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All-Atom Contacts	Clashscore, all atoms:	0.8	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	29	14.15%	Goal: <0.3%
	Favored rotamers	154	75.12%	Goal: >98%
	Ramachandran outliers	6	2.64%	Goal: <0.05%
	Ramachandran favored	201	88.55%	Goal: >98%
	MolProbity score [^]	2.21		64 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	8	3.67%	Goal: 0
	Bad bonds:	0 / 1906	0.00%	Goal: 0%
	Bad angles:	18 / 2575	0.70%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	0 / 8	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	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: Clashscore: 83.62 Outliers: 6 of 227 Poor rotamers: 29 of 205 Outliers: 8 of 218 Outliers: 0 of 229 Outliers: 16 of 228 Non-Trans: 0 of 228									
20	ILE	23.64	-	-	OUTLIER (0.1%) chi angles: 265.7,182.7	0.28Å	-	OUTLIER(S) worst is C-CA-CB: 4.2 σ	-
21	LYS	50.69	-	Allowed (0.87%) General / -40.1,118.2	Favored (32.8%) <i>mtmt</i> chi angles: 287.7,173.5,280.9,172.7	0.10Å	-	-	-
22	ALA	19.75	-	Favored (2.63%) General / -48.9,-60.6	-	0.12Å	-	-	-
23	GLY	22.3	-	Favored (24.31%) Glycine / -80.7,-35.8	-	-	-	-	-
24	PRO	125.66	-	Favored (56.1%) Trans-Pro / -66.2,-21.0	Favored (7.9%) <i>Cg_exo</i> chi angles: 323.8	0.05Å	-	-	-
				Favored	Favored (42.2%)				

25	MET	46.45	-	(5.09%) Pre-Pro / -50.9,150.6	<i>mtm</i> chi angles: 277.7,192.5,285.2	0.08Å	-	-	-
26	PRO	86.37	-	Allowed (1.31%) Trans-Pro / -77.8,89.8	Favored (59.3%) <i>Cg_endo</i> chi angles: 32	0.05Å	-	-	-
27	LYS	38.12	-	Favored (64.61%) General / -52.3,-43.7	Favored (19%) <i>mtmm</i> chi angles: 300.9,170.4,304.3,301	0.06Å	-	-	-
28	HIS	56.4	-	Favored (18.42%) General / -124.0,113.5	Favored (11.9%) <i>t</i> - <i>170</i> chi angles: 181.4,176	0.08Å	-	-	-
29	ILE	39.9	-	Favored (7.91%) Ile or Val / -98.7,146.6	Favored (74.5%) <i>mt</i> chi angles: 300.1,174.7	0.07Å	-	-	-
30	ALA	35.16	-	Favored (5.23%) General / -125.7,97.6	-	0.05Å	-	-	-
31	PHE	57.83	-	Favored (29.42%) General / -87.8,120.7	Favored (61.4%) <i>m</i> - <i>80</i> chi angles: 305.9,100.5	0.10Å	-	-	-
32	ILE	159.94	-	Favored (17.42%) Ile or Val / -100.6,105.3	Allowed (0.4%) <i>tt</i> chi angles: 163.6,170.8	0.16Å	-	-	-
33	MET	80.72	-	Favored (12.04%) General / -65.2,120.1	Favored (60.1%) <i>mtt</i> chi angles: 298,182.4,173.9	0.08Å	-	-	-
34	ASP	73.54	-	Favored (44.22%) General / -149.0,159.4	Favored (27.9%) <i>t0</i> chi angles: 199.8,3.1	0.06Å	-	-	-
35	GLY	38.43	-	Favored (57.31%) Glycine / 95.4,10.1	-	-	-	-	-
36	ASN	43.14	-	Favored (87.21%) General / -65.3,-37.5	Favored (2.5%) <i>m110</i> chi angles: 315.3,71.9	0.15Å	-	-	-
37	ARG	94.09	-	Favored (39.6%) General / -80.9,-22.5	Favored (6.8%) <i>ttt180</i> chi angles: 198.6,177,202.5,223.9	0.17Å	-	-	-
38	ARG	107.27	-	Favored (87.1%) General / -67.0,-39.2	Favored (47.7%) <i>mtt90</i> chi angles: 299.8,175.4,174,111.5	0.10Å	-	-	-

39	TYR	37.54	-	Favored (72.51%) General / -71.0,-38.2	Favored (87.1%) <i>t80</i> chi angles: 180.7,76.4	0.04Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 83.62				Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229
				Non-Trans: 0 of 228					
40	ALA	27.59	-	Favored (66.08%) General / -56.9,-32.7	-	0.06Å	-	-	-
41	LYS	91.73	-	Favored (73.4%) General / -66.2,-32.1	Allowed (1.4%) <i>tptp</i> chi angles: 184,67.4,226.8,77.7	0.11Å	-	-	-
42	LYS	91.28	-	Favored (67.91%) General / -72.7,-37.6	Favored (52.5%) <i>mtmt</i> chi angles: 295.8,190.9,291.4,177.3	0.12Å	-	-	-
43	CYS	58.04	-	Favored (51.53%) General / -78.6,-19.9	Favored (14.7%) <i>m</i> chi angles: 310	0.10Å	-	-	-
44	GLN	65.91	-	Favored (10.85%) General / 65.3,30.9	OUTLIER (0%) chi angles: 232.3,316.6,120.5	0.14Å	-	-	-
45	VAL	38.5	-	Favored (12.22%) Ile or Val / -117.7,166.2	Favored (67.1%) <i>t</i> chi angles: 179.1	0.12Å	-	-	-
46	GLU	78.33	-	Favored (31.4%) General / -76.9,157.5	Favored (2.9%) <i>tp30</i> chi angles: 185.8,51.8,113.9	0.06Å	-	OUTLIER(S) worst is C-N- CA: 5.3 σ	-
47	ARG	185.53	-	OUTLIER (0.04%) General / -56.5,0.0	OUTLIER (0%) chi angles: 71.2,205.2,110.3,136.9	0.10Å	-	-	-
48	GLN	47.19	-	Favored (32.26%) General / -84.5,-20.0	Favored (79.1%) <i>mt0</i> chi angles: 295.6,184.1,347.9	0.17Å	-	-	-
49	GLU	108.83	-	Favored (78.68%) General / -56.1,-44.1	OUTLIER (0.3%) chi angles: 160.8,287.9,296.6	0.07Å	-	-	-
50	GLY	21.77	-	Favored (8.52%) Glycine / -67.1,0.1	-	-	-	-	-
51	HIS	66.26	-	Favored (10.92%)	Favored (2.7%) <i>m-70</i>	0.12Å	-	-	-

				General / -101.2,-31.6	chi angles: 318.6,321				
52	SER	73.09	-	Favored (68.26%) General / -67.7,-47.8	Favored (52.5%) <i>m</i> chi angles: 300.7	0.08Å	-	-	-
53	GLN	81.23	-	Favored (59.5%) General / -74.5,-25.7	Favored (18.4%) <i>tp40</i> chi angles: 171.4,49.2,17.3	0.13Å	-	-	-
54	GLY	44.78	-	Favored (71.42%) Glycine / -54.9,-40.2	-	-	-	-	-
55	PHE	104.14	0.42Å CD1 with 100 LYS HE2	Favored (73.76%) General / -68.9,-44.1	OUTLIER (0.2%) chi angles: 97.2,74.6	0.17Å	-	-	-
56	ASN	65.29	-	Favored (79.08%) General / -56.1,-44.4	Favored (7.6%) <i>t0</i> chi angles: 165.7,264.8	0.05Å	-	-	-
57	LYS	132.64	-	Favored (88.36%) General / -66.6,-39.4	OUTLIER (0%) chi angles: 225.4,291.4,95.7,163.4	0.05Å	-	-	-
58	LEU	46.79	-	Favored (68.54%) General / -55.0,-50.6	Favored (69.2%) <i>tp</i> chi angles: 177.2,63.5	0.04Å	-	-	-
59	ALA	31.08	-	Favored (86.57%) General / -59.5,-47.2	-	0.07Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 83.62				Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229
									Non-Trans: 0 of 228
60	GLU	96.63	-	Favored (86.29%) General / -67.2,-40.8	Favored (15.4%) <i>tp30</i> chi angles: 175.3,44.3,33.9	0.15Å	-	-	-
61	THR	99.88	-	Favored (83.49%) General / -57.1,-44.7	OUTLIER (0.1%) chi angles: 270.7	0.18Å	-	-	-
62	LEU	92.65	-	Favored (75.24%) General / -66.6,-33.2	Allowed (0.6%) <i>mp</i> chi angles: 275.4,37.5	0.09Å	-	-	-
63	ARG	96.87	-	Favored (68.35%) General / -72.1,-40.2	Favored (13.9%) <i>ttp80</i> chi angles: 194.6,218,59.7,65	0.05Å	-	-	-

64	TRP 141.47	-	Favored (83.78%) General / -67.9,-39.1	Favored (26.7%) <i>t</i> - 100 chi angles: 179.5,281.6	0.12Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.0 σ	-
65	CYS 29.36	-	Favored (64.76%) General / -55.8,-33.9	Favored (44.1%) <i>m</i> chi angles: 284	0.12Å	-	-	-
66	LEU 119.74	-	Favored (92.57%) General / -65.4,-39.7	Favored (56.4%) <i>tp</i> chi angles: 181.6,57.9	0.08Å	-	-	-
67	ASN 93.22	-	Favored (32.27%) General / -83.6,-22.6	Allowed (0.3%) <i>p0</i> chi angles: 61.4,249.7	0.20Å	-	OUTLIER(S) worst is CA- CB-CG: 4.7 σ	-
68	LEU 108.71	-	Favored (15.49%) General / -90.6,-34.5	Favored (3.3%) <i>tt</i> chi angles: 194.6,145.8	0.14Å	-	-	-
69	GLY 38.41	-	Favored (4.92%) Glycine / 111.2,25.7	-	-	-	-	-
70	ILE 126.46	-	Favored (30.48%) Ile or Val / -79.2,133.2	Favored (37.6%) <i>mm</i> chi angles: 304.4,306.1	0.05Å	-	-	-
71	LEU 69.62	-	Favored (8.26%) General / -85.5,-49.2	Favored (8.8%) <i>mt</i> chi angles: 317.3,180.9	0.10Å	-	-	-
72	GLU 81.06	-	Favored (46.08%) General / -123.1,148.1	Allowed (1.9%) <i>mp0</i> chi angles: 265.7,83.4,23.7	0.11Å	-	-	-
73	VAL 45.43	-	Favored (17.2%) Ile or Val / -142.6,128.3	OUTLIER (0.2%) chi angles: 149.7	0.09Å	-	-	-
74	THR 109.79	-	Favored (51.41%) General / -111.2,135.6	Favored (10.7%) <i>t</i> chi angles: 186.6	0.13Å	-	-	-
75	VAL 46.1	-	Favored (74.59%) Ile or Val / -123.0,127.1	OUTLIER (0.2%) chi angles: 148.8	0.10Å	-	-	-
76	TYR 169.54	-	Favored (13.15%) General / -90.7,100.3	Allowed (0.3%) <i>t80</i> chi angles: 209.7,358.7	0.03Å	-	-	-
77	ALA 66.17	-	Favored (12.08%) General /	-	0.08Å	-	-	-

					-103.3,-28.1								
78	PHE	112.99	-		Favored (20.97%) General / -159.5,151.7	Favored (48.2%) <i>t80</i> chi angles: 184.4,62.6	0.03Å	-	-	-			
79	SER	132.05	0.42Å HA with 156 TYR O		Favored (45.08%) General / -135.2,158.2	Favored (42.2%) <i>t</i> chi angles: 178.3	0.11Å	-	-	-			
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides				
Avg: 83.62				Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228			
80	ILE	138.09	-		Favored (30.02%) Ile or Val / -70.9,-27.4	Favored (22.6%) <i>mt</i> chi angles: 311.1,177.9	0.10Å	-	-	-			
81	GLU	170.75	-		Favored (88.53%) General / -66.7,-40.6	Allowed (1.7%) <i>tp30</i> chi angles: 198.9,69.7,111.1	0.14Å	-	-	-			
82	ASN	216.87	-		Favored (35.69%) General / -73.2,-4.9	Favored (67.1%) <i>m-40</i> chi angles: 287.9,307.1	0.11Å	-	-	-			
83	PHE	181.42	-		Favored (60.29%) General / -75.8,-13.0	Favored (71.8%) <i>t80</i> chi angles: 184.2,252.5	0.13Å	-	-	-			
84	LYS	170.56	-		Favored (8.16%) General / -88.5,15.3	OUTLIER (0%) chi angles: 277,74.8,75,276.1	0.13Å	-	-	-			
85	ARG	171.09	-		Favored (9.09%) General / -71.2,172.5	Favored (81.7%) <i>mtt180</i> chi angles: 290.7,181.3,181.8,198.1	0.05Å	-	-	-			
86	SER	85.67	-		Allowed (1.73%) General / -45.0,142.8	Favored (4.6%) <i>m</i> chi angles: 311.4	0.09Å	-	-	-			
87	LYS	125.34	-		Favored (79.2%) General / -59.2,-38.1	Favored (43.6%) <i>tttp</i> chi angles: 175.9,166.2,171.4,64.5	0.21Å	-	-	-			
88	SER	32.87	-		Favored (59.22%) General / -51.9,-39.5	Favored (51.9%) <i>p</i> chi angles: 56.7	0.08Å	-	-	-			
89	GLU	163.12	-		Favored (74.49%) General / -69.0,-43.6	OUTLIER (0%) chi angles: 252.4,297.1,246.2	0.12Å	-	-	-			
					Favored								

90	VAL	104.43	-	Favored (61.17%) Ile or Val / -71.7,-46.5	Favored (3.3%) <i>m</i> chi angles: 309.7	0.28Å	-	-	-
91	ASP	69.22	-	Favored (97.29%) General / -64.1,-41.4	Allowed (0.8%) <i>m</i> -30 chi angles: 302.2,31.1	0.11Å	-	-	-
92	GLY	22.82	-	Favored (72.94%) Glycine / -70.4,-27.3	-	-	-	-	-
93	LEU	66.25	-	Favored (68.8%) General / -72.1,-34.6	Favored (10.3%) <i>mt</i> chi angles: 282.4,154.5	0.13Å	-	-	-
94	MET	109.79	-	Favored (62.55%) General / -65.0,-51.3	Favored (68.4%) <i>mtt</i> chi angles: 293.6,176.6,185.3	0.12Å	-	-	-
95	ASP	72.33	-	Favored (15.11%) General / -63.1,-56.6	Favored (18.2%) <i>t70</i> chi angles: 175.8,83.2	0.13Å	-	-	-
96	LEU	135.95	-	Favored (81.12%) General / -64.6,-35.5	Favored (47.9%) <i>mt</i> chi angles: 296.6,165.2	0.18Å	-	-	-
97	ALA	27.64	-	Favored (99.96%) General / -62.9,-43.0	-	0.07Å	-	-	-
98	ARG	98.95	-	Favored (66.41%) General / -69.5,-28.9	OUTLIER (0%) chi angles: 186,262.3,22.1,264.7	0.11Å	-	-	-
99	GLN	110.6	-	Favored (18.24%) General / -70.5,-53.0	Favored (3.2%) <i>tt0</i> chi angles: 205.1,183.2,119.1	0.06Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 83.62			Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
100	LYS	246.81	0.42Å HE2 with 55 PHE CD1	OUTLIER (0.01%) General / -178.2,0.2	Favored (8.2%) <i>ptmt</i> chi angles: 66.4,191,307.2,182.5	0.14Å	-	-	-
101	PHE	166.33	-	Favored (72%) General / -64.5,-31.0	Favored (27.8%) <i>t80</i> chi angles: 163,250.6	0.20Å	-	-	-
102	SER	100.55	-	Favored (3.02%) General / -113.4,38.0	Favored (25%) <i>p</i> chi angles: 78.5	0.14Å	-	OUTLIER(S) worst is C-N-CA: 5.5 σ	-

103	ARG 318.05	-	Favored (4.48%) General / 73.7,12.8	OUTLIER (0%) chi angles: 65.3,54.7,59.3,145.9	0.33Å	-	-	-
104	LEU 248.73	-	Allowed (0.09%) General / -82.8,-149.7	Allowed (0.8%) <i>mm</i> chi angles: 290.6,315.6	0.33Å	-	OUTLIER(S) worst is C-N- CA: 5.2 σ	-
105	MET 160.58	-	OUTLIER (0.01%) General / -11.6,-65.4	Favored (48.5%) <i>tpp</i> chi angles: 187.8,71.3,80.8	0.21Å	-	-	-
106	GLU 83.44	-	Favored (39.96%) General / -78.8,-37.9	Allowed (0.4%) <i>tm</i> - 30 chi angles: 203.7,309.4,291.9	0.09Å	-	-	-
107	GLU 71.44	-	Favored (42.28%) General / -79.8,-23.4	Favored (2.9%) <i>mt</i> - 10 chi angles: 268.6,201.1,26.1	0.06Å	-	-	-
108	LYS 148.79	-	Favored (50.31%) General / -49.8,-45.9	Favored (47.9%) <i>pttt</i> chi angles: 70.1,188.3,170.4,184.5	0.20Å	-	-	-
109	GLU 75.86	-	Favored (42.87%) General / -79.3,-24.3	OUTLIER (0%) chi angles: 135.9,295.2,327.8	0.21Å	-	-	-
110	LYS 42.43	-	Favored (66.48%) General / -71.8,-31.3	Favored (11.7%) <i>mttp</i> chi angles: 292.7,151.7,190.9,66.7	0.10Å	-	-	-
111	LEU 98.76	-	Favored (68.76%) General / -70.2,-31.4	Favored (5.3%) <i>mp</i> chi angles: 279,72.2	0.14Å	-	-	-
112	GLN 84.21	-	Favored (77.57%) General / -68.1,-35.0	Favored (89.6%) <i>mt0</i> chi angles: 298.1,172,317	0.12Å	-	-	-
113	LYS 101.02	-	Favored (69.92%) General / -65.8,-29.4	Favored (13.2%) <i>mmtp</i> chi angles: 308.9,297.1,162,57	0.14Å	-	-	-
114	HIS 100.14	-	Favored (60.5%) General / -74.8,-12.9	Favored (4.6%) <i>t-90</i> chi angles: 198.5,314.3	0.04Å	-	OUTLIER(S) worst is CA- CB-CG: 7.8 σ	-
115	GLY 29.32	-	Favored (84.83%) Glycine / 66.4,33.4	-	-	-	-	-
116	VAL 54.56	-	Favored (6.88%) Ile or Val /	OUTLIER (0.1%) chi angles: 146.2	0.11Å	-	-	-

-83.0,146.5

117	CYS	52.86	-	Favored (7.54%) General / -107.9,97.9	Favored (20.4%) <i>t</i> chi angles: 191.1	0.05Å	-	-	-
118	ILE	71.89	-	Favored (37.53%) Ile or Val / -127.5,144.4	Favored (12.9%) <i>tt</i> chi angles: 184.6,160.2	0.08Å	-	-	-
119	ARG	174.03	-	Favored (14.62%) General / -153.1,174.1	OUTLIER (0%) chi angles: 94.2,300.9,116.5,155.5	0.22Å	-	-	-

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120	VAL	99.09	-	Allowed (0.96%) Ile or Val / -73.8,173.0	Allowed (1.5%) <i>p</i> chi angles: 78.5	0.18Å	-	-	-	-
121	LEU	115.08	-	Favored (2.64%) General / -158.4,113.7	Favored (2.6%) <i>tp</i> chi angles: 182.7,39	0.09Å	-	-	-	-
122	GLY	27	-	Favored (24.88%) Glycine / 156.4,173.4	-	-	-	-	-	-
123	ASP	83.59	-	Favored (31.28%) General / -79.0,151.9	Favored (38.9%) <i>t0</i> chi angles: 192.3,355.8	0.06Å	-	-	-	-
124	LEU	101.71	-	Favored (56.38%) General / -76.0,-26.2	OUTLIER (0.2%) chi angles: 220,168.1	0.08Å	-	-	-	-
125	HIS	85.86	-	Favored (2.56%) General / -66.5,109.0	Favored (94.8%) <i>m-70</i> chi angles: 303.7,294.3	0.04Å	-	OUTLIER(S) worst is C-N-CA: 4.1 σ	-	-
126	LEU	245.68	-	Allowed (0.14%) General / 84.6,19.8	Allowed (0.9%) <i>mm</i> chi angles: 293.2,313.6	0.21Å	-	-	-	-
127	LEU	76.51	-	Favored (61.97%) Pre-Pro / -100.0,118.2	Favored (21.3%) <i>tp</i> chi angles: 189.8,57.1	0.11Å	-	-	-	-
128	PRO	88.69	-	Favored (23.1%) Trans-Pro / -77.0,143.4	Favored (67.6%) <i>Cg_endo</i> chi angles: 31.3	0.02Å	-	-	-	-
				Favored						

129	LEU	85.18	-	Favored (82.42%) General / -66.3,-36.2	Favored (35.8%) <i>tp</i> chi angles: 185.5,56.7	0.09Å	-	-	-
130	ASP	89.82	-	Favored (96.49%) General / -64.4,-41.6	Favored (22.8%) <i>p0</i> chi angles: 58,334	0.08Å	-	-	-
131	LEU	38.13	-	Favored (83.9%) General / -57.7,-46.8	Favored (2.2%) <i>tp</i> chi angles: 189.5,88.7	0.03Å	-	-	-
132	GLN	43.97	-	Favored (95.31%) General / -63.5,-39.8	Favored (28.5%) <i>mt0</i> chi angles: 284.4,169.1,100.8	0.10Å	-	-	-
133	GLU	69.96	-	Favored (97.17%) General / -64.0,-42.7	Favored (12%) <i>tm-30</i> chi angles: 189.6,291.7,328.3	0.07Å	-	-	-
134	LEU	53.28	-	Favored (69.51%) General / -68.1,-30.4	Favored (52.2%) <i>mt</i> chi angles: 301.5,184.9	0.17Å	-	-	-
135	ILE	91.94	-	Favored (97.07%) Ile or Val / -62.1,-43.0	Favored (11%) <i>mm</i> chi angles: 289.8,286	0.12Å	-	-	-
136	ALA	24.6	-	Favored (95.9%) General / -63.6,-40.0	-	0.09Å	-	-	-
137	GLN	64.47	-	Favored (82.41%) General / -59.4,-39.2	Favored (79.8%) <i>mt0</i> chi angles: 293.2,183.1,358.7	0.09Å	-	-	-
138	ALA	37.75	-	Favored (67.9%) General / -63.0,-51.1	-	0.08Å	-	-	-
139	VAL	30.64	-	Favored (70.58%) Ile or Val / -59.8,-37.3	Favored (48.4%) <i>t</i> chi angles: 169.2	0.15Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
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Avg: 83.62	Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
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140	GLN	89.19	-	Favored (72%) General / -57.1,-37.5	Allowed (0.6%) <i>tm130</i> chi angles: 207.2,301.1,117.9	0.12Å	-	-	-
141	ALA	57.16	-	Favored (17.55%) General /	-	0.10Å	-	-	-

				-92.3,-27.6				
				Favored				
142	THR	160.99	-	(60.66%)	OUTLIER (0%)	0.24Å	-	-
				General /	chi angles: 250.5			
				-56.5,-28.8				
				Favored	Favored (46.6%)			
143	LYS	97.47	-	(11.9%)	<i>mtmt</i>	0.10Å	-	-
				General /	chi angles:			
				-49.7,-31.8	296,180.3,298.2,188.9			
				Favored	Favored (9.8%)			
144	ASN	52.24	-	(22.34%)	<i>m110</i>	0.03Å	-	-
				General /	chi angles: 303.7,81.2			
				-109.6,16.2				
				Favored	Favored (22.8%) <i>m-</i>			
145	TYR	81.1	-	(14.8%)	<i>10</i>	0.08Å	-	-
				General /	chi angles: 292.8,161.6			
				-120.0,165.3				
				OUTLIER				
146	ASN	185.82	-	(0%)	Favored (7.5%) <i>p0</i>	0.17Å	-	-
				General /	chi angles: 49.3,6.8			
				166.3,25.4				
				Favored	OUTLIER (0%)			
147	LYS	116.48	-	(57.63%)	chi angles:	0.09Å	-	-
				General /	286.3,68.2,263.3,176.9			
				-78.6,-16.2				
				Allowed				
148	CYS	78.16	-	(0.26%)	Favored (47.4%) <i>t</i>	0.06Å	-	-
				General /	chi angles: 179.5			
				-176.0,133.2				
				Favored				
149	PHE	56.99	-	(47.7%)	Favored (11.4%) <i>t80</i>	0.06Å	-	-
				General /	chi angles: 187.2,108.6			
				-104.5,134.4				
				Favored				
150	LEU	54.8	-	(52.16%)	Favored (60.3%) <i>mt</i>	0.05Å	-	-
				General /	chi angles: 304.4,181.8			
				-131.6,150.4				
				Favored				
151	ASN	60.46	-	(44.8%)	Favored (76.1%) <i>m-</i>	0.12Å	-	-
				General /	<i>40</i>			
				-121.0,124.4	chi angles: 294.7,348.4			
				Favored				
152	VAL	53.8	-	(5.08%)	Favored (85.3%) <i>t</i>	0.03Å	-	-
				Ile or Val /	chi angles: 177.6			
				-92.1,95.0				
				Favored				
153	CYS	52.84	-	(8.94%)	Favored (61.5%) <i>m</i>	0.07Å	-	-
				General /	chi angles: 300.6			
				-79.3,102.9				
				Favored				
154	PHE	142.34	-	(35.31%)	Favored (10%) <i>t80</i>	0.04Å	-	-
				General /	chi angles: 192.8,288			
				-136.5,132.4				
				Favored				
155	ALA	51.37	-	(21.87%)	-	0.09Å	-	-
				General /				

156	TYR	75.18	0.42Å O with 79 SER HA	59.8,33.9 Favored (21.91%) General / -96.3,149.2	Favored (84.9%) <i>t80</i> chi angles: 179.8,83.6	0.06Å	-	-	-
157	THR	67.95	-	Allowed (0.47%) General / -172.0,121.8	OUTLIER (0.1%) chi angles: 275	0.05Å	-	-	-
158	SER	84.63	-	Favored (74.01%) General / -61.6,-33.5	Favored (94%) <i>p</i> chi angles: 64.2	0.15Å	-	-	-
159	ARG	80.19	-	Allowed (0.21%) General / -74.5,17.4	Favored (18.9%) <i>ptt-90</i> chi angles: 75.9,190.4,187.8,255.9	0.25Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 83.62	Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
160	HIS	69.86	-	Allowed (1.25%) General / -139.5,-9.7	OUTLIER (0%) chi angles: 237.7,59.4	0.21Å	-	-	-
161	GLU	40.66	-	Favored (70.61%) General / -70.5,-42.9	Favored (4.5%) <i>tt0</i> chi angles: 204.9,200.1,352.9	0.09Å	-	-	-
162	ILE	114.64	-	Favored (79.09%) Ile or Val / -65.5,-37.0	Favored (4.2%) <i>pt</i> chi angles: 68,188.6	0.21Å	-	-	-
163	SER	25.6	-	Favored (83.72%) General / -66.2,-36.7	Favored (73%) <i>p</i> chi angles: 59.3	0.13Å	-	-	-
164	ASN	25.29	-	Favored (45.35%) General / -78.6,-26.0	Favored (3.4%) <i>m-40</i> chi angles: 298.7,18.8	0.13Å	-	-	-
165	ALA	27.2	-	Favored (86.39%) General / -65.2,-45.1	-	0.05Å	-	-	-
166	VAL	77.38	-	Favored (50.52%) Ile or Val / -65.7,-30.6	Allowed (0.4%) <i>p</i> chi angles: 85.5	0.26Å	-	-	-
167	ARG	101.62	-	Favored (67.78%) General / -68.2,-29.0	Favored (4%) <i>tpm170</i> chi angles: 186.4,56.8,265.6,189.1	0.12Å	-	-	-

168	GLU	31.59	-	Favored (70.83%) General / -70.7,-42.2	OUTLIER (0%) chi angles: 192.2,269.7,52.8	0.13Å	-	-	-
169	MET	27.87	-	Favored (84.45%) General / -58.5,-41.1	Allowed (0.6%) <i>mpp</i> chi angles: 287.4,109.7,87.5	0.14Å	-	-	-
170	ALA	22.97	-	Favored (64.43%) General / -69.4,-26.0	-	0.12Å	-	-	-
171	TRP	32	-	Favored (69.42%) General / -65.4,-28.7	Favored (73.4%) <i>m100</i> chi angles: 292,116	0.21Å	-	-	-
172	GLY	15.12	-	Favored (9.01%) Glycine / -82.3,-41.9	-	-	-	-	-
173	VAL	25.04	-	Favored (82.57%) Ile or Val / -68.6,-41.0	Favored (73.9%) <i>t</i> chi angles: 178.4	0.17Å	-	-	-
174	GLU	58.08	-	Favored (58.97%) General / -75.6,-19.9	Favored (66.1%) <i>mt</i> - <i>10</i> chi angles: 293.9,162.8,15.9	0.07Å	-	-	-
175	GLN	74.23	-	Favored (16.27%) General / -113.5,4.5	Favored (23.9%) <i>mt0</i> chi angles: 297.3,184.6,113.9	0.08Å	-	-	-
176	GLY	18.73	-	Favored (59.73%) Glycine / 75.8,29.1	-	-	-	-	-
177	LEU	46.99	-	Favored (11.7%) General / -118.6,1.9	Favored (14.4%) <i>mt</i> chi angles: 313.5,174.5	0.06Å	-	-	-
178	LEU	56.54	-	Favored (13.92%) General / -159.1,141.4	Favored (5.2%) <i>tp</i> chi angles: 194.6,81.1	0.11Å	-	-	-
179	ASP	44.92	-	Favored (30.55%) Pre-Pro / -96.6,146.0	Favored (56.2%) <i>t0</i> chi angles: 177.9,2.7	0.11Å	-	OUTLIER(S) worst is CA- CB-CG: 5.9 σ	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 83.62				Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
					Favored (32.39%)	Favored (9.5%)				

180	PRO	65.4	-	Trans-Pro / -52.5,-27.5	Cg _{exo} chi angles: 324.2	0.07Å	-	-	-
181	SER	67.26	-	Favored (66.52%) General / -58.3,-30.2	Favored (10.7%) <i>m</i> chi angles: 308	0.11Å	-	-	-
182	ASP	51.31	-	Favored (24.26%) General / -70.0,-5.2	Favored (7.3%) <i>m</i> - 30 chi angles: 309.7,338.2	0.07Å	-	-	-
183	ILE	75.08	-	Allowed (0.17%) Ile or Val / -76.7,63.4	Favored (93.8%) <i>mt</i> chi angles: 294.8,167	0.16Å	-	-	-
184	SER	79.03	-	Favored (11.11%) General / -92.3,168.8	Favored (9.9%) <i>t</i> chi angles: 191	0.04Å	-	-	-
185	GLU	72.66	-	Favored (90.08%) General / -60.5,-40.1	OUTLIER (0%) chi angles: 110,77.5,14.1	0.15Å	-	-	-
186	SER	70.87	-	Favored (79.38%) General / -68.0,-36.1	Favored (23.7%) <i>p</i> chi angles: 53.4	0.09Å	-	-	-
187	LEU	140.02	-	Favored (50.65%) General / -78.4,-20.7	OUTLIER (0.1%) chi angles: 299.5,218.7	0.21Å	-	-	-
188	LEU	72.96	-	Favored (91.54%) General / -59.0,-45.0	Favored (5.9%) <i>mp</i> chi angles: 266.1,63.1	0.13Å	-	-	-
189	ASP	35.81	-	Favored (78.58%) General / -65.9,-34.6	Favored (27.9%) <i>m</i> - 30 chi angles: 293.8,285.3	0.20Å	-	-	-
190	LYS	68.33	-	Favored (76.39%) General / -56.5,-48.8	Favored (5.6%) <i>tpp</i> chi angles: 180.2,199.1,74.5,75.5	0.07Å	-	-	-
191	CYS	75.51	-	Favored (42.91%) General / -79.3,-24.2	Favored (54.5%) <i>m</i> chi angles: 302.5	0.09Å	-	-	-
192	LEU	55.65	-	Favored (45.29%) General / -67.2,152.7	Favored (21.1%) <i>mt</i> chi angles: 288.7,157.9	0.08Å	-	-	-
193	TYR	45.28	-	Favored (75.19%) General / -61.8,-34.0	Favored (4.2%) <i>t80</i> chi angles: 192.3,114.3	0.09Å	-	-	-

194	THR	135.08	-	Favored (3.2%) General / -95.3,27.6	Favored (8.1%) <i>t</i> chi angles: 193.3	0.22Å	-	-	-
195	ASN	90.8	-	Favored (3.18%) General / -41.5,-45.4	Favored (28.7%) <i>p0</i> chi angles: 56.1,12.6	0.14Å	-	OUTLIER(S) worst is CA- CB-CG: 4.1 σ	-
196	ARG	115.13	-	Favored (2.26%) General / -75.0,84.0	OUTLIER (0%) chi angles: 198.5,291.2,91.9,198.3	0.07Å	-	-	-
197	SER	90.23	-	Allowed (0.73%) Pre-Pro / -179.4,154.2	Favored (40%) <i>t</i> chi angles: 177.9	0.09Å	-	-	-
198	PRO	72.55	-	Favored (8.45%) Trans-Pro / -85.9,170.7	Favored (8.4%) <i>Cg_endo</i> chi angles: 39.4	0.07Å	-	-	-
199	HIS	89.01	-	Favored (99.11%) Pre-Pro / -66.6,147.1	Favored (66.8%) <i>m90</i> chi angles: 291.5,73.6	0.03Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
Avg: 83.62			Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
200	PRO	122.94	-	Favored (74.2%) Trans-Pro / -58.5,149.6	Favored (4%) <i>Cg_exo</i> chi angles: 323.1	0.05Å	-	-	-
201	ASP	63.69	-	Favored (9.93%) General / -94.8,-40.0	Favored (10.1%) <i>m-30</i> chi angles: 283.1,19.7	0.06Å	-	-	-
202	ILE	93.63	-	Favored (11.17%) Ile or Val / -150.1,135.7	Favored (10.7%) <i>tt</i> chi angles: 201,168.7	0.12Å	-	-	-
203	LEU	99.6	-	Favored (51.51%) General / -104.3,131.6	Favored (5.6%) <i>tt</i> chi angles: 188.8,144.9	0.10Å	-	-	-
204	ILE	106.77	-	Favored (65.45%) Ile or Val / -112.5,130.8	Favored (33.2%) <i>mm</i> chi angles: 309.1,304.5	0.12Å	-	-	-
205	ARG	93.68	-	Favored (7.5%) General / -131.1,105.1	Favored (52.6%) <i>ttt180</i> chi angles: 191.3,160,177.5,177.6	0.06Å	-	-	-
206	THR	47.29	-	Favored (54.13%) General /	Favored (14.1%) <i>p</i> chi angles: 47.5	0.04Å	-	OUTLIER(S) worst is C-N- CA: 5.7 σ	-

-69.4,140.9

OUTLIER

207	SER	80.64	-	(0.04%) General / 90.0,19.0 Favored (85.38%) Glycine / 77.8,11.5	Favored (68.2%) <i>p</i> chi angles: 72.2	0.31Å	-	-	-
208	GLY	29.06	-	(6.17%) General / -81.5,88.6	Allowed (1.8%) <i>mm</i> - 30 chi angles: 276.2,281.7,39.7	0.06Å	-	-	-
209	GLU	85.58	-	(0.06%) lle or Val / -64.9,86.0	Favored (6.1%) <i>p</i> chi angles: 58.9	0.17Å	-	-	-
210	VAL	112.57	-	Allowed (1.08%) General / -176.7,153.1	Allowed (0.4%) <i>mtm110</i> chi angles: 255.4,140.8,292.6,124.1	0.07Å	-	-	-
211	ARG	177.53	-	Favored (27.96%) General / -81.1,-38.0	Favored (91.9%) <i>mt</i> chi angles: 291.2,172.8	0.09Å	-	-	-
212	LEU	66.55	-	Favored (28.33%) General / 53.2,45.6	Favored (48.4%) <i>m</i> chi angles: 291.1	0.15Å	-	-	-
213	SER	66.43	-	Favored (14.7%) General / 61.8,38.7	Allowed (1.3%) <i>m</i> - 30 chi angles: 300.7,49.2	0.09Å	-	-	-
214	ASP	106.44	-	Favored (17.74%) General / -100.4,106.2	Favored (3.9%) <i>t80</i> chi angles: 190.3,27.9	0.04Å	-	-	-
215	PHE	80.77	-	Favored (17.73%) General / 49.0,50.5	OUTLIER (0.2%) chi angles: 301.4,216.6	0.10Å	-	-	-
216	LEU	71.62	-	Favored (64.97%) General / -52.0,-47.3	Favored (60%) <i>tp</i> chi angles: 180.7,58.7	0.09Å	-	-	-
217	LEU	74.59	-	Favored (58.36%) General / -74.2,-43.1	Favored (62.1%) <i>t</i> - 100 chi angles: 183,265	0.06Å	-	OUTLIER(S) worst is CE3- CD2-CG: 5.0 σ	-
218	TRP	68.25	-	Favored (77.11%) General / -68.2,-43.8	Favored (10.4%) <i>mp10</i> chi angles: 306.7,81.4,0.5	0.14Å	-	-	-
219	GLN	101.42	-						

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

		Avg: 83.62	Clashscore: 0.8	Outliers: 6 of 227	Poor rotamers: 29 of 205	Outliers: 8 of 218	Outliers: 0 of 229	Outliers: 16 of 229	Non-Trans: 0 of 228
220	THR	167.95	-	Favored (58.22%) General / -82.1,-5.2	OUTLIER (0%) chi angles: 217.4	0.19Å	-	-	-
221	SER	89.87	-	Favored (69.53%) General / -58.9,-32.4	Favored (89.6%) <i>p</i> chi angles: 66.8	0.11Å	-	-	-
222	HIS	138.29	-	Allowed (1.08%) General / -90.9,31.4	Allowed (1.7%) <i>m90</i> chi angles: 301.5,44.9	0.07Å	-	OUTLIER(S) worst is CA-CB-CG: 8.4 σ	-
223	SER	80.7	-	Favored (29.21%) General / -138.1,164.4	Favored (23.8%) <i>t</i> chi angles: 184.6	0.11Å	-	-	-
224	CYS	70.71	-	Favored (8.66%) General / -93.2,171.9	Favored (30.7%) <i>t</i> chi angles: 189.2	0.07Å	-	-	-
225	LEU	83.49	-	Favored (41.63%) General / -146.4,154.4	Allowed (1.8%) <i>mp</i> chi angles: 311.5,89.6	0.08Å	-	-	-
226	VAL	99.51	-	Allowed (1.78%) Ile or Val / -152.9,129.2	Favored (9.8%) <i>p</i> chi angles: 62.9	0.12Å	-	-	-
227	PHE	47.73	-	Allowed (0.9%) General / -105.1,70.5	Allowed (1.9%) <i>m-80</i> chi angles: 324.7,285.9	0.07Å	-	-	-
228	GLN	50.74	-	Favored (77.39%) Pre-Pro / -56.7,138.5	Favored (28.6%) <i>mt0</i> chi angles: 302.2,189.9,256.4	0.05Å	-	-	-
229	PRO	124.45	-	Favored (9.91%) Trans-Pro / -77.6,-23.3	Favored (47.5%) <i>Cg_endo</i> chi angles: 33.3	0.08Å	-	-	-
230	VAL	90.33	-	Favored (18.35%) Ile or Val / -64.5,141.3	Favored (7.1%) <i>p</i> chi angles: 68.6	0.10Å	-	-	-
231	LEU	99.8	0.42Å HB2 with 234 GLU OE1	Favored (21.72%) General / -81.4,164.9	OUTLIER (0%) chi angles: 300.3,35	0.04Å	-	-	-
232	TRP	71.59	-	Favored (97.77%) Pre-Pro / -55.4,-47.8	Favored (67.9%) <i>t-100</i> chi angles: 181.4,261.7	0.22Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.7 σ	-

233	PRO	76.42	-	Favored (62.14%) Trans-Pro / -61.4,-38.8	Favored (59.7%) <i>Cg_exo</i> chi angles: 328.4	0.08Å	-	-	-
234	GLU	91.99	0.42Å OE1 with 231 LEU HB2	Favored (38.13%) General / -88.7,-14.1	Allowed (0.9%) <i>mp0</i> chi angles: 324.3,88.6,304.7	0.14Å	-	-	-
235	TYR	92.64	-	Allowed (0.4%) General / -52.8,109.4	Favored (36.5%) <i>t80</i> chi angles: 175.6,58	0.08Å	-	-	-
236	THR	48.68	-	Allowed (1.77%) General / -80.4,-168.6	Favored (69.9%) <i>p</i> chi angles: 62.3	0.16Å	-	-	-
237	PHE	154.88	-	Favored (22.69%) General / -87.2,-27.9	Favored (40.7%) <i>p90</i> chi angles: 60.5,82.7	0.12Å	-	-	-
238	TRP	56.58	-	Favored (75.31%) General / -55.4,-43.5	Favored (37.4%) <i>m100</i> chi angles: 309.7,92	0.12Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.4 σ	-
239	ASN	33.61	-	Favored (60.04%) General / -76.2,-15.4	Favored (35%) <i>m110</i> chi angles: 302.9,115.4	0.11Å	-	-	-
<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: 83.62</div> <div>Clashscore: 0.8</div> <div>Outliers: 6 of 227</div> <div>Poor rotamers: 29 of 205</div> <div>Outliers: 8 of 218</div> <div>Outliers: 0 of 229</div> <div>Outliers: 16 of 229</div> <div>Non-Trans: 0 of 228</div> </div>									
240	LEU	49.42	-	Favored (28.56%) General / -78.5,-42.8	Favored (7.5%) <i>tp</i> chi angles: 177.5,45.4	0.11Å	-	-	-
241	PHE	166.79	-	Favored (45.5%) General / -79.4,-21.6	Favored (3%) <i>p90</i> chi angles: 81.9,79	0.26Å	-	OUTLIER(S) worst is CA- CB-CG: 4.8 σ	-
242	GLU	67.85	-	Favored (73.93%) General / -70.6,-37.7	OUTLIER (0.2%) chi angles: 151,273.3,303.8	0.20Å	-	-	-
243	ALA	28.23	-	Favored (98.08%) General / -61.8,-41.7	-	0.06Å	-	-	-
244	ILE	40.47	-	Favored (80.3%) Ile or Val / -68.6,-39.4	Favored (39.9%) <i>mt</i> chi angles: 287.9,158.3	0.12Å	-	-	-
				Favored (67.6%)	Favored (6%) <i>tt</i>				

245	LEU	39.09	-	General / -54.4,-40.0	chi angles: 190.1,148.9	0.05Å	-	-	-
246	GLN	60.03	-	Allowed (0.52%) General / -69.4,8.9	Favored (31.5%) <i>mt0</i> chi angles: 296.2,150.1,5.5	0.04Å	-	-	-
247	PHE	36.59	-	Allowed (1.47%) General / -139.0,-5.4	Favored (58.9%) <i>t80</i> chi angles: 186.3,91.3	0.06Å	-	-	-
248	GLN	108.76	-	-	Favored (2.6%) <i>pp30</i> chi angles: 55.7,75.6,60.2	0.04Å	-	-	-

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