



Viewing cep290_mb_522-689-FFX1FH_reg-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.8	99 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	9	5.81%	Goal: <0.3%
	Favored rotamers	126	81.29%	Goal: >98%
	Ramachandran outliers	4	2.41%	Goal: <0.05%
	Ramachandran favored	151	90.96%	Goal: >98%
	MolProbity score^	2.04		74 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	4.32%	Goal: 0
	Bad bonds:	0 / 1371	0.00%	Goal: 0%
	Bad angles:	12 / 1824	0.66%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 2	0.00%	Expected: ≤1 per chain, or ≤5%
	Twisted Peptides:	1 / 167	0.60%	Goal: 0

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	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 102.92	Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167
522	ASN	44.67	-	-	OUTLIER (0.2%) chi angles: 61.5,117.2	0.02Å	-	-	-
523	SER	66.93	-	Favored (12.24%) General / -51.4,-28.2	Favored (14.2%) <i>p</i> chi angles: 51.5	0.12Å	-	-	-
524	LYS	108.36	-	Favored (68.2%) General / -55.6,-37.4	Favored (48.6%) <i>t</i> <i>t</i> <i>t</i> <i>m</i> chi angles: 186.1,178.7,183.3,285.2	0.18Å	-	-	-
525	HIS	63.32	-	Favored (69.12%) General / -68.8,-30.6	Favored (3%) <i>m</i> -70 chi angles: 262.7,293.2	0.20Å	-	-	-
526	LEU	39.98	-	Favored (77.05%) General / -69.5,-40.5	Favored (68.4%) <i>tp</i> chi angles: 179.7,62.5	0.05Å	-	-	-

527	LYS 125.99	-	Favored (28.41%) General / -93.1,-13.5	Favored (9.9%) <i>tptp</i> chi angles: 179.6,63,199.8,74.7	0.12Å	-	-	-
528	GLN 119.23	-	Favored (7.84%) General / -91.9,-46.4	Favored (7.8%) <i>mm110</i> chi angles: 279.8,307,139.3	0.12Å	-	OUTLIER(S) worst is C-N- CA: 4.1 σ	-
529	GLN 337.23	-	OUTLIER (0%) General / 139.8,156.1	Favored (22.1%) <i>tt0</i> chi angles: 165.2,187.4,2.3	0.08Å	-	-	-
530	GLN 313.1	-	Allowed (0.33%) General / -143.4,-69.5	Favored (15.2%) <i>tp-</i> <i>100</i> chi angles: 179.2,56.7,266.4	0.12Å	-	-	Twisted nonPRO omega= 149.39
531	TYR 334.86	-	Allowed (1.62%) General / -129.3,58.3	Favored (5.9%) <i>p90</i> chi angles: 61.1,289.5	0.05Å	-	-	-
532	ARG 250.29	-	Favored (2.94%) General / -133.6,-172.3	Favored (27.7%) <i>mmt180</i> chi angles: 298.6,299.3,168.5,169.9	0.22Å	-	-	-
533	ALA 76.23	-	Favored (73.21%) General / -56.0,-40.3	-	0.14Å	-	-	-
534	GLU 103.31	-	Favored (79.79%) General / -66.8,-45.0	Allowed (0.7%) <i>tp30</i> chi angles: 194.6,84.9,305.6	0.05Å	-	-	-
535	ASN 77.87	-	Favored (76.43%) General / -64.7,-33.6	Favored (7.8%) <i>t0</i> chi angles: 177.9,237.8	0.10Å	-	-	-
536	GLN 91.65	-	Favored (73.06%) General / -67.8,-32.5	Favored (7.1%) <i>tp40</i> chi angles: 179.2,66.8,105.1	0.13Å	-	-	-
537	ILE 86.12	-	Favored (53.41%) Ile or Val / -73.7,-39.8	Favored (18.8%) <i>pt</i> chi angles: 71.6,173	0.32Å	-	OUTLIER(S) worst is N- CA-CB: 4.4 σ	-
538	LEU 45.06	-	Favored (79.93%) General / -62.5,-35.6	Favored (28.7%) <i>mt</i> chi angles: 308.3,184.6	0.13Å	-	-	-
539	LEU 127.11	-	Favored (68.02%) General / -72.6,-35.8	Favored (49.2%) <i>tp</i> chi angles: 183.7,59.5	0.04Å	-	-	-
540	LYS 114.55	-	Favored (62.36%) General / -74.8,-33.9	Favored (30.1%) <i>tptt</i> chi angles: 182.6,51.5,183,168.9	0.14Å	-	-	-

541	GLU	96.37	-	Favored (73.65%) General / -69.9,-42.2	Favored (8.3%) <i>pt0</i> chi angles: 53.7,189,333.2	0.20Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 102.92			Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167
542	ILE	105.19	-	Favored (74.75%) Ile or Val / -64.2,-35.7	Favored (42.7%) <i>pt</i> chi angles: 61.5,174.5	0.26Å	-	-	-
543	GLU	85.57	-	Favored (54.73%) General / -76.4,-25.5	OUTLIER (0%) chi angles: 168.1,275.5,75	0.20Å	-	-	-
544	SER	50.05	-	Favored (62.51%) General / -70.7,-21.7	Favored (46.6%) <i>m</i> chi angles: 290.8	0.12Å	-	-	-
545	LEU	152.65	-	Favored (39.33%) General / -55.4,-26.0	Favored (15.6%) <i>tp</i> chi angles: 193.1,61.3	0.08Å	-	-	-
546	GLU	142.1	-	Favored (82.3%) General / -62.3,-36.5	Favored (3.9%) <i>tp30</i> chi angles: 177.3,56.7,341.7	0.06Å	-	-	-
547	GLU	196.14	0.42Å OE2 with 554 LYS NZ	Favored (6.81%) General / -82.7,63.4	Allowed (0.6%) <i>mm-30</i> chi angles: 252.3,287.3,104.2	0.11Å	-	OUTLIER(S) worst is C-N- CA: 7.0 σ	-
548	GLU	135.62	-	OUTLIER (0.01%) General / -15.5,-63.6	Favored (4.3%) <i>tt0</i> chi angles: 178.6,205.5,105.2	0.12Å	-	-	-
549	ARG	235.37	0.41Å HD2 with 667 VAL HG22	Favored (2.45%) General / -140.9,91.9	Allowed (1.4%) <i>mtp180</i> chi angles: 296.3,123.2,71.2,210.4	0.02Å	-	-	-
550	LEU	138.61	-	Allowed (0.1%) General / -29.9,-66.1	Favored (3.7%) <i>tt</i> chi angles: 188.5,139.7	0.10Å	-	-	-
551	ASP	52.98	-	Favored (68.47%) General / -65.9,-27.8	Allowed (1.3%) <i>m-30</i> chi angles: 294.8,45.5	0.08Å	-	-	-
552	LEU	182	-	Favored (32.02%) General / -80.5,-37.1	OUTLIER (0.2%) chi angles: 294.3,286.7	0.04Å	-	-	-
553	LYS	97.85	-	Favored (82.91%)	Favored (68.6%) <i>mmtt</i>	0.11Å	-	-	-

				General /	chi angles:				
				-68.0,-40.5	302.2,298.8,184.2,190.1				
554	LYS	144.47	0.42Å NZ with 547 GLU OE2	Favored (77.4%)	Favored (17.6%) <i>mmtm</i>	0.16Å	-	-	-
				General / -55.6,-45.4	chi angles: 305.6,304.7,166.7,289.6				
555	LYS	89.41	0.41Å O with 562 GLU HB3	Favored (3.15%)	Favored (34.1%) <i>mttp</i>	0.13Å	-	-	-
				General / -56.7,-60.7	chi angles: 285.7,168.7,186.3,71.9				
556	ILE	156.05	-	Favored (4.25%) Ile or Val / -94.8,-31.2	Favored (18.7%) <i>pt</i> chi angles: 57.8,160.7	0.24Å	-	-	-
557	ARG	209.16	-	Favored (2.65%)	Favored (18.8%) <i>ttm170</i>	0.10Å	-	-	-
				General / -126.5,-32.4	chi angles: 182.2,185,279.3,200.3				
558	GLN	235.68	-	Favored (6.32%)	Favored (74.3%) <i>mt0</i>	0.07Å	-	-	-
				General / -89.7,178.2	chi angles: 294.8,168.6,9.5				
559	MET	295.71	-	Allowed (1.23%)	Favored (5.4%) <i>ttt</i>	0.04Å	-	-	-
				General / -70.7,96.6	chi angles: 191.7,149.5,182.7				
560	ALA	250.04	-	Allowed (0.35%)	-	0.18Å	-	-	-
				General / -151.4,-150.6					
561	GLN	141.94	-	Favored (74.32%)	Favored (35.8%) <i>mm110</i>	0.16Å	-	-	-
				General / -63.5,-49.2	chi angles: 295.8,300.6,106.6				
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 102.92			Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167
562	GLU	96.89	0.41Å HB3 with 555 LYS O	Favored (63.41%)	Favored (90.1%) <i>tt0</i>	0.15Å	-	-	-
				General / -73.4,-41.4	chi angles: 184.9,174.3,2				
563	ARG	114.28	-	Favored (83.44%)	Favored (2.6%) <i>tmm160</i>	0.21Å	-	OUTLIER(S) worst is N-CA-CB: 4.0 σ	-
				General / -59.9,-38.9	chi angles: 190.5,273,274.1,164.3				
564	GLY	19.39	-	Favored (93.87%)	-	-	-	-	-
				Glycine / -58.5,-45.9					
565	LYS	43.44	-	Favored (87.73%)	Favored (96.8%) <i>mttt</i>	0.12Å	-	-	-
				General / -64.5,-37.5	chi angles: 295.3,178.4,185.9,182.4				

566	ARG	69.32	-	Favored (74.06%) General / -70.6,-37.9	Favored (40.3%) <i>mtt180</i> chi angles: 291.2,180.8,172.9,214.2	0.12Å	-	-	-
567	SER	64.13	-	Favored (65.3%) General / -72.7,-31.7	Favored (10.2%) <i>p</i> chi angles: 50.1	0.18Å	-	-	-
568	ALA	29.59	-	Favored (73.43%) General / -66.9,-46.9	-	0.09Å	-	-	-
569	THR	90.86	-	Favored (87.81%) General / -59.2,-41.2	Favored (6.6%) <i>p</i> chi angles: 45.5	0.18Å	-	-	-
570	SER	68.82	-	Favored (77.47%) General / -65.8,-34.1	Favored (12.4%) <i>p</i> chi angles: 50.8	0.17Å	-	-	-
571	GLY	17.6	-	Favored (59.54%) Glycine / -74.1,-31.5	-	-	-	-	-
572	LEU	44.25	-	Favored (87.25%) General / -63.7,-46.1	Favored (34.6%) <i>mt</i> chi angles: 307.6,174.5	0.13Å	-	-	-
573	THR	97.9	-	Favored (75.96%) General / -65.3,-33.4	Favored (15.6%) <i>p</i> chi angles: 48.5	0.23Å	-	-	-
574	THR	91.71	-	Favored (92.71%) General / -65.5,-40.3	Favored (4.4%) <i>p</i> chi angles: 44.1	0.22Å	-	-	-
575	GLU	35.96	-	Favored (94.67%) General / -64.6,-40.0	Allowed (1.8%) <i>tt0</i> chi angles: 206.9,206.9,321.8	0.18Å	-	-	-
576	ASP	34.75	-	Favored (60.89%) General / -51.1,-49.4	Favored (42.5%) <i>m-30</i> chi angles: 302.8,338.5	0.11Å	-	-	-
577	LEU	88.22	-	Favored (89.9%) General / -58.7,-43.4	Favored (5.7%) <i>mp</i> chi angles: 266.9,65.3	0.13Å	-	-	-
578	ASN	41.6	-	Favored (61.67%) General / -72.5,-26.2	Favored (35%) <i>m110</i> chi angles: 304.9,126.6	0.11Å	-	-	-
579	LEU	89.86	-	Favored (53.23%) General /	Favored (22.6%) <i>mt</i> chi angles: 306.8,169.2	0.10Å	-	-	-

-77.5,-31.2

580	THR	103.35	-	Favored (58.59%) General / -76.1,-31.0	Favored (57.2%) <i>m</i> chi angles: 303.7	0.13Å	-	-	-
581	GLU	60.2	-	Favored (68.18%) General / -71.5,-32.5	Favored (4.2%) <i>pt0</i> chi angles: 82.5,182.3,113.8	0.18Å	-	-	-

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Avg: 102.92				Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167

582	ASN	28.19	-	Favored (83.19%) General / -62.3,-47.7	Allowed (1.5%) <i>m-40</i> chi angles: 267.3,253	0.11Å	-	-	-
583	ILE	89.95	-	Favored (79.71%) Ile or Val / -62.0,-50.5	Favored (3.1%) <i>tt</i> chi angles: 208,173.6	0.26Å	-	-	-
584	SER	78.21	-	Favored (92.3%) General / -59.2,-44.0	Favored (60.7%) <i>m</i> chi angles: 298.8	0.07Å	-	-	-
585	GLN	84.01	-	Favored (77.41%) General / -65.1,-34.0	Favored (55.4%) <i>mt0</i> chi angles: 282.8,189.9,41.8	0.12Å	-	-	-
586	GLY	29.97	-	Favored (65.5%) Glycine / -86.0,-15.2	-	-	-	-	-
587	ASP	74.11	-	Favored (57.69%) General / -77.0,-8.6	Favored (67.7%) <i>m-30</i> chi angles: 299.5,324.3	0.10Å	-	-	-
588	ARG	141.43	-	Allowed (0.12%) General / -67.0,74.7	Favored (54.4%) <i>mtm180</i> chi angles: 299.5,181.3,297.4,152.5	0.04Å	-	OUTLIER(S) worst is NE- CZ-NH2: 4.2 σ	-
589	ILE	163.66	-	Favored (6.99%) Ile or Val / -89.3,-20.9	Allowed (1.2%) <i>pp</i> chi angles: 68.7,94.1	0.22Å	-	-	-
590	SER	37.88	-	Favored (97.92%) General / -60.8,-43.5	Favored (18.8%) <i>p</i> chi angles: 52.6	0.06Å	-	-	-
591	GLU	34.01	-	Favored (88.61%) General / -58.5,-42.9	Favored (87.1%) <i>mt-10</i> chi angles: 289.3,177.2,331.6	0.04Å	-	-	-
				Favored	Favored (81.7%)				

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				-146.8,20.2				
				OUTLIER				
605	ALA 108.71	-		(0.02%)	-	0.11Å	-	-
				General /				
				-66.9,-85.7				
				OUTLIER	Favored (3.1%) <i>pt0</i>			
606	GLN 180.07	-		(0%)	chi angles:	0.17Å	-	-
				General /	47.8,183.1,249.3			
				179.9,-113.7				
				Allowed	Favored (80.2%) <i>p</i>			
607	SER 92.77	-		(0.12%)	chi angles: 61.4	0.15Å	-	-
				General /				
				-89.3,-92.6				
				Allowed	Favored (4.4%) <i>tttm</i>			
608	LYS 162.32	0.41Å	HG2 with	(0.38%)	chi angles:	0.07Å	-	-
			608 LYS O	General /	202,195.3,156.1,295.8			
				-155.1,12.9				
				Favored	Favored (25.8%) <i>m-</i>			
609	ASN 102.21	-		(60.21%)	40	0.09Å	-	OUTLIER(S)
				General /	chi angles: 311.5,294.4			worst is C-N-
				-74.0,-42.6				CA: 4.6 σ
				Favored	Favored (4.5%) <i>mp0</i>			
610	GLU 105.64	-		(46.47%)	chi angles:	0.07Å	-	-
				General /	312.9,90.3,310.1			
				-75.5,-5.7				
				Favored	Favored (47.6%) <i>m-</i>			
611	PHE 75.48	-		(59.06%)	80	0.11Å	-	-
				General /	chi angles: 284.7,77.3			
				-83.2,-9.7				
				Favored	Favored (7.6%) <i>mp</i>			
612	LEU 139.52	-		(22.62%)	chi angles: 279.6,64.1	0.15Å	-	-
				General /				
				-84.7,-35.4				
				Favored	Favored (69.3%) <i>m</i>			
613	SER 189.5	-		(16.06%)	chi angles: 296.6	0.06Å	-	-
				General /				
				-59.3,154.6				
				Allowed	Allowed (1.5%)			
614	ARG 317.93	-		(0.52%)	<i>tpt90</i>	0.12Å	-	OUTLIER(S)
				General /	chi angles:			worst is C-N-
				-173.1,133.2	200.3,70.9,214.9,86.9			CA: 4.7 σ
				Favored	OUTLIER (0.2%)			
615	GLU 123.01	-		(5.05%)	chi angles:	0.07Å	-	-
				General /	159.2,51.1,322.4			
				-44.0,-54.9				
				Favored	Allowed (0.6%) <i>mm</i>			
616	LEU 69.22	-		(75.11%)	chi angles: 295.6,319.2	0.15Å	-	-
				General /				
				-60.0,-35.5				
				Favored	Favored (31.7%) <i>mm</i>			
617	ILE 88.33	-		(27.85%)	chi angles: 297.5,293	0.13Å	-	-
				Ile or Val /				
				-76.8,-37.2				
				Favored	OUTLIER (0.1%)			
618	GLU 108.29	-		(76.61%)	chi angles:	0.11Å	-	-
				General /				

-69.4,-41.2 177.3,14.2,245

619	LYS	78.66	-	Favored (90.88%) General / -60.0,-41.0	Allowed (0.4%) <i>tmm</i> chi angles: 215.7,160.7,315.7,315.7	0.13Å	-	-	-
620	GLU	120.08	-	Favored (75.25%) General / -63.6,-33.3	OUTLIER (0.2%) chi angles: 234.3,298.8,288.6	0.11Å	-	OUTLIER(S) worst is C-N- CA: 4.6 σ	-
621	ARG	164.6	-	Favored (72.19%) General / -65.3,-31.2	Favored (9.2%) <i>tmm170</i> chi angles: 211.3,183.6,294.4,144.4	0.06Å	-	-	-

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Avg: 102.92			Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167
622	ASP	78.07	-	Favored (97.01%) General / -63.0,-40.2	OUTLIER (0%) chi angles: 240.8,300.6	0.09Å	-	-	-
623	LEU	85.43	-	Favored (45.11%) General / -78.7,-29.0	Favored (5.1%) <i>mp</i> chi angles: 285.2,69.9	0.17Å	-	-	-
624	GLU	118.62	-	Favored (67.29%) General / -71.8,-32.2	OUTLIER (0.3%) chi angles: 106.5,168.3,297.1	0.18Å	-	-	-
625	ARG	109.43	-	Favored (72.51%) General / -56.2,-39.4	Favored (4.2%) <i>ptt-90</i> chi angles: 92.2,202.9,203.6,287.4	0.15Å	-	-	-
626	SER	88.12	-	Favored (52.59%) General / -79.1,-18.8	Favored (71.7%) <i>m</i> chi angles: 296	0.16Å	-	-	-
627	ARG	86.45	-	Favored (3.73%) General / -106.5,-47.6	Favored (85.2%) <i>mtm180</i> chi angles: 300.9,165.4,294.2,174.8	0.06Å	-	-	-
628	THR	151.47	-	Favored (14.97%) General / -91.0,-34.9	OUTLIER (0.2%) chi angles: 210	0.18Å	-	-	-
629	VAL	155.91	-	Favored (5.17%) Ile or Val / -90.9,-56.4	Allowed (0.7%) <i>m</i> chi angles: 314	0.38Å	-	OUTLIER(S) worst is N-CA-CB: 4.1 σ	-
630	ILE	150.51	-	Favored (20.78%) Ile or Val / -78.9,-49.1	Favored (10.4%) <i>pt</i> chi angles: 73.9,177.7	0.31Å	-	-	-

631	ALA	42.96	-	Favored (42.2%) General / -71.2,-49.6	-	0.11Å	-	-	-
632	LYS	106.71	-	Favored (90.36%) General / -66.0,-42.1	Favored (2.7%) <i>tpp</i> chi angles: 188.7,196.1,58.3,45.7	0.07Å	-	-	-
633	PHE	43.86	-	Favored (54.89%) General / -77.2,-30.9	Favored (96.7%) <i>m</i> - 80 chi angles: 292.9,89.9	0.20Å	-	-	-
634	GLN	50.8	-	Favored (95.98%) General / -64.5,-40.6	Favored (7.8%) <i>mt</i> 0 chi angles: 284,162.8,222.6	0.12Å	-	-	-
635	ASN	29.63	-	Favored (75.74%) General / -66.7,-46.4	Favored (46.5%) <i>m</i> - 40 chi angles: 294,359.2	0.11Å	-	-	-
636	LYS	90.89	-	Favored (84.46%) General / -64.2,-36.5	Favored (17.6%) <i>tptp</i> chi angles: 178.4,63.2,177.7,73.1	0.09Å	-	-	-
637	LEU	122.3	-	Favored (80.78%) General / -59.5,-48.7	Allowed (0.9%) <i>tm</i> chi angles: 184.4,276.7	0.04Å	-	-	-
638	LYS	59.49	-	Favored (90.08%) General / -58.7,-44.0	Favored (28.1%) <i>tttm</i> chi angles: 181.1,184,165.2,287.9	0.12Å	-	-	-
639	GLU	67.81	-	Favored (76.6%) General / -55.7,-43.5	Favored (61%) <i>mt</i> - 10 chi angles: 292.1,159,13.7	0.04Å	-	-	-
640	LEU	32.75	-	Favored (82.13%) General / -67.5,-37.0	Favored (75.8%) <i>mt</i> chi angles: 294.7,167.4	0.05Å	-	-	-
641	VAL	27.66	-	Favored (65.7%) Ile or Val / -64.6,-33.8	Favored (94.1%) <i>t</i> chi angles: 174.7	0.19Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 102.92				Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167

642	GLU	29.7	-	Favored (25.26%) General / -84.2,-31.0	Favored (18.6%) <i>mt</i> - 10 chi angles: 284.6,158.1,322.2	0.14Å	-	-	-
				Favored (96.91%)	Favored (26.3%) <i>tp</i> 30				

643	GLU	26.29	-	General / -64.3,-40.9	chi angles: 180.1,47.1,35.9	0.08Å	-	-	-
644	ASN	96.16	-	Favored (65.76%) General / -67.2,-23.2	Favored (13.1%) <i>p0</i> chi angles: 67.7,64.8	0.31Å	-	OUTLIER(S) worst is CA- CB-CG: 7.2 σ	-
645	LYS	129.16	-	Favored (73.78%) General / -69.4,-43.2	Favored (13.5%) <i>mmtm</i> chi angles: 306.6,306.9,166.8,281.4	0.17Å	-	-	-
646	GLN	80.68	-	Favored (76.31%) General / -67.6,-34.1	Allowed (1%) <i>pt0</i> chi angles: 89.4,158.3,3.5	0.22Å	-	-	-
647	LEU	44.3	-	Favored (80.93%) General / -68.0,-37.0	Favored (74.7%) <i>mt</i> chi angles: 300.8,173.3	0.11Å	-	-	-
648	GLU	64.6	-	Favored (69.69%) General / -66.2,-48.8	Favored (4.6%) <i>tp30</i> chi angles: 165.2,44.2,65.6	0.11Å	-	-	-
649	GLU	65.93	-	Favored (75.49%) General / -61.0,-34.9	Favored (29.2%) <i>mm-30</i> chi angles: 296.2,319.3,309.5	0.12Å	-	-	-
650	GLY	34.03	-	Favored (64.69%) Glycine / -62.7,-23.0	-	-	-	-	-
651	MET	87.5	-	Favored (31.59%) General / -80.2,-38.1	Favored (15.7%) <i>mtm</i> chi angles: 299.5,202.2,270.4	0.07Å	-	-	-
652	LYS	46.7	-	Favored (74.13%) General / -60.9,-34.1	Favored (36.7%) <i>mttp</i> chi angles: 302,190.5,187.7,71	0.18Å	-	-	-
653	GLU	40.6	-	Favored (18.01%) General / -47.8,-52.6	Favored (32.4%) <i>mt-10</i> chi angles: 287.4,177.7,248.4	0.15Å	-	-	-
654	ILE	97.16	-	Favored (16.36%) Ile or Val / -76.7,-26.4	Favored (16.5%) <i>mm</i> chi angles: 308.9,310.3	0.14Å	-	-	-
655	LEU	131.01	-	Favored (79.27%) General / -66.3,-35.0	Favored (81.7%) <i>mt</i> chi angles: 300.5,175.4	0.14Å	-	-	-
656	GLN	25.91	-	Favored (99.3%) General / -62.8,-41.5	Favored (82.4%) <i>mt0</i> chi angles: 292,176.5,25.6	0.09Å	-	-	-
				Favored					

657	ALA	28.87	-	(97.3%) General / -64.0,-40.8	-	0.09Å	-	-	-
658	ILE	93.74	-	Favored (82.87%) Ile or Val / -65.5,-38.6	Allowed (0.6%) <i>tt</i> chi angles: 204.6,189.4	0.22Å	-	-	-
659	LYS	134.72	0.50Å NZ with 660 GLU OE2	Favored (71.9%) General / -54.7,-42.9	Favored (7.1%) <i>tppp</i> chi angles: 182.7,183.9,59,52.1	0.05Å	-	-	-
660	GLU	41.1	0.50Å OE2 with 659 LYS NZ	Favored (59.97%) General / -75.7,-36.2	Favored (26.5%) <i>mm-30</i> chi angles: 283.5,314.6,315.7	0.19Å	-	-	-
661	MET	123.09	-	Favored (24.88%) General / -97.5,14.9	Favored (48%) <i>mtt</i> chi angles: 298.4,189.2,175.2	0.07Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 102.92	Clashscore: 1.8	Outliers: 4 of 166	Poor rotamers: 9 of 155	Outliers: 7 of 162	Outliers: 0 of 168	Outliers: 12 of 168	Non-Trans: 1 of 167
662	GLN	134.93	-	Favored (38.38%) General / -82.3,-19.9	Favored (5.7%) <i>tt0</i> chi angles: 182.1,151,257.2	0.06Å	-	-	-
663	LYS	283.71	-	Favored (6.36%) General / -90.5,78.4	Favored (10.7%) <i>pttm</i> chi angles: 45.8,174.5,185.7,294.3	0.07Å	-	-	-
664	ASP	196.82	-	Favored (35.05%) Pre-Pro / -116.7,145.3	Favored (2.6%) <i>m-30</i> chi angles: 317.7,306.5	0.08Å	-	-	-
665	PRO	82.41	-	Favored (19.57%) Trans-Pro / -74.9,-17.6	Favored (20.4%) <i>Cg_endo</i> chi angles: 36.9	0.07Å	-	-	-
666	ASP	51.07	-	Favored (57.76%) General / -75.8,-20.9	Allowed (0.9%) <i>m-30</i> chi angles: 315.7,63.6	0.05Å	-	-	-
667	VAL	41.76	0.41Å HG22 with 549 ARG HD2	Favored (82.04%) Ile or Val / -64.5,-38.2	Favored (57.1%) <i>t</i> chi angles: 170.4	0.07Å	-	-	-
668	LYS	80.05	-	Favored (62.77%) General / -73.0,-42.8	Favored (5.1%) <i>tppp</i> chi angles: 182.9,194,60.6,53.3	0.04Å	-	-	-
669	GLY	210.81	-	Favored (21.33%) Glycine /	-	-	-	-	-

64.6,-171.1

Favored

(5.28%)

Glycine /

85.3,-27.1

Favored

(85.31%)

General /

-60.1,-39.1

Favored

(61.89%)

General /

-55.5,-31.2

Favored

(64.98%)

General /

-57.4,-30.4

Favored

(65.99%)

General /

-59.7,-26.9

Favored

(75.13%)

Ile or Val /

-67.0,-35.6

Favored

(2.57%)

Pre-Pro /

-71.7,-33.4

Favored

(72.72%)

Trans-Pro /

-63.0,-33.9

Favored

(81.96%)

General /

-63.4,-35.9

Favored

(77.04%)

General /

-55.9,-47.6

Favored

(97.87%)

General /

-62.8,-43.8

Favored

(85.68%)

General /

-58.4,-41.7

Favored (35.2%)

mm-30

chi angles:

308.6,306,310.7

Allowed (1.7%) *p*

chi angles: 41.5

Favored (30.9%) *m*

chi angles: 302.8

Favored (75.5%) *mt*

chi angles: 300,172.3

Favored (3.8%) *mt*

chi angles: 302.2,143.5

Favored (13.1%) *tt*

chi angles: 198.7,170.6

Favored (45.8%)

Cg_exo

chi angles: 327.5

Favored (20.5%) *m*

chi angles: 304.6

Allowed (1.5%) *mp*

chi angles: 268.8,79.1

Allowed (1.2%) *tt0*

chi angles:

187.5,219.9,335.2

Favored (5.8%)

mmt-90

chi angles:

301.7,299.6,155.5,281.3

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
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Avg: 102.92
 Clashscore: 1.8
 Outliers: 4 of 166
 Poor rotamers: 9 of 155
 Outliers: 7 of 162
 Outliers: 0 of 168
 Outliers: 12 of 168
 Outliers: 12 of 167
 Trans: 1 of 167

682	LEU 134.53	-	Favored (69.97%) General / -70.9,-42.4	Favored (17.5%) <i>tp</i> chi angles: 191.3,68.7	0.07Å	-	-	-
683	VAL 34.75	-	Favored (87.09%) Ile or Val / -58.5,-43.6	Favored (24.2%) <i>t</i> chi angles: 164.9	0.10Å	-	-	-
684	ASN 77.82	-	Favored (18.2%) General / -74.4,-0.7	Favored (19.6%) <i>m-40</i> chi angles: 306.5,338.5	0.10Å	-	-	-
685	ALA 36.12	-	Favored (40.47%) General / -102.0,5.2	-	0.03Å	-	-	-
686	ILE 111.65	-	Favored (32.49%) Ile or Val / -117.0,142.1	Favored (15.9%) <i>mm</i> chi angles: 314,304.8	0.10Å	-	-	-
687	GLU 77.31	-	Favored (58.01%) General / -62.2,136.6	Favored (15%) <i>mt-10</i> chi angles: 307.7,191.4,84.2	0.12Å	-	-	-
688	SER 61.66	-	Favored (57.4%) General / -78.3,-7.6	Favored (27.6%) <i>p</i> chi angles: 54.3	0.09Å	-	OUTLIER(S) worst is C-N- CA: 5.5 σ	-
689	LYS 47.78	-	-	Allowed (1.3%) <i>tppp</i> chi angles: 177.5,209.7,51.6,50.1	0.15Å	-	-	-

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