



Viewing iqcb1_mb_365_560-FFX1FH_reg-multi.table

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All-Atom Contacts	Clashscore, all atoms:	4.24	96 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	7	4.12%	Goal: <0.3%
	Favored rotamers	151	88.82%	Goal: >98%
	Ramachandran outliers	4	2.06%	Goal: <0.05%
	Ramachandran favored	175	90.21%	Goal: >98%
	MolProbity score^	2.22	63 rd percentile* (N=27675, 0Å - 99Å)	
	Cβ deviations >0.25Å	5	2.63%	Goal: 0
	Bad bonds:	0 / 1653	0.00%	Goal: 0%
	Bad angles:	14 / 2212	0.63%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 6	0.00%	Expected: ≤1 per chain, or ≤5%

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	C β deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195
365	GLU	77.57	-	-	-	Favored (9.4%) <i>pt0</i> chi angles: 65.6,168.2,336.1	0.18Å	-	-	-
366	LEU	36.58	-	-	Favored (62.12%) General / -53.2,-51.5	Favored (53.6%) <i>tp</i> chi angles: 179.7,65.4	0.06Å	-	-	-
367	GLN	94.21	-	-	Favored (79.89%) General / -61.1,-36.5	Favored (24.8%) <i>pt0</i> chi angles: 68.4,178.5,296.3	0.13Å	-	-	-
368	LEU	49.41	-	-	Favored (79.14%) General / -63.8,-47.9	Allowed (1.5%) <i>tt</i> chi angles: 199.8,177.9	0.04Å	-	-	-
369	SER	74.84	-	-	Favored (67.17%) General / -70.0,-30.0	Favored (30.7%) <i>m</i> chi angles: 302.9	0.09Å	-	-	-
					Favored	Favored (90.1%)				

370	MET	45.44	-	(21.75%) General / -81.5,-41.4	<i>mtp</i> chi angles: 297.1,182.2,71.9	0.09Å	-	-	-
371	LEU	51.98	-	Favored (11.68%) General / -90.8,98.3	Favored (87.5%) <i>mt</i> chi angles: 295.6,178.5	0.07Å	-	-	-
372	GLU	47.76	-	Favored (2.07%) General / -50.1,151.2	Favored (35%) <i>mt-10</i> chi angles: 290.3,165.7,306.8	0.15Å	-	-	-
373	ILE	105.46	-	Allowed (1.6%) Ile or Val / -63.5,113.8	Favored (19.6%) <i>pt</i> chi angles: 58.3,161	0.11Å	-	-	-
374	VAL	104.06	-	Favored (12%) Ile or Val / -99.7,144.6	Favored (3.1%) <i>p</i> chi angles: 74.6	0.14Å	-	-	-
375	HIS	121.2	-	Favored (3%) Pre-Pro / -151.1,101.8	Favored (81.1%) <i>m90</i> chi angles: 294.4,82.4	0.09Å	-	-	-
376	PRO	75.79	-	Favored (29.04%) Trans-Pro / -72.0,137.4	Favored (52.9%) <i>Cg_endo</i> chi angles: 32.7	0.03Å	-	-	-
377	GLY	46.58	-	Favored (3.23%) Glycine / -61.5,110.6	-	-	-	-	-
378	GLN	74.51	-	Favored (28.85%) General / -80.2,153.1	Favored (36.4%) <i>mt0</i> chi angles: 296.3,178.3,100.9	0.06Å	-	-	-
379	VAL	225.24	-	Favored (3.11%) Ile or Val / -61.3,157.5	Favored (29%) <i>m</i> chi angles: 298.3	0.11Å	-	-	-
380	GLU	114.84	0.43Å HB2 with 506 HIS CE1	Favored (84.58%) General / -61.2,-37.9	Favored (58.5%) <i>tt0</i> chi angles: 194.6,182.8,353.7	0.04Å	-	-	-
381	LYS	246.14	-	Favored (6.07%) General / -80.3,67.3	Favored (83.4%) <i>tttt</i> chi angles: 188.3,177.7,176,180.4	0.10Å	-	-	-
382	HIS	276.1	-	OUTLIER (0%) General / -174.7,-103.1	Favored (26.4%) <i>t-90</i> chi angles: 198.3,300.1	0.03Å	-	-	-
383	TYR	137.34	-	Favored (60.96%) General / -73.9,-27.3	Favored (83.7%) <i>m-80</i> chi angles: 300.2,284.1	0.08Å	-	-	-
384	ARG	205.59	0.41Å HG2 with	Favored (2.95%)	Favored (53.7%) <i>ttp80</i>	0.15Å	-	-	-

384 ARG O

General /

chi angles:

71.3,28.6

193.4,184,60.7,65.7

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195
385	GLU	113.15	-		Favored (63.87%) General / -56.5,-31.3	Favored (8.2%) <i>pt0</i> chi angles: 69.7,170.7,42.8	0.05Å	-	-	-
386	MET	145.21	-		Favored (61.56%) General / -71.9,-24.0	Favored (2.3%) <i>tpt</i> chi angles: 212.5,74.7,215.4	0.06Å	-	-	-
387	GLU	78.2	-		Favored (20.45%) General / -91.0,-23.4	Favored (39.3%) <i>tp30</i> chi angles: 170.6,70.2,28.3	0.18Å	-	-	-
388	GLU	133.85	-		Favored (65.02%) General / -69.4,-27.1	Favored (48.3%) <i>mm-30</i> chi angles: 293.7,288.3,307.5	0.04Å	-	-	-
389	LYS	131.62	-		Allowed (1.66%) General / -39.2,129.9	Favored (86%) <i>tttt</i> chi angles: 181.2,178,179.9,178.3	0.04Å	-	-	-
390	SER	76.78	-		Favored (55.78%) General / -52.7,-35.6	Favored (54.7%) <i>p</i> chi angles: 57.1	0.12Å	-	-	-
391	ALA	36.98	-		Favored (16.97%) General / -48.9,-36.4	-	0.07Å	-	-	-
392	LEU	117.69	-		Favored (83.01%) General / -67.9,-38.4	Allowed (0.9%) <i>mm</i> chi angles: 289,293	0.12Å	-	-	-
393	ILE	314.24	-		Allowed (0.81%) Ile or Val / -83.9,72.5	Favored (82.5%) <i>mt</i> chi angles: 293.6,174.2	0.13Å	-	-	-
394	ILE	274.56	-	0.43Å HG21 with 397 HIS CD2	Favored (4.2%) Ile or Val / -85.0,95.2	Favored (16.2%) <i>tt</i> chi angles: 190.9,173.5	0.24Å	-	-	-
395	GLN	62.51	-		Favored (8.82%) General / -44.9,-43.2	Favored (77.3%) <i>mt0</i> chi angles: 292.7,184.8,357.7	0.12Å	-	-	-
396	LYS	76.43	-		Favored (98.61%) General / -63.5,-41.2	Favored (98.4%) <i>mttt</i> chi angles: 292.4,180,178.8,178.5	0.17Å	-	-	-
0.43Å				Favored	Favored (8.6%) <i>m-</i>	OUTLIER(S)				

397	HIS	78.18	CD2 with 394 ILE HG21	(64.63%) General / -68.8,-48.1	70 chi angles: 294.1,337.6	0.16Å	-	worst is CA- CB-CG: 4.5 σ	-
398	TRP	71.09	-	Favored (70.49%) General / -60.4,-31.6	Favored (57.6%) <i>m</i> - 10 chi angles: 298.2,348.5	0.15Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.8 σ	-
399	ARG	69.17	-	Favored (96.29%) General / -61.2,-41.2	Favored (81.9%) <i>ttt180</i> chi angles: 184.9,172.3,177.5,176.8	0.08Å	-	-	-
400	GLY	26.61	-	Favored (79.93%) Glycine / -60.0,-33.7	-	-	-	-	-
401	TYR	104.5	-	Favored (84.56%) General / -67.0,-42.8	Favored (2.5%) <i>m</i> - 80 chi angles: 285.6,49.8	0.13Å	-	-	-
402	ARG	128.79	-	Favored (65.15%) General / -73.7,-37.5	Favored (97.4%) <i>mtt180</i> chi angles: 296.4,179.7,178.7,183.7	0.16Å	-	-	-
403	GLU	87.16	-	Favored (88.94%) General / -66.1,-42.6	Favored (8.3%) <i>pt0</i> chi angles: 57.4,177.9,291.3	0.18Å	-	-	-
404	ARG	130.8	-	Favored (91.57%) General / -65.5,-39.1	Favored (55.5%) <i>mmt-90</i> chi angles: 297.5,279.5,174.7,285.4	0.13Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88			Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195
405	LYS	67.07	-	Favored (88.14%) General / -62.9,-37.7	Favored (6.4%) <i>tpp</i> chi angles: 184.2,192.7,62.9,56.3	0.11Å	-	-	-
406	ASN	38.43	-	Favored (58.33%) General / -78.0,-16.2	Favored (62.8%) <i>m</i> - 40 chi angles: 296.4,350	0.16Å	-	-	-
407	PHE	89.54	-	Favored (42.3%) General / -79.5,-32.1	Favored (79.3%) <i>m</i> - 80 chi angles: 295.3,287.7	0.13Å	-	-	-
408	HIS	55.51	-	Favored (60.79%) General / -72.8,-23.6	Favored (21.8%) <i>t</i> - 170 chi angles: 189.1,181.6	0.11Å	-	OUTLIER(S) worst is CA- CB-CG: 4.8 σ	-
409	GLN	50.49	-	Favored (16.42%) General /	Favored (61.8%) <i>tt0</i> chi angles: 189.8,178.2,351.5	0.14Å	-	-	-

-99.0,-21.0

410	GLN 120.23	-	Favored (61.02%) General / -73.5,-13.2	Favored (8.2%) <i>tp</i> - <i>100</i> chi angles: 190.6,53.6,226.6	0.09Å	-	-	-
411	ARG 154.11	-	Favored (9.66%) General / -52.1,-25.8	Favored (33.1%) <i>mmt180</i> chi angles: 294.2,308.3,173.6,190.5	0.18Å	-	-	-
412	GLN 243.25	-	Favored (34.81%) General / -91.1,134.1	Favored (11.8%) <i>tp</i> - <i>100</i> chi angles: 185,61.1,279.8	0.09Å	-	-	-
413	SER 202.6	-	Favored (11.64%) General / -156.0,177.2	Favored (10.6%) <i>t</i> chi angles: 190	0.05Å	-	-	-
414	LEU 45.44	-	Favored (63.09%) General / -72.9,-42.9	Favored (54.8%) <i>mt</i> chi angles: 305.1,175.6	0.10Å	-	-	-
415	ILE 40.76	-	Favored (15.71%) Ile or Val / -113.4,149.9	Favored (92.3%) <i>mt</i> chi angles: 297.5,172.4	0.10Å	-	-	-
416	GLU 160.38	-	Favored (2.69%) General / -99.9,83.2	Allowed (0.9%) <i>mt</i> - <i>10</i> chi angles: 323.4,204.8,45.1	0.04Å	-	-	-
417	TYR 131.32	0.46Å O with 418 LYS HG3	Favored (3.21%) General / -68.4,-59.4	Favored (83.8%) <i>t80</i> chi angles: 177.4,84.7	0.19Å	-	OUTLIER(S) worst is C-N- CA: 4.9 σ	-
418	LYS 228.95	0.46Å HG3 with 417 TYR O	Allowed (0.15%) General / -172.4,100.9	Favored (41%) <i>mttp</i> chi angles: 289.8,178.1,191,64.5	0.11Å	-	-	-
419	ALA 273.54	-	Favored (28.19%) General / -159.6,156.6	-	0.10Å	-	-	-
420	ALA 115.96	-	Favored (18.09%) General / -87.2,-36.2	-	0.06Å	-	-	-
421	VAL 61.81	-	Favored (6.06%) Ile or Val / -98.2,-19.2	Favored (7.3%) <i>t</i> chi angles: 190.8	0.23Å	-	-	-
422	THR 120.99	-	Favored (96.74%) General / -63.9,-43.2	Favored (69.2%) <i>p</i> chi angles: 62.4	0.12Å	-	-	-
423	LEU 52.32	-	Favored (73.36%)	Favored (15.1%) <i>tp</i> chi angles: 192.5,69.1	0.12Å	-	-	-

General /
-60.8,-33.6Favored
(90.05%)
General /
-66.3,-40.8Favored (3%) *tp-100*
chi angles:
190.4,79.4,307.3

0.04Å

-

-

-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
			Avg: 114.88	Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195
424		GLN	120.61	-	Favored (90.05%) General / -66.3,-40.8	Favored (3%) <i>tp-100</i> chi angles: 190.4,79.4,307.3	0.04Å	-	-	-
425		ARG	75.34	-	Favored (84.16%) General / -62.9,-36.7	Favored (58.5%) <i>tp-170</i> chi angles: 180.1,181.2,66.1,179.4	0.10Å	-	-	-
426		ALA	38.64	-	Favored (80.87%) General / -66.7,-35.7	-	0.16Å	-	-	-
427		ALA	44.2	-	Favored (99.53%) General / -63.1,-42.7	-	0.08Å	-	-	-
428		LEU	129.69	-	Favored (96.87%) General / -61.4,-41.2	Favored (19.7%) <i>tp</i> chi angles: 189.1,69.8	0.07Å	-	-	-
429		LYS	88.02	-	Favored (79.95%) General / -59.8,-37.7	Favored (52.6%) <i>mtmt</i> chi angles: 295.5,179.9,288.2,187.3	0.17Å	-	-	-
430		PHE	153.45	-	Favored (79.05%) General / -66.1,-34.9	Favored (50.3%) <i>m-80</i> chi angles: 283.7,282	0.16Å	-	-	-
431		LEU	84.56	-	Favored (75.04%) General / -69.8,-41.3	Favored (6.7%) <i>mp</i> chi angles: 275.8,68.7	0.11Å	-	-	-
432		ALA	35.71	-	Favored (80.14%) General / -65.4,-46.5	-	0.04Å	-	-	-
433		LYS	62.5	-	Favored (86.07%) General / -61.8,-37.9	Favored (47.3%) <i>mtmt</i> chi angles: 291.1,175.4,292.8,180.8	0.11Å	-	-	-
434		CYS	77.48	0.41Å O with 438 LYS HG2	Favored (52.34%) General / -61.2,-53.8	Favored (58.1%) <i>t</i> chi angles: 182.7	0.10Å	-	-	-
435		ARG	82.41	-	Favored (71.98%) General / -58.9,-34.7	Favored (80.5%) <i>ttt180</i> chi angles: 186.1,182,176.2,180.7	0.13Å	-	-	-

436	LYS	70.5	-	Favored (60.77%) General / -74.5,-14.0	Favored (11.1%) <i>tmm</i> chi angles: 182.7,175.6,284.6,303.1	0.07Å	-	-	-
437	LYS	83.05	-	Favored (15.58%) General / -109.5,-5.9	Favored (72.6%) <i>mmtt</i> chi angles: 298.2,293.4,185.2,178	0.11Å	-	-	-
438	LYS	152.96	0.41Å HG2 with 434 CYS O	Favored (43.43%) General / -79.0,-25.5	OUTLIER (0%) chi angles: 305.8,300.7,256.2,57.5	0.12Å	-	OUTLIER(S) worst is C-N- CA: 4.1 σ	-
439	LYS	205.75	-	Favored (3.66%) General / -122.6,-177.5	Favored (11.3%) <i>tptp</i> chi angles: 181.7,61,194.9,72.1	0.15Å	-	-	-
440	LEU	280.8	0.47Å HD13 with 441 PHE N	Favored (51%) General / -115.3,138.4	Allowed (0.7%) <i>tm</i> chi angles: 193.7,295.1	0.11Å	-	-	-
441	PHE	283.97	0.47Å N with 440 LEU HD13	Allowed (0.07%) General / -177.3,108.3	Favored (31.5%) <i>p90</i> chi angles: 54.6,94.6	0.07Å	-	-	-
442	ALA	288.51	-	Allowed (0.47%) Pre-Pro / 178.0,153.5	-	0.11Å	-	-	-
443	PRO	210.74	-	Favored (2.27%) Trans-Pro / -65.8,112.6	Favored (38.5%) <i>Cg_exo</i> chi angles: 327	0.06Å	-	-	-
444	TRP	268.99	-	Favored (8.91%) General / -148.9,178.2	Allowed (0.5%) <i>m-10</i> chi angles: 258.6,14.2	0.06Å	-	-	-
<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>Cis Peptides</div> </div>									
<div> <div>Avg: 114.88</div> <div>Clashscore: 4.24</div> <div>Outliers: 4 of 194</div> <div>Poor rotamers: 7 of 170</div> <div>Outliers: 5 of 190</div> <div>Outliers: 0 of 196</div> <div>Outliers: 14 of 196</div> <div>Non-Trans: 0 of 195</div> </div>									
445	ARG	279.84	-	Favored (22.66%) General / -109.4,154.4	Favored (39%) <i>mmm160</i> chi angles: 295.1,293,293.7,173.1	0.06Å	-	-	-
446	GLY	94.06	-	Favored (4.78%) Glycine / 152.1,148.2	-	-	-	-	-
447	LEU	142.07	-	Favored (30.55%) General / -75.3,-46.9	Allowed (1.2%) <i>tm</i> chi angles: 187.3,280.7	0.07Å	-	-	-
448	GLN	228.31	-	Favored (28.23%) General /	Favored (17.9%) <i>mm-40</i> chi angles:	0.10Å	-	-	-

				-100.4,145.4	289.7,291.1,22.8				
449	GLU 221.74	-		Favored (20.14%) General / -72.3,121.9	Favored (4%) <i>mt-10</i> chi angles: 275.9,208.1,343.7	0.15Å	-	-	-
450	LEU 192.21	-		Favored (3.75%) General / -77.2,79.9	Allowed (1.1%) <i>mm</i> chi angles: 290.8,309.6	0.11Å	-	-	-
451	THR 115.71	-		Favored (70.23%) General / -61.0,-30.4	Favored (2.2%) <i>t</i> chi angles: 199.1	0.24Å	-	-	-
452	ASP 175.51	-		Favored (28.51%) General / -95.1,116.3	Favored (14.6%) <i>t70</i> chi angles: 184.7,279.9	0.07Å	-	-	-
453	ALA 89.69	0.42Å O with 454 ARG HB2		Favored (34.27%) General / -82.5,-24.0	-	0.10Å	-	OUTLIER(S) worst is C-N- CA: 4.4 σ	-
454	ARG 283.75	0.42Å HB2 with 453 ALA O		OUTLIER (0%) General / 164.8,33.6	Favored (14.3%) <i>tpp-160</i> chi angles: 195.7,58.5,63.3,182	0.14Å	-	-	-
455	ARG 293.3	-		Favored (4.25%) General / -156.9,120.7	Favored (38.2%) <i>mmt180</i> chi angles: 293,301.6,171.7,184.9	0.09Å	-	-	-
456	VAL 256.69	-		Favored (5.21%) lle or Val / -107.4,163.7	Favored (31.1%) <i>t</i> chi angles: 185.6	0.15Å	-	-	-
457	GLU 101.5	-		Favored (4.43%) General / 62.4,48.9	Favored (20.7%) <i>tt0</i> chi angles: 189.6,200.7,356.2	0.08Å	-	-	-
458	LEU 178.76	-		Favored (60.4%) General / -51.2,-41.7	Allowed (1%) <i>mm</i> chi angles: 292.1,302.3	0.16Å	-	-	-
459	LYS 128.35	-		Favored (77.68%) General / -60.2,-49.4	Favored (99%) <i>mttt</i> chi angles: 293.9,180.7,177.6,179.4	0.19Å	-	-	-
460	LYS 116.33	-		Favored (61.14%) General / -72.4,-22.2	Favored (96.1%) <i>mttt</i> chi angles: 295.1,179.2,184.3,172.3	0.11Å	-	-	-
461	ARG 122.43	-		Favored (59.91%) General / -77.6,-11.9	Favored (2.2%) <i>mpt90</i> chi angles: 290.3,77.1,175.3,79.2	0.17Å	-	-	-
462	VAL 41.14	-		Favored (17.57%) lle or Val /	Favored (96.7%) <i>t</i> chi angles: 175.7	0.07Å	-	OUTLIER(S) worst is C-N-	-

-76.8,-52.1

CA: 4.9 σ

463	ASP	38.25	-	Favored (66.89%) General / -52.9,-48.7	OUTLIER (0%) chi angles: 333.3,346.3	0.06Å	-	OUTLIER(S) worst is CA- CB-CG: 6.7 σ	-
464	ASP	38.34	-	Favored (85.75%) General / -64.7,-45.7	Favored (26.5%) <i>t0</i> chi angles: 187.1,43.6	0.08Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195
465	TYR	68.83	-	Favored (75.04%) General / -55.0,-46.6	Favored (52.6%) <i>t80</i> chi angles: 184.5,94.7	0.05Å	-	-	-	
466	VAL	43	-	Favored (90.29%) Ile or Val / -61.5,-48.1	Favored (86.2%) <i>t</i> chi angles: 173.7	0.12Å	-	-	-	
467	ARG	150.35	-	Favored (70.79%) General / -60.4,-31.9	Favored (87%) <i>mtm180</i> chi angles: 293.2,179.3,292.1,171	0.15Å	-	-	-	
468	ARG	39.18	-	Favored (60.04%) General / -74.5,-20.3	Favored (86.6%) <i>mtt-85</i> chi angles: 295.7,170.8,189.8,279.6	0.09Å	-	OUTLIER(S) worst is CD-NE-CZ: 5.6 σ	-	
469	HIS	46.98	-	Favored (32.02%) General / -82.9,-25.8	Favored (47.6%) <i>m90</i> chi angles: 284.3,69.4	0.20Å	-	OUTLIER(S) worst is CA-CB-CG: 4.5 σ	-	
470	LEU	95.99	0.41Å O with 474 MET HB3	Favored (31.4%) General / -78.8,-41.0	Favored (6.6%) <i>mp</i> chi angles: 281.8,66	0.11Å	-	-	-	
471	GLY	42.09	-	Favored (23.83%) Glycine / -73.9,-46.3	-	-	-	-	-	
472	SER	88.56	-	Allowed (0.22%) Pre-Pro / -84.6,-64.8	Favored (72%) <i>m</i> chi angles: 295.9	0.25Å	-	-	-	
473	PRO	214.25	-	Favored (19.9%) Trans-Pro / -55.6,-48.5	OUTLIER (0.1%) chi angles: 320.2	0.07Å	-	-	-	
474	MET	108.5	0.41Å HB3 with 470 LEU O	Favored (6.42%) General / -81.0,-53.5	Favored (26%) <i>ttt</i> chi angles: 192.2,180.5,181.5	0.20Å	-	-	-	

475	SER	59.19	-	Favored (82.61%) General / -68.1,-38.8	Favored (29.5%) <i>m</i> chi angles: 303.1	0.27Å	-	-	-
476	ASP	78.27	-	Favored (52.66%) General / -67.7,-51.2	Favored (22.7%) <i>t70</i> chi angles: 179.4,53.7	0.11Å	-	-	-
477	VAL	44	-	Favored (80.9%) Ile or Val / -67.7,-38.7	Favored (4.4%) <i>t</i> chi angles: 192	0.19Å	-	-	-
478	VAL	50.97	-	Favored (54.07%) Ile or Val / -64.3,-31.6	Favored (90.9%) <i>t</i> chi angles: 174.3	0.22Å	-	-	-
479	SER	30.37	-	Favored (93.21%) General / -59.6,-45.0	Favored (23%) <i>t</i> chi angles: 185.1	0.10Å	-	-	-
480	ARG	131.86	-	Favored (86.82%) General / -66.9,-41.8	Favored (71.3%) <i>mtt90</i> chi angles: 293.2,183,186.5,76.4	0.15Å	-	-	-
481	GLU	61.33	-	Favored (87.38%) General / -64.5,-37.4	Favored (14.1%) <i>mm-30</i> chi angles: 299,291.3,279.6	0.07Å	-	-	-
482	LEU	103.62	-	Favored (58.05%) General / -75.5,-26.4	Favored (29.1%) <i>tp</i> chi angles: 185.2,68.7	0.12Å	-	-	-
483	HIS	52.44	-	Favored (77.35%) General / -69.7,-39.0	Favored (51.9%) <i>t-90</i> chi angles: 183.1,284.5	0.12Å	-	-	-
484	ALA	32.47	-	Favored (96.37%) General / -60.4,-42.6	-	0.08Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88			Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196	Non-Trans: 0 of 195

485	GLN	56.73	0.51Å O with 489 ARG HD3	Favored (95.32%) General / -64.8,-42.0	Favored (23.5%) <i>mt0</i> chi angles: 294.2,178.5,231.3	0.12Å	-	-	-
486	ALA	36.86	-	Favored (82.36%) General / -68.1,-40.6	-	0.13Å	-	-	-
487	GLN	78.43	-	Favored (63.63%)	Favored (61.1%) <i>tt0</i> chi angles:	0.08Å	-	-	-

				General / -73.4,-41.2	187.3,169.9,353.4				
488	GLU	82.55	-	Favored (43.57%) General / -80.5,-20.5	Favored (7.5%) <i>pt0</i> chi angles: 76.4,184.8,36.2	0.21Å	-	-	-
489	ARG	112.05	0.51Å HD3 with 485 GLN O	Favored (28.69%) General / -76.9,-45.2	Favored (11%) <i>mpt180</i> chi angles: 273.2,51.1,174.8,177.8	0.12Å	-	-	-
490	LEU	104.01	-	Favored (14.7%) General / -52.8,-56.6	Favored (4.6%) <i>tt</i> chi angles: 191.5,161.2	0.05Å	-	-	-
491	GLN	105.91	-	Favored (5.1%) General / -76.5,-55.9	Favored (4.8%) <i>pt0</i> chi angles: 72.1,176.1,252.5	0.16Å	-	-	-
492	HIS	98.29	0.52Å HA with 501 GLU HG3	Favored (38.69%) General / -81.6,-21.1	Favored (21.5%) <i>m170</i> chi angles: 302.8,139.8	0.30Å	-	OUTLIER(S) worst is CA- CB-CG: 6.1 σ	-
493	TYR	292.34	0.62Å HA with 498 ALA HB2	OUTLIER (0%) General / 152.9,137.5	Favored (85.6%) <i>t80</i> chi angles: 177.8,73.2	0.10Å	-	-	-
494	PHE	285.55	-	Favored (10.24%) General / -145.4,175.5	Favored (24.9%) <i>t80</i> chi angles: 190.5,58.1	0.04Å	-	-	-
495	MET	240.8	-	Favored (21.68%) General / -50.2,135.2	Favored (12.5%) <i>tpt</i> chi angles: 181.7,56.4,182.4	0.05Å	-	-	-
496	GLY	106.42	-	Favored (15.39%) Glycine / 86.6,-138.0	-	-	-	-	-
497	ARG	301.82	-	Favored (29.79%) General / -91.6,140.4	Favored (30.5%) <i>mmt180</i> chi angles: 291.1,292.1,186.6,162.2	0.08Å	-	-	-
498	ALA	226.96	0.62Å HB2 with 493 TYR HA	Favored (55.07%) General / -62.5,133.5	-	0.12Å	-	-	-
499	LEU	221.38	-	Favored (77.78%) General / -68.4,-35.5	Favored (9.4%) <i>mt</i> chi angles: 309.1,191.9	0.19Å	-	-	-
500	GLU	67.43	-	Allowed (0.52%) General / -101.3,-78.6	Favored (61.7%) <i>mt-10</i> chi angles: 299.7,175.5,26.9	0.07Å	-	-	-
501	GLU	96.84	0.52Å HG3 with	Allowed (0.64%) General /	Favored (6.1%) <i>mm-30</i> chi angles:	0.06Å	-	-	-

492 HIS HA

-66.6,5.1

303.6,261.4,11.6

502	ARG	171.9	-	Favored (2.01%) General / -126.5,-39.5	Favored (73%) <i>ttt180</i> chi angles: 191.4,181.3,177,187.1	0.14Å	-	-	-
503	ALA	56.69	-	Favored (27.73%) General / -76.0,-46.7	-	0.06Å	-	-	-
504	GLN	108.39	-	Favored (39.82%) General / -80.0,-33.1	Favored (5%) <i>tt0</i> chi angles: 200.1,176.5,118.4	0.11Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196
									Non-Trans: 0 of 195
505	GLN	105.31	-	Favored (71.89%) General / -63.7,-30.8	Favored (10.4%) <i>tt0</i> chi angles: 184.3,173.7,115.9	0.19Å	-	-	-
506	HIS	81.03	0.43Å CE1 with 380 GLU HB2	Favored (87.1%) General / -62.5,-37.7	Favored (44.2%) <i>t-90</i> chi angles: 200.8,288.2	0.15Å	-	OUTLIER(S) worst is CA- CB-CG: 5.7 σ	-
507	ARG	107.36	-	Favored (70.77%) General / -62.6,-50.5	Favored (79.5%) <i>ttt180</i> chi angles: 180.4,181.9,178.3,178	0.11Å	-	-	-
508	GLU	87.24	0.40Å HG2 with 515 SER HB2	Favored (4.39%) General / -45.3,-56.9	Favored (4.9%) <i>tt0</i> chi angles: 164.5,197.4,315.2	0.06Å	-	-	-
509	ALA	44.06	-	Allowed (1.36%) General / -38.2,-54.7	-	0.08Å	-	-	-
510	LEU	65.3	-	Favored (61.87%) General / -74.4,-40.6	Favored (38.1%) <i>tp</i> chi angles: 180.1,68.5	0.04Å	-	-	-
511	ILE	103.41	-	Favored (20.96%) Ile or Val / -62.8,126.4	Favored (25.5%) <i>mm</i> chi angles: 291.9,294.2	0.09Å	-	-	-
512	ALA	20.22	-	Favored (51.2%) General / -74.3,-7.0	-	0.07Å	-	-	-
513	GLN	35.27	-	Favored (46.18%) General / -91.7,-8.7	Favored (26.1%) <i>mt0</i> chi angles: 306.3,183.6,253.5	0.07Å	-	-	-

514	ILE	177.65	-	Allowed (0.26%) Ile or Val / -142.5,-15.6	Favored (3%) <i>tt</i> chi angles: 196.8,182.1	0.17Å	-	-	-
515	SER	160.29	0.40Å HB2 with 508 GLU HG2	Allowed (0.12%) General / -138.6,-129.3	Allowed (1.5%) <i>t</i> chi angles: 202.4	0.22Å	-	-	-
516	THR	137.4	0.49Å HA with 519 GLU OE2	Favored (73.26%) General / -60.9,-33.5	Favored (10.1%) <i>t</i> chi angles: 186.2	0.34Å	-	OUTLIER(S) worst is N- CA-CB: 4.2 σ	-
517	ASN	73.81	-	Favored (24.93%) General / -82.3,4.2	Favored (81.3%) <i>m-40</i> chi angles: 291.2,315.5	0.21Å	-	-	-
518	VAL	48.43	-	Favored (18.44%) Ile or Val / -79.7,-50.1	Favored (71.5%) <i>t</i> chi angles: 178.6	0.07Å	-	-	-
519	GLU	35.23	0.49Å OE2 with 516 THR HA	Favored (79.03%) General / -56.0,-45.4	Favored (3.1%) <i>mt-10</i> chi angles: 307.6,152.6,49	0.04Å	-	-	-
520	GLN	53.67	-	Favored (70.6%) General / -70.4,-32.8	Favored (78.8%) <i>mt0</i> chi angles: 297.1,176.3,46	0.14Å	-	-	-
521	LEU	135.09	-	Favored (43.94%) General / -79.2,-31.6	Favored (15.6%) <i>tp</i> chi angles: 190.8,71.2	0.09Å	-	-	-
522	MET	111.58	-	Favored (64.12%) General / -73.9,-33.7	Favored (20.7%) <i>mmt</i> chi angles: 297.1,292.5,191.7	0.14Å	-	-	-
523	LYS	111.22	-	Favored (11.76%) General / -94.8,-36.3	Allowed (0.9%) <i>mtpm</i> chi angles: 293.5,175.7,69.8,279.2	0.11Å	-	-	-
524	ALA	63.43	-	Allowed (1.79%) Pre-Pro / -78.8,-46.8	-	0.28Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196
									Non-Trans: 0 of 195
525	PRO	159.6	-	Favored (27.37%) Trans-Pro / -61.1,-43.9	OUTLIER (0.1%) chi angles: 321.3	0.05Å	-	-	-
				Favored					

526	SER	77.53	-	(61.13%) General / -63.4,-52.5	Favored (36.6%) <i>p</i> chi angles: 55.5	0.09Å	-	-	-
527	LEU	152.18	-	Favored (71.45%) General / -69.4,-32.5	Favored (39.2%) <i>mt</i> chi angles: 306.1,173	0.15Å	-	-	-
528	LYS	135.02	-	Favored (57.57%) General / -75.5,-25.9	Favored (11.6%) <i>tptp</i> chi angles: 186.6,68.2,196,75.9	0.15Å	-	-	-
529	GLU	51.18	-	Favored (63.74%) General / -73.5,-40.7	Favored (13.4%) <i>tm</i> - 30 chi angles: 186.2,282.7,345.5	0.09Å	-	-	-
530	ALA	35.3	-	Favored (87.92%) General / -59.8,-46.9	-	0.03Å	-	-	-
531	GLU	82.75	0.52Å O with 535 PRO HD2	Favored (59.99%) General / -74.7,-20.2	Favored (6.8%) <i>tm</i> - 30 chi angles: 172.4,283.3,328.1	0.19Å	-	-	-
532	GLY	33.86	-	Favored (85.98%) Glycine / -61.6,-33.8	-	-	-	-	-
533	LYS	134.09	-	Favored (7.92%) General / -86.8,-48.8	Favored (14.5%) <i>mtmt</i> chi angles: 296.5,167.5,297,205.4	0.04Å	-	-	-
534	GLU	78.44	-	Favored (49.93%) Pre-Pro / -58.2,-55.0	Favored (34.4%) <i>mt</i> - 10 chi angles: 291.1,168.3,51.5	0.11Å	-	-	-
535	PRO	155.34	0.52Å HD2 with 531 GLU O	Favored (67.2%) Trans-Pro / -51.9,-37.6	OUTLIER (0%) chi angles: 315.6	0.07Å	-	-	-
536	GLU	107.84	-	Favored (74.54%) General / -69.6,-34.7	Favored (48.2%) <i>tp30</i> chi angles: 187.8,57.1,31.9	0.16Å	-	-	-
537	LEU	87.23	-	Favored (76.11%) General / -69.5,-35.9	Allowed (1.2%) <i>mm</i> chi angles: 280.7,306.6	0.14Å	-	-	-
538	PHE	87.83	-	Favored (70.24%) General / -71.8,-36.5	Favored (69.1%) <i>t80</i> chi angles: 185.6,85.7	0.06Å	-	-	-
539	LEU	151.77	-	Favored (72.64%) General / -71.0,-37.8	Favored (27.7%) <i>tp</i> chi angles: 188.6,62.3	0.04Å	-	-	-

540	SER	79.59	-	Favored (57.97%) General / -75.3,-21.9	Favored (80.6%) <i>p</i> chi angles: 61.5	0.13Å	-	-	-
541	ARG	163.35	-	Favored (41.03%) General / -64.4,-53.9	Favored (49.6%) <i>mmt180</i> chi angles: 297,293.4,177.4,178	0.14Å	-	-	-
542	SER	93	-	Favored (55.56%) General / -76.9,-20.9	Favored (13%) <i>p</i> chi angles: 81.3	0.20Å	-	-	-
543	ARG	113.03	-	Allowed (0.56%) Pre-Pro / -81.9,-56.4	Favored (70.6%) <i>mmt-90</i> chi angles: 294,288.8,171.6,279.7	0.24Å	-	-	-
544	PRO	109.78	-	Favored (15.39%) Trans-Pro / -64.3,-43.0	OUTLIER (0%) chi angles: 319.6	0.07Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 114.88				Clashscore: 4.24	Outliers: 4 of 194	Poor rotamers: 7 of 170	Outliers: 5 of 190	Outliers: 0 of 196	Outliers: 14 of 196
545	VAL	87.92	-	Favored (34.14%) Ile or Val / -55.8,-33.4	Allowed (1%) <i>p</i> chi angles: 80.2	0.18Å	-	-	-
546	ALA	54.39	-	Favored (54.64%) General / -81.2,-4.2	-	0.14Å	-	OUTLIER(S) worst is C-N- CA: 4.1 σ	-
547	ALA	56.57	-	OUTLIER (0%) General / 121.7,167.1	-	0.17Å	-	-	-
548	LYS	66.9	-	Favored (55.98%) General / -76.8,-20.8	Favored (99.1%) <i>mttt</i> chi angles: 295.3,178.4,179.2,178.9	0.16Å	-	-	-
549	ALA	38.28	-	Favored (59.76%) General / -77.1,-11.0	-	0.06Å	-	-	-
550	LYS	156.51	-	Favored (60.42%) General / -73.7,-20.9	Favored (10.6%) <i>tptp</i> chi angles: 183.1,178.4,157.1,51.9	0.05Å	-	-	-
551	GLN	70.07	-	Favored (74.65%) General / -55.0,-44.7	Favored (14.8%) <i>tp-100</i> chi angles: 183.6,64,267.2	0.12Å	-	-	-
				Favored					

552	ALA	37.82	-	(73.8%) General / -62.9,-32.5	-	0.09Å	-	-	-
553	HIS	122.07	-	Favored (46.07%) General / -84.8,1.6	Favored (65.6%) <i>m90</i> chi angles: 299.9,78.6	0.06Å	-	-	-
554	LEU	167.58	-	Favored (43.73%) General / -83.8,-16.7	Favored (25.2%) <i>mt</i> chi angles: 300.7,189.4	0.14Å	-	-	-
555	THR	42.49	-	Favored (83.88%) General / -61.9,-37.2	Favored (6%) <i>m</i> chi angles: 313.8	0.08Å	-	-	-
556	THR	111.87	-	Favored (6.48%) General / -79.2,-53.9	Favored (51.8%) <i>p</i> chi angles: 56.5	0.14Å	-	-	-
557	LEU	98.98	-	Favored (85.5%) General / -61.7,-47.4	Favored (5.4%) <i>mt</i> chi angles: 297.3,200.7	0.16Å	-	-	-
558	LYS	256.63	-	Allowed (0.12%) General / 79.0,151.7	Favored (21.6%) <i>mtmm</i> chi angles: 293.2,169.5,292.1,300.3	0.12Å	-	-	-
559	HIS	88.64	-	Favored (7.25%) General / -82.0,-52.2	Favored (5.2%) <i>t-90</i> chi angles: 178.3,297.4	0.13Å	-	-	-
560	ILE	122.97	-	-	OUTLIER (0.1%) chi angles: 73.2,284.6	0.17Å	-	-	-

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