



# Viewing cep290\_mb\_522-689H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	80.43		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	2	1.29%	Goal: <1%
	Ramachandran outliers	5	3.01%	Goal: <0.05%
	Ramachandran favored	156	93.98%	Goal: >98%
	MolProbity score <sup>^</sup>	2.86		29 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.62%	Goal: 0
	Bad backbone bonds:	0 / 1371	0.00%	Goal: 0%
	Bad backbone angles:	22 / 1824	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: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
522	ASN	44.67	-	-	92.4% ( <i>m</i> -20) chi angles: 291.4,325.7	0.087Å	-	-
523	SER	66.93	-	Favored (68.23%) General / -63.8,-25.5	94.1% ( <i>p</i> ) chi angles: 65	0.116Å	-	-
524	LYS	108.36	0.407Å HB2 with 524 LYS NZ	Favored (91.02%) General / -60.2,-40.8	3.7% ( <i>ttmp</i> ?) chi angles: 191.9,167.2,298.3,80.8	0.087Å	-	-
525	HIS	63.32	0.774Å O with 532 ARG HD2	Favored (95.94%) General / -61.6,-45.0	83% ( <i>m</i> -70) chi angles: 290.8,265.8	0.104Å	-	OUTLIER(S) worst is CD2-NE2-CE1: 4.338 σ

526	LEU	39.98	1.115Å HA with 532 ARG HD3	Favored (79.19%) General / -59.9,-49.0	64.6% ( <i>tp</i> ) chi angles: 179.8,62.8	0.108Å	-	-
527	LYS	125.99	0.41Å O with 534 GLU HB2	Favored (60.58%) General / -65.9,-51.2	74.7% ( <i>mmtt</i> ) chi angles: 298.9,301.7,179.7,179.1	0.114Å	-	-
528	GLN	119.23	0.701Å O with 534 GLU HB3	Favored (4.44%) General / -63.0,-59.7	26.8% ( <i>mt-30</i> ) chi angles: 292.9,177.5,145.2	0.154Å	-	-
529	GLN	337.23	1.053Å HB3 with 686 ILE HG13	OUTLIER (0.01%) General / 156.5,163.6	51.9% ( <i>tt0</i> ) chi angles: 183,189.2,345.9	0.147Å	-	OUTLIER(S) worst is C-N- CA: 6.983 $\sigma$
530	GLN	313.1	0.847Å HB3 with 532 ARG HG3	OUTLIER (0.01%) General / -174.6,-131.3	14.1% ( <i>tt0</i> ) chi angles: 180.1,171.7,126.1	0.144Å	-	OUTLIER(S) worst is C-N- CA: 8.013 $\sigma$
531	TYR	334.86	0.561Å H with 530 GLN HG2	Favored (8.29%) General / -85.5,82.5	27.8% ( <i>p90</i> ) chi angles: 58.3,281.9	0.038Å	-	OUTLIER(S) worst is N-CA- C: 4.2 $\sigma$
532	ARG	250.29	1.115Å HD3 with 526 LEU HA	Favored (4.04%) General / -128.0,-177.2	89.1% ( <i>mtt-85</i> ) chi angles: 295.8,196.1,185.6,271.4	0.132Å	-	-
533	ALA	76.23	-	Favored (94.24%) General / -60.7,-45.4	-	0.087Å	-	-
534	GLU	103.31	0.701Å HB3 with 528 GLN O	Favored (97.47%) General / -64.0,-41.2	2.5% ( <i>tp10</i> ) chi angles: 185.9,91.1,280.7	0.088Å	-	-
535	ASN	77.87	0.55Å HB2 with 529 GLN HG3	Favored (93.59%) General / -64.5,-39.3	9.2% ( <i>t-20</i> ) chi angles: 177.7,228.4	0.131Å	-	OUTLIER(S) worst is CA-CB- CG: 5.653 $\sigma$
536	GLN	91.65	-	Favored (98.6%) General / -60.9,-42.8	6.1% ( <i>tt0</i> ) chi angles: 177.5,190.8,155.8	0.125Å	-	-
537	ILE	86.12	0.822Å O with 540 LYS HG3	Favored (94.06%) Isoleucine or valine /	46.7% ( <i>pt</i> ) chi angles: 62,169	0.053Å	-	-

538	LEU	45.06	0.667Å O with 541 GLU HG2	-64.0,-41.9 Favored (91.36%) General / -63.3,-38.5	89.1% ( <i>mt</i> ) chi angles: 298,180.2	0.076Å	-	-		
539	LEU	127.11	0.414Å O with 542 ILE HG12	Favored (97.42%) General / -62.5,-44.0	52.4% ( <i>tp</i> ) chi angles: 179.9,67.3	0.12Å	-	-		
540	LYS	114.55	0.822Å HG3 with 537 ILE O	Favored (97.31%) General / -64.1,-41.0	0% chi angles: 79.8,79.8,179,178.4	0.085Å	-	-		
541	GLU	96.37	0.941Å HG3 with 675 ILE HD13	Favored (94.36%) General / -64.0,-43.9	18.6% ( <i>pt-20</i> ) chi angles: 58.8,185.9,339.2	0.081Å	-	-		
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	
Avg:			102.92	Clashscore:	80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
542	ILE	105.19	0.837Å HG23 with 675 ILE HG21	Favored (92.8%) Isoleucine or valine / -64.1,-41.5	46.8% ( <i>pt</i> ) chi angles: 60.3,170.6	0.042Å	-	-		
543	GLU	85.57	0.504Å N with 542 ILE HG13	Favored (76.67%) General / -66.1,-33.8	67.8% ( <i>tt0</i> ) chi angles: 195,168.8,359.1	0.039Å	-	-		
544	SER	50.05	-	Favored (54.75%) General / -61.8,-17.1	60.6% ( <i>p</i> ) chi angles: 72.4	0.124Å	-	-		
545	LEU	152.65	-	Favored (69.01%) General / -63.3,-27.0	65.5% ( <i>tp</i> ) chi angles: 177.8,64	0.117Å	-	-		
546	GLU	142.1	0.476Å HA with 546 GLU OE1	Favored (71.03%) General / -53.9,-45.0	3.8% ( <i>tp10</i> ) chi angles: 179.7,72.3,316	0.099Å	-	-		
547	GLU	196.14	-	Favored (3.01%) General / -68.0,108.3	59.4% ( <i>mm-40</i> ) chi angles: 291.9,286,357.4	0.104Å	-	-		
			0.746Å	Favored	33.1% ( <i>tt0</i> )					

548	GLU 135.62	O with 549 ARG HG3	(79.84%) General / -61.0,-48.9	chi angles: 189.9,170.8,51.4	0.092Å	-	-
549	ARG 235.37	0.908Å HB3 with 552 LEU HD23	Allowed (1.99%) General / -156.1,100.0	13.6% ( <i>mtp180</i> ) chi angles: 297.2,140.1,86.1,208.1	0.104Å	-	-
550	LEU 138.61	0.549Å O with 550 LEU HD13	Favored (82.56%) General / -65.0,-46.1	3% ( <i>tm?</i> ) chi angles: 187.6,291.7	0.077Å	-	-
551	ASP 52.98	-	Favored (75.34%) General / -65.1,-48.0	77.1% ( <i>m-20</i> ) chi angles: 297.3,346	0.144Å	-	-
552	LEU 182	0.908Å HD23 with 549 ARG HB3	Favored (83.15%) General / -66.2,-44.7	3% ( <i>mm?</i> ) chi angles: 290,296.9	0.147Å	-	-
553	LYS 97.85	0.866Å HB3 with 558 GLN HG2	Favored (96.89%) General / -60.7,-42.2	73.2% ( <i>mmtt</i> ) chi angles: 293.2,302.6,174.2,183.1	0.082Å	-	-
554	LYS 144.47	1.03Å HA with 558 GLN HB2	Favored (78.79%) General / -59.4,-49.2	31.2% ( <i>mmtp</i> ) chi angles: 288.9,299.2,180,73.5	0.114Å	-	-
555	LYS 89.41	0.663Å O with 562 GLU HB3	Favored (48.3%) General / -60.6,-54.2	47.3% ( <i>mttp</i> ) chi angles: 293.7,163.5,185.4,70.9	0.077Å	-	OUTLIER(S) worst is C-N- CA: 5.07 $\sigma$
556	ILE 156.05	0.886Å HG13 with 557 ARG H	Allowed (0.15%) Isoleucine or valine / -76.9,-74.2	38.9% ( <i>pt</i> ) chi angles: 60.3,166.3	0.131Å	-	-
557	ARG 209.16	0.886Å H with 556 ILE HG13	Favored (9.49%) General / -84.1,-48.8	36.8% ( <i>ttm180</i> ) chi angles: 175.5,179.4,289.4,189.8	0.1Å	-	-
558	GLN 235.68	1.03Å HB2 with 554 LYS HA	Favored (11.83%) General / -62.8,161.9	39.3% ( <i>mm-40</i> ) chi angles: 301.2,301.1,357	0.084Å	-	-
559	MET 295.71	0.638Å HB2 with 563 ARG HH21	Favored (4.03%) General / -56.9,117.5	24% ( <i>ttt</i> ) chi angles: 188.8,174.9,189.3	0.131Å	-	-

560	ALA	250.04	0.583Å HB3 with 554 LYS O	Allowed (0.19%) General / -176.7,-167.6	-	0.114Å	-	-	
561	GLN	141.94	0.614Å HA with 561 GLN OE1	Favored (89.23%) General / -62.4,-46.3	10.4% ( <i>mm</i> -40) chi angles: 292.6,298.1,54.6	0.075Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
562	GLU	96.89	0.968Å HB2 with 654 ILE HG21	Favored (83.46%) General / -67.6,-41.7	37.7% ( <i>tt0</i> ) chi angles: 184.6,179.6,296.5	0.129Å	-	-	
563	ARG	114.28	0.638Å HH21 with 559 MET HB2	Favored (99.91%) General / -63.0,-43.0	4% ( <i>tmm</i> _?) chi angles: 181.3,262.3,274,186.5	0.119Å	-	-	
564	GLY	19.39	-	Favored (98.68%) Glycine / -62.3,-40.2	-	-	-	-	
565	LYS	43.44	-	Favored (88.41%) General / -66.4,-38.8	93.2% ( <i>mttt</i> ) chi angles: 289.2,170.2,178.9,184.9	0.084Å	-	-	
566	ARG	69.32	0.802Å O with 569 THR HG22	Favored (96.72%) General / -63.8,-40.5	80.4% ( <i>mtt180</i> ) chi angles: 281.9,195.2,168.8,180	0.104Å	-	-	
567	SER	64.13	-	Favored (88.49%) General / -64.8,-37.7	97.3% ( <i>p</i> ) chi angles: 64.7	0.072Å	-	-	
568	ALA	29.59	0.528Å O with 572 LEU HG	Favored (94.43%) General / -62.9,-39.4	-	0.07Å	-	-	
569	THR	90.86	0.802Å HG22 with 566 ARG O	Favored (94.59%) General / -64.6,-39.9	10.3% ( <i>t</i> ) chi angles: 192.6	0.064Å	-	-	
570	SER	68.82	0.849Å O with 573 THR HG22	Favored (87.43%) General /	70% ( <i>m</i> ) chi angles: 297.3	0.095Å	-	-	

571	GLY	17.6	0.787Å O with 574 THR HG22	-66.7,-38.8 Favored (98.33%) Glycine / -63.7,-40.2	-	-	-	-
572	LEU	44.25	0.528Å HG with 568 ALA O	Favored (83.81%) General / -62.4,-36.9	83.9% ( <i>mt</i> ) chi angles: 295.1,180.2	0.11Å	-	-
573	THR	97.9	0.849Å HG22 with 570 SER O	Favored (89.01%) General / -66.6,-40.5	5.3% ( <i>t</i> ) chi angles: 197.2	0.096Å	-	-
574	THR	91.71	0.787Å HG22 with 571 GLY O	Favored (92.91%) General / -63.8,-38.9	8.8% ( <i>t</i> ) chi angles: 193.1	0.067Å	-	-
575	GLU	35.96	0.595Å O with 579 LEU HD13	Favored (84.13%) General / -63.8,-36.5	99.8% ( <i>mt-10</i> ) chi angles: 292.6,177.8,349.1	0.019Å	-	-
576	ASP	34.75	0.62Å OD1 with 637 LEU HD22	Favored (85.19%) General / -60.9,-38.3	73.6% ( <i>m-20</i> ) chi angles: 291.3,319.5	0.117Å	-	-
577	LEU	88.22	0.763Å O with 580 THR HG22	Favored (99.92%) General / -62.8,-42.9	10.7% ( <i>mp</i> ) chi angles: 278.3,59.1	0.105Å	-	-
578	ASN	41.6	0.776Å O with 581 GLU HG2	Favored (99.27%) General / -62.1,-42.5	6.4% ( <i>m120</i> ) chi angles: 288.8,169.7	0.076Å	-	OUTLIER(S) worst is CA-CB- CG: 5.152 σ
579	LEU	89.86	0.723Å HD21 with 636 LYS HE2	Favored (91.7%) General / -65.5,-39.4	8.9% ( <i>mp</i> ) chi angles: 284.8,63	0.084Å	-	-
580	THR	103.35	0.79Å O with 583 ILE HG22	Favored (81.22%) General / -64.8,-35.5	11.9% ( <i>t</i> ) chi angles: 191.6	0.074Å	-	-
581	GLU	60.2	0.776Å HG2 with 578 ASN O	Favored (90.91%) General / -65.0,-38.4	12.6% ( <i>pt-20</i> ) chi angles: 67.8,179,63.1	0.101Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

		Avg: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
582	ASN	28.19	0.536Å O with 585 GLN HG2	Favored (98.63%) General / -63.5,-41.4	83% ( <i>m-20</i> ) chi angles: 289.7,316	0.071Å	-	OUTLIER(S) worst is CA-CB- CG: 4.544 σ
583	ILE	89.95	0.79Å HG22 with 580 THR O	Favored (90.01%) Isoleucine or valine / -62.6,-40.9	16.7% ( <i>tt</i> ) chi angles: 196.3,168.7	0.067Å	-	-
584	SER	78.21	0.549Å O with 587 ASP HB2	Favored (93.12%) General / -61.2,-45.8	60.5% ( <i>m</i> ) chi angles: 299.1	0.09Å	-	-
585	GLN	84.01	0.536Å HG2 with 582 ASN O	Favored (86.39%) General / -64.9,-37.1	13.1% ( <i>pt20</i> ) chi angles: 62.5,179.9,118.2	0.059Å	-	-
586	GLY	29.97	-	Favored (75.36%) Glycine / -61.0,-31.2	-	-	-	-
587	ASP	74.11	0.549Å HB2 with 584 SER O	Favored (65.69%) General / -60.8,-24.3	83.9% ( <i>m-20</i> ) chi angles: 281.6,348.5	0.085Å	-	OUTLIER(S) worst is CA-CB- CG: 6.035 σ
588	ARG	141.43	-	Allowed (1.36%) General / -75.9,60.5	74.1% ( <i>mtt-85</i> ) chi angles: 278.1,188.9,178,261.5	0.168Å	-	-
589	ILE	163.66	0.831Å HB with 625 ARG HD2	Favored (61.13%) Isoleucine or valine / -69.6,-34.3	2% ( <i>pp</i> ) chi angles: 66.4,80.3	0.079Å	-	-
590	SER	37.88	0.649Å N with 589 ILE HD12	Favored (66.36%) General / -57.2,-32.4	94.9% ( <i>p</i> ) chi angles: 64.9	0.1Å	-	-
591	GLU	34.01	-	Favored (83.81%) General / -63.7,-36.4	46.3% ( <i>mt-10</i> ) chi angles: 292.5,187.6,274.6	0.079Å	-	-
592	ARG	83.04	0.911Å HE with 621 ARG HG2	Favored (92.85%) General / -59.4,-44.5	83% ( <i>mtt85</i> ) chi angles: 292,181.5,170.3,87.2	0.152Å	-	-

593	LYS	89.98	0.52Å O with 596 LEU HB3	Favored (86.27%) General / -64.5,-37.1	57.3% ( <i>tttm</i> ) chi angles: 189,164.5,183.7,286.4	0.079Å	-	-	
594	LEU	92.58	-	Favored (89.91%) General / -61.7,-39.0	86.5% ( <i>mt</i> ) chi angles: 296.8,180.7	0.11Å	-	-	
595	ASP	80	0.411Å O with 598 SER HB2	Favored (76.36%) General / -62.8,-34.0	12.7% ( <i>t70</i> ) chi angles: 189.6,282.5	0.079Å	-	OUTLIER(S) worst is CA-CB- CG: 4.378 σ	
596	LEU	127.21	0.558Å C with 596 LEU HD13	Favored (77.74%) General / -56.8,-41.5	2% ( <i>tm?</i> ) chi angles: 173.2,282.2	0.107Å	-	-	
597	LEU	45.34	-	Favored (82.14%) General / -62.5,-36.3	87.6% ( <i>mt</i> ) chi angles: 299.1,180	0.14Å	-	-	
598	SER	97.73	0.411Å HB2 with 595 ASP O	Favored (3.24%) General / -66.0,-1.6	73.2% ( <i>m</i> ) chi angles: 295.4	0.092Å	-	-	
599	LEU	134.48	0.932Å HD13 with 615 GLU HB2	Favored (71.16%) General / -59.0,-33.8	63.1% ( <i>tp</i> ) chi angles: 179.9,63.3	0.099Å	-	-	
600	LYS	84.31	-	Favored (69.56%) General / -58.7,-32.9	38.7% ( <i>ttmt</i> ) chi angles: 180,175.4,299.3,176.4	0.133Å	-	-	
601	ASN	88.45	-	Favored (62.82%) General / -58.2,-26.4	21.2% ( <i>t-20</i> ) chi angles: 195.1,303.6	0.062Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 102.92		Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
602	MET	131.24	-	-	Favored (82.18%) General / -57.6,-42.0	47.4% ( <i>ttp</i> ) chi angles: 181.5,168.3,59.5	0.051Å	-	-
603	SER	51.37	-	-	Favored (49.1%)	94.7% ( <i>p</i> )	0.082Å	-	OUTLIER(S) worst is C-N-



			General / -60.0,-54.2	chi angles: 63.5			CA: 4.156 $\sigma$
604	GLU 133.75	-	Favored (57.14%) General / -76.6,-8.4	24.9% ( <i>pt-20</i> ) chi angles: 61.1,180,1	0.089Å	-	-
605	ALA 108.71	0.465Å O with 606 GLN HB3	Allowed (1.85%) General / -48.9,-61.8	-	0.079Å	-	-
606	GLN 180.07	0.465Å HB3 with 605 ALA O	OUTLIER (0%) General / 151.8,-138.1	3.2% ( <i>pt20</i> ) chi angles: 55.7,191.7,192.7	0.15Å	-	-
607	SER 92.77	0.462Å N with 606 GLN HG3	OUTLIER (0%) General / -57.7,-94.0	38.2% ( <i>p</i> ) chi angles: 53.6	0.033Å	-	-
608	LYS 162.32	0.505Å HG3 with 611 PHE HB2	OUTLIER (0.01%) General / -172.3,16.6	55.7% ( <i>tttm</i> ) chi angles: 184.1,168.9,171.1,291.7	0.101Å	-	-
609	ASN 102.21	-	Favored (77.13%) General / -69.2,-41.3	20% ( <i>t-20</i> ) chi angles: 180.8,295.6	0.081Å	-	OUTLIER(S) worst is CA-CB- CG: 4.552 $\sigma$
610	GLU 105.64	0.535Å HA with 610 GLU OE1	Favored (72.33%) General / -68.8,-32.6	47.9% ( <i>mm-40</i> ) chi angles: 301.6,303.4,354.4	0.083Å	-	-
611	PHE 75.48	0.505Å HB2 with 608 LYS HG3	Favored (67.7%) General / -56.0,-36.3	12.2% ( <i>m-85</i> ) chi angles: 270.3,77.9	0.113Å	-	OUTLIER(S) worst is CA-CB- CG: 5.034 $\sigma$
612	LEU 139.52	-	Favored (79.33%) General / -57.6,-40.6	69.9% ( <i>tp</i> ) chi angles: 177.8,62.5	0.107Å	-	-
613	SER 189.5	-	Favored (49.85%) General / -61.5,146.1	67% ( <i>m</i> ) chi angles: 296.4	0.092Å	-	-
614	ARG 317.93	0.598Å HB3 with 617 ILE HG12	Favored (47.25%) General / -136.6,148.0	32.7% ( <i>tpt85</i> ) chi angles: 197.2,73.5,186.4,86.4	0.093Å	-	-
615	GLU 123.01	0.932Å HB2 with 599 LEU HD13	Favored (89.9%) General / -65.0,-44.2	15.3% ( <i>tp10</i> ) chi angles: 157.2,67.9,27.8	0.102Å	-	-

616	LEU	69.22	0.667Å H with 616 LEU HD22	Favored (97.63%) General / -64.0,-41.1	1.8% ( <i>mm?</i> ) chi angles: 298.9,299.7	0.073Å	-	-
617	ILE	88.33	0.598Å HG12 with 614 ARG HB3	Favored (91.83%) Isoleucine or valine / -64.2,-41.2	42.3% ( <i>mm</i> ) chi angles: 296.4,299.9	0.063Å	-	-
618	GLU	108.29	0.672Å OE2 with 592 ARG HB3	Favored (98.39%) General / -62.3,-41.3	3.8% ( <i>tm-20</i> ) chi angles: 201.5,291.5,299.8	0.077Å	-	-
619	LYS	78.66	-	Favored (94.51%) General / -64.2,-43.6	73.1% ( <i>tttt</i> ) chi angles: 197.3,163.2,179.5,176.6	0.06Å	-	-
620	GLU	120.08	-	Favored (78.5%) General / -63.9,-34.7	3.6% ( <i>tm-20</i> ) chi angles: 195.6,290.6,295.7	0.081Å	-	-
621	ARG	164.6	0.911Å HG2 with 592 ARG HE	Favored (84.03%) General / -59.8,-39.1	46.3% ( <i>ttm180</i> ) chi angles: 184.6,172.9,295.4,124.4	0.074Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
622	ASP	78.07	0.581Å O with 625 ARG HG2	Favored (96.67%) General / -62.2,-44.4	43.6% ( <i>m-20</i> ) chi angles: 281.9,321.6	0.106Å	-	OUTLIER(S) worst is CA-CB- CG: 4.248 σ	
623	LEU	85.43	0.458Å N with 623 LEU HD12	Favored (97.68%) General / -63.9,-41.7	6.4% ( <i>mp</i> ) chi angles: 290.9,63.8	0.117Å	-	-	
624	GLU	118.62	0.816Å HG2 with 621 ARG HA	Favored (69.73%) General / -65.0,-28.8	12% ( <i>pt-20</i> ) chi angles: 71.3,159.5,11.4	0.143Å	-	-	
625	ARG	109.43	0.831Å HD2 with 589 ILE HB	Favored (92.03%) General / -59.4,-42.5	12% ( <i>ptt-85</i> ) chi angles: 73.1,205.7,209,279.5	0.136Å	-	-	
			0.573Å	Favored (57.39%)	82.8% ( <i>p</i> )				

626	SER	88.12	O with 630 ILE HG12	General / -65.0,-52.2	chi angles: 69.3	0.091Å	-	-
627	ARG	86.45	0.779Å O with 631 ALA HB3	Favored (8.44%) General / -62.9,-58.1	77.7% ( <i>mtm180</i> ) chi angles: 297.8,179.3,303.2,188.1	0.074Å	-	-
628	THR	151.47	0.788Å HG22 with 624 GLU O	Favored (3.99%) General / -71.2,-58.0	9% ( <i>t</i> ) chi angles: 183.5	0.079Å	-	OUTLIER(S) worst is C-N- CA: 4.157 $\sigma$
629	VAL	155.91	0.78Å HG22 with 625 ARG O	Favored (13.75%) Isoleucine or valine / -69.4,-55.9	33.7% ( <i>m</i> ) chi angles: 299.4	0.135Å	-	OUTLIER(S) worst is C-N- CA: 4.661 $\sigma$
630	ILE	150.51	0.678Å O with 634 GLN HG3	Favored (21.09%) Isoleucine or valine / -73.6,-52.5	36.3% ( <i>pt</i> ) chi angles: 66.4,169	0.115Å	-	-
631	ALA	42.96	0.779Å HB3 with 627 ARG O	Favored (68.02%) General / -66.3,-49.1	-	0.074Å	-	-
632	LYS	106.71	0.537Å HB3 with 628 THR O	Favored (75.93%) General / -64.7,-48.1	53.1% ( <i>tppt</i> ) chi angles: 188.8,71.6,173.3,182	0.095Å	-	-
633	PHE	43.86	0.546Å HB2 with 629 VAL O	Favored (91.07%) General / -65.8,-42.1	68.5% ( <i>m-85</i> ) chi angles: 285.7,85.8	0.086Å	-	OUTLIER(S) worst is CA-CB- CG: 6.341 $\sigma$
634	GLN	50.8	0.678Å HG3 with 630 ILE O	Favored (95.47%) General / -60.8,-41.3	27% ( <i>mt-30</i> ) chi angles: 289.2,183.5,173.1	0.118Å	-	-
635	ASN	29.63	-	Favored (98.87%) General / -62.8,-41.0	82% ( <i>m-20</i> ) chi angles: 283.4,350.7	0.082Å	-	OUTLIER(S) worst is CA-CB- CG: 4.847 $\sigma$
636	LYS	90.89	0.723Å HE2 with 579 LEU HD21	Favored (98.92%) General / -61.8,-42.3	52.1% ( <i>mtpt</i> ) chi angles: 297.5,159.5,65,182.8	0.118Å	-	-
637	LEU	122.3	0.62Å HD22 with 576 ASP OD1	Favored (99.31%) General / -61.4,-43.2	3.1% ( <i>tm?</i> ) chi angles: 180.9,288.4	0.052Å	-	-

638	LYS	59.49	-	Favored (96.11%) General / -63.3,-40.0	49.5% ( <i>tttm</i> ) chi angles: 179.8,167.4,169,287.4	0.106Å	-	-
639	GLU	67.81	-	Favored (89.47%) General / -62.8,-38.1	50.4% ( <i>tt0</i> ) chi angles: 192,167.9,23.8	0.055Å	-	-
640	LEU	32.75	0.556Å HD12 with 576 ASP OD1	Favored (95.04%) General / -63.8,-39.8	79.7% ( <i>mt</i> ) chi angles: 293.6,180.3	0.094Å	-	-
641	VAL	27.66	0.768Å HA with 644 ASN ND2	Favored (93.06%) Isoleucine or valine / -62.7,-41.6	94.6% ( <i>t</i> ) chi angles: 176.8	0.075Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
642	GLU	29.7	-	Favored (92.6%) General / -65.3,-39.5	93.7% ( <i>mt-10</i> ) chi angles: 287,180.5,339.3	0.084Å	-	-
643	GLU	26.29	0.704Å O with 646 GLN HG2	Favored (92.99%) General / -64.0,-39.0	99.5% ( <i>mt-10</i> ) chi angles: 293.2,180.1,355.4	0.071Å	-	-
644	ASN	96.16	0.768Å ND2 with 641 VAL HA	Favored (78.03%) General / -64.8,-34.3	21.6% ( <i>p30</i> ) chi angles: 65.1,54.6	0.128Å	-	-
645	LYS	129.16	-	Favored (99.87%) General / -62.6,-42.9	17.9% ( <i>tppt?</i> ) chi angles: 178.6,63.1,68.7,179.5	0.074Å	-	-
646	GLN	80.68	0.704Å HG2 with 643 GLU O	Favored (95.79%) General / -65.0,-41.0	14.4% ( <i>pt20</i> ) chi angles: 66.4,174.1,50.3	0.109Å	-	-
647	LEU	44.3	0.462Å N with 646 GLN HG3	Favored (82.84%) General / -62.8,-36.4	68.8% ( <i>mt</i> ) chi angles: 290.7,180.1	0.071Å	-	-
			0.693Å	Favored	15.1% ( <i>tp10</i> )			

648	GLU	64.6	HA with 651 MET CE	(92.7%) General / -59.5,-42.7 Favored	chi angles: 173.1,81.6,39.2	0.116Å	-	-
649	GLU	65.93	0.703Å HA with 652 LYS HD2	(97.1%) General / -63.9,-40.7 Favored	86.4% ( <i>tt0</i> ) chi angles: 185.2,177.4,352.3	0.067Å	-	-
650	GLY	34.03	-	(96.03%) Glycine / -63.0,-38.1 Favored	-	-	-	-
651	MET	87.5	0.693Å CE with 648 GLU HA	(74.79%) General / -60.9,-34.6 Favored	75.4% ( <i>mtm</i> ) chi angles: 289.3,183.8,281.8	0.073Å	-	-
652	LYS	46.7	0.703Å HD2 with 649 GLU HA	(87.87%) General / -62.8,-37.7 Favored	84.9% ( <i>mttt</i> ) chi angles: 297.7,162.4,178.9,173.4	0.032Å	-	-
653	GLU	40.6	-	(99.12%) General / -63.2,-41.3 Favored	95.4% ( <i>mt-10</i> ) chi angles: 291.7,180.2,336.7	0.144Å	-	-
654	ILE	97.16	0.968Å HG21 with 562 GLU HB2	(77.24%) Isoleucine or valine / -61.2,-37.3 Favored	49.9% ( <i>mm</i> ) chi angles: 301.4,299	0.097Å	-	-
655	LEU	131.01	0.772Å O with 658 ILE HG22	(98.05%) General / -62.6,-40.8 Favored	3% ( <i>tm?</i> ) chi angles: 183.7,291.1	0.088Å	-	-
656	GLN	25.91	-	(92.78%) General / -62.3,-39.4 Favored	93.1% ( <i>mt-30</i> ) chi angles: 293.4,181.8,345	0.093Å	-	-
657	ALA	28.87	0.497Å CB with 555 LYS HD3	(99.2%) General / -62.6,-41.9 Favored	-	0.079Å	-	-
658	ILE	93.74	0.86Å HG13 with 552 LEU HD12	(81.38%) Isoleucine or valine / -63.0,-38.2 Favored	19.5% ( <i>tt</i> ) chi angles: 192.3,169.9	0.114Å	-	-
659	LYS	134.72	0.455Å N with 658 ILE HG23	(82.48%) General / Favored	4% ( <i>tppt?</i> ) chi angles: 165.4,64.2,109.4,167.2	0.1Å	-	-

660	GLU	41.1	-	-57.2,-43.2 Favored (74.05%) General / -62.6,-49.7	44.9% ( <i>tt0</i> ) chi angles: 180.2,181,66.1	0.129Å	-	-	
661	MET	123.09	0.656Å HG3 with 555 LYS HZ3	Favored (67.71%) General / -70.0,-30.4	25.9% ( <i>mmt</i> ) chi angles: 301.1,296.9,172.3	0.069Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 102.92			Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168	
662	GLN	134.93	0.716Å HG3 with 549 ARG NH2	Favored (75.56%) General / -55.9,-42.1	19.4% ( <i>tt0</i> ) chi angles: 192.3,164.1,261.8	0.027Å	-	-	
663	LYS	283.71	0.737Å HD2 with 663 LYS O	Favored (20.43%) General / -77.8,118.8	0% chi angles: 53.8,79.3,177.1,299.2	0.111Å	-	-	
664	ASP	196.82	-	Favored (12.78%) Pre-proline / -147.5,138.1	46.8% ( <i>m-20</i> ) chi angles: 285,312.7	0.113Å	-	-	
665	PRO	82.41	-	Favored (77.54%) Trans-proline / -60.4,-24.4	61.3% ( <i>Cg_endo</i> ) chi angles: 27.4	0.048Å	-	-	
666	ASP	51.07	-	Favored (71.31%) General / -63.2,-30.1	5.8% ( <i>m-20</i> ) chi angles: 281.1,28.9	0.1Å	-	OUTLIER(S) worst is CA-CB- CG: 4.784 σ	
667	VAL	41.76	-	Favored (86.93%) Isoleucine or valine / -57.8,-46.6	92.4% ( <i>t</i> ) chi angles: 177	0.103Å	-	-	
668	LYS	80.05	-	Favored (76.72%) General / -60.1,-49.7	78.9% ( <i>tttt</i> ) chi angles: 172.1,178.1,167.5,184.3	0.158Å	-	-	
669	GLY	210.81	-	Favored (32.33%) Glycine / 68.9,-174.9	-	-	-	-	
				Favored					

670	GLY	225.26	-	(25.88%) Glycine / 92.8,-24.0	-	-	-	-
671	GLU	130.72	-	Favored (77.68%) General / -65.2,-34.1	87.4% ( <i>tt0</i> ) chi angles: 180.1,175.2,353.6	0.111Å	-	-
672	THR	132.11	-	Favored (73.49%) General / -64.5,-32.0	63.6% ( <i>p</i> ) chi angles: 64.8	0.072Å	-	-
673	SER	94.07	0.488Å O with 677 PRO HD2	Favored (27.2%) General / -54.5,-25.7	68.1% ( <i>m</i> ) chi angles: 296.2	0.087Å	-	-
674	LEU	126.44	0.748Å O with 674 LEU HD13	Favored (72.45%) General / -60.5,-33.3	3.1% ( <i>tm?</i> ) chi angles: 184.2,290.7	0.081Å	-	-
675	ILE	63.82	0.941Å HD13 with 541 GLU HG3	Favored (83.11%) Isoleucine or valine / -56.8,-45.6	78.7% ( <i>mt</i> ) chi angles: 301.1,168.6	0.098Å	-	-
676	ILE	122.45	1.103Å HA with 679 LEU HD13	Favored (54.89%) Pre-proline / -62.8,-39.6	18% ( <i>tt</i> ) chi angles: 181.3,167.5	0.254Å	-	OUTLIER(S) worst is CA-C- N: 4.07 $\sigma$
677	PRO	124.85	1.054Å HD3 with 676 ILE HG23	Favored (63.84%) Trans-proline / -64.5,-24.1	82% ( <i>Cg_exo</i> ) chi angles: 330.7	0.121Å	-	-
678	SER	72.12	0.561Å HB2 with 675 ILE O	Favored (79.16%) General / -66.0,-34.9	69.3% ( <i>m</i> ) chi angles: 296	0.118Å	-	-
679	LEU	85.31	1.103Å HD13 with 676 ILE HA	Favored (99.16%) General / -61.5,-42.7	6.7% ( <i>mp</i> ) chi angles: 289.4,62.2	0.176Å	-	-
680	GLU	35.38	-	Favored (97.22%) General / -61.8,-44.3	87.1% ( <i>mt-10</i> ) chi angles: 294.3,177.4,14	0.135Å	-	-
681	ARG	46.15	-	Favored (96.37%) General / -62.3,-44.5	86% ( <i>mtt-85</i> ) chi angles: 299.7,193.8,180.5,284	0.115Å	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 102.92	Clashscore: 80.43	Outliers: 5 of 166	Poor rotamers: 2 of 155	Outliers: 1 of 162	Outliers: 0 of 168	Outliers: 21 of 168
682	LEU	134.53	0.574Å HD21 with 534 GLU HB3	Favored (91.46%) General / -66.0,-40.6	34.3% ( <i>tp</i> ) chi angles: 188.4,62	0.06Å	-	-
683	VAL	34.75	0.758Å HG23 with 679 LEU O	Favored (82.6%) Isoleucine or valine / -63.5,-38.6	95.9% ( <i>t</i> ) chi angles: 178.3	0.08Å	-	-
684	ASN	77.82	-	Favored (85.78%) General / -57.9,-43.2	46.2% ( <i>t30</i> ) chi angles: 181,60.9	0.089Å	-	OUTLIER(S) worst is CA-CB- CG: 4.343 $\sigma$
685	ALA	36.12	-	Favored (93.93%) General / -63.4,-39.2	-	0.083Å	-	-
686	ILE	111.65	1.053Å HG13 with 529 GLN HB3	Favored (30.54%) Isoleucine or valine / -68.0,134.2	48.3% ( <i>mm</i> ) chi angles: 304.6,302	0.073Å	-	-
687	GLU	77.31	-	Favored (55.9%) General / -68.1,138.6	53.5% ( <i>mt-10</i> ) chi angles: 295.7,179.9,52.7	0.11Å	-	-
688	SER	61.66	-	Favored (89.99%) General / -64.3,-38.1	47.6% ( <i>t</i> ) chi angles: 180	0.117Å	-	-
689	LYS	47.78	-	-	48.9% ( <i>tttp</i> ) chi angles: 181.8,166.8,180.4,76.6	0.109Å	-	-

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