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All-Atom Contacts	Clashscore, all atoms:	33.22	13 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	0.53%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	203	97.60%	Goal: >98%
	MolProbity score^	2.09		71 st percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.50%	Goal: 0
	Bad backbone bonds:	0 / 1681	0.00%	Goal: 0%
	Bad backbone angles:	26 / 2302	1.13%	Goal: <0.1%

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
		Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
24	GLN	81.62	-	-	5.3% (<i>pp0?</i>) chi angles: 64.4,84.3,43.9	0.037Å	-	-
25	VAL	85.44	0.431Å O with 25 VAL HG13	Favored (18.55%) Isoleucine or valine / -70.9,140.3	14.3% (<i>p</i>) chi angles: 64.6	0.083Å	-	-
26	ASN	52.34	-	Favored (55.73%) General / -68.4,141.4	44.1% (<i>t30</i>) chi angles: 179.9,52	0.099Å	-	OUTLIER(S) worst is CA-CB-CG: 4.621 σ
27	ARG	99.93	0.539Å HE with 60 MET HB2	Favored (52.22%) General /	34.7% (<i>mtm-85</i>) chi angles: 292.6,163.2,285.1,256.8	0.115Å	-	-

28	LEU	86.21	0.535Å N with 28 LEU HD22	-122.3,140.8 Favored (80.66%) Pre-proline / -77.6,156.5	1.9% (<i>mm?</i>) chi angles: 290.7,289.9	0.089Å	-	-
29	PRO	83.6	0.59Å HG2 with 107 VAL HG23	Favored (41.84%) Trans-proline / -75.0,159.1	13.1% (<i>Cg_endo</i>) chi angles: 15.8	0.09Å	-	-
30	PHE	57.73	-	Favored (49.5%) General / -135.2,148.0	36.2% (<i>p90</i>) chi angles: 55.4,82.3	0.077Å	-	OUTLIER(S) worst is CA- CB-CG: 4.656 σ
31	PHE	97.12	0.838Å CZ with 107 VAL HG13	Favored (38.23%) General / -79.0,139.2	79.9% (<i>m-85</i>) chi angles: 289.4,279.7	0.201Å	-	-
32	THR	82.88	0.604Å OG1 with 56 LEU HB2	Favored (19.5%) General / -88.5,-30.3	67% (<i>p</i>) chi angles: 64.6	0.065Å	-	-
33	ASN	73.23	0.912Å HD21 with 56 LEU H	Favored (57.24%) General / -58.8,138.4	60.2% (<i>m-80</i>) chi angles: 301.1,282.9	0.073Å	-	OUTLIER(S) worst is CA- CB-CG: 5.243 σ
34	HIS	57.37	-	Favored (71.37%) General / -67.7,-31.4	85.9% (<i>t60</i>) chi angles: 182.7,72.6	0.104Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.442 σ
35	PHE	96.1	-	Favored (66.99%) General / -61.4,-25.2	16.2% (<i>p90</i>) chi angles: 54.8,74.2	0.192Å	-	-
36	PHE	79.92	-	Favored (76.17%) General / -57.7,-39.0	53.9% (<i>m-85</i>) chi angles: 283.1,278.3	0.066Å	-	OUTLIER(S) worst is CA- CB-CG: 7.194 σ
37	ASP	76.11	-	Favored (2.97%) General / -72.0,-59.0	76.8% (<i>m-20</i>) chi angles: 290.7,356.5	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 5.42 σ
38	THR	158.65	0.88Å HG23 with 39 TYR H	Allowed (0.07%) General / -77.2,-84.4	4.7% (<i>t</i>) chi angles: 175.3	0.074Å	-	-
39	TYR	80.9	0.88Å H with 38 THR HG23	Allowed (1.5%) General / -179.3,167.3	41.1% (<i>p90</i>) chi angles: 60.7,82.6	0.084Å	-	-

40	LEU	63.86	-	Favored (45.92%) General / -119.7,124.3	59.4% (<i>tp</i>) chi angles: 179.9,60.2	0.067Å	-	-	
41	LEU	43.91	-	Favored (48.39%) General / -103.5,124.2	57% (<i>tp</i>) chi angles: 179.7,65.7	0.1Å	-	-	
42	ILE	42.97	-	Favored (73.01%) Isoleucine or valine / -124.9,128.2	70.9% (<i>mt</i>) chi angles: 301.7,166.4	0.079Å	-	-	
43	SER	92.25	-	Favored (42.59%) General / -74.0,147.9	78.9% (<i>p</i>) chi angles: 70.1	0.103Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
44	GLU	80.4		0.537Å CG with 125 VAL HG22	Favored (65.46%) General / -67.1,-18.8	15.5% (<i>pt-20</i>) chi angles: 56,183.2,328.9	0.095Å	-	-
45	ASP	152.55		0.72Å CG with 125 VAL HG11	Favored (69.87%) General / -62.0,-28.9	86.1% (<i>m-20</i>) chi angles: 294.7,346.4	0.221Å	-	OUTLIER(S) worst is CA- CB-CG: 5.394 σ
46	THR	61.33	-		Favored (10.49%) Pre-proline / -48.2,123.2	89.2% (<i>m</i>) chi angles: 302.6	0.05Å	-	-
47	PRO	140.82	-		Favored (41.3%) Trans-proline / -73.2,146.6	10.1% (<i>Cg_endo</i>) chi angles: 11.3	0.154Å	-	-
48	VAL	96.22		0.857Å HG11 with 92 PRO HD3	Favored (18.5%) Isoleucine or valine / -69.6,140.6	17.6% (<i>m</i>) chi angles: 291.6	0.052Å	-	-
49	GLY	22.83	-		Favored (61.56%) Glycine / 99.2,-13.7	-	-	-	-
					Favored				

50	SER	32.5	-	(20.94%) General / -85.1,156.7	47.4% (t) chi angles: 180.1	0.087Å	-	-
51	SER	48.87	-	Favored (35.04%) General / -88.9,131.6	95.9% (p) chi angles: 63.7	0.093Å	-	-
52	VAL	66.44	-	Favored (22.12%) Isoleucine or valine / -79.5,-47.4	85.1% (t) chi angles: 179	0.049Å	-	-
53	THR	116.4	-	Favored (3.3%) General / -168.4,-177.7	14.8% (t) chi angles: 187.2	0.096Å	-	-
54	GLN	51.47	O with 56 LEU HD22	0.578Å Favored (51.93%) General / -126.3,131.1	66.4% (tt0) chi angles: 180,180.1,0.1	0.13Å	-	-
55	LEU	110.31	HD21 with 105 PHE CG	0.618Å Favored (41.54%) General / -75.8,139.1	5.2% (mp) chi angles: 298.5,79.6	0.139Å	-	-
56	LEU	103.98	H with 33 ASN HD21	0.912Å Favored (50.06%) General / -120.9,142.1	2.6% (mm?) chi angles: 293.6,300.3	0.124Å	-	-
57	ALA	38.19	-	Favored (44.42%) General / -151.1,158.7	-	0.1Å	-	-
58	GLN	46.46	-	Favored (50.46%) General / -130.6,139.7	7.9% (tt0) chi angles: 180,179.1,174.7	0.073Å	-	-
59	ASP	91.47	-	Favored (40.73%) General / -122.8,123.3	9.8% (t70) chi angles: 190.3,297.9	0.087Å	-	-
60	MET	90.65	0.685Å CE with 60 MET HA	Favored (75.38%) General / -63.5,-33.3	10% (mmp) chi angles: 295.2,293.6,73.4	0.059Å	-	-
61	ASP	88.61	0.48Å O with 62 ASN HB2	Favored (63.51%) General / -69.7,-20.4	70.9% (m-20) chi angles: 300.1,329.8	0.064Å	-	OUTLIER(S) worst is CA- CB-CG: 6.606 σ
			0.48Å	Favored				OUTLIER(S)

62	ASN	60.37	HB2 with 61 ASP O	(2.21%) General / 71.0,32.9 Favored (82.33%) Pre-proline / -77.2,154.2	89.7% (<i>m</i> -20) chi angles: 291.1,321.7	0.085Å	-	worst is CA- CB-CG: 4.799 σ
63	ASP	52.47	-		79.7% (<i>m</i> -20) chi angles: 293.1,325	0.131Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
64	PRO	67.81	-	Favored (60.86%) Trans-proline / -69.5,146.2	88.4% (<i>Cg_exo</i>) chi angles: 331.4	0.082Å	-	-
65	LEU	73.97	-	Favored (32.38%) General / -120.8,156.2	85.7% (<i>mt</i>) chi angles: 296.8,180.9	0.106Å	-	-
66	VAL	49.27	-	Favored (66.57%) Isoleucine or valine / -124.6,134.5	89.5% (<i>t</i>) chi angles: 175.3	0.091Å	-	-
67	PHE	139.58	0.823Å CD2 with 107 VAL HG12	Favored (33.78%) General / -113.2,149.3	85% (<i>m</i> -85) chi angles: 290,86.4	0.107Å	-	OUTLIER(S) worst is CA- CB-CG: 4.698 σ
68	GLY	27.81	-	Favored (29.07%) Glycine / -157.6,-175.9	-	-	-	-
69	VAL	90.38	0.417Å O with 69 VAL HG13	Favored (51.19%) Isoleucine or valine / -128.0,139.7	14.9% (<i>p</i>) chi angles: 63.7	0.075Å	-	-
70	SER	38.32	-	Favored (54.95%) General / -119.3,134.9	47.4% (<i>t</i>) chi angles: 180.1	0.099Å	-	-
71	GLY	23.09	-	Favored (6.49%) Glycine / 115.5,138.4	-	-	-	-
72	GLU	44.49	-	Favored (72.76%) General /	11.6% (<i>pt</i> -20) chi angles: 63.7,189.6,63.3	0.069Å	-	-

73	GLU	37.49	-	-67.1,-46.9 Favored (85.02%) General / -67.1,-42.2	60.8% (<i>mt-10</i>) chi angles: 294.3,170.7,312.2	0.044Å	-	-
74	ALA	26.68	-	Favored (92.69%) General / -62.9,-38.9	-	0.085Å	-	-
75	SER	33.46	-	Favored (67.66%) General / -67.3,-28.0	94.1% (<i>p</i>) chi angles: 66.9	0.081Å	-	-
76	ARG	149.79	-	Favored (82.39%) General / -63.9,-47.0	23.6% (<i>mmt85</i>) chi angles: 287.8,280.1,185.9,85.5	0.11Å	-	-
77	PHE	69.43	-	Favored (50.27%) General / -75.9,-42.0	96.7% (<i>m-85</i>) chi angles: 292.9,276.2	0.06Å	-	OUTLIER(S) worst is CA- CB-CG: 7.954 σ
78	PHE	64.16	-	Favored (46.61%) General / -121.1,146.5	93.2% (<i>m-85</i>) chi angles: 299.1,282.3	0.125Å	-	OUTLIER(S) worst is CA- CB-CG: 5.359 σ
79	ALA	37.6	0.756Å HB3 with 88 TRP CE2	Favored (48.49%) General / -121.1,144.5	-	0.112Å	-	-
80	VAL	39.09	-	Favored (72.46%) Isoleucine or valine / -125.0,131.5	91.9% (<i>t</i>) chi angles: 177	0.083Å	-	-
81	GLU	48.49	-	Favored (90.6%) Pre-proline / -73.2,125.8	93.7% (<i>mt-10</i>) chi angles: 292.3,176.2,7.2	0.087Å	-	-
82	PRO	162.43	-	Favored (31.87%) Trans-proline / -59.7,-44.4	35% (<i>Cg_exo</i>) chi angles: 338.3	0.097Å	-	-
83	ASP	66.86	-	Favored (55.76%) General / -71.5,-47.4	11.7% (<i>m-20</i>) chi angles: 293.4,16	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 4.447 σ

Alt Res High B Clash > 0.4Å Ramachandran Rotamer C β deviation Bond lengths Bond angles

		Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
84	THR	83.11	-	Favored (15.46%) General / -87.0,-39.7	71.7% (<i>p</i>) chi angles: 63.8	0.069Å	-	-
85	GLY	32.71	0.476Å O with 55 LEU HD12	Favored (64.29%) Glycine / 92.6,6.1	-	-	-	-
86	VAL	37.48	-	Favored (27.01%) Isoleucine or valine / -69.1,136.1	73.1% (<i>t</i>) chi angles: 173.1	0.083Å	-	-
87	VAL	42.35	0.522Å CG2 with 55 LEU HD11	Favored (54.89%) Isoleucine or valine / -107.7,132.6	65.8% (<i>t</i>) chi angles: 179.7	0.12Å	-	-
88	TRP	70.58	0.756Å CE2 with 79 ALA HB3	Favored (42.57%) General / -129.9,157.3	47.8% (<i>p-90</i>) chi angles: 55.8,278.7	0.081Å	-	-
89	LEU	69.41	-	Favored (29.29%) General / -93.1,116.7	43.8% (<i>tp</i>) chi angles: 185.1,65.1	0.048Å	-	-
90	ARG	152.38	-	Favored (54.65%) General / -76.0,-40.1	7.1% (<i>mtm180</i>) chi angles: 289.4,233,303.9,152	0.101Å	-	-
91	GLN	86.67	-	Favored (66.14%) Pre-proline / -136.9,160.5	77.6% (<i>mt-30</i>) chi angles: 295,191.4,336.3	0.099Å	-	-
92	PRO	79.58	0.857Å HD3 with 48 VAL HG11	Favored (46.71%) Trans-proline / -69.6,141.7	86% (<i>Cg_exo</i>) chi angles: 331.2	0.186Å	-	-
93	LEU	58.13	-	Favored (25.93%) General / -84.4,149.6	84.8% (<i>mt</i>) chi angles: 295.2,180	0.12Å	-	-
94	ASP	68.71	1.069Å HB3 with 97 THR HG22	Favored (7.11%) General / -138.6,110.3	64.9% (<i>t0</i>) chi angles: 183.8,2.1	0.118Å	-	-

95	ARG	140.18	0.957Å HD3 with 124 ASP HB2	Favored (78.05%) General / -64.5,-34.4	48.4% (<i>ttp85</i>) chi angles: 184.3,203.1,62.4,81.6	0.132Å	-	-
96	GLU	108.85	-	Favored (96.03%) General / -62.2,-40.5	11.5% (<i>mp0</i>) chi angles: 281.8,66.8,53.9	0.056Å	-	-
97	THR	131.16	1.069Å HG22 with 94 ASP HB3	Favored (13.05%) General / -73.1,-52.8	15.2% (<i>t</i>) chi angles: 187.9	0.063Å	-	-
98	LYS	87.73	0.585Å N with 97 THR HG23	Favored (6.21%) General / -152.6,120.7	35.9% (<i>ttmt</i>) chi angles: 185.8,166.8,290.1,179.8	0.091Å	-	-
99	SER	69.66	-	Favored (26.11%) General / -82.5,-36.7	83.3% (<i>p</i>) chi angles: 60.8	0.066Å	-	-
100	GLU	67.79	-	Favored (41.53%) General / -143.0,152.0	6.3% (<i>pt-20</i>) chi angles: 62.1,158.5,300.2	0.119Å	-	-
101	PHE	69.04	-	Favored (11.26%) General / -165.8,172.9	47% (<i>p90</i>) chi angles: 56.5,87	0.067Å	-	OUTLIER(S) worst is CA- CB-CG: 4.134 σ
102	THR	38.29	-	Favored (39.29%) General / -117.6,150.3	70.9% (<i>p</i>) chi angles: 64	0.093Å	-	-
103	VAL	42.3	-	Favored (32.35%) Isoleucine or valine / -136.9,163.6	28.2% (<i>m</i>) chi angles: 296.7	0.106Å	-	-
<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> <div> <div>Avg: 75.22</div> <div>Clashscore: 33.22</div> <div>Outliers: 0 of 208</div> <div>Poor rotamers: 1 of 187</div> <div>Outliers: 1 of 199</div> <div>Outliers: 0 of 210</div> <div>Outliers: 25 of 210</div> </div>								
104	GLU	36.81	0.53Å HG2 with 117 LYS HG2	Favored (54.46%) General / -123.7,136.4	54.3% (<i>mt-10</i>) chi angles: 295.3,180.8,45.5	0.108Å	-	-
								OUTLIER(S) worst is CA-

105	PHE	56.99	CG with 55 LEU HD21	General / -114.5,155.1	72.4% (<i>m</i> -85) chi angles: 289.9,285.6	0.127Å	-	CB-CG: 5.009 σ
106	SER	46.61	-	Favored (49.28%) General / -133.0,155.4	92.7% (<i>p</i>) chi angles: 63.1	0.095Å	-	-
107	VAL	140.28	0.838Å HG13 with 31 PHE CZ	Favored (32.14%) Isoleucine or valine / -140.1,142.2	13.7% (<i>m</i>) chi angles: 306.6	0.127Å	-	-
108	SER	60.68	-	Favored (37.25%) General / -139.5,141.7	48.5% (<i>t</i>) chi angles: 179.5	0.102Å	-	-
109	ASP	128.21	-	Favored (54.19%) General / -86.3,0.3	53.3% (<i>p</i> 30) chi angles: 58.8,5.3	0.171Å	-	-
110	HIS	110.97	-	Allowed (1.27%) General / 78.7,-10.9	76.4% (<i>m</i> -70) chi angles: 283,275.6	0.103Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.354 σ
111	GLN	91.36	-	Favored (12.78%) General / -85.8,-44.1	44.1% (<i>mt</i> -30) chi angles: 296.3,162.3,77	0.002Å	-	-
112	GLY	28.45	-	Favored (31.66%) Glycine / -152.8,174.0	-	-	-	-
113	VAL	94.2	0.53Å HG22 with 114 ILE N	Favored (20.11%) Isoleucine or valine / -141.2,153.3	10.4% (<i>p</i>) chi angles: 61.1	0.065Å	-	-
114	ILE	101.58	0.64Å O with 114 ILE HD12	Favored (33.8%) Isoleucine or valine / -125.8,145.1	2.4% (<i>pp</i>) chi angles: 60.7,76.7	0.039Å	-	-
115	THR	40.22	-	Favored (53.1%) General / -124.7,140.2	76.7% (<i>p</i>) chi angles: 61.7	0.091Å	-	-
116	ARG	84.23	-	Favored (39.12%) General /	52.9% (<i>mmt</i> -85) chi angles:	0.065Å	-	-

-138.6,142.9 300.5,282.3,170.1,250.6

117	LYS	82.7	0.53Å HG2 with 104 GLU HG2	Favored (24.96%) General / -85.6,150.0	44.3% (<i>mtmt</i>) chi angles: 294,176.7,303.1,170.5	0.106Å	-	-
118	VAL	44.96	-	Favored (54.92%) Isoleucine or valine / -130.0,138.1	69.2% (<i>t</i>) chi angles: 173.5	0.123Å	-	-
119	ASN	46.36	-	Favored (38.21%) General / -92.2,129.4	80.6% (<i>m-20</i>) chi angles: 293.3,307.9	0.137Å	-	-
120	ILE	63.75	-	Favored (66.66%) Isoleucine or valine / -116.4,132.2	96.7% (<i>mt</i>) chi angles: 294.8,169.8	0.048Å	-	-
121	GLN	35.64	-	Favored (52.21%) General / -116.9,137.4	55.1% (<i>tt0</i>) chi angles: 180,176.3,332.8	0.083Å	-	-
122	VAL	37.68	-	Favored (55%) Isoleucine or valine / -101.8,127.7	87.1% (<i>t</i>) chi angles: 177.3	0.077Å	-	-
123	GLY	29.62	-	Favored (18.82%) Glycine / -86.1,142.1	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
124	ASP	65.62	0.957Å HB2 with 95 ARG HD3	Favored (28.74%) General / -82.3,147.6	25.9% (<i>t0</i>) chi angles: 188.6,41.5	0.114Å	-	-	
125	VAL	73.03	0.72Å HG11 with 45 ASP CG	Favored (17.02%) Isoleucine or valine / -142.4,165.2	35.5% (<i>m</i>) chi angles: 297.9	0.134Å	-	-	
126	ASN	78.77	-	Favored (7.48%) General / -84.0,84.8	63.7% (<i>t30</i>) chi angles: 189.3,28.6	0.094Å	-	-	

127	ASP	214.23	-	Favored (21.52%) General / -86.3,-31.4	11.2% (<i>m</i> -20) chi angles: 305,274.3	0.255Å	-	OUTLIER(S) worst is CB- CA-C: 5.432 σ
128	ASN	82.64	0.526Å HD22 with 159 PRO HG2	Favored (43.48%) General / -113.8,144.2	79.7% (<i>m</i> -20) chi angles: 300.3,308	0.096Å	-	OUTLIER(S) worst is CA- CB-CG: 4.33 σ
129	ALA	46.45	-	Favored (24.66%) Pre-proline / -87.6,166.5	-	0.108Å	-	-
130	PRO	69.46	-	Favored (65.47%) Trans-proline / -70.4,151.7	74.1% (<i>Cg_exo</i>) chi angles: 332.3	0.102Å	-	-
131	THR	37.29	-	Favored (53.85%) General / -117.4,127.2	92.7% (<i>m</i>) chi angles: 300.3	0.089Å	-	-
132	PHE	61.66	0.787Å CE2 with 218 THR HG23	Favored (28.34%) General / -81.2,151.0	83.1% (<i>m</i> -85) chi angles: 289.2,276.2	0.129Å	-	-
133	HIS	53.81	-	Favored (37.45%) General / -122.7,154.9	96.4% (<i>m</i> -70) chi angles: 301.7,286	0.094Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.477 σ
134	ASN	69.5	-	Favored (13.18%) General / 63.3,34.4	29.8% (<i>m</i> 120) chi angles: 290.1,111.9	0.073Å	-	OUTLIER(S) worst is CA- CB-CG: 5.572 σ
135	GLN	65.35	0.776Å HB3 with 136 PRO HA	Favored (46.94%) Pre-proline / -79.1,165.7	39.8% (<i>mt</i> -30) chi angles: 291.9,183.3,102.9	0.098Å	-	-
136	PRO	153.58	0.776Å HA with 135 GLN HB3	Favored (90.26%) Cis-proline / -76.5,163.2	57.8% (<i>Cg_exo</i>) chi angles: 334.4	0.105Å	-	-
137	TYR	83.63	0.441Å HB3 with 222 LEU CD1	Favored (51.43%) General / -108.2,125.3	58.3% (<i>m</i> -85) chi angles: 298.6,297.4	0.2Å	-	-
138	SER	34.64	-	Favored (25.67%) General / -152.5,147.0	90% (<i>p</i>) chi angles: 65.3	0.109Å	-	-

139	VAL	92.47	0.422Å HG22 with 140 ARG N	Favored (15.49%) Isoleucine or valine / -147.9,149.3	7.2% (<i>p</i>) chi angles: 58.1	0.069Å	-	-
140	ARG	104.86	0.652Å HD2 with 225 ILE O	Favored (56.51%) General / -115.4,129.2	16.4% (<i>tpt180</i>) chi angles: 184.6,68,174.7,269.4	0.099Å	-	-
141	ILE	52.97	-	Favored (73.86%) Pre-proline / -135.7,151.2	44.3% (<i>pt</i>) chi angles: 63.4,168.6	0.067Å	-	-
142	PRO	66.58	-	Favored (53.22%) Trans-proline / -72.8,152.9	75.5% (<i>Cg_exo</i>) chi angles: 333.1	0.094Å	-	-
143	GLU	72.48	0.814Å HG2 with 229 VAL HG22	Favored (67.66%) General / -66.5,-27.3	17% (<i>pt-20</i>) chi angles: 63.3,180.9,314.9	0.083Å	-	-
<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>								
<div> <div>Avg: 75.22</div> <div>Clashscore: 33.22</div> <div>Outliers: 0 of 208</div> <div>Poor rotamers: 1 of 187</div> <div>Outliers: 1 of 199</div> <div>Outliers: 0 of 210</div> <div>Outliers: 25 of 210</div> </div>								
144	ASN	105.61	-	Allowed (1.24%) General / -95.6,36.8	31.1% (<i>p-10</i>) chi angles: 63.8,332.5	0.087Å	-	-
145	THR	54.8	-	Favored (83.11%) Pre-proline / -71.9,135.2	91.3% (<i>m</i>) chi angles: 300.6	0.086Å	-	-
146	PRO	137.42	-	Favored (61.56%) Trans-proline / -69.6,146.7	5.8% (<i>Cg_endo</i>) chi angles: 8.2	0.168Å	-	-
147	VAL	92.76	-	Favored (19.02%) Isoleucine or valine / -68.8,140.4	16.9% (<i>m</i>) chi angles: 291	0.067Å	-	-
148	GLY	31.18	-	Favored (48.92%) Glycine / 104.8,-10.7	-	-	-	-
Favored								

149	THR	52.32	-	(69.73%) Pre-proline / -79.0,130.5	87.4% (<i>m</i>) chi angles: 301.9	0.068Å	-	-
150	PRO	104.56	-	Favored (5%) Trans-proline / -77.8,120.1	11% (<i>Cg_endo</i>) chi angles: 14.2	0.171Å	-	-
151	ILE	120.32	-	Favored (13.11%) Isoleucine or valine / -89.7,-40.6	45.8% (<i>pt</i>) chi angles: 63.5,170.4	0.137Å	-	-
152	PHE	96.34	-	Favored (38.27%) General / -156.9,159.5	36.4% (<i>t80</i>) chi angles: 195,83.5	0.121Å	-	-
153	ILE	108.94	0.484Å O with 153 ILE HG23	Favored (57.14%) Isoleucine or valine / -130.1,123.9	17.3% (<i>tt</i>) chi angles: 195.2,169.6	0.06Å	-	-
154	VAL	52.51	-	Favored (2.93%) Isoleucine or valine / -90.5,158.0	30.9% (<i>m</i>) chi angles: 296.9	0.077Å	-	-
155	ASN	56.83	-	Favored (25.76%) General / -142.3,133.2	23.4% (<i>t-20</i>) chi angles: 187,271.8	0.073Å	-	-
156	ALA	40.66	-	Favored (41.9%) General / -142.9,152.3	-	0.102Å	-	-
157	THR	40.26	-	Favored (32.4%) General / -133.0,162.2	62.4% (<i>p</i>) chi angles: 62.3	0.102Å	-	-
158	ASP	72	-	Favored (6.63%) Pre-proline / -144.3,121.8	31.1% (<i>t0</i>) chi angles: 193.4,323.8	0.094Å	-	-
159	PRO	91.11	0.526Å HG2 with 128 ASN HD22	Favored (30.74%) Trans-proline / -71.4,-17.1	43.2% (<i>Cg_endo</i>) chi angles: 24.3	0.118Å	-	-
160	ASP	58.09	-	Favored (34.52%) General / -67.9,157.6	69.7% (<i>m-20</i>) chi angles: 291.6,313.6	0.069Å	-	OUTLIER(S) worst is CA- CB-CG: 5.142 σ

161	LEU	53.93	-	Favored (24.09%) General / -83.6,153.8	83.4% (<i>mt</i>) chi angles: 298.1,181.8	0.066Å	-	-	
162	GLY	28.45	-	Favored (38.55%) Glycine / 67.2,-141.0	-	-	-	-	
163	ALA	38.26	-	Favored (72.72%) General / -60.6,-33.5	-	0.09Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
164	GLY	44.72	-	Favored (72.62%) Glycine / -60.3,-31.1	-	-	-	-	-
165	GLY	64.96	-	Favored (63.64%) Glycine / -74.6,-28.3	-	-	-	-	-
166	SER	109.85	-	Favored (32.24%) General / -84.4,139.4	78.8% (<i>p</i>) chi angles: 59.4	0.096Å	-	-	-
167	VAL	51.87	-	Favored (35.29%) Isoleucine or valine / -120.1,142.6	93.9% (<i>t</i>) chi angles: 176.9	0.067Å	-	-	-
168	LEU	55.4	-	Favored (47.56%) General / -120.3,145.0	79% (<i>mt</i>) chi angles: 294.2,180.7	0.083Å	-	-	-
169	TYR	59.58	-	Favored (43.64%) General / -117.7,146.6	92.8% (<i>m-85</i>) chi angles: 300.3,279.8	0.18Å	-	-	-
170	SER	41.36	-	Favored (32.88%) General / -159.3,158.7	86.3% (<i>p</i>) chi angles: 61.3	0.113Å	-	-	-
171	PHE	58.66	0.546Å CE2 with 180	Favored (27.77%)	69.7% (<i>m-85</i>)	0.133Å	-	OUTLIER(S) worst is CA- CB-CG: 4.921	

			ILE HB	General / -90.2,142.4	chi angles: 289.8,286.9			σ
172	GLN	58.33	-	Favored (23.24%) Pre-proline / -126.4,115.8	41.1% (<i>tt0</i>) chi angles: 178.8,180,300.2	0.111Å	-	-
173	PRO	74.31	-	Favored (34.24%) Cis-proline / -78.9,178.4	19.6% (<i>Cg_endo</i>) chi angles: 17.6	0.053Å	-	-
174	PRO	62.21	-	Favored (96.52%) Trans-proline / -61.9,146.3	80.5% (<i>Cg_exo</i>) chi angles: 330.6	0.142Å	-	-
175	SER	38.11	-	Favored (40.97%) General / -107.2,139.9	47.7% (<i>t</i>) chi angles: 179.9	0.098Å	-	-
176	GLN	137.76	0.623Å HG3 with 177 PHE CD1	Favored (67.7%) General / -72.1,-33.3	0% chi angles: 71.3,98.4,255.7	0.073Å	-	-
177	PHE	93.29	0.623Å CD1 with 176 GLN HG3	Favored (46.97%) General / -76.7,-40.9	92.8% (<i>m-85</i>) chi angles: 291.9,87.2	0.096Å	-	OUTLIER(S) worst is CA- CB-CG: 8.481 σ
178	PHE	78.45	0.456Å CD2 with 203 LEU HD11	Favored (50.9%) General / -129.0,149.3	82.1% (<i>m-85</i>) chi angles: 302.9,273.4	0.123Å	-	OUTLIER(S) worst is CA- CB-CG: 5.783 σ
179	ALA	43.33	0.852Å HB2 with 190 ILE HD11	Favored (38.48%) General / -120.5,152.1	-	0.107Å	-	-
180	ILE	51.1	0.546Å HB with 171 PHE CE2	Favored (56.58%) Isoleucine or valine / -133.7,130.9	21.4% (<i>tt</i>) chi angles: 187.8,168	0.061Å	-	-
181	ASP	49.52	0.585Å HB3 with 184 ARG HB2	Favored (42.1%) General / -69.7,130.3	21.1% (<i>t0</i>) chi angles: 189.5,315.9	0.067Å	-	-
182	SER	48.92	-	Favored (75.02%) General / -63.6,-49.0	87.7% (<i>p</i>) chi angles: 65.5	0.073Å	-	-
				Favored				

183	ALA	54.9	-	(21.39%) General / -74.5,-49.6	-	0.074Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
184	ARG	122.23	0.585Å HB2 with 181 ASP HB3	Favored (64.82%) General / -73.3,-39.9	61.9% (<i>mtp180</i>) chi angles: 297,172.4,82.2,175	0.057Å	-	-
185	GLY	28.9	-	Favored (72.86%) Glycine / 86.3,11.2	-	-	-	-
186	ILE	56.27	-	Favored (33.54%) Isoleucine or valine / -86.7,131.9	90.8% (<i>mt</i>) chi angles: 298.3,167.9	0.058Å	-	-
187	VAL	49.9	-	Favored (32.65%) Isoleucine or valine / -101.9,136.7	87.5% (<i>t</i>) chi angles: 178.9	0.081Å	-	-
188	THR	121.47	0.542Å CG2 with 179 ALA HB3	Favored (48.44%) General / -131.4,154.6	9.2% (<i>t</i>) chi angles: 180.2	0.052Å	-	-
189	VAL	77.26	-	Favored (25.64%) Isoleucine or valine / -87.5,113.9	70.1% (<i>t</i>) chi angles: 173.4	0.08Å	-	-
190	ILE	235.96	0.852Å HD11 with 179 ALA HB2	Favored (14.14%) Isoleucine or valine / -83.3,-38.1	37.3% (<i>mm</i>) chi angles: 305.8,295.7	0.057Å	-	-
191	ARG	142.54	0.593Å HG3 with 192 GLU N	Favored (41.5%) General / -134.0,159.2	6.7% (<i>tpp180</i>) chi angles: 180.2,76.8,71.7,143.9	0.119Å	-	-
192	GLU	72.8	0.593Å N with 191 ARG HG3	Favored (58.18%) General / -64.2,137.9	24.6% (<i>pt-20</i>) chi angles: 67.6,174.3,9.2	0.148Å	-	-
				Favored				

193	LEU	116.33	0.448Å HD22 with 226 ILE HD12	(13.56%) General / -95.3,162.7	4.6% (<i>mp</i>) chi angles: 302.2,81	0.108Å	-	-
194	ASP	66.27	0.761Å HB3 with 197 THR HG22	Favored (5.44%) General / -148.5,113.4	56.2% (<i>t0</i>) chi angles: 190.6,351.5	0.092Å	-	-
195	TYR	55.37	0.408Å CZ with 199 GLN HG3	Favored (93.52%) General / -62.6,-39.4	86.9% (<i>t80</i>) chi angles: 177,83.2	0.075Å	-	-
196	GLU	104.79	-	Favored (83.7%) General / -58.4,-40.9	14.7% (<i>mp0</i>) chi angles: 280.6,62.8,44.2	0.035Å	-	-
197	THR	120.01	0.761Å HG22 with 194 ASP HB3	Favored (15%) General / -74.7,-51.1	14.9% (<i>t</i>) chi angles: 188.6	0.084Å	-	-
198	THR	51.94	0.582Å N with 197 THR HG23	Favored (18.64%) General / -138.1,122.7	88.8% (<i>m</i>) chi angles: 300.9	0.082Å	-	-
199	GLN	105.07	0.408Å HG3 with 195 TYR CZ	Favored (44.74%) General / -77.2,-40.6	10.6% (<i>mp0</i>) chi angles: 300.1,75.7,65.3	0.07Å	-	-
200	ALA	41.48	-	Favored (41.43%) General / -148.4,155.6	-	0.099Å	-	-
201	TYR	131.03	-	Favored (52.05%) General / -122.9,141.3	97.2% (<i>m-85</i>) chi angles: 296.1,89.7	0.162Å	-	-
202	GLN	51.67	-	Favored (12.91%) General / -118.1,106.5	78.1% (<i>mm-40</i>) chi angles: 301.3,297.3,333.8	0.131Å	-	-
203	LEU	50.11	0.456Å HD11 with 178 PHE CD2	Favored (33.61%) General / -106.0,143.8	76.5% (<i>mt</i>) chi angles: 299.1,183	0.103Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 1 of	Outliers:	Outliers:	Outliers:
			75.22	33.22	208	187	1 of 199	0 of 210	25 of 210

204	THR	33.55	-	Favored (42.36%) General / -98.8,122.7	85.6% (<i>m</i>) chi angles: 301.4	0.113Å	-	-
205	VAL	35.6	-	Favored (48.19%) Isoleucine or valine / -102.6,132.7	70.1% (<i>t</i>) chi angles: 173.6	0.087Å	-	-
206	ASN	46.65	-	Favored (55.55%) General / -110.1,128.7	32.3% (<i>t-20</i>) chi angles: 184.7,306	0.097Å	-	-
207	ALA	43.48	0.488Å HB3 with 218 THR HG22	Favored (41.14%) General / -117.1,121.4	-	0.123Å	-	-
208	THR	42.76	0.424Å HG22 with 209 ASP O	Favored (51.17%) General / -128.9,141.8	89.5% (<i>m</i>) chi angles: 300.8	0.082Å	-	-
209	ASP	70.36	0.424Å O with 208 THR HG22	Favored (20.92%) General / -83.0,163.5	24.4% (<i>p30</i>) chi angles: 58.3,30.1	0.106Å	-	-
210	GLN	122.57	-	Favored (57.48%) General / -80.0,-15.3	16.2% (<i>mm100</i>) chi angles: 296.2,318.7,107.3	0.19Å	-	-
211	ASP	87.47	-	Favored (8.4%) General / -46.1,127.2	11.4% (<i>t70</i>) chi angles: 189,289.1	0.054Å	-	-
212	LYS	81.41	-	Favored (70.72%) General / -65.9,-48.6	51.5% (<i>mttp</i>) chi angles: 297.8,165.8,179.9,68.8	0.091Å	-	-
213	THR	131.14	-	Favored (11.52%) General / -69.7,-54.9	66.9% (<i>p</i>) chi angles: 62.1	0.07Å	-	-
214	ARG	164.59	0.57Å HA with 214 ARG NE	Favored (6.62%) Pre-proline / -141.2,99.0	5.4% (<i>tpm_?</i>) chi angles: 183.9,69.1,295.1,159.4	0.09Å	-	-
215	PRO	82.52	-	Favored (28.43%) Trans-proline / -78.1,153.2	10.3% (<i>Cg_endo</i>) chi angles: 13.4	0.111Å	-	-

216	LEU	56.57	-	Favored (50.06%) General / -124.6,144.6	88% (<i>mt</i>) chi angles: 296.1,179.8	0.095Å	-	-
217	SER	90.84	-	Favored (45.05%) General / -131.2,156.6	53.7% (<i>p</i>) chi angles: 55	0.059Å	-	-
218	THR	112.63	0.787Å HG23 with 132 PHE CE2	Favored (41.47%) General / -138.5,146.1	6.5% (<i>t</i>) chi angles: 194.9	0.078Å	-	-
219	LEU	46.72	-	Favored (34.06%) General / -114.5,151.0	88.8% (<i>mt</i>) chi angles: 298.1,180.3	0.115Å	-	-
220	ALA	32.88	0.519Å HB2 with 132 PHE CD2	Favored (40.79%) General / -146.1,153.5	-	0.111Å	-	-
221	ASN	55.36	-	Favored (35.02%) General / -102.8,141.8	26.9% (<i>t-20</i>) chi angles: 182.7,257	0.079Å	-	-
222	LEU	62.85	0.441Å CD1 with 137 TYR HB3	Favored (35.46%) General / -122.5,121.0	63.6% (<i>tp</i>) chi angles: 178.3,60.6	0.101Å	-	-
223	ALA	37.28	-	Favored (50.03%) General / -103.1,128.3	-	0.098Å	-	-
<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>								
Avg: 75.22			Clashscore: 33.22	Outliers: 0 of 208	Poor rotamers: 1 of 187	Outliers: 1 of 199	Outliers: 0 of 210	Outliers: 25 of 210
224	ILE	100.15	-	Favored (56.07%) Isoleucine or valine / -113.4,117.7	4.6% (<i>mp</i>) chi angles: 298,82.9	0.115Å	-	-
225	ILE	98.57	0.652Å O with 140 ARG HD2	Favored (43.8%) Isoleucine or valine / -99.1,132.8	51.4% (<i>mm</i>) chi angles: 302.2,301.2	0.06Å	-	-
			0.448Å	Favored				

226	ILE	105.11	HD12 with 193 LEU HD22	(54.98%) Isoleucine or valine / -101.2,126.8	50% (<i>mm</i>) chi angles: 301.3,300.2	0.081Å	-	-
227	THR	41.17	0.545Å HA with 140 ARG HH21	Favored (35.11%) General / -83.3,130.9	86% (<i>m</i>) chi angles: 301.3	0.082Å	-	-
228	ASP	44.94	-	Favored (39.88%) General / -76.3,133.9	58.8% (<i>t0</i>) chi angles: 188.9,1.6	0.078Å	-	-
229	VAL	106.42	0.814Å HG22 with 143 GLU HG2	Favored (19.76%) Isoleucine or valine / -119.9,160.9	27.3% (<i>m</i>) chi angles: 296	0.046Å	-	-
230	GLN	133.03	-	Allowed (1.1%) General / -72.3,85.8	42.4% (<i>tp60</i>) chi angles: 178.3,69.9,16.8	0.094Å	-	-
231	ASP	152.15	0.587Å OD1 with 229 VAL HG23	Favored (66.6%) General / -72.5,-33.0	81.5% (<i>m-20</i>) chi angles: 284.5,355.8	0.164Å	-	-
232	MET	125.71	-	Favored (8.95%) General / -58.9,120.4	2% (<i>mpt?</i>) chi angles: 291.2,71.3,181.3	0.119Å	-	-
233	ASP	26.11	-	-	51.1% (<i>m-20</i>) chi angles: 285.5,314.1	0.1Å	-	OUTLIER(S) worst is CA- CB-CG: 4.276 σ

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