



# Viewing iqcb1\_mb\_365\_560H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	92.7	0 <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	5	2.94%	Goal: <1%
	Ramachandran outliers	4	2.06%	Goal: <0.05%
	Ramachandran favored	178	91.75%	Goal: >98%
	MolProbity score^	3.28		14 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 1653	0.00%	Goal: 0%
	Bad backbone angles:	23 / 2212	1.04%	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: 114.88			Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
365	GLU	77.57	-	-	20.3% ( <i>pt</i> -20) chi angles: 58.6,184.4,347	0.035Å	-	-
366	LEU	36.58	0.61Å O with 370 MET HG3	Favored (91.09%) General / -63.3,-45.5	64.6% ( <i>tp</i> ) chi angles: 179.7,62	0.108Å	-	-
367	GLN	94.21	-	Favored (82.5%) General / -68.2,-39.0	29.4% ( <i>pt</i> 20) chi angles: 65.1,180,309.2	0.084Å	-	-
368	LEU	49.41	0.529Å O with 368 LEU HD23	Favored (78.47%) General / -62.3,-48.8	3.3% ( <i>tt</i> ) chi angles: 188.7,179.8	0.066Å	-	-

369	SER	74.84	-	Favored (83.32%) General / -67.8,-41.3	69.3% ( <i>m</i> ) chi angles: 297.1	0.084Å	-	-
370	MET	45.44	0.61Å HG3 with 366 LEU O	Favored (99.03%) General / -61.9,-42.4	91.5% ( <i>mtp</i> ) chi angles: 293.4,185.3,70.5	0.08Å	-	-
371	LEU	51.98	0.457Å HD23 with 531 GLU OE2	Favored (44.57%) General / -97.2,129.4	81.8% ( <i>mt</i> ) chi angles: 293.9,180	0.09Å	-	-
372	GLU	47.76	-	Favored (12.83%) General / -88.9,167.9	64.1% ( <i>mt-10</i> ) chi angles: 291.7,180.1,308.7	0.109Å	-	-
373	ILE	105.46	0.617Å O with 373 ILE HG13	Favored (35.66%) Isoleucine or valine / -73.8,130.9	45.3% ( <i>pt</i> ) chi angles: 62.1,167.7	0.083Å	-	-
374	VAL	104.06	0.483Å O with 374 VAL HG13	Favored (67.1%) Isoleucine or valine / -124.1,134.2	14.9% ( <i>p</i> ) chi angles: 63.7	0.074Å	-	-
375	HIS	121.2	-	Favored (8.5%) Pre-proline / -137.9,102.0	79.1% ( <i>m80</i> ) chi angles: 297.5,85.1	0.111Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.425 σ
376	PRO	75.79	-	Favored (85.38%) Trans-proline / -56.7,138.5	76.1% ( <i>Cg_endo</i> ) chi angles: 29.7	0.046Å	-	-
377	GLY	46.58	-	Favored (23.18%) Glycine / -70.5,133.0	-	-	-	-
378	GLN	74.51	0.424Å NE2 with 383 TYR CD2	Favored (6.8%) General / -93.6,175.3	26.1% ( <i>mt-30</i> ) chi angles: 295.2,172.6,135.6	0.073Å	-	-
379	VAL	225.24	-	Favored (3.97%) Isoleucine or valine / -82.4,155.8	27.7% ( <i>m</i> ) chi angles: 295.7	0.071Å	-	-
380	GLU	114.84	0.831Å HB2 with 506	Favored (97.74%)	73.6% ( <i>tt0</i> ) chi angles:	0.127Å	-	-

			HIS NE2	General / -63.8,-42.2	183.8,180.4,20.5			
381	LYS	246.14	0.762Å HA with 381 LYS NZ	Allowed (0.76%) General / -69.2,95.7	0% chi angles: 199.6,83.7,337.2,286.3	0.125Å	-	-
382	HIS	276.1	0.601Å HB2 with 381 LYS O	OUTLIER (0%) General / 154.5,-115.8	12.1% ( <i>t60</i> ) chi angles: 197.1,96.1	0.142Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.415 σ
383	TYR	137.34	0.509Å CD2 with 382 HIS CD2	Favored (77.23%) General / -62.0,-35.0	70.6% ( <i>m-85</i> ) chi angles: 290.7,288	0.094Å	-	-
384	ARG	205.59	0.847Å O with 387 GLU HG2	Favored (2.19%) General / 69.3,36.8	87.5% ( <i>mtt-85</i> ) chi angles: 301.1,172.2,186,263.9	0.089Å	-	-
<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: 114.88</div> <div>Clashscore: 92.7</div> <div>Outliers: 4 of 194</div> <div>Poor rotamers: 5 of 170</div> <div>Outliers: 0 of 190</div> <div>Outliers: 0 of 196</div> <div>Outliers: 22 of 196</div> </div>								
385	GLU	113.15	-	Favored (79.09%) General / -65.9,-34.9	26.4% ( <i>pt-20</i> ) chi angles: 61.6,178.9,17.3	0.087Å	-	-
386	MET	145.21	0.942Å HE3 with 509 ALA HB1	Favored (81.13%) General / -63.9,-35.6	7.3% ( <i>tpt</i> ) chi angles: 208.3,71.1,188.6	0.063Å	-	-
387	GLU	78.2	0.847Å HG2 with 384 ARG O	Favored (72.53%) General / -62.6,-31.6	25.6% ( <i>pt-20</i> ) chi angles: 67.6,179.9,1.9	0.096Å	-	-
388	GLU	133.85	-	Favored (68.43%) General / -64.5,-26.4	23.4% ( <i>tp10</i> ) chi angles: 183.4,71.4,45.2	0.077Å	-	-
389	LYS	131.62	0.908Å HB3 with 392 LEU HD23	Allowed (1.03%) General / -39.0,134.4	35.5% ( <i>ttmt</i> ) chi angles: 180.8,168,286.2,179.6	0.085Å	-	-
390	SER	76.78	0.41Å O with 393 ILE HG22	Favored (66.38%) General / -66.5,-24.6	47.4% ( <i>t</i> ) chi angles: 180.1	0.101Å	-	-
			0.694Å	Favored				

391	ALA	36.98	H with 389 LYS HG2	(85.04%) General / -60.6,-38.5 Favored	-	0.099Å	-	-
392	LEU	117.69	0.908Å HD23 with 389 LYS HB3	(80.8%) General / -60.7,-37.1 Favored	2.9% ( <i>mm?</i> ) chi angles: 285.9,290.2	0.071Å	-	-
393	ILE	314.24	0.572Å O with 393 ILE HG23	(19.38%) Isoleucine or valine / -85.4,110.3 Favored	0% chi angles: 182.3,289.4	0.026Å	-	-
394	ILE	274.56	0.749Å HD13 with 397 HIS CG	(45.52%) Isoleucine or valine / -111.8,113.9 Favored	20.8% ( <i>tt</i> ) chi angles: 188.7,166.5	0.069Å	-	-
395	GLN	62.51	0.701Å O with 399 ARG HG3	(81.42%) General / -68.5,-38.8 Favored	98.3% ( <i>mt-30</i> ) chi angles: 295.1,180.1,331.9	0.119Å	-	-
396	LYS	76.43	-	(87.98%) General / -62.6,-46.5 Favored	58% ( <i>tptt</i> ) chi angles: 185,66.3,180.2,179.9	0.076Å	-	-
397	HIS	78.18	0.749Å CG with 394 ILE HD13	(96.19%) General / -62.9,-44.4 Favored	63.3% ( <i>m170</i> ) chi angles: 288,166.9	0.072Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.446 σ
398	TRP	71.09	-	(88.93%) General / -66.4,-39.2 Favored	46.3% ( <i>m0</i> ) chi angles: 289.9,358.2	0.055Å	-	-
399	ARG	69.17	0.701Å HG3 with 395 GLN O	(76.3%) General / -60.9,-35.3 Favored	20.5% ( <i>mtp-105</i> ) chi angles: 293.3,175.9,73.1,268.4	0.075Å	-	-
400	GLY	26.61	0.519Å O with 403 GLU HG2	(97.48%) Glycine / -61.8,-39.5 Favored	-	-	-	-
401	TYR	104.5	0.878Å HE2 with 489 ARG HG3	(77.34%) General / -64.7,-47.7 Favored	23.9% ( <i>m-85</i> ) chi angles: 284.9,68.7	0.095Å	-	-
402	ARG	128.79	0.648Å HG2 with 399 ARG O	(98.62%) General / Favored	5.9% ( <i>ptm180</i> ) chi angles: 60.9,210.6,310.2,132.2	0.033Å	-	-

403	GLU	87.16	0.519Å HG2 with 400 GLY O	-62.2,-41.7 Favored (90.85%) General / -61.4,-39.5	12% ( <i>pt-20</i> ) chi angles: 62.4,168.5,309.1	0.089Å	-	-	
404	ARG	130.8	0.425Å N with 403 GLU HG3	Favored (98.47%) General / -63.5,-42.8	34.2% ( <i>mmt180</i> ) chi angles: 290.1,288.1,177.2,171.6	0.071Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 114.88	Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
405	LYS	67.07	0.882Å HE2 with 489 ARG HH21	Favored (91.34%) General / -65.6,-39.1	63.3% ( <i>mttm</i> ) chi angles: 292.8,166.8,179.9,295.2	0.099Å	-	-	
406	ASN	38.43	0.505Å O with 410 GLN HB2	Favored (74.76%) General / -58.0,-37.7	85.9% ( <i>m-20</i> ) chi angles: 290,319.1	0.082Å	-	OUTLIER(S) worst is CA-CB- CG: 4.23 σ	
407	PHE	89.54	0.693Å O with 410 GLN HB3	Favored (97.21%) General / -64.0,-42.6	96.1% ( <i>m-85</i> ) chi angles: 292.4,276.8	0.126Å	-	OUTLIER(S) worst is CA-CB- CG: 5.163 σ	
408	HIS	55.51	0.496Å O with 411 ARG HB2	Favored (94.43%) General / -62.3,-45.2	53.4% ( <i>m170</i> ) chi angles: 299.4,161.2	0.058Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.447 σ	
409	GLN	50.49	0.79Å O with 412 GLN HG2	Favored (68.42%) General / -69.0,-30.1	80.7% ( <i>mt-30</i> ) chi angles: 294.1,180,28.4	0.072Å	-	-	
410	GLN	120.23	0.693Å HB3 with 407 PHE O	Favored (63.05%) General / -60.1,-22.6	5.1% ( <i>tp-100</i> ) chi angles: 180,67.5,194.7	0.097Å	-	-	
411	ARG	154.11	0.904Å HA with 419 ALA HB1	Favored (56.59%) General / -52.5,-36.9	30% ( <i>mmt180</i> ) chi angles: 287.3,305.7,173.7,194.9	0.03Å	-	-	
412	GLN	243.25	0.905Å CA with 421 VAL HB	Favored (37.81%) General / -76.2,130.2	15.7% ( <i>pt20</i> ) chi angles: 66.2,180.2,47.2	0.162Å	-	-	
			0.571Å	Favored (25.72%)	49.9% ( <i>m</i> )				

413	SER	202.6	H with 422 THR HG22	General / -155.0,168.8	chi angles: 289.6	0.122Å	-	-
414	LEU	45.44	-	Favored (86.56%) General / -65.4,-44.7	90.1% ( <i>mt</i> ) chi angles: 297.4,180.1	0.089Å	-	-
415	ILE	40.76	0.49Å HG22 with 416 GLU N	Favored (24.4%) Isoleucine or valine / -120.8,147.8	86.1% ( <i>mt</i> ) chi angles: 298.7,167	0.093Å	-	-
416	GLU	160.38	1.084Å HG2 with 422 THR HB	Favored (5.29%) General / -102.8,93.8	88.2% ( <i>mt-10</i> ) chi angles: 302.2,179.9,4.1	0.185Å	-	-
417	TYR	131.32	0.703Å O with 418 LYS HG3	Favored (64.97%) General / -66.6,-49.8	92.8% ( <i>m-85</i> ) chi angles: 293.3,280.2	0.147Å	-	-
418	LYS	228.95	0.703Å HG3 with 417 TYR O	Allowed (0.11%) General / -176.8,116.2	93.3% ( <i>mttt</i> ) chi angles: 291.3,168.7,177.4,180.1	0.158Å	-	-
419	ALA	273.54	0.904Å HB1 with 411 ARG HA	Favored (13.96%) General / -164.0,153.2	-	0.041Å	-	-
420	ALA	115.96	0.871Å H with 411 ARG HD2	Favored (16.33%) General / -65.6,-55.7	-	0.092Å	-	-
421	VAL	61.81	0.905Å HB with 412 GLN CA	Favored (42.32%) Isoleucine or valine / -72.7,-32.8	65.4% ( <i>t</i> ) chi angles: 179.7	0.11Å	-	-
422	THR	120.99	1.084Å HB with 416 GLU HG2	Favored (79.38%) General / -59.8,-37.5	41.6% ( <i>p</i> ) chi angles: 54.4	0.124Å	-	-
423	LEU	52.32	0.662Å HB3 with 420 ALA O	Favored (85.64%) General / -63.8,-37.0	57% ( <i>tp</i> ) chi angles: 181.8,64.2	0.089Å	-	-
424	GLN	120.61	0.486Å HB3 with 421 VAL O	Favored (98.16%) General / -61.5,-42.0	5.8% ( <i>tp60</i> ) chi angles: 180.5,82,314.1	0.092Å	-	-

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Avg: 114.88			Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
425	ARG	75.34	-	Favored (80.62%) General / -63.8,-35.4	61.1% ( <i>ttt85</i> ) chi angles: 182.7,178.7,180,86.2	0.09Å	-	-
426	ALA	38.64	0.549Å HB3 with 423 LEU O	Favored (84.79%) General / -61.7,-37.6	-	0.088Å	-	-
427	ALA	44.2	0.451Å HA with 430 PHE HD2	Favored (89.63%) General / -61.2,-39.2	-	0.095Å	-	-
428	LEU	129.69	-	Favored (83.56%) General / -62.0,-37.1	50.6% ( <i>tp</i> ) chi angles: 184,63.7	0.065Å	-	-
429	LYS	88.02	-	Favored (78.47%) General / -64.1,-34.6	74.5% ( <i>mmtt</i> ) chi angles: 299.2,302.8,178.6,180	0.068Å	-	-
430	PHE	153.45	0.509Å HA with 433 LYS HE3	Favored (96.18%) General / -63.1,-44.3	68.3% ( <i>m-85</i> ) chi angles: 285.3,270.9	0.098Å	-	OUTLIER(S) worst is CA-CB- CG: 5.656 σ
431	LEU	84.56	0.472Å N with 431 LEU HD12	Favored (97.26%) General / -64.1,-41.5	6.3% ( <i>mp</i> ) chi angles: 290,60.8	0.065Å	-	-
432	ALA	35.71	0.519Å O with 436 LYS HG3	Favored (93.67%) General / -62.5,-45.3	-	0.088Å	-	-
433	LYS	62.5	0.509Å HE3 with 430 PHE HA	Favored (85.45%) General / -67.4,-39.9	47.5% ( <i>mtmt</i> ) chi angles: 293.8,168.8,284.9,180.5	0.096Å	-	-
434	CYS	77.48	0.836Å O with 438 LYS HG2	Favored (99.17%) General / -61.2,-42.8	51.9% ( <i>t</i> ) chi angles: 179.9	0.091Å	-	-
435	ARG	82.41	-	Favored (88.53%) General /	94.7% ( <i>mtm-85</i> ) chi angles:	0.122Å	-	-

				-64.4,-45.2	291.6,193.1,295.3,265.3				
436	LYS	70.5	0.519Å HG3 with 432 ALA O	Favored (91.29%) General / -59.7,-45.7	45.9% ( <i>mtpt</i> ) chi angles: 299.8,164.4,82.2,179.6	0.085Å	-	-	
437	LYS	83.05	0.592Å O with 453 ALA HB2	Favored (77.75%) General / -65.2,-34.2	50.4% ( <i>pttt</i> ) chi angles: 66.6,165.1,180.3,168.1	0.089Å	-	-	
438	LYS	152.96	0.836Å HG2 with 434 CYS O	Favored (81.72%) General / -56.7,-44.7	1.7% ( <i>mmmp?</i> ) chi angles: 294.5,297.6,253.7,60.5	0.093Å	-	-	
439	LYS	205.75	-	Allowed (0.96%) General / -106.4,-163.8	63% ( <i>mttm</i> ) chi angles: 288.9,169.1,179.6,298.3	0.079Å	-	-	
440	LEU	280.8	1.103Å HB2 with 451 THR HA	Favored (5.92%) General / -136.5,105.5	3.3% ( <i>tm?</i> ) chi angles: 182.2,287.7	0.062Å	-	-	
441	PHE	283.97	0.442Å O with 442 ALA HB2	Favored (4.27%) General / -157.8,122.2	33.7% ( <i>p90</i> ) chi angles: 53.4,82.8	0.134Å	-	-	
442	ALA	288.51	0.442Å HB2 with 441 PHE O	Allowed (0.11%) Pre-proline / 166.7,159.8	-	0.111Å	-	-	
443	PRO	210.74	0.408Å O with 444 TRP CD1	Favored (20.37%) Trans-proline / -71.4,132.2	87.7% ( <i>Cg_exo</i> ) chi angles: 331.3	0.157Å	-	-	
444	TRP	268.99	0.408Å CD1 with 443 PRO O	Favored (2.18%) General / -170.5,-176.6	4.9% ( <i>m0</i> ) chi angles: 267.4,3.1	0.174Å	-	-	OUTLIER(S) worst is N-CA- CB: 4.142 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	
		Avg: 114.88	Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196	
445	ARG	279.84	-	Favored (51.78%) General / -116.7,138.0 Allowed (1.7%)	45.4% ( <i>ptt85</i> ) chi angles: 56,182.9,169.3,83.2	0.131Å	-	-	



446	GLY	94.06	-	Glycine / 170.3,134.1	-	-	-	-
447	LEU	142.07	0.545Å C with 447 LEU HD13	Favored (83.67%) General / -65.2,-45.8	3% ( <i>tm?</i> ) chi angles: 180.4,288.4	0.063Å	-	-
448	GLN	228.31	0.428Å HG2 with 447 LEU HD12	Favored (50.67%) General / -110.5,135.8	15.8% ( <i>mm-40</i> ) chi angles: 292.9,282.9,52.4	0.146Å	-	-
449	GLU	221.74	0.586Å HB3 with 440 LEU HD12	Favored (46.27%) General / -72.8,138.1	99.5% ( <i>mt-10</i> ) chi angles: 293.4,179.8,352.5	0.133Å	-	-
450	LEU	192.21	0.555Å N with 450 LEU HD22	Favored (6.13%) General / -96.9,92.5	1.5% ( <i>mm?</i> ) chi angles: 294.5,292.2	0.088Å	-	-
451	THR	115.71	1.103Å HA with 440 LEU HB2	Favored (93.6%) General / -64.8,-43.3	81.4% ( <i>p</i> ) chi angles: 61.1	0.072Å	-	-
452	ASP	175.51	0.446Å OD1 with 454 ARG HA	Allowed (1.29%) General / -70.8,96.8	9.3% ( <i>t0</i> ) chi angles: 179.9,310.8	0.102Å	-	-
453	ALA	89.69	0.592Å HB2 with 437 LYS O	Favored (65.71%) General / -62.5,-51.9	-	0.134Å	-	-
454	ARG	283.75	0.487Å HG3 with 454 ARG O	OUTLIER (0.02%) General / -176.6,60.6	4.1% ( <i>ptm-85</i> ) chi angles: 61.1,184.5,298.5,252.7	0.063Å	-	-
455	ARG	293.3	0.582Å HD2 with 438 LYS HD2	Favored (20.81%) General / -162.1,169.5	94.6% ( <i>mtt-85</i> ) chi angles: 291.2,178.3,180,269.2	0.113Å	-	-
456	VAL	256.69	0.601Å HG12 with 457 GLU N	Allowed (1.17%) Isoleucine or valine / -157.0,164.3	75.9% ( <i>t</i> ) chi angles: 179.3	0.094Å	-	-
457	GLU	101.5	0.601Å N with 456 VAL HG12	Favored (16.32%) General / 52.5,51.3	57% ( <i>mt-10</i> ) chi angles: 295,171.5,308.1	0.088Å	-	-

458	LEU	178.76	0.634Å HB3 with 438 LYS NZ	Favored (89.48%) General / -66.3,-39.5	1.8% ( <i>mm?</i> ) chi angles: 296.3,296.5	0.087Å	-	-
459	LYS	128.35	0.828Å HD2 with 460 LYS N	Favored (98.18%) General / -61.2,-43.9	0.1% chi angles: 58.2,78.1,180,175.7	0.082Å	-	-
460	LYS	116.33	0.828Å N with 459 LYS HD2	Favored (86.56%) General / -65.8,-37.5	52.1% ( <i>tptt</i> ) chi angles: 187.8,63.3,185.4,172.8	0.088Å	-	-
461	ARG	122.43	0.537Å HD3 with 457 GLU O	Favored (84.01%) General / -62.3,-37.1	2.8% ( <i>mpt_?</i> ) chi angles: 288.2,67.6,179.4,88.1	0.08Å	-	-
462	VAL	41.14	-	Favored (84.08%) Isoleucine or valine / -58.0,-43.0	87.6% ( <i>t</i> ) chi angles: 175.1	0.076Å	-	-
463	ASP	38.25	-	Favored (93.34%) General / -63.3,-39.0	91.8% ( <i>m-20</i> ) chi angles: 290,336.5	0.094Å	-	OUTLIER(S) worst is CA-CB- CG: 4.077 $\sigma$
464	ASP	38.34	0.697Å O with 467 ARG HG2	Favored (76.32%) General / -68.3,-34.5	93.5% ( <i>m-20</i> ) chi angles: 292.5,337.3	0.089Å	-	OUTLIER(S) worst is CA-CB- CG: 4.561 $\sigma$
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
Avg: 114.88			Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
465	TYR	68.83	0.651Å CZ with 434 CYS HB2	Favored (75.61%) General / -62.9,-49.2	83.5% ( <i>t80</i> ) chi angles: 180.7,82.9	0.115Å	-	-
466	VAL	43	0.546Å O with 470 LEU HD13	Favored (92.16%) Isoleucine or valine / -63.8,-41.3	99% ( <i>t</i> ) chi angles: 176.4	0.067Å	-	-
467	ARG	150.35	0.697Å HG2 with 464 ASP O	Favored (92.14%) General / -61.5,-39.8	5.1% ( <i>ptm105</i> ) chi angles: 60.7,183.9,289.3,88.2	0.079Å	-	-
468	ARG	39.18	0.546Å HG3 with 464 ASP O	Favored (99.81%) General /	94.2% ( <i>mtt-85</i> ) chi angles: 302.6,185.1,184.2,277	0.056Å	-	-

469	HIS	46.98	0.573Å O with 473 PRO HD2	-62.4,-43.0 Favored (99.72%) General / -63.0,-42.3	25.2% ( <i>m80</i> ) chi angles: 283.9,61.1	0.058Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.515 $\sigma$
470	LEU	95.99	0.659Å O with 474 MET HB3	Favored (81.52%) General / -62.1,-48.1	8.7% ( <i>mp</i> ) chi angles: 284.5,60.7	0.09Å	-	-
471	GLY	42.09	-	Favored (23.9%) Glycine / -67.1,-53.9	-	-	-	-
472	SER	88.56	0.769Å HB2 with 473 PRO HD3	Allowed (1.92%) Pre-proline / -68.1,-64.4	70.5% ( <i>m</i> ) chi angles: 297.6	0.152Å	-	-
473	PRO	214.25	0.769Å HD3 with 472 SER HB2	Favored (4.95%) Trans-proline / -67.0,-44.6	73.4% ( <i>Cg_exo</i> ) chi angles: 332.4	0.159Å	-	-
474	MET	108.5	0.659Å HB3 with 470 LEU O	Favored (53.47%) General / -68.8,-50.1	20.1% ( <i>ttt</i> ) chi angles: 193.2,174.9,191.1	0.067Å	-	-
475	SER	59.19	-	Favored (52.01%) General / -73.7,-45.5	3.9% ( <i>p</i> ) chi angles: 89.6	0.143Å	-	-
476	ASP	78.27	-	Favored (85.28%) General / -61.2,-47.6	60.5% ( <i>t0</i> ) chi angles: 188.8,358.5	0.085Å	-	OUTLIER(S) worst is CA-CB- CG: 4.155 $\sigma$
477	VAL	44	0.667Å O with 480 ARG HG2	Favored (88.79%) Isoleucine or valine / -67.1,-43.2	90.3% ( <i>t</i> ) chi angles: 177.1	0.08Å	-	-
478	VAL	50.97	0.558Å HG23 with 474 MET O	Favored (57.31%) Isoleucine or valine / -62.3,-33.1	54.8% ( <i>t</i> ) chi angles: 169.3	0.08Å	-	-
479	SER	30.37	-	Favored (93.69%) General / -59.8,-44.9	67.8% ( <i>m</i> ) chi angles: 296.2	0.077Å	-	-
480	ARG	131.86	0.667Å HG2 with 477	Favored (98.87%)	12.3% ( <i>ptp180</i> ) chi angles:	0.108Å	-	-

			VAL O	General / -62.5,-41.5	61.1,170,52.7,187			
481	GLU	61.33	0.575Å OE2 with 477 VAL HG12	Favored (94.53%) General / -64.8,-43.0	38.4% ( <i>mt-10</i> ) chi angles: 292.6,159.6,36	0.097Å	-	-
482	LEU	103.62	0.776Å O with 482 LEU HD13	Favored (80%) General / -64.8,-35.1	3.1% ( <i>tm?</i> ) chi angles: 186.5,290.8	0.056Å	-	-
483	HIS	52.44	-	Favored (93.13%) General / -61.6,-40.0	66.9% ( <i>m170</i> ) chi angles: 294.1,167.3	0.075Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.406 σ
484	ALA	32.47	-	Favored (94.18%) General / -59.7,-43.1	-	0.092Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 114.88	Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
485	GLN	56.73	0.678Å HG2 with 489 ARG NH1	Favored (78.68%) General / -69.0,-40.8	27.7% ( <i>mt-30</i> ) chi angles: 296.6,179.9,210.7	0.064Å	-	-
486	ALA	36.86	-	Favored (88.94%) General / -60.6,-46.8	-	0.081Å	-	-
487	GLN	78.43	0.717Å HA with 487 GLN HE21	Favored (84.96%) General / -65.7,-44.8	3.2% ( <i>mm-40</i> ) chi angles: 291.3,290.9,246.5	0.067Å	-	-
488	GLU	82.55	0.526Å HG3 with 489 ARG HD2	Favored (78.54%) General / -67.2,-44.9	12.2% ( <i>pt-20</i> ) chi angles: 58.9,186,75.1	0.071Å	-	-
489	ARG	112.05	0.882Å HH21 with 405 LYS HE2	Favored (96.62%) General / -63.7,-40.4	11.1% ( <i>mpt_?</i> ) chi angles: 277.1,69.5,178.3,160.8	0.118Å	-	-
490	LEU	104.01	1.126Å HG with 499 LEU HD12	Favored (14.52%) General / -59.8,-57.1	3.7% ( <i>tt</i> ) chi angles: 182.8,175.6	0.057Å	-	-
491	GLN	105.91	0.602Å HG3 with 492	Favored (15.84%)	28.6% ( <i>pt20</i> ) chi angles:	0.099Å	-	-

			HIS N	General / -72.4,-52.5	65.3,174.2,313.6			
492	HIS	98.29	0.672Å HB2 with 401 TYR OH	Favored (6.13%) General / -68.3,-57.3	66.4% ( <i>m170</i> ) chi angles: 291.8,169	0.103Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.438 σ
493	TYR	292.34	0.869Å HA with 498 ALA CB	Allowed (0.08%) General / 179.0,132.8	54.6% ( <i>t80</i> ) chi angles: 168.8,84.7	0.089Å	-	-
494	PHE	285.55	0.591Å HD1 with 489 ARG HG2	Favored (6.33%) General / -140.9,-179.9	55.9% ( <i>t80</i> ) chi angles: 189.9,72.9	0.089Å	-	OUTLIER(S) worst is CA-CB- CG: 5.235 σ
495	MET	240.8	0.466Å N with 494 PHE CD2	Favored (28.04%) General / -58.7,148.8	67.6% ( <i>ttp</i> ) chi angles: 180,180,67.4	0.11Å	-	-
496	GLY	106.42	-	Favored (45.7%) Glycine / 80.7,-163.2	-	-	-	-
497	ARG	301.82	0.509Å HD3 with 503 ALA HB2	Favored (48.61%) General / -72.5,143.0	7.8% ( <i>ptp180</i> ) chi angles: 60.2,171.9,65.5,161	0.115Å	-	-
498	ALA	226.96	0.869Å CB with 493 TYR HA	Favored (57.28%) General / -67.3,140.4	-	0.134Å	-	OUTLIER(S) worst is C-N- CA: 4.865 σ
499	LEU	221.38	1.126Å HD12 with 490 LEU HG	Allowed (0.78%) General / -65.9,-64.8	31% ( <i>mt</i> ) chi angles: 292,188.7	0.111Å	-	-
500	GLU	67.43	-	Favored (4.5%) General / -78.4,-56.4	87.4% ( <i>mt-10</i> ) chi angles: 289.9,190.8,354.6	0.102Å	-	-
501	GLU	96.84	0.546Å HB2 with 492 HIS O	Favored (33.03%) General / -69.4,-51.8	55.7% ( <i>mm-40</i> ) chi angles: 289.5,283.3,319.9	0.087Å	-	-
502	ARG	171.9	0.779Å H with 498 ALA HB3	Favored (50.34%) General / -63.7,-53.5	0% chi angles: 193.3,254.4,92.7,141.9	0.07Å	-	-
503	ALA	56.69	0.509Å HB2 with 497	Favored (60.37%)	-	0.076Å	-	-

			ARG HD3	General / -69.6,-48.4 Favored (72.04%) General / -68.7,-32.3	11.5% ( <i>tt0</i> ) chi angles: 186.9,164.1,126.3	0.091Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 114.88	Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
505		GLN	105.31	0.402Å HB2 with 501 GLU O	Favored (71.5%) General / -61.6,-31.4	32.5% ( <i>tt0</i> ) chi angles: 186.9,176,96.4	0.091Å	-	-
506		HIS	81.03	0.831Å NE2 with 380 GLU HB2	Favored (90.53%) General / -59.2,-42.3	53% ( <i>t-80</i> ) chi angles: 192.3,270.9	0.08Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.435 σ
507		ARG	107.36	0.8Å O with 511 ILE HG12	Favored (88.68%) General / -58.9,-42.1	57.4% ( <i>mtp180</i> ) chi angles: 292.2,159.3,50.4,195.1	0.103Å	-	-
508		GLU	87.24	0.889Å HA with 514 ILE HG21	Favored (96.06%) General / -60.3,-43.7	32% ( <i>tt0</i> ) chi angles: 175,181.2,288.2	0.129Å	-	-
509		ALA	44.06	0.942Å HB1 with 386 MET HE3	Favored (92.97%) General / -59.6,-45.1	-	0.077Å	-	-
510		LEU	65.3	-	Favored (77.31%) General / -68.6,-43.0	64.4% ( <i>tp</i> ) chi angles: 179.7,61.9	0.104Å	-	-
511		ILE	103.41	1.108Å HB with 514 ILE HG22	Favored (4.16%) Isoleucine or valine / -55.5,121.9	42.2% ( <i>mm</i> ) chi angles: 296.2,299.2	0.071Å	-	-
512		ALA	20.22	1.092Å HA with 517 ASN HB2	Favored (96.94%) General / -64.1,-40.7	-	0.098Å	-	-
513		GLN	35.27	0.544Å O with 518 VAL HG22	Favored (81.56%) General / -65.2,-46.2	46.8% ( <i>mt-30</i> ) chi angles: 297.5,179.6,261.3	0.085Å	-	-

514	ILE	177.65	1.108Å HG22 with 511 ILE HB	Favored (21.23%) Isoleucine or valine / -80.7,-46.3	19.3% ( <i>tt</i> ) chi angles: 191,164.9	0.217Å	-	OUTLIER(S) worst is C-N- CA: 4.474 σ
515	SER	160.29	0.652Å HB2 with 508 GLU HG2	Allowed (0.28%) General / -122.5,-121.0	12.2% ( <i>t</i> ) chi angles: 191.1	0.091Å	-	-
516	THR	137.4	0.756Å HG21 with 386 MET HE1	Favored (78.25%) General / -57.1,-41.0	12.6% ( <i>t</i> ) chi angles: 185.7	0.044Å	-	-
517	ASN	73.81	1.092Å HB2 with 512 ALA HA	Favored (69.49%) General / -62.9,-27.6	44.1% ( <i>m-20</i> ) chi angles: 279.2,301.9	0.114Å	-	OUTLIER(S) worst is CA-CB- CG: 6.526 σ
518	VAL	48.43	0.544Å HG22 with 513 GLN O	Favored (76.92%) Isoleucine or valine / -57.8,-50.6	61.3% ( <i>t</i> ) chi angles: 180.1	0.241Å	-	-
519	GLU	35.23	-	Favored (99.41%) General / -63.0,-41.1	94.4% ( <i>mt-10</i> ) chi angles: 293.7,180.5,5.2	0.116Å	-	-
520	GLN	53.67	-	Favored (89.03%) General / -65.7,-43.5	77.7% ( <i>mt-30</i> ) chi angles: 292.2,183.7,46.6	0.091Å	-	-
521	LEU	135.09	0.718Å O with 525 PRO HD2	Favored (95.11%) General / -64.9,-41.9	57.9% ( <i>tp</i> ) chi angles: 181,64.4	0.089Å	-	-
522	MET	111.58	-	Favored (75.82%) General / -63.2,-49.0	18.3% ( <i>mmt</i> ) chi angles: 289.4,291.8,192.5	0.093Å	-	-
523	LYS	111.22	-	Favored (55.44%) General / -72.6,-46.2	8.1% ( <i>mtpm?</i> ) chi angles: 290.5,166,63.5,289.4	0.079Å	-	-
524	ALA	63.43	0.751Å HB3 with 525 PRO HD3	Favored (75.23%) Pre-proline / -63.7,-49.8	-	0.108Å	-	-

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles

Avg: Clashscore: Outliers: 4 of Poor rotamers: 5 of Outliers: Outliers: Outliers: 22

		114.88	92.7	194	170	0 of 190	0 of 196	of 196
525	PRO	159.6	0.751Å HD3 with 524 ALA HB3	Favored (39.09%) Trans-proline / -66.5,-32.9	71.1% ( <i>Cg_exo</i> ) chi angles: 327.9	0.218Å	-	-
526	SER	77.53	-	Favored (45.87%) General / -67.9,-51.6	96.8% ( <i>p</i> ) chi angles: 63.9	0.077Å	-	-
527	LEU	152.18	-	Favored (87.18%) General / -67.0,-40.7	79.9% ( <i>mt</i> ) chi angles: 296.5,182.1	0.058Å	-	-
528	LYS	135.02	-	Favored (91.41%) General / -63.0,-38.5	22.6% ( <i>tmm</i> ) chi angles: 185.7,162.9,295.9,294.3	0.056Å	-	-
529	GLU	51.18	-	Favored (77.81%) General / -68.8,-36.0	89% ( <i>mt-10</i> ) chi angles: 293.3,189.6,343	0.068Å	-	-
530	ALA	35.3	-	Favored (94.5%) General / -64.9,-42.7	-	0.071Å	-	-
531	GLU	82.75	0.764Å O with 535 PRO HD2	Favored (65.25%) General / -67.7,-20.3	56.5% ( <i>mt-10</i> ) chi angles: 291.3,180.1,298.1	0.074Å	-	-
532	GLY	33.86	-	Favored (95.21%) Glycine / -62.2,-45.8	-	-	-	-
533	LYS	134.09	0.542Å O with 537 LEU HD23	Favored (71.71%) General / -70.3,-42.8	6.3% ( <i>tppm?</i> ) chi angles: 189.7,165.3,65.4,290	0.058Å	-	-
534	GLU	78.44	0.792Å HB2 with 535 PRO HD3	Favored (81.61%) Pre-proline / -61.6,-50.6	25.7% ( <i>mt-10</i> ) chi angles: 301.8,157.5,45.5	0.048Å	-	-
535	PRO	155.34	0.792Å HD3 with 534 GLU HB2	Favored (37.51%) Trans-proline / -69.8,-17.1	85.3% ( <i>Cg_exo</i> ) chi angles: 328.8	0.219Å	-	-
536	GLU	107.84	-	Favored (64.92%)	40.3% ( <i>mm-40</i> ) chi angles:	0.101Å	-	-



537	LEU	87.23	0.542Å HD23 with 533 LYS O	General / -72.7,-41.9 Favored (77.71%) General / -68.4,-43.2	278,292.2,293.8 2.6% ( <i>mm?</i> ) chi angles: 289.9,293.5	0.088Å	-	-
538	PHE	87.83	-	Favored (98.86%) General / -62.6,-41.3	79.9% ( <i>t80</i> ) chi angles: 181.7,83.8	0.081Å	-	OUTLIER(S) worst is CA-CB- CG: 4.842 σ
539	LEU	151.77	0.558Å C with 539 LEU HD13	Favored (78.81%) General / -62.8,-48.5	3.1% ( <i>tm?</i> ) chi angles: 180.3,286.8	0.027Å	-	-
540	SER	79.59	0.715Å O with 544 PRO HD2	Favored (67.04%) General / -66.0,-25.3	47.6% ( <i>t</i> ) chi angles: 180	0.088Å	-	-
541	ARG	163.35	0.618Å O with 545 VAL HB	Favored (75.55%) General / -63.1,-49.1	12.2% ( <i>tpp180</i> ) chi angles: 204.8,80.9,56.2,171.8	0.145Å	-	-
542	SER	93	0.767Å O with 545 VAL HG12	Favored (66.99%) General / -71.6,-42.9	95.9% ( <i>p</i> ) chi angles: 64.8	0.075Å	-	-
543	ARG	113.03	0.621Å HB2 with 544 PRO HD3	Favored (56.25%) Pre-proline / -63.3,-53.1	81.4% ( <i>mmt-85</i> ) chi angles: 289.8,282.2,175,271.1	0.132Å	-	-
544	PRO	109.78	0.715Å HD2 with 540 SER O	Favored (22.01%) Trans-proline / -71.9,-23.5	98.8% ( <i>Cg_exo</i> ) chi angles: 329.4	0.18Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 114.88				Clashscore: 92.7	Outliers: 4 of 194	Poor rotamers: 5 of 170	Outliers: 0 of 190	Outliers: 0 of 196	Outliers: 22 of 196
545	VAL	87.92	0.767Å HG12 with 542 SER O	Favored (80.85%) Isoleucine or valine / -66.0,-37.9	9.2% ( <i>p</i> ) chi angles: 70.9	0.067Å	-	-	
546	ALA	54.39	0.856Å HB3 with 550 LYS HG2	Favored (65.11%) General / -60.8,-52.4 OUTLIER	-	0.071Å	-	-	

547	ALA	56.57	0.691Å O with 550 LYS HB3	(0.01%) General / 155.0,169.0	-	0.155Å	-	-
548	LYS	66.9	-	Favored (77.29%) General / -69.6,-39.2	36.1% ( <i>ttpt</i> ) chi angles: 187.9,164,61.2,181.3	0.067Å	-	-
549	ALA	38.28	-	Favored (70.17%) General / -60.7,-30.7	-	0.105Å	-	-
550	LYS	156.51	0.986Å HZ1 with 557 LEU HD12	Favored (60.81%) General / -57.6,-25.9	25.3% ( <i>tptp</i> ) chi angles: 179.8,67.2,169.3,46.3	0.108Å	-	-
551	GLN	70.07	0.88Å HA with 554 LEU CD1	Favored (87.62%) General / -58.1,-44.0	24.2% ( <i>tp60</i> ) chi angles: 181.4,92.3,55.4	0.108Å	-	-
552	ALA	37.82	-	Favored (97.69%) General / -63.9,-41.8	-	0.094Å	-	-
553	HIS	122.07	-	Favored (65.94%) General / -67.2,-24.9	62.6% ( <i>t60</i> ) chi angles: 186.5,84.2	0.09Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.406 σ
554	LEU	167.58	0.88Å CD1 with 551 GLN HA	Favored (67.77%) General / -59.3,-29.7	79.1% ( <i>mt</i> ) chi angles: 294,180.6	0.123Å	-	-
555	THR	42.49	-	Favored (77.08%) General / -55.8,-43.6	93.4% ( <i>m</i> ) chi angles: 300.2	0.095Å	-	-
556	THR	111.87	-	Favored (73.78%) General / -65.6,-48.0	43% ( <i>p</i> ) chi angles: 67.5	0.077Å	-	-
557	LEU	98.98	0.986Å HD12 with 550 LYS HZ1	Favored (91.8%) General / -65.4,-39.1	29.5% ( <i>mt</i> ) chi angles: 290.5,188.1	0.098Å	-	-
558	LYS	256.63	0.513Å HB3 with 560 ILE HD13	OUTLIER (0.03%) General / 68.5,121.0	93.3% ( <i>mttt</i> ) chi angles: 291.9,168.9,179.3,181.6	0.087Å	-	-

559	HIS	88.64	0.538Å CD2 with 539 LEU HD11	Favored (87.68%) General / -64.9,-45.0	65.4% ( <i>t</i> -80) chi angles: 188.5,279.7	0.089Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.414 σ
560	ILE	122.97	0.683Å H with 560 ILE HD13	-	0.2% chi angles: 64.6,296.8	0.092Å	-	-

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