041Å	-	-
A 320	VAL	50	-	Favored (2.28%) Isoleucine or valine / -69.6,109.3	8.1% ( <i>p</i> ) chi angles: 59.6	0.054Å	-	-
A 321	ASP	50	-	OUTLIER (0.01%) General / 107.6,-34.2	43.5% ( <i>t0</i> ) chi angles: 188.4,328.9	0.074Å	-	OUTLIER(S) worst is CA- CB-CG: 6.289 $\sigma$
A 322	ASN	99.99	-	Allowed (0.25%) General /	66.2% ( <i>m-80</i> ) chi angles: 297.2,281.3	0.039Å	-	-

A 323	TYR	99.99	0.701Å CD1 with A 318 ASP HA	-142.1,-148.8 Favored (30.46%) General / -159.7,157.9	99.1% ( <i>m</i> -85) chi angles: 296.7,276.1	0.066Å	-	-
A 324	THR	50	-	Favored (46.88%) General / -129.0,154.2	90.5% ( <i>m</i> ) chi angles: 302.3	0.08Å	-	-
A 325	CYS	50	-	Favored (55.49%) General / -113.2,132.4	89.1% ( <i>m</i> ) chi angles: 291.9	0.054Å	-	-
A 326	HIS	50	0.644Å HB3 with A 315 THR OG1	Favored (6.1%) General / -102.2,95.1	16.2% ( <i>t</i> -160) chi angles: 175.4,205.8	0.092Å	OUTLIER(S) worst is CD2-- NE2: 4.234 σ	OUTLIER(S) worst is CB- CG-CD2: 4.419 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118
A 327	CYS	50	-	Favored (47.85%) General / -71.7,147.0	54.3% ( <i>m</i> ) chi angles: 306.6	0.017Å	-	-
A 328	TRP	50	0.494Å HB3 with A 329 PRO HD2	Favored (84.79%) Pre-proline / -72.0,159.7	99.2% ( <i>m</i> 95) chi angles: 293.1,98.7	0.035Å	-	-
A 329	PRO	50	0.494Å HD2 with A 328 TRP HB3	Favored (4.27%) Trans-proline / -60.2,117.5	79% ( <i>Cg_endo</i> ) chi angles: 29.8	0.024Å	-	-
A 330	GLY	50	-	Favored (23.61%) Glycine / 114.2,-4.5	-	-	-	-
A 331	TYR	50	-	Favored (52.96%) General / -126.6,139.8	78.4% ( <i>m</i> -85) chi angles: 303.5,283.4	0.03Å	-	-
A 332	THR	50	-	Favored (14.98%) General / -135.4,171.1	14.9% ( <i>t</i> ) chi angles: 188.7	0.089Å	-	-
A 333	GLY	50	-	Favored (16.74%)	-	-	-	-

				Glycine / 111.1,160.4				
A 334	ALA	50	-	Favored (65.91%) General / -58.9,-28.2	-	0.014Å	-	-
A 335	GLN	50	-	Favored (11.4%) General / -121.4,17.8	86.1% ( <i>mt-30</i> ) chi angles: 295.7,179.9,297.8	0.016Å	-	-
A 336	CYS	50	-	Favored (26.7%) General / 57.2,35.8	19.9% ( <i>m</i> ) chi angles: 312.2	0.022Å	-	-
A 337	GLU	50	-	Favored (58.62%) General / -86.5,-7.2	1.6% ( <i>pm0</i> ) chi angles: 60.5,272.3,79.6	0.122Å	-	-
A 338	ILE	50	-	Favored (53.47%) Isoleucine or valine / -101.9,122.0	75.3% ( <i>mt</i> ) chi angles: 300.7,175.8	0.036Å	-	-
A 339	ASP	50	-	Favored (10.78%) General / -86.1,98.2	39.6% ( <i>t0</i> ) chi angles: 182.9,24.6	0.015Å	-	-
A 340	LEU	50	0.42Å HD22 with A 342 GLU OE2	Favored (15.19%) General / -53.2,124.7	7.7% ( <i>tt</i> ) chi angles: 189.5,160.9	0.057Å	-	-
A 341	ASN	50	-	Favored (10.44%) General / -85.9,97.8	56% ( <i>t-20</i> ) chi angles: 191.2,345.6	0.038Å	-	-
A 342	GLU	50	0.42Å OE2 with A 340 LEU HD22	Favored (17.06%) General / -71.6,-2.4	46% ( <i>mp0</i> ) chi angles: 290.7,74.4,21.1	0.075Å	-	-
A 343	CYS	50	-	Favored (24.56%) General / -108.6,5.0	95.6% ( <i>m</i> ) chi angles: 291.1	0.065Å	-	-
A 344	ASN	50	-	Favored (72.93%) General / -64.8,-31.6	20.4% ( <i>t-20</i> ) chi angles: 189.1,293.3	0.009Å	-	-
.				Favored				

A 345	SER	50	-	(28.35%) General / -95.3,12.6 Favored	78.9% ( <i>p</i> ) chi angles: 59.5	0.02Å	-	-
A 346	ASN	50	-	(3.16%) Pre-proline / 47.7,68.8	26.6% ( <i>m120</i> ) chi angles: 299.1,132.7	0.011Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118
A 347	PRO	50	0.873Å HG3 with A 361 LYS HD2	Favored (7.82%) Trans-proline / -75.7,-28.7	34.8% ( <i>Cg_endo</i> ) chi angles: 37	0.048Å	-	-
A 348	CYS	50	-	Favored (35.43%) General / -77.2,129.1	59.6% ( <i>m</i> ) chi angles: 304.7	0.042Å	-	-
A 349	GLN	50	-	Favored (19.12%) General / -106.2,155.8	83.9% ( <i>mt-30</i> ) chi angles: 300.1,182.1,354.7	0.056Å	-	-
A 350	SER	50	0.638Å HB3 with A 389 PHE CE2	Allowed (1.21%) General / 63.1,60.3	29.3% ( <i>m</i> ) chi angles: 304.2	0.147Å	-	-
A 351	ASN	50	-	Favored (5.48%) General / 55.8,22.4	94.6% ( <i>m-20</i> ) chi angles: 293.5,337.8	0.019Å	-	-
A 352	GLY	50	-	Favored (46.02%) Glycine / -71.0,149.4	-	-	-	-
A 353	GLU	50	0.956Å HG3 with A 384 ILE HG13	Favored (37.04%) General / -96.5,136.4	3.9% ( <i>pt-20</i> ) chi angles: 40.7,167.6,329.9	0.124Å	-	-
A 354	CYS	50	-	Favored (41.64%) General / -105.7,138.6	26.9% ( <i>t</i> ) chi angles: 190.3	0.06Å	-	-
A 355	VAL	50	0.694Å HG11 with A 363 TYR CB	Favored (53.8%) Isoleucine or valine / -111.1,116.9	8.2% ( <i>p</i> ) chi angles: 59.6	0.1Å	-	-

A 356	GLU	50	-	Favored (6.31%) General / -77.9,100.3	11.5% ( <i>tm-20</i> ) chi angles: 182.5,287.1,322.8	0.117Å	-	-
A 357	LEU	50	0.658Å HD21 with A 363 TYR CD1	Favored (6.45%) General / -110.0,173.2	73.4% ( <i>mt</i> ) chi angles: 293.2,181.3	0.082Å	-	-
A 358	SER	50	-	Favored (4.17%) General / -73.9,102.7	32.3% ( <i>t</i> ) chi angles: 184.3	0.025Å	-	-
A 359	SER	50	0.484Å HB2 with A 329 PRO O	Favored (2.33%) General / 76.2,15.4	32.6% ( <i>t</i> ) chi angles: 184.1	0.013Å	-	-
A 360	GLU	50	-	Favored (17.61%) General / -166.0,165.9	16.7% ( <i>pt-20</i> ) chi angles: 65.3,174.8,335.6	0.008Å	-	-
A 361	LYS	50	0.873Å HD2 with A 347 PRO HG3	Favored (5.77%) General / -123.1,32.2	22% ( <i>pttp</i> ) chi angles: 61.9,187.5,182.1,68	0.069Å	-	-
A 362	GLN	50	0.739Å HA with A 382 VAL O	Favored (14.82%) General / -118.3,108.2	94.1% ( <i>mt-30</i> ) chi angles: 294.3,183.6,331.6	0.076Å	-	-
A 363	TYR	99.99	0.709Å CE2 with A 365 ARG HG3	Favored (42.88%) General / -117.3,147.1	55.7% ( <i>t80</i> ) chi angles: 189.6,71.6	0.165Å	-	OUTLIER(S) worst is CG- CD2-CE2: 4.42 σ
A 364	GLY	99.99	-	Favored (8.11%) Glycine / -131.4,135.2	-	-	-	-
A 365	ARG	99.99	0.709Å HG3 with A 363 TYR CE2	Favored (49.69%) General / -120.0,141.5	59.1% ( <i>mtt-85</i> ) chi angles: 280.9,167.6,190.8,291.1	0.125Å	-	-
A 366	ILE	99.99	0.456Å HG22 with A 367 THR N	Favored (22.82%) Isoleucine or valine / -133.6,168.9	69.7% ( <i>mt</i> ) chi angles: 301.6,176.9	0.089Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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		Avg: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118
A 367	THR 99.99	0.456Å N with A 366 ILE HG22	Favored (4.83%) General / -163.4,134.9	86.7% ( <i>m</i> ) chi angles: 301.2	0.095Å	-	-	
A 368	GLY 99.99	-	Favored (7.04%) Glycine / -138.7,134.9	-	-	-	-	
A 369	LEU 99.99	-	Favored (56.33%) Pre-proline / -129.7,86.2	96.5% ( <i>mt</i> ) chi angles: 295.9,176.7	0.074Å	-	-	
A 370	PRO 99.99	0.713Å HB3 with A 375 TYR CE2	Favored (5.38%) Trans-proline / -83.7,131.5	59.1% ( <i>Cg_endo</i> ) chi angles: 26.8	0.146Å	-	-	
A 371	SER 99.99	-	Allowed (1.3%) General / -151.4,-161.3	90.4% ( <i>p</i> ) chi angles: 65.3	0.067Å	-	-	
A 372	SER 99.99	-	Favored (84.88%) General / -66.3,-37.2	78.1% ( <i>p</i> ) chi angles: 59	0.012Å	-	-	
A 373	PHE 99.99	-	Favored (56.26%) General / -74.6,-43.3	97.1% ( <i>m-85</i> ) chi angles: 293.6,274.5	0.037Å	-	-	
A 374	SER 99.99	-	OUTLIER (0.01%) General / 172.9,-147.3	88% ( <i>p</i> ) chi angles: 61.7	0.027Å	-	-	
A 375	TYR 99.99	0.713Å CE2 with A 370 PRO HB3	Favored (43.2%) General / -136.7,142.2	88.5% ( <i>m-85</i> ) chi angles: 300.1,89.6	0.086Å	-	-	
A 376	HIS 99.99	-	Favored (11.77%) General / -123.2,107.5	97.2% ( <i>m-70</i> ) chi angles: 293.9,283.9	0.022Å	OUTLIER(S) worst is CG-- ND1: 4.406 σ	OUTLIER(S) worst is CB- CG-CD2: 4.134 σ	
A 377	GLU 99.99	-	Favored (45.38%) General / -119.8,146.8	86.5% ( <i>tt0</i> ) chi angles: 180.6,178.2,8.8	0.088Å	-	-	
A 378	ALA 99.99	-	Favored (20.12%) General / -120.1,120.1	99.9% ( <i>mt</i> ) chi angles: 179.9,179.9	0.056Å	-	-	

A 378	ALA	99.99	-	(29.12%) General / -154.6,151.7	-	0.056Å	-	-
A 379	SER	99.99	-	Favored (30.36%) General / -161.4,161.9	83.2% ( <i>p</i> ) chi angles: 60.8	0.044Å	-	-
A 380	GLY	99.99	-	Favored (7.34%) Glycine / -161.0,141.4	-	-	-	-
A 381	TYR	99.99	0.463Å C with A 382 VAL CG1	Favored (37.52%) General / -139.4,141.5	97.2% ( <i>m-85</i> ) chi angles: 295.6,270.3	0.284Å	-	OUTLIER(S) worst is C-CA- CB: 6.225 $\sigma$
A 382	VAL	99.99	0.835Å HG11 with A 384 ILE HG12	Favored (11.8%) Isoleucine or valine / -140.0,172.8	1.6% ( <i>m</i> ) chi angles: 321.1	0.197Å	OUTLIER(S) worst is N-- CA: 5.112 $\sigma$	OUTLIER(S) worst is CA- CB-CG2: 8.267 $\sigma$
A 383	CYS	50	0.744Å O with A 382 VAL HA	OUTLIER (0.01%) General / -1.7,108.6	73.8% ( <i>m</i> ) chi angles: 296.8	0.09Å	-	-
A 384	ILE	50	0.956Å HG13 with A 353 GLU HG3	Favored (2.51%) Isoleucine or valine / -84.3,89.2	0.1% chi angles: 333.3,215.7	0.274Å	-	OUTLIER(S) worst is CB- CG1-CD1: 9.391 $\sigma$
A 385	CYS	50	-	Favored (57.8%) General / -62.8,136.3	62.2% ( <i>m</i> ) chi angles: 303.4	0.057Å	-	-
A 386	GLN	50	0.863Å NE2 with A 387 PRO HD2	Favored (89.03%) Pre-proline / -69.2,136.4	72.5% ( <i>tp60</i> ) chi angles: 185.4,63.3,55.3	0.065Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118
A 387	PRO	50	0.863Å HD2 with A 386 GLN NE2	Favored (3.2%) Trans-proline / -41.4,127.7	43.9% ( <i>Cg_exo</i> ) chi angles: 326.2	0.067Å	-	-
A 388	GLY	50	0.762Å O with A 398 VAL HG12	Favored (22.96%) Glycine / 111.8,-19.8	-	-	-	-



A 389	PHE	50	0.638Å CE2 with A 350 SER HB3	Favored (42.03%) General / -117.8,148.5	1.4% ( <i>m-30</i> ) chi angles: 293.5,34.1	0.044Å	-	-
A 390	THR	50	-	Favored (31.19%) General / -145.4,164.5	81.9% ( <i>p</i> ) chi angles: 60.9	0.024Å	-	-
A 391	GLY	50	-	Favored (15.57%) Glycine / 117.4,171.4	-	-	-	-
A 392	ILE	50	0.594Å HG13 with A 393 HIS ND1	Favored (69.75%) Isoleucine or valine / -64.3,-34.5	42.1% ( <i>pt</i> ) chi angles: 59.4,174.8	0.074Å	-	-
A 393	HIS	50	0.594Å ND1 with A 392 ILE HG13	Favored (20.3%) General / -111.8,8.0	58.3% ( <i>m80</i> ) chi angles: 304.3,98.7	0.063Å	OUTLIER(S) worst is CG-- ND1: 4.309 σ	-
A 394	CYS	50	-	Favored (28.1%) General / 57.5,38.9	56.6% ( <i>m</i> ) chi angles: 306	0.026Å	-	-
A 395	GLU	50	-	Favored (30.44%) General / -84.0,-24.7	16.8% ( <i>pm0</i> ) chi angles: 69.4,285.9,356.6	0.086Å	-	-
A 396	GLU	50	-	Favored (32.63%) General / -89.5,122.4	45.5% ( <i>tt0</i> ) chi angles: 179.4,180.2,68.7	0.046Å	-	-
A 397	ASP	50	-	Favored (9.77%) General / -83.4,99.0	44.3% ( <i>t0</i> ) chi angles: 187.4,329	0.048Å	-	-
A 398	VAL	50	0.762Å HG12 with A 388 GLY O	Allowed (1.13%) Isoleucine or valine / -43.6,128.6	9.9% ( <i>p</i> ) chi angles: 60.8	0.081Å	-	-
A 399	ASN	50	-	Favored (10.62%) General / -87.7,96.9	52.2% ( <i>t30</i> ) chi angles: 183.4,54.2	0.051Å	-	-
A 400	GLU	50	0.503Å CE2 with A	Favored (62.45%)	16.9% ( <i>mp0</i> ) chi angles:	0.067Å	-	-

A 400	GLU	50	-	398 VAL HG13	Favored (62.43%) General / -63.8,-16.9	Chi angles: 278.2,68.9,40	0.007 Å	-	-
A 401	CYS	50	-	-	Favored (59.29%) General / -82.0,-10.3	73.3% (m) chi angles: 296.9	0.017 Å	-	-
A 402	SER	50	-	-	Favored (86.73%) General / -62.7,-37.5	26.5% (t) chi angles: 185.6	0.02 Å	-	-
A 403	SER	50	-	-	Favored (39.58%) General / -83.0,1.5	71.5% (p) chi angles: 57.8	0.01 Å	-	-
A 404	ASN	50	-	-	Allowed (1.49%) Pre-proline / 53.1,71.2	31.4% (t-20) chi angles: 184.8,305	0.069 Å	-	-
A 405	PRO	50	-	-	Favored (10.29%) Trans-proline / -72.4,-32.4	88.2% (Cg_endo) chi angles: 31.8	0.052 Å	-	-
A 406	CYS	50	-	-	Favored (9.73%) General / -75.4,110.3	28.1% (m) chi angles: 310.5	0.028 Å	-	-
#	Alt Res	High B	Clash > 0.4 Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	
		Avg: 60.17	Clashscore: 37.9	Outliers: 3 of 116	Poor rotamers: 1 of 104	Outliers: 2 of 107	Outliers: 6 of 118	Outliers: 8 of 118	
A 407	GLN	50	-	-	Favored (36.34%) General / -71.1,158.5	85.6% (mt-30) chi angles: 295.4,181,298	0.026 Å	-	-
A 408	ASN	50	-	-	Favored (20.11%) General / 60.8,32.5	33.1% (m120) chi angles: 292.7,115.9	0.048 Å	-	-
A 409	GLY	50	-	-	Favored (10.44%) Glycine / 55.9,59.5	-	-	-	-
A 410	GLY	50	-	-	Favored (18.15%) Glycine / -92.5,146.4	-	-	-	-
		0.666 Å		Favored					

A 411	THR	50	0.000 Å OG1 with A 422 HIS HB3	Favored (45.66%) General / -71.7,133.5	71.6% ( <i>p</i> ) chi angles: 61.9	0.023 Å	-	-
A 412	CYS	50	-	Favored (53.81%) General / -112.5,134.8	48.8% ( <i>t</i> ) chi angles: 182.5	0.07 Å	-	-
A 413	GLU	50	0.687 Å HB3 with A 420 THR OG1	Favored (36.72%) General / -121.1,120.9	4.9% ( <i>tm-20</i> ) chi angles: 173.8,297.6,322.5	0.122 Å	-	-
A 414	ASN	50	-	Favored (43.98%) General / -73.6,136.1	51.3% ( <i>t30</i> ) chi angles: 184.4,58.7	0.045 Å	-	-
A 415	LEU	50	0.623 Å HB3 with A 416 PRO HD2	Allowed (0.14%) Pre-proline / -127.1,-168.1	37.1% ( <i>mt</i> ) chi angles: 288.5,184.6	0.139 Å	-	-
A 416	PRO	50	0.623 Å HD2 with A 415 LEU HB3	Allowed (0.74%) Trans-proline / -88.7,114.4	65.9% ( <i>Cg_endo</i> ) chi angles: 33.9	0.023 Å	-	-
A 417	GLY	50	-	Favored (57.63%) Glycine / 54.9,34.5	-	-	-	-
A 418	ASN	50	-	Favored (4.92%) General / -167.7,146.9	25% ( <i>t-20</i> ) chi angles: 185.9,298.5	0.086 Å	-	-
A 419	TYR	50	-	Favored (34.84%) General / -123.1,156.5	55.5% ( <i>p90</i> ) chi angles: 62.6,269.8	0.049 Å	-	-
A 420	THR	50	0.687 Å OG1 with A 413 GLU HB3	Favored (18.03%) General / -125.7,114.0	63.5% ( <i>p</i> ) chi angles: 62.2	0.047 Å	-	-
A 421	CYS	50	-	Favored (34.42%) General / -89.1,124.5	88.3% ( <i>m</i> ) chi angles: 292	0.02 Å	-	-
A 422	HIS	50	0.666 Å HB3 with A 411 THR OG1	Favored (4.6%) General / -103.6,92.8	14.8% ( <i>t-160</i> ) chi angles: 174,206.3	0.113 Å	OUTLIER(S) worst is CD2-- NE2: 4.341 σ	OUTLIER(S) worst is CB- CG-CD2: 4.72 σ

A 423	CYS	50	-	favoured (98.84%) Pre-proline / -64.8,144.3	82.7% ( <i>m</i> ) chi angles: 299.9	0.026Å	-	-
A 424	PRO	99.99	-	-	74.9% ( <i>Cg_endo</i> ) chi angles: 33.3	0.014Å	-	-

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