



# Viewing cngb3\_mb\_465-636H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	104.5	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	3.33%	Goal: <1%
	Ramachandran outliers	3	1.76%	Goal: <0.05%
	Ramachandran favored	157	92.35%	Goal: >98%
	MolProbity score^	3.35		12 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 1382	0.00%	Goal: 0%
	Bad backbone angles:	24 / 1868	1.28%	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: 100.32	Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
465	TYR	76.46	-	-	92.6% ( <i>m-85</i> ) chi angles: 291.6,276.9	0.042Å	-	OUTLIER(S) worst is CA-CB-CG: 4.186 σ
466	MET	32.81	0.65Å SD with 479 VAL HG11	Favored (95.09%) General / -63.6,-39.7	77.4% ( <i>mtm</i> ) chi angles: 292.8,179.8,286	0.099Å	-	-
467	ASN	93.52	-	Favored (63.64%) General / -63.3,-52.0	2.5% ( <i>p30</i> ) chi angles: 60.8,105.9	0.069Å	-	-
468	ASN	80.76	-	Favored (72.25%) General /	17.2% ( <i>p-10</i> ) chi angles: 64.1,303.6	0.102Å	-	-

469	TYR	97.41	-	-67.9,-46.2 Favored (11.88%) General / -67.1,-56.0	65.1% ( <i>m-85</i> ) chi angles: 285.3,277.5	0.091Å	-	OUTLIER(S) worst is C-N- CA: 5.036 $\sigma$
470	SER	240.49	0.411Å C with 472 PRO HD2	Favored (2.49%) General / -165.0,129.4	46.6% ( <i>t</i> ) chi angles: 180.5	0.093Å	-	-
471	ILE	220.1	-	Favored (6.64%) Pre-proline / -71.3,-38.3	48.7% ( <i>mm</i> ) chi angles: 300.2,300.5	0.069Å	-	OUTLIER(S) worst is CA-C- N: 4.131 $\sigma$
472	PRO	191.85	0.578Å HG2 with 475 VAL CG2	Allowed (0.18%) Trans-proline / -36.6,117.9	56.4% ( <i>Cg_endo</i> ) chi angles: 25.9	0.195Å	-	-
473	LYS	117.13	-	Favored (77.53%) General / -62.8,-34.5	32.1% ( <i>mmmt</i> ) chi angles: 300.2,299.6,288.6,179.7	0.123Å	-	-
474	LEU	133.42	0.507Å N with 474 LEU HD22	Favored (92.68%) General / -59.9,-42.0	2.1% ( <i>mm?</i> ) chi angles: 292.1,293.5	0.113Å	-	-
475	VAL	55.27	0.578Å CG2 with 472 PRO HG2	Favored (79.07%) Isoleucine or valine / -69.8,-44.3	94.4% ( <i>t</i> ) chi angles: 175.8	0.067Å	-	-
476	GLN	91.11	0.737Å O with 479 VAL HG12	Favored (99.23%) General / -61.8,-42.6	40.7% ( <i>tt0</i> ) chi angles: 179.9,180.1,298.7	0.085Å	-	-
477	LYS	60.2	0.662Å O with 480 ARG HG2	Favored (88.62%) General / -65.5,-44.0	59.8% ( <i>tttm</i> ) chi angles: 180.4,166.2,179.9,297.3	0.089Å	-	-
478	ARG	121.87	-	Favored (95.29%) General / -62.6,-39.9	51.7% ( <i>mtm180</i> ) chi angles: 284.6,180,285.5,203.8	0.057Å	-	-
479	VAL	94.56	0.737Å HG12 with 476 GLN O	Favored (95.17%) Isoleucine or valine / -64.4,-42.4	7.1% ( <i>p</i> ) chi angles: 69.5	0.077Å	-	-
480	ARG	159.42	0.662Å HG2 with 477 LYS O	Favored (91.4%) General /	10.8% ( <i>ptm180</i> ) chi angles: 61.9,194.3,308.9,124.5	0.096Å	-	-

481	THR	98.79	0.587Å HG23 with 477 LYS O	Favored (93.53%) General / -66.0,-40.7 -63.6,-39.1	62.7% ( <i>p</i> ) chi angles: 62.8	0.084Å	-	-
482	TRP	94.31	0.72Å HE1 with 544 LEU HB2	Favored (93.36%) General / -62.3,-39.6	25.8% ( <i>t90</i> ) chi angles: 180.1,44.6	0.08Å	-	-
483	TYR	46.03	0.579Å O with 487 TRP HE3	Favored (98.74%) General / -60.9,-42.7	54.8% ( <i>t80</i> ) chi angles: 181.2,273.3	0.07Å	-	-
484	GLU	41.96	-	Favored (90.76%) General / -63.7,-45.3	99.2% ( <i>mt-10</i> ) chi angles: 292.3,173.5,356.8	0.089Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
Avg: 100.32			Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
485	TYR	59.78	0.539Å CE2 with 613 PHE CE2	Favored (87.19%) General / -66.8,-38.8	83.6% ( <i>m-85</i> ) chi angles: 290.5,280.3	0.08Å	-	OUTLIER(S) worst is CA- CB-CG: 4.11 $\sigma$
486	THR	53.46	0.893Å HA with 544 LEU HD12	Favored (4.87%) General / -68.2,-58.2	87.8% ( <i>m</i> ) chi angles: 301.1	0.067Å	-	-
487	TRP	110.19	0.897Å HE1 with 492 MET HA	Favored (65.21%) General / -73.5,-38.7	19.1% ( <i>m-90</i> ) chi angles: 286.7,259.1	0.075Å	-	-
488	ASP	55.74	0.401Å O with 489 SER HB3	Favored (12.29%) General / 58.1,48.9	89.3% ( <i>m-20</i> ) chi angles: 287.1,353.2	0.085Å	-	OUTLIER(S) worst is CA- CB-CG: 4.554 $\sigma$
489	SER	109.81	0.401Å HB3 with 488 ASP O	Favored (7.26%) General / 67.7,9.7	47.4% ( <i>t</i> ) chi angles: 180.1	0.073Å	-	-
490	GLN	220.23	0.552Å O with 487 TRP HB3	Favored (34.63%) General / -77.7,150.1	54.9% ( <i>tt0</i> ) chi angles: 180.3,180,57.2	0.131Å	-	-
491	ARG	188.01	0.581Å HG2 with 492	Favored (36.32%) General /	39.8% ( <i>ttm180</i> ) chi angles:	0.118Å	-	-

			MET N	-69.2,157.7	175.1,190,292.3,121.7			
492	MET	50.74	0.897Å HA with 487 TRP HE1	Favored (57.27%) General / -67.3,140.8	98.2% ( <i>mtp</i> ) chi angles: 294.2,179.9,68.3	0.089Å	-	-
493	LEU	54.95	-	Favored (35.8%) General / -117.7,152.1	89% ( <i>mt</i> ) chi angles: 298.5,180	0.142Å	-	-
494	ASP	86.32	-	Allowed (1.26%) General / -107.8,79.2	39.8% ( <i>m-20</i> ) chi angles: 287.4,8.6	0.154Å	-	-
495	GLU	104.66	0.688Å O with 499 LEU HD23	Favored (88.5%) General / -64.2,-37.7	57% ( <i>mm-40</i> ) chi angles: 293.7,289.7,298.4	0.098Å	-	-
496	SER	75.85	0.555Å O with 500 LYS HB2	Favored (66.95%) General / -58.2,-52.1	70.8% ( <i>m</i> ) chi angles: 295.8	0.08Å	-	-
497	ASP	46.22	-	Favored (58.89%) General / -68.0,-49.9	10.6% ( <i>t0</i> ) chi angles: 192.8,304.6	0.071Å	-	-
498	LEU	50.73	0.828Å O with 501 THR HG22	Favored (70.48%) General / -65.8,-48.8	83.6% ( <i>mt</i> ) chi angles: 294.7,180	0.056Å	-	-
499	LEU	101.96	0.809Å HD12 with 511 ALA HB1	Favored (83.77%) General / -65.8,-36.5	1.9% ( <i>mm?</i> ) chi angles: 290,289	0.05Å	-	-
500	LYS	118.13	0.555Å HB2 with 496 SER O	Favored (76.98%) General / -62.9,-34.2	22.6% ( <i>tpp</i> ) chi angles: 188.5,162.9,72.7,85.6	0.079Å	-	-
501	THR	106.65	0.881Å CG2 with 502 LEU HD12	Favored (81.18%) General / -66.9,-36.0	6.2% ( <i>t</i> ) chi angles: 195.4	0.075Å	-	-
502	LEU	112.83	0.914Å HB3 with 506 VAL CG1	Favored (59.97%) Pre-proline / -73.2,164.6	7.9% ( <i>mp</i> ) chi angles: 287,66.2	0.104Å	-	-
503	PRO	148.8	0.537Å O with 506	Favored (37.41%)	73.6% ( <i>Cg_exo</i> )	0.088Å	-	-

			VAL HG12	Trans-proline / -73.7,163.4	chi angles: 333.7			
504	THR	32.08	0.725Å HG22 with 508 LEU HD13	Favored (93.64%) General / -63.3,-44.9	85.2% ( <i>m</i> ) chi angles: 301.6	0.074Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.32	Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
505	THR	89.44	0.547Å HG23 with 506 VAL N	Favored (93.23%) General / -60.2,-45.4	11.6% ( <i>t</i> ) chi angles: 185	0.043Å	-	-
506	VAL	92.54	0.914Å CG1 with 502 LEU HB3	Favored (77.04%) Isoleucine or valine / -65.0,-36.1	9.4% ( <i>p</i> ) chi angles: 60.5	0.053Å	-	-
507	GLN	83.39	0.807Å HE21 with 511 ALA HB2	Favored (82.93%) General / -62.0,-47.9	0.5% chi angles: 291.7,259.1,228.2	0.142Å	-	-
508	LEU	104.53	0.725Å HD13 with 504 THR HG22	Favored (26.88%) General / -63.5,-55.1	9.1% ( <i>mp</i> ) chi angles: 282.5,57.7	0.079Å	-	OUTLIER(S) worst is C-N- CA: 4.084 σ
509	ALA	56.74	0.736Å HA with 515 ASN HD22	Favored (16.6%) General / -68.7,-54.4	-	0.09Å	-	-
510	LEU	190.57	0.555Å HB3 with 506 VAL O	Favored (3.57%) General / -76.6,-57.9	4.6% ( <i>tt</i> ) chi angles: 192.4,175.5	0.078Å	-	-
511	ALA	221.96	0.993Å HB3 with 514 VAL HG23	OUTLIER (0.02%) General / -28.6,103.5	-	0.106Å	-	-
512	ILE	201.22	0.556Å O with 512 ILE HG23	OUTLIER (0%) Isoleucine or valine / 17.1,85.3	17.9% ( <i>tt</i> ) chi angles: 181.6,166.8	0.074Å	-	-
513	ASP	201.63	0.812Å HB3 with 516 PHE O	Allowed (1.55%) General / 39.8,60.9	88.8% ( <i>m-20</i> ) chi angles: 284.7,340.1	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 5.047 σ
514	VAL	121.88	0.993Å HG23 with 511 ALA HB3	Allowed (0.4%) Isoleucine or valine / -60.4,-66.3	12.1% ( <i>t</i> ) chi angles: 160.8	0.175Å	-	-

515	ASN	77.09	0.736Å HD22 with 509 ALA HA	Favored (87.26%) General / -66.0,-38.0	50.9% ( <i>m-20</i> ) chi angles: 280.4,303.7	0.071Å	-	OUTLIER(S) worst is CA- CB-CG: 6.495 σ
516	PHE	195.07	0.812Å O with 513 ASP HB3	Favored (3.54%) General / -72.6,103.3	60.6% ( <i>t80</i> ) chi angles: 188.2,83.2	0.084Å	-	OUTLIER(S) worst is CA- CB-CG: 6.559 σ
517	SER	268.21	-	Allowed (0.74%) General / -163.4,-162.5	22.7% ( <i>t</i> ) chi angles: 186.6	0.069Å	-	-
518	ILE	233.12	1.082Å HD13 with 565 LYS HA	Allowed (0.1%) Isoleucine or valine / -86.4,52.8	39.3% ( <i>pt</i> ) chi angles: 61.4,166.1	0.058Å	-	-
519	ILE	122.5	0.742Å HD12 with 533 ILE HD13	Favored (67.25%) Isoleucine or valine / -72.1,-42.8	15.7% ( <i>tt</i> ) chi angles: 182.3,174.6	0.075Å	-	-
520	SER	74.62	0.598Å N with 519 ILE HG23	Favored (73.64%) General / -64.5,-32.1	47.3% ( <i>t</i> ) chi angles: 180.1	0.078Å	-	-
521	LYS	123.2	-	Favored (81.15%) General / -64.9,-35.4	35.4% ( <i>mtp</i> ) chi angles: 296.4,297.6,180.3,65.1	0.111Å	-	-
522	VAL	105.96	0.955Å HG11 with 525 PHE HD2	Favored (50.48%) Isoleucine or valine / -99.6,129.2	8.7% ( <i>p</i> ) chi angles: 60.1	0.064Å	-	-
523	ASP	40.14	0.618Å HA with 526 LYS HG2	Favored (73.73%) General / -65.8,-32.3	3.4% ( <i>m-20</i> ) chi angles: 288.6,33.2	0.098Å	-	OUTLIER(S) worst is CA- CB-CG: 4.187 σ
524	LEU	114.03	0.775Å HD13 with 522 VAL CG2	Favored (86.38%) General / -58.8,-47.0	5.2% ( <i>mp</i> ) chi angles: 294.4,64.2	0.138Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg:	Clashscore:	Outliers: 3 of	Poor rotamers: 5 of	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
100.32	104.5	170	150			

525	PHE	86.76	1.068Å HB3 with 533 ILE HD12	Favored (47.48%) General /	53.5% ( <i>m-85</i> ) chi angles: 290.6,297.5	0.11Å	-	OUTLIER(S) worst is CA- CB-CG: 7.922
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				-75.7,-43.4				$\sigma$
526	LYS	143.12	0.618Å HG2 with 523 ASP HA	Favored (70.97%) General / -54.4,-42.8	0% chi angles: 60.6,171.4,297.1,77.4	0.062Å	-	-
527	GLY	39.91	0.505Å N with 526 LYS HG3	Favored (63.19%) Glycine / -71.4,-36.3	-	-	-	-
528	CYS	101.26	0.429Å SG with 525 PHE HA	Favored (23.27%) General / -72.9,166.3	24% ( <i>p</i> ) chi angles: 67.8	0.111Å	-	-
529	ASP	97.16	-	Favored (51.16%) General / -67.5,148.7	57.2% ( <i>p30</i> ) chi angles: 64.6,5.6	0.138Å	-	-
530	THR	110.26	0.68Å O with 533 ILE HG22	Favored (72.53%) General / -63.6,-31.4	13.6% ( <i>t</i> ) chi angles: 186.5	0.067Å	-	-
531	GLN	77.03	0.978Å HA with 534 TYR CE2	Favored (96.34%) General / -63.8,-43.4	58.4% ( <i>tt0</i> ) chi angles: 191,180,350.1	0.063Å	-	-
532	MET	77.62	0.5Å HA with 631 TYR CE2	Favored (86.8%) General / -62.5,-46.8	11.7% ( <i>ttt</i> ) chi angles: 173.3,196.9,180.2	0.159Å	-	-
533	ILE	102.85	1.068Å HD12 with 525 PHE HB3	Favored (98.55%) Isoleucine or valine / -63.0,-45.5	18.4% ( <i>tt</i> ) chi angles: 194.3,168.8	0.1Å	-	-
534	TYR	182.02	0.978Å CE2 with 531 GLN HA	Favored (77.94%) General / -64.2,-34.4	12.6% ( <i>p90</i> ) chi angles: 65.3,73.4	0.234Å	-	OUTLIER(S) worst is N-CA- CB: 4.063 $\sigma$
535	ASP	51.36	0.471Å O with 539 ARG HG2	Favored (88.25%) General / -61.2,-38.9	50.8% ( <i>t0</i> ) chi angles: 192,0.3	0.078Å	-	-
536	MET	172.35	0.613Å CE with 627 ILE HD13	Favored (70.39%) General / -70.9,-42.1	40.3% ( <i>tpp</i> ) chi angles: 194.3,77.1,79	0.082Å	-	-
537	LEU	114.98	0.718Å HD13 with	Favored (84.36%)	8.8% ( <i>mp</i> )	0.08Å	-	-

			533 ILE O	General / -62.9,-36.8 Favored (88.2%) General / -61.8,-38.5 Favored (63.96%) General / -70.6,-27.3 Favored (38.27%) General / -71.1,157.4 Favored (50.66%) General / -127.2,131.6 Favored (39.8%) General / -76.5,137.8 Favored (23.16%) Isoleucine or valine / -144.9,141.6 Favored (42.12%) General / -114.4,145.2	chi angles: 278.9,53.7  60.5% ( <i>tp</i> ) chi angles: 179.7,64.5  22.1% ( <i>mmm-85</i> ) chi angles: 306.5,309.5,285.8,257.5  88.8% ( <i>mt</i> ) chi angles: 298.5,180.1  27.3% ( <i>mtmm</i> ) chi angles: 293.8,166.9,283.2,284  73.4% ( <i>m</i> ) chi angles: 295.3  93.6% ( <i>t</i> ) chi angles: 176.9  46.3% ( <i>mt</i> ) chi angles: 292.3,185.7	0.094Å	-	-	
538	LEU	143.31	-						
539	ARG	153.25	0.945Å HB3 with 623 THR HG21						
540	LEU	63.35	0.531Å HB3 with 617 LEU HB3						
541	LYS	89.03	-						
542	SER	84.28	-						
543	VAL	40.74	0.424Å CG1 with 545 TYR CE1						
544	LEU	156.28	0.893Å HD12 with 486 THR HA						
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.32		Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
545	TYR	113.97	0.576Å HB3 with 549 ASP OD2						
546	LEU	95.02	0.603Å N with 546 LEU HD22						
547	PRO	144.95	-						



548	GLY	31.08	-	Favored (49.63%) Glycine / 94.4,-20.2	-	-	-	-
549	ASP	106.62	0.605Å O with 609 VAL HG23	Favored (45.45%) General / -71.0,150.7	56.3% ( <i>p30</i> ) chi angles: 60.7,6.5	0.115Å	-	-
550	PHE	63.85	-	Favored (25.06%) General / -98.0,113.2	38.3% ( <i>m-85</i> ) chi angles: 279.1,276.1	0.114Å	-	OUTLIER(S) worst is CA- CB-CG: 4.455 σ
551	VAL	100.78	0.808Å CG2 with 608 VAL HB	Favored (79.34%) Isoleucine or valine / -70.0,-43.3	27.4% ( <i>m</i> ) chi angles: 295.9	0.051Å	-	-
552	CYS	51.07	0.562Å N with 551 VAL HG23	Favored (47.4%) General / -138.7,151.8	85.1% ( <i>m</i> ) chi angles: 295.6	0.1Å	-	-
553	LYS	145.27	0.413Å HB3 with 556 GLU HG2	Favored (45.1%) General / -121.5,147.9	17% ( <i>ttmm</i> ) chi angles: 200.8,162.8,291.5,296.2	0.063Å	-	-
554	LYS	216.98	0.732Å HE2 with 605 THR O	Favored (16.01%) General / -61.6,-56.8	57.7% ( <i>tttm</i> ) chi angles: 193.1,165.7,180.6,295.5	0.065Å	-	-
555	GLY	131.1	-	Favored (69.98%) Glycine / -64.6,-25.1	-	-	-	-
556	GLU	109.62	0.773Å O with 603 ARG HB3	Favored (12.75%) General / -58.9,155.6	16.4% ( <i>mm-40</i> ) chi angles: 296,291.3,21.4	0.082Å	-	-
557	ILE	123.96	0.828Å HD12 with 599 GLY O	Favored (20.41%) Isoleucine or valine / -102.2,106.8	28.5% ( <i>mm</i> ) chi angles: 305.2,310	0.086Å	-	-
558	GLY	61.45	0.6Å H with 603 ARG HG2	Favored (20.55%) Glycine / -73.4,135.2	-	-	-	OUTLIER(S) worst is C-N- CA: 4.697 σ
559	LYS	164.69	0.813Å O with 621 LYS HG3	Favored (20.71%) General /	0% chi angles: 301.9,68.6,178,287.4	0.084Å	-	-

560	GLU	108.99	0.652Å HB2 with 619 LEU O	Favored (16.55%) General / -154.8,173.4	25% ( <i>pt-20</i> ) chi angles: 61.3,182.1,24	0.063Å	-	-
561	MET	100.93	-	Favored (11.55%) General / -123.0,169.0	25.3% ( <i>ptm</i> ) chi angles: 58.9,180,279.7	0.073Å	-	-
562	TYR	71.19	0.789Å CE2 with 618 THR HG22	Favored (51.55%) General / -130.7,151.1	35.4% ( <i>m-85</i> ) chi angles: 299.8,74.4	0.13Å	-	-
563	ILE	89.67	0.852Å HA with 589 VAL HG12	Favored (59.26%) Isoleucine or valine / -120.3,135.8	2% ( <i>mp</i> ) chi angles: 296.8,66.7	0.103Å	-	-
564	ILE	122.09	0.905Å HD13 with 616 LEU HD22	Favored (21.17%) Isoleucine or valine / -93.2,109.0	36.1% ( <i>mm</i> ) chi angles: 302.5,293.5	0.138Å	-	-
<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: 100.32</div> <div>Clashscore: 104.5</div> <div>Outliers: 3 of 170</div> <div>Poor rotamers: 5 of 150</div> <div>Outliers: 0 of 158</div> <div>Outliers: 0 of 172</div> <div>Outliers: 22 of 172</div> </div>								
565	LYS	87.15	1.082Å HA with 518 ILE HD13	Favored (28.67%) General / -72.4,-50.2	56.5% ( <i>tttm</i> ) chi angles: 194.5,166,187.4,298.5	0.064Å	-	-
566	HIS	57.87	0.614Å HB3 with 615 ASN OD1	Favored (12.14%) General / -158.8,138.8	77.7% ( <i>t60</i> ) chi angles: 184.9,77.6	0.088Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.569 σ
567	GLY	29.33	-	Favored (12.64%) Glycine / 130.9,170.2	-	-	-	-
568	GLU	63.51	-	Favored (52.78%) General / -124.2,140.6	56% ( <i>mt-10</i> ) chi angles: 292.8,177.3,300.7	0.122Å	-	-
569	VAL	52.11	0.466Å HG22 with 584 LEU O	Favored (29.54%) Isoleucine or valine / -136.6,145.9	15.5% ( <i>m</i> ) chi angles: 289.7	0.073Å	-	-

570	GLN 100.11	0.684Å HG2 with 609 VAL HG12	Favored (47.31%) General / -111.0,138.5	2.3% ( <i>pt20</i> ) chi angles: 64.7,181,167.1	0.09Å	-	-
571	VAL 110.02	1.027Å HB with 583 THR HG22	Favored (55.7%) Isoleucine or valine / -101.7,126.2	7.6% ( <i>p</i> ) chi angles: 59.1	0.052Å	-	-
572	LEU 57.36	0.527Å O with 606 ALA HB1	Favored (36.19%) General / -110.5,146.3	87.6% ( <i>mt</i> ) chi angles: 296.3,180	0.085Å	-	-
573	GLY 65.73	-	Favored (40.22%) Glycine / -175.8,-172.1	-	-	-	-
574	GLY 60.33	0.458Å N with 575 PRO HD2	Favored (99.79%) Glycine / -62.5,-41.5	-	-	-	-
575	PRO 82.65	0.458Å HD2 with 574 GLY N	Favored (22.08%) Trans-proline / -75.1,169.7	8.4% ( <i>Cg_endo</i> ) chi angles: 10.4	0.099Å	-	-
576	ASP 129.42	-	Favored (9.1%) General / -54.9,121.6	16.6% ( <i>p-10</i> ) chi angles: 61.7,309.1	0.072Å	-	-
577	GLY 40.63	-	Favored (20.41%) Glycine / -79.5,138.5	-	-	-	-
578	THR 136.38	0.57Å O with 571 VAL HG12	Favored (15%) General / -154.6,174.4	82.6% ( <i>p</i> ) chi angles: 60.6	0.085Å	-	-
579	LYS 149.2	0.783Å O with 584 LEU HA	Favored (69.39%) General / -68.9,-30.8	0.5% chi angles: 290.2,67,180.1,298.9	0.085Å	-	-
580	VAL 127.33	0.568Å O with 580 VAL HG13	Favored (20.43%) Isoleucine or valine / -90.6,109.1	7.2% ( <i>p</i> ) chi angles: 58.1	0.054Å	-	-
581	LEU 289.52	0.977Å HB3 with 571 VAL HG11	OUTLIER (0.03%) General / -176.0,-149.1	26.7% ( <i>tp</i> ) chi angles: 191,61	0.08Å	-	-

582	VAL	184.77	0.845Å H with 581 LEU HG	Favored (82.01%) Isoleucine or valine / -61.0,-39.4	13.6% ( <i>p</i> ) chi angles: 62.9	0.051Å	-	-	
583	THR	251.32	1.027Å HG22 with 571 VAL HB	Favored (28.21%) General / -102.6,146.4	5.2% ( <i>t</i> ) chi angles: 197.4	0.071Å	-	-	
584	LEU	179.05	0.783Å HA with 579 LYS O	Allowed (0.05%) General / -150.3,-131.4	2.8% ( <i>mp</i> ) chi angles: 303.7,70.9	0.165Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 100.32	Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172	Outliers: 22 of 172
585	LYS	120.81	0.837Å HG2 with 586 ALA H	Allowed (1.59%) General / -111.7,-170.1	35.6% ( <i>ttmt</i> ) chi angles: 193.9,173.6,302.6,176.7	0.11Å	-	-	
586	ALA	42.77	0.837Å H with 585 LYS HG2	Favored (48.16%) General / -56.9,140.6	-	0.081Å	-	-	
587	GLY	26.55	-	Favored (65.24%) Glycine / 95.3,-14.4	-	-	-	-	
588	SER	83.88	0.546Å HB2 with 584 LEU HD13	Favored (11.56%) General / -91.4,168.4	82.6% ( <i>p</i> ) chi angles: 69.4	0.118Å	-	-	
589	VAL	43.83	0.852Å HG12 with 563 ILE HA	Favored (22.77%) Isoleucine or valine / -141.1,157.9	29.4% ( <i>m</i> ) chi angles: 296.8	0.1Å	-	-	
590	PHE	70.55	0.874Å HE2 with 564 ILE HD11	Favored (38.74%) General / -155.8,164.3	38.7% ( <i>p90</i> ) chi angles: 54.9,84.3	0.063Å	-	OUTLIER(S) worst is CA- CB-CG: 5.693 σ	
591	GLY	40.75	-	Favored (56.64%) Glycine / 97.6,7.7	-	-	-	-	
592	GLU	156.88	0.817Å HA with 595	Favored (69.08%)	1.8% ( <i>mp0</i> ) chi angles:	0.205Å	-	OUTLIER(S) worst is CB-	

			LEU HD23	General / -71.3,-32.9	301.3,86.9,270.7				CG-CD: 4.322 $\sigma$
593	ILE	55.51	0.444Å HG22 with 603 ARG NH2	Favored (80.47%) Isoleucine or valine / -56.1,-44.9	79.7% ( <i>mt</i> ) chi angles: 300.2,167.1	0.071Å	-	-	
594	SER	93.85	0.621Å HB2 with 603 ARG HD3	Favored (70.47%) General / -63.9,-29.3	90.6% ( <i>p</i> ) chi angles: 62.6	0.108Å	-	-	
595	LEU	112	0.876Å HG with 624 LEU HD22	Favored (93%) General / -64.0,-44.3	3.6% ( <i>mm?</i> ) chi angles: 288.2,303.9	0.149Å	-	-	
596	LEU	57.19	-	Favored (15.52%) General / -72.5,-52.5	89.1% ( <i>mt</i> ) chi angles: 298.2,180.1	0.056Å	-	-	
597	ALA	37.72	-	Favored (93.73%) General / -65.4,-41.3	-	0.089Å	-	-	
598	ALA	45.17	-	Favored (18.81%) General / 61.6,31.7	-	0.075Å	-	-	
599	GLY	61.1	0.971Å HA3 with 603 ARG HH11	Allowed (0.46%) Glycine / -59.0,104.0	-	-	-	-	
600	GLY	102.85	0.457Å O with 557 ILE HG13	Favored (61.74%) Glycine / -71.9,-35.0	-	-	-	-	
601	GLY	144.49	0.584Å O with 557 ILE HD11	Favored (2.23%) Glycine / -95.7,-107.3	-	-	-	-	
602	ASN	182.57	0.585Å O with 599 GLY HA3	Favored (54.44%) General / -62.6,133.1	4.3% ( <i>m120</i> ) chi angles: 289.6,54.6	0.078Å	-		OUTLIER(S) worst is CA- CB-CG: 5.174 $\sigma$
603	ARG	267.67	0.971Å HH11 with 599 GLY HA3	Allowed (0.17%) General / -137.8,-112.2	0.2% chi angles: 190.5,47.9,275.5,119.3	0.094Å	-	-	
604	ARG	116.08	0.546Å HB2 with 554	Favored (3.47%)	38.5% ( <i>mmt180</i> ) chi angles:	0.1Å	-	-	

				LYS O	General / -48.0,120.4	296,291.4,187.3,199.7			
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
				Avg: 100.32	Clashscore: 104.5	Outliers: 3 of 170	Poor rotamers: 5 of 150	Outliers: 0 of 158	Outliers: 0 of 172
605	THR	49.55		0.732Å O with 554 LYS HE2	Favored (75.33%) General / -69.9,-41.0	66.7% ( <i>p</i> ) chi angles: 63.1	0.072Å	-	-
606	ALA	53		0.527Å HB1 with 572 LEU O	Favored (4.27%) General / -136.3,-176.2	-	0.1Å	-	-
607	ASN	51.03		-	Favored (31.86%) General / -111.3,148.9	70.1% ( <i>m-80</i> ) chi angles: 295.7,286.7	0.16Å	-	-
608	VAL	56.3		0.808Å HB with 551 VAL CG2	Favored (61.14%) Isoleucine or valine / -130.4,126.4	66.9% ( <i>t</i> ) chi angles: 179.6	0.065Å	-	-
609	VAL	96.47		0.684Å HG12 with 570 GLN HG2	Favored (43.81%) Isoleucine or valine / -125.6,142.0	11.4% ( <i>p</i> ) chi angles: 66.6	0.072Å	-	-
610	ALA	46.76		-	Favored (22.05%) General / -75.6,121.2	-	0.082Å	-	-
611	HIS	111.19		-	Favored (63.28%) General / -74.4,-34.1	13.3% ( <i>t60</i> ) chi angles: 197,94.9	0.09Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.457 σ
612	GLY	24.29		-	Favored (13.95%) Glycine / -143.2,-172.1	-	-	-	-
613	PHE	54.53		0.539Å CE2 with 485 TYR CE2	Favored (49.54%) General / -63.5,131.9	83.8% ( <i>m-85</i> ) chi angles: 293.5,82	0.113Å	-	OUTLIER(S) worst is CA- CB-CG: 5.738 σ
614	ALA	44.01		-	Favored (50.75%) General / -126.1,144.4	-	0.112Å	-	-

615	ASN	101.06	0.628Å HA with 544 LEU HD23	Favored (48.6%) General / -114.8,123.2	16.8% ( <i>p-10</i> ) chi angles: 55.7,324.8	0.114Å	-	-
616	LEU	70.34	0.905Å HD22 with 564 ILE HD13	Favored (28.07%) General / -129.7,162.6	68.1% ( <i>mt</i> ) chi angles: 304.2,182.5	0.14Å	-	-
617	LEU	93.1	0.531Å HB3 with 540 LEU HB3	Favored (40.12%) General / -124.2,123.4	5.3% ( <i>mp</i> ) chi angles: 294.1,63.9	0.109Å	-	-
618	THR	111.56	0.789Å HG22 with 562 TYR CE2	Favored (15.7%) General / -95.8,157.9	43.4% ( <i>p</i> ) chi angles: 67.3	0.111Å	-	-
619	LEU	59.31	0.784Å HD11 with 623 THR CG2	Favored (23.1%) General / -137.3,125.5	59.5% ( <i>tp</i> ) chi angles: 180.1,64.5	0.097Å	-	-
620	ASP	41.12	0.496Å HA with 560 GLU HB3	Favored (23.39%) General / -80.2,164.3	52.9% ( <i>p-10</i> ) chi angles: 61.9,352.9	0.098Å	-	-
621	LYS	63.02	0.813Å HG3 with 559 LYS O	Favored (95.44%) General / -61.9,-40.4	59.7% ( <i>mtpt</i> ) chi angles: 292.8,166.6,68,180.8	0.122Å	-	-
622	LYS	89.66	0.445Å HD2 with 622 LYS N	Favored (87.22%) General / -61.7,-47.0	3% ( <i>mptp?</i> ) chi angles: 287.4,66.7,184.4,73.7	0.059Å	-	-
623	THR	47.38	0.945Å HG21 with 539 ARG HB3	Favored (87.59%) General / -65.6,-37.8	55% ( <i>m</i> ) chi angles: 294.6	0.132Å	-	-
624	LEU	46.92	0.876Å HD22 with 595 LEU HG	Favored (89.73%) General / -59.5,-46.1	61% ( <i>tp</i> ) chi angles: 177.9,65.5	0.117Å	-	-
<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:</div> <div>Clashscore:</div> <div>Outliers: 3 of</div> <div>Poor rotamers: 5 of</div> <div>Outliers: 0 of 158</div> <div>Outliers: 0 of 172</div> <div>Outliers: 22 of 172</div> </div>								
<div> <div>100.32</div> <div>104.5</div> <div>170</div> <div>150</div> <div></div> <div></div> <div></div> </div>								
625	GLN	111.94	0.837Å O with 629	Favored (85.31%) General /	62% ( <i>tp60</i> ) chi angles: 184.3,74,61	0.089Å	-	-

			VAL HG23	-65.3,-36.8					
626	GLU	70.8	0.684Å HG2 with 539 ARG HH12	Favored (92.81%) General / -62.5,-45.5	30.8% ( <i>tp10</i> ) chi angles: 172.4,79.8,8.3	0.1Å	-	-	
627	ILE	88.89	0.635Å HG22 with 624 LEU O	Favored (90.84%) Isoleucine or valine / -66.4,-44.1	21% ( <i>tt</i> ) chi angles: 189.9,167.2	0.051Å	-	-	
628	LEU	47.32	0.547Å N with 627 ILE HG23	Favored (78.96%) General / -63.1,-35.0	83.2% ( <i>mt</i> ) chi angles: 295.9,180.9	0.072Å	-	-	
629	VAL	23.88	0.837Å HG23 with 625 GLN O	Favored (93.3%) Isoleucine or valine / -59.3,-44.9	88.1% ( <i>t</i> ) chi angles: 175.2	0.085Å	-	-	
630	HIS	76.13	0.539Å C with 632 PRO HD3	Favored (65.81%) General / -66.1,-50.0	9.1% ( <i>t60</i> ) chi angles: 191.8,108.1	0.091Å	-		OUTLIER(S) worst is CD2- NE2-CE1: 4.376 σ
631	TYR	72.75	0.691Å OH with 531 GLN HG2	Favored (23.93%) Pre-proline / -115.5,89.9	70.2% ( <i>m-85</i> ) chi angles: 305.7,277.2	0.165Å	-	-	
632	PRO	69.95	0.539Å HD3 with 630 HIS C	Favored (33.81%) Trans-proline / -68.9,-24.2	83% ( <i>Cg_exo</i> ) chi angles: 331.8	0.168Å	-	-	
633	ASP	79.73	-	Favored (76.65%) General / -63.2,-34.0	51.6% ( <i>t0</i> ) chi angles: 183.3,14.9	0.1Å	-		OUTLIER(S) worst is CA- CB-CG: 4.146 σ
634	SER	90.68	-	Favored (66%) General / -64.2,-20.4	36% ( <i>m</i> ) chi angles: 303.6	0.085Å	-	-	
635	GLU	37.55	-	Favored (87.94%) General / -60.6,-39.4	87% ( <i>tt0</i> ) chi angles: 187.3,173.7,356.7	0.08Å	-	-	
636	ARG	66.46	-	-	77.7% ( <i>mmt-85</i> ) chi angles: 299.4,302.1,177.2,279.1	0.125Å	-	-	

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