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All-Atom Contacts	Clashscore, all atoms:	94.26		0 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	12	4.65%	Goal: <1%
	Ramachandran outliers	3	1.06%	Goal: <0.05%
	Ramachandran favored	273	96.81%	Goal: >98%
	MolProbity score [^]	3.14		18 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.37%	Goal: 0
	Bad backbone bonds:	0 / 2392	0.00%	Goal: 0%
	Bad backbone angles:	47 / 3228	1.46%	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: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258 0% chi angles: 74.6,294.1,174.5	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
1	MET	120.85	-	-		0.092Å	-	-
2	ASN	75.98	-	Favored (70.69%) General / -67.3,-30.8	26.6% (t-20) chi angles: 200.9,340.9	0.064Å	-	-
3	ARG	122.54	0.534Å HD2 with 25 GLU HB3	Favored (65.43%) General / -67.4,-19.7	15.9% (ttp-105) chi angles: 186.1,152.6,65.1,266.5	0.16Å	-	-
4	TYR	141.56	-	Favored (40.28%) General / -95.7,133.0 Favored	61% (m-85) chi angles: 306.3,273.1	0.092Å	-	OUTLIER(S) worst is CA-CB-CG: 4.572 σ

5	THR	111.38	-	(8.51%) General / -127.1,174.9	14.7% (<i>t</i>) chi angles: 189	0.092Å	-	-
6	THR	92.69	0.55Å O with 6 THR HG22	Favored (23.76%) General / 50.8,47.9	53.9% (<i>m</i>) chi angles: 304.6	0.041Å	-	-
7	MET	82.7	1.014Å HB3 with 19 LEU HD11	Favored (27.95%) General / -78.9,124.2	76.5% (<i>mtm</i>) chi angles: 295.5,180.3,290.4	0.106Å	-	-
8	ARG	108.28	0.765Å O with 19 LEU HG	Favored (54.41%) General / -122.8,134.7	36.6% (<i>ptt180</i>) chi angles: 63.8,173.1,186.1,173.1	0.106Å	-	-
9	GLN	47.93	-	Favored (23.05%) General / -77.3,121.0	56.1% (<i>tt0</i>) chi angles: 179.9,180,333.5	0.11Å	-	-
10	LEU	62.56	-	Favored (45.26%) General / -76.7,-41.4	67.8% (<i>mt</i>) chi angles: 298.6,184.4	0.049Å	-	-
11	GLY	22.01	-	Favored (33.62%) Glycine / 161.8,-161.9	-	-	-	-
12	ASP	38.06	-	Favored (53.34%) General / -105.0,129.7	68% (<i>m-20</i>) chi angles: 295.9,306.5	0.118Å	-	-
13	GLY	29.03	-	Favored (27.11%) Glycine / -101.8,-166.2	-	-	-	-
14	THR	66.43	0.494Å HG21 with 160 VAL HG12	Favored (60.66%) General / -63.2,-52.8	84.8% (<i>m</i>) chi angles: 301.5	0.084Å	-	-
15	TYR	98.21	0.873Å CE1 with 150 LEU HD22	Favored (62.49%) General / -74.8,-35.8	98.6% (<i>m-85</i>) chi angles: 297.7,273.2	0.041Å	-	OUTLIER(S) worst is CA- CB-CG: 5.882 σ
16	GLY	33.75	-	Favored (31.3%) Glycine / 171.0,-159.3	-	-	-	-

17	SER	27.67	-	(51.04%) General / -66.2,149.0 Favored	90.8% (<i>p</i>) chi angles: 65.8	0.086Å	-	-
18	VAL	33.91	-	(39.63%) Isoleucine or valine / -121.8,142.1 Favored	91.7% (<i>t</i>) chi angles: 177	0.086Å	-	-
19	LEU	123.69	1.014Å HD11 with 7 MET HB3	(43.78%) General / -145.6,158.8 Favored	5.6% (<i>tt</i>) chi angles: 179.2,165.8	0.071Å	-	-
20	MET	152.56	0.831Å N with 19 LEU HD23	(53.74%) General / -121.2,139.2 Favored	0% chi angles: 76.9,79.3,174.1	0.068Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
21	GLY	22.38	-	Favored (22.45%) Glycine / -143.1,176.8	-	-	-	-
22	LYS	102.96	-	Favored (55.63%) General / -109.8,129.4	33.8% (<i>ttpt</i>) chi angles: 180,161.9,54.8,183.3	0.07Å	-	-
23	SER	90.22	-	Favored (27.5%) General / -83.0,121.8	47.7% (<i>t</i>) chi angles: 179.9	0.112Å	-	-
24	ASN	80.28	-	Favored (83.2%) General / -66.3,-36.5	42.2% (<i>t30</i>) chi angles: 191.7,61.1	0.069Å	-	OUTLIER(S) worst is CA- CB-CG: 4.294 σ
25	GLU	79.44	0.658Å HG3 with 26 SER N	Favored (39.01%) General / -64.3,-54.1	16.8% (<i>pt-20</i>) chi angles: 62.7,168.6,352.1	0.087Å	-	-
26	SER	49.52	0.658Å N with 25 GLU HG3	Favored (44.67%) General / -78.9,-34.8	89.4% (<i>p</i>) chi angles: 62.3	0.062Å	-	-
27	GLY	24.6	-	Favored (79.23%) Glycine / 89.5,0.6	-	-	-	-

28	GLU	55.51	-	Favored (18.67%) General / -87.9,158.5	49.2% (<i>mt-10</i>) chi angles: 291.9,177.4,65	0.119Å	-	-
29	LEU	144.63	-	Favored (38.82%) General / -78.3,140.6	53.5% (<i>mt</i>) chi angles: 287.8,180.1	0.136Å	-	-
30	VAL	47.46	-	Favored (31.84%) Isoleucine or valine / -132.9,165.6	28.6% (<i>m</i>) chi angles: 295.3	0.111Å	-	-
31	ALA	34.35	-	Favored (40.25%) General / -108.8,141.8	-	0.112Å	-	-
32	ILE	48.33	0.529Å CG2 with 76 TYR HD2	Favored (75.28%) Isoleucine or valine / -122.5,128.1	97.4% (<i>mt</i>) chi angles: 293,167.4	0.105Å	-	-
33	LYS	58.43	-	Favored (43.77%) General / -121.8,124.3	87% (<i>mttt</i>) chi angles: 291.5,178.9,173.4,195.4	0.093Å	-	-
34	ARG	162.5	0.415Å HG3 with 74 HIS NE2	Favored (33.82%) General / -86.9,132.4	0.4% chi angles: 184.7,244.8,272.8,89.5	0.125Å	-	-
35	MET	178.27	0.661Å SD with 75 LEU HG	Favored (22.04%) General / -109.6,110.8	25.4% (<i>ptm</i>) chi angles: 61.2,186.9,298.3	0.088Å	-	-
36	LYS	178.26	0.828Å CG with 38 LYS HE3	Favored (36.88%) General / -79.5,136.3	0.5% chi angles: 184.2,58.8,95.6,277	0.09Å	-	-
37	ARG	130.87	0.74Å C with 38 LYS HD2	Favored (50.18%) General / -131.8,153.4	15.7% (<i>ptt180</i>) chi angles: 62.6,164.8,179.9,122.7	0.144Å	-	-
38	LYS	152.34	0.828Å HE3 with 36 LYS CG	Favored (5.65%) General / -147.7,113.3	0.3% chi angles: 291.6,67.8,172.2,291.1	0.145Å	-	-
39	PHE	315.91	0.885Å	Favored (10.63%)	81% (<i>t80</i>)	0.101Å	-	OUTLIER(S) worst is CA-

				CE2 with 41 SER HB2		General / -163.1,146.2	chi angles: 173.1,81.3		CB-CG: 5.023 σ	
40	TYR	288.27	-			Favored (44.72%) General / -130.8,131.6	90.7% (<i>t80</i>) chi angles: 180.3,77.3	0.093Å	-	-
#	Alt Res	High B		Clash > 0.4Å		Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 100.17		Clashscore: 94.26		Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
41	SER	192		0.885Å HB2 with 39 PHE CE2		Favored (18.56%) General / -149.2,170.4	47.6% (<i>t</i>) chi angles: 180	0.129Å	-	-
42	TRP	154.01	-			Favored (81.07%) General / -62.5,-48.1	56.1% (<i>t-105</i>) chi angles: 179.9,269.5	0.105Å	-	-
43	ASP	194.63	-			Favored (39.92%) General / -75.0,130.8	18.8% (<i>p-10</i>) chi angles: 62.4,313.9	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 4.126 σ
44	GLU	107.11	-			Favored (70.73%) General / -70.2,-32.7	63.6% (<i>tt0</i>) chi angles: 182,179.5,29.7	0.066Å	-	-
45	CYS	99.82	-			Favored (6.88%) General / -53.1,149.3	52% (<i>t</i>) chi angles: 180	0.08Å	-	-
46	MET	306.03		0.947Å HA with 46 MET HE3		Favored (5.1%) General / -118.0,176.7	3.5% (<i>tpt</i>) chi angles: 187.4,68.1,281.9	0.085Å	-	-
47	ASN	165.14		0.778Å H with 46 MET HG3		Favored (3.21%) General / -84.9,54.8	9% (<i>m-20</i>) chi angles: 297.3,13.7	0.094Å	-	OUTLIER(S) worst is CA- CB-CG: 4.778 σ
48	LEU	95.21		0.659Å H with 48 LEU HD12		Favored (72.9%) General / -69.3,-43.9	3.1% (<i>mp</i>) chi angles: 300.7,66	0.154Å	-	-
49	ARG	87.22	-			Favored (97.19%) General / -64.1,-41.7	1.6% (<i>tmt_?</i>) chi angles: 195.4,253.4,181.1,136	0.053Å	-	-
				0.546Å		Favored	6.8% (<i>mm-40</i>)			

50	GLU	72.42	HB2 with 47 ASN HB3	(85.53%) General / -62.8,-47.0	chi angles: 289.8,286.2,73.5	0.073Å	-	-
51	VAL	103.21	0.886Å HG21 with 77 PHE HE1	Favored (73.77%) Isoleucine or valine / -66.8,-35.0	7.7% (<i>p</i>) chi angles: 59.2	0.082Å	-	-
52	LYS	95.64	0.423Å N with 51 VAL HG13	Favored (72.39%) General / -61.2,-32.6	59.9% (<i>tttm</i>) chi angles: 186.2,165.8,180.1,289.6	0.078Å	-	-
53	SER	77.79	-	Favored (67.58%) General / -61.9,-25.5	66.3% (<i>m</i>) chi angles: 296.5	0.086Å	-	-
54	LEU	73	0.674Å HA with 57 LEU HD23	Favored (66.48%) General / -63.5,-21.7	62.4% (<i>mt</i>) chi angles: 290.9,181.5	0.088Å	-	-
55	LYS	74.08	-	Favored (65.15%) General / -57.8,-29.8	59.8% (<i>mtpt</i>) chi angles: 293.5,167,62.3,180	0.083Å	-	-
56	LYS	80.34	-	Favored (71.24%) General / -62.4,-30.5	80.4% (<i>tttt</i>) chi angles: 188.7,165.6,180.3,179.7	0.073Å	-	-
57	LEU	118.54	1.08Å HD12 with 116 ILE HG22	Allowed (0.12%) General / -66.5,86.8	0.8% chi angles: 295,285.3	0.16Å	-	-
58	ASN	71.43	-	Favored (18.22%) General / -115.0,109.5	29.4% (<i>t-20</i>) chi angles: 194.4,313.2	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 4.221 σ
59	HIS	55.5	0.556Å HE1 with 111 GLN HE21	Favored (27.52%) General / -156.1,152.1	61.7% (<i>t-80</i>) chi angles: 186.5,273.8	0.087Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.402 σ
60	ALA	50.59	0.477Å O with 140 LYS HG2	Favored (82.47%) General / -61.0,-37.5	-	0.082Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg:	Clashscore:	Outliers: 3 of	Poor rotamers: 12 of	Outliers:	Outliers:	Outliers:
100.17	94.26	282	258	1 of 271	0 of 284	43 of 284

61	ASN 112.81	0.56Å HD22 with 111 GLN HB3	Favored (55.53%) General / -79.1,-6.0 Favored (39.83%) Isoleucine or valine / -117.4,140.6	92.2% (<i>m-20</i>) chi angles: 291.2,347.4	0.081Å	-	OUTLIER(S) worst is CA- CB-CG: 6.902 σ
62	VAL 108.45	-	Favored (24.95%) Isoleucine or valine / -69.2,124.4	35.9% (<i>m</i>) chi angles: 297.6	0.075Å	-	-
63	ILE 120.35	0.65Å HD11 with 82 MET SD	Favored (36.94%) General / -78.9,135.2	30.5% (<i>mm</i>) chi angles: 294,293.2	0.114Å	-	-
64	LYS 104.31	-	Favored (16.57%) General / -89.2,104.0	33.3% (<i>mtmt</i>) chi angles: 288.4,161.4,271.4,183.8	0.061Å	-	-
65	LEU 70.78	0.536Å HD13 with 79 PHE CZ	Favored (51.83%) General / -75.0,-43.8	66.9% (<i>tp</i>) chi angles: 177.7,63.6	0.123Å	-	-
66	LYS 87.57	-	Favored (24.07%) General / -157.9,151.8	44.9% (<i>mttp</i>) chi angles: 288.8,172,164.5,81.4	0.083Å	-	-
67	GLU 57.51	-	Favored (69.95%) Isoleucine or valine / -114.1,123.6	52.1% (<i>mt-10</i>) chi angles: 295.8,175.4,51.3	0.075Å	-	-
68	VAL 44.32	-	Favored (63.64%) Isoleucine or valine / -121.0,120.9	98.6% (<i>t</i>) chi angles: 176.4	0.108Å	-	-
69	ILE 48.98	-	Favored (10.78%) General / -122.0,105.9	89.6% (<i>mt</i>) chi angles: 298.8,169	0.087Å	-	-
70	ARG 150.58	-	Favored (43.5%) General / -141.6,151.8	49.6% (<i>ttp85</i>) chi angles: 195,177.8,84.1,85	0.085Å	-	-
71	GLU 104.99	-		4.7% (<i>tp10</i>) chi angles: 200.9,74.8,271.3	0.085Å	-	-

72	ASN	63.62	-	Favored (24.53%) General / 57.1,34.2	12% (<i>m120</i>) chi angles: 296.5,153.8	0.132Å	-	-
73	ASP	85.73	-	Favored (25.54%) General / 55.1,35.8	46% (<i>t0</i>) chi angles: 193.7,3	0.059Å	-	OUTLIER(S) worst is CA- CB-CG: 4.186 σ
74	HIS	115.04	0.641Å ND1 with 76 TYR HE1	Favored (43.42%) General / -123.9,151.5	7.1% (<i>t-160</i>) chi angles: 206.2,190.5	0.173Å	-	OUTLIER(S) worst is CA- CB-CG: 5.085 σ
75	LEU	119.69	0.661Å HG with 35 MET SD	Favored (45.48%) General / -124.6,126.2	0.6% chi angles: 196.1,306.6	0.183Å	-	-
76	TYR	118.93	0.641Å HE1 with 74 HIS ND1	Favored (52.81%) General / -126.6,139.9	11.8% (<i>m-85</i>) chi angles: 274.8,66.2	0.193Å	-	-
77	PHE	131.62	0.886Å HE1 with 51 VAL HG21	Favored (44.88%) General / -111.4,141.5	45.9% (<i>m-85</i>) chi angles: 297.4,301.9	0.364Å	-	OUTLIER(S) worst is CB- CA-C: 6.158 σ
78	ILE	107.3	0.434Å CD1 with 32 ILE HG12	Favored (65.33%) Isoleucine or valine / -113.2,121.4	50.6% (<i>mm</i>) chi angles: 302.9,300.1	0.1Å	-	-
79	PHE	75.22	0.536Å CZ with 65 LEU HD13	Favored (19.64%) General / -123.0,163.9	76.5% (<i>m-85</i>) chi angles: 287.6,276.6	0.166Å	-	-
80	GLU	55.63	-	Favored (57.04%) General / -62.8,143.9	84.5% (<i>tt0</i>) chi angles: 179.9,185.7,0.7	0.127Å	-	-
<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: 100.17</div> <div>Clashscore: 94.26</div> <div>Outliers: 3 of 282</div> <div>Poor rotamers: 12 of 258</div> <div>Outliers: 1 of 271</div> <div>Outliers: 0 of 284</div> <div>Outliers: 43 of 284</div> </div>								
81	TYR	72.26	-	Favored (42.15%) General / -99.8,134.8	90.9% (<i>t80</i>) chi angles: 178.7,75.7	0.057Å	-	-
82	MET	98.43	0.801Å SD with 140	Favored (43.07%)	70.5% (<i>mtp</i>) chi angles:	0.105Å	-	-

		LYS HB2	General / -130.4,129.4	298.5,182.5,88.5			
83	LYS	124.87 -	Favored (73.03%) General / -65.3,-48.4	58.7% (<i>tptt</i>) chi angles: 175.8,66.7,179.6,180	0.083Å	-	-
84	GLU	129.87 0.411Å HA with 84 GLU OE1	Favored (7.73%) General / -100.3,171.5	64.9% (<i>mm-40</i>) chi angles: 299.8,309,332.6	0.08Å	-	-
85	ASN	73.27 0.601Å HD21 with 88 GLN CG	Favored (38.56%) General / -142.1,161.2	8.5% (<i>p30</i>) chi angles: 60.5,89.6	0.08Å	-	-
86	LEU	61.74 -	Favored (98.34%) General / -61.4,-43.7	59.8% (<i>tp</i>) chi angles: 182.2,62.3	0.058Å	-	-
87	TYR	139.42 0.834Å CE1 with 91 LYS HD3	Favored (82.36%) General / -63.0,-47.6	87.2% (<i>t80</i>) chi angles: 179.6,81.9	0.079Å	-	-
88	GLN	121.32 0.601Å CG with 85 ASN HD21	Favored (95.33%) General / -64.3,-43.3	30.1% (<i>mm100</i>) chi angles: 297.9,295.8,120.4	0.088Å	-	-
89	LEU	109.27 0.819Å HD11 with 97 PHE HZ	Allowed (1.52%) General / -64.3,-62.6	60.8% (<i>tp</i>) chi angles: 179.9,64.2	0.063Å	-	-
90	MET	238.88 0.83Å CE with 193 LEU HD23	Favored (5.46%) General / -75.5,-55.7	5.1% (<i>ppp?</i>) chi angles: 72.9,85,69.3	0.182Å	-	-
91	LYS	62.44 0.834Å HD3 with 87 TYR CE1	Favored (19.44%) General / -67.9,-54.4	61.7% (<i>mtpt</i>) chi angles: 290.9,170.5,64.8,180	0.12Å	-	-
92	ASP	80.39 -	Favored (2.54%) General / -73.2,-59.8	71.8% (<i>m-20</i>) chi angles: 292.1,357.5	0.064Å	-	OUTLIER(S) worst is CA- CB-CG: 5.705 σ
93	ARG	157 0.622Å HB3 with 89 LEU O	Favored (19.18%) General / -68.7,-53.9	4.9% (<i>tpp180</i>) chi angles: 184.2,69.9,72.1,136.3	0.084Å	-	-
		0.988Å HB2 with 97	Favored (7.03%)	75.6% (<i>m-20</i>)			OUTLIER(S) worst is CA-

94	ASN	63.35	PHE CE2	General / -131.0,104.3	chi angles: 292.2,301.8	0.099Å	-	CB-CG: 4.152 σ
95	LYS	131.89	0.805Å HE2 with 96 LEU HD21	Favored (66.92%) General / -68.6,-28.5	0% chi angles: 53.3,294.7,191.5,180.3	0.068Å	-	-
96	LEU	101.75	0.805Å HD21 with 95 LYS HE2	Favored (72.28%) General / -64.3,-31.2	2% (<i>mm?</i>) chi angles: 295.6,297.3	0.103Å	-	-
97	PHE	143.47	0.988Å CE2 with 94 ASN HB2	Allowed (0.15%) Pre-proline / -25.6,129.0	26.1% (<i>m-85</i>) chi angles: 276.7,291.1	0.166Å	-	OUTLIER(S) worst is CA- CB-CG: 4.551 σ
98	PRO	132.14	-	Favored (57.25%) Trans-proline / -72.1,155.2	76.5% (<i>Cg_exo</i>) chi angles: 333.2	0.128Å	-	-
99	GLU	74.15	-	Favored (78.78%) General / -63.3,-34.9	71.8% (<i>tt0</i>) chi angles: 183.5,175,338.6	0.07Å	-	-
100	SER	68.36	-	Favored (97.73%) General / -62.9,-40.5	47.7% (<i>t</i>) chi angles: 179.9	0.087Å	-	-

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Avg: 100.17				Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
101	VAL	45.37	-	-	Favored (93.32%) Isoleucine or valine / -65.0,-41.9	78.1% (<i>t</i>) chi angles: 172.7	0.063Å	-	-
102	ILE	50.83	1.107Å HG23 with 193 LEU HD13	-	Favored (98.58%) Isoleucine or valine / -61.3,-45.5	96.9% (<i>mt</i>) chi angles: 292.9,169.3	0.101Å	-	-
103	ARG	62.74	0.737Å HH21 with 284 PHE HA	-	Favored (97.8%) General / -63.2,-40.6	77.4% (<i>ttt180</i>) chi angles: 179.9,181.6,172.8,181.4	0.096Å	-	-
104	ASN	84.34	-	-	Favored (94.62%) General / -63.9,-43.9	0.6% chi angles: 193.8,181.1	0.09Å	-	-

105	ILE	109.83	1.079Å HD11 with 193 LEU HD12	Favored (87.46%) Isoleucine or valine / -64.8,-40.0	17.1% (<i>pt</i>) chi angles: 68.5,160.3	0.116Å	-	-
106	MET	71.57	0.645Å N with 105 ILE HG13	Favored (98.45%) General / -61.9,-43.6	19.9% (<i>ttt</i>) chi angles: 178.8,190.7,171.7	0.127Å	-	-
107	TYR	46.13	-	Favored (87.62%) General / -62.3,-46.7	81.7% (<i>t80</i>) chi angles: 180.8,83.6	0.098Å	-	-
108	GLN	112.1	0.722Å NE2 with 139 VAL HG23	Favored (84.07%) General / -65.9,-36.7	22.8% (<i>pt20</i>) chi angles: 58.4,193.6,333.5	0.145Å	-	OUTLIER(S) worst is CB- CG-CD: 4.634 σ
109	ILE	106.79	0.745Å HD12 with 186 VAL HG23	Favored (96.62%) Isoleucine or valine / -64.7,-43.8	29.7% (<i>pt</i>) chi angles: 61.3,179.9	0.109Å	-	-
110	LEU	120.92	1.059Å HD23 with 279 LEU HD23	Favored (94.48%) General / -64.0,-39.6	57.8% (<i>tp</i>) chi angles: 180,65.2	0.093Å	-	-
111	GLN	100.51	0.56Å HB3 with 61 ASN HD22	Favored (96.53%) General / -64.3,-42.4	33.5% (<i>tt0</i>) chi angles: 180.4,167.3,285.5	0.069Å	-	-
112	GLY	23.69	-	Favored (97.78%) Glycine / -64.5,-42.0	-	-	-	-
113	LEU	144.54	0.98Å HD13 with 144 PHE HZ	Favored (99.55%) General / -62.9,-41.8	4.3% (<i>mm?</i>) chi angles: 276.6,291.6	0.136Å	-	-
114	ALA	27.48	-	Favored (93%) General / -61.0,-40.3	-	0.094Å	-	-
115	PHE	46.75	0.467Å CZ with 119 HIS CE1	Favored (78.94%) General / -60.1,-49.1	84.9% (<i>t80</i>) chi angles: 178.8,83.5	0.088Å	-	-
116	ILE	141.84	1.08Å HG22 with 57 LEU HD12	Favored (85.4%) Isoleucine or valine / -67.0,-40.4	2.6% (<i>pp</i>) chi angles: 57.9,77.3	0.138Å	-	-
				Favored	OUTLIER(S)			

117	HIS	52.21	0.836Å N with 116 ILE HD12	(86.51%) General / -62.0,-37.9	43.1% (<i>m170</i>) chi angles: 288.9,151.4	0.096Å	-	worst is CD2- NE2-CE1: 4.474 σ
118	LYS	112.81	-	Favored (81.72%) General / -61.0,-37.2	6% (<i>tppm?</i>) chi angles: 189.9,165.1,81.9,293.4	0.074Å	-	-
119	HIS	104.68	0.467Å CE1 with 115 PHE CZ	Favored (62.32%) General / -71.5,-17.9	42.7% (<i>m80</i>) chi angles: 280.3,74.1	0.09Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.469 σ
120	GLY	31.07	-	Favored (48%) Glycine / 88.2,20.8	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
121	PHE	92.16	0.599Å O with 116 ILE HD13	Favored (55.68%) General / -110.1,129.5	69.9% (<i>m-85</i>) chi angles: 287.8,81.9	0.098Å	-	OUTLIER(S) worst is CA- CB-CG: 6.276 σ
122	PHE	118.34	0.703Å HE2 with 179 SER HB3	Favored (43.02%) General / -111.6,143.1	77.6% (<i>m-85</i>) chi angles: 301.4,84.9	0.096Å	-	OUTLIER(S) worst is CA- CB-CG: 7.01 σ
123	HIS	101.44	0.827Å CE1 with 125 ASP HB3	Favored (4.26%) General / -75.8,-56.9	47.2% (<i>t-80</i>) chi angles: 193.1,268	0.063Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.418 σ
124	ARG	162.53	-	Allowed (0.18%) General / 77.3,-27.2	87.2% (<i>mtt180</i>) chi angles: 298.4,173.5,179.6,200.9	0.084Å	-	OUTLIER(S) worst is C-N- CA: 4.614 σ
125	ASP	185.43	0.827Å HB3 with 123 HIS CE1	Favored (42.48%) General / -101.5,6.7	21.6% (<i>t0</i>) chi angles: 204.6,10.4	0.084Å	-	-
126	MET	119.2	0.56Å HE2 with 113 LEU HD21	Favored (30.42%) General / -51.8,134.7	85.9% (<i>mmm</i>) chi angles: 293.8,287.4,282.3	0.1Å	-	-
127	LYS	130.86	0.48Å O with 130 ASN HB3	Favored (24.18%) Pre-proline / -161.2,160.6 Favored	27.9% (<i>pttt</i>) chi angles: 45.2,180.1,163.4,195.5	0.116Å	-	-

128	PRO	92.38	0.728Å HG3 with 189 ILE HG13	(77.93%) Trans-proline / -62.5,-28.7	84.4% (<i>Cg_exo</i>) chi angles: 331	0.147Å	-	-
129	GLU	154.2	-	Favored (73.75%) General / -64.3,-32.2	24.4% (<i>tp10</i>) chi angles: 195.3,75.7,359.3	0.081Å	-	OUTLIER(S) worst is C-N- CA: 5.05 σ
130	ASN	206.52	0.516Å HD21 with 143 ASP HB2	Favored (59.86%) General / -74.7,-20.4	20.2% (<i>t-20</i>) chi angles: 189.2,284.1	0.188Å	-	-
131	LEU	75.91	0.666Å HD11 with 189 ILE HD13	Favored (17.07%) General / -95.2,105.2	44.5% (<i>mt</i>) chi angles: 301.5,187.7	0.091Å	-	-
132	LEU	104.19	0.622Å HB3 with 82 MET HB2	Favored (18.87%) General / -89.2,156.3	1.5% (<i>mm?</i>) chi angles: 291.9,288.6	0.083Å	-	-
133	CYS	59.83	0.6Å C with 82 MET HE2	Favored (50.95%) General / -130.6,143.7	72.3% (<i>m</i>) chi angles: 297.1	0.112Å	-	-
134	MET	116.04	0.672Å N with 82 MET HE2	Favored (10.57%) General / -142.0,118.0	64.9% (<i>ttp</i>) chi angles: 183.8,175.9,68.3	0.093Å	-	-
135	GLY	167.49	-	Favored (16.88%) Glycine / 106.0,-150.4	-	-	-	-
136	PRO	325.01	-	Favored (29.23%) Trans-proline / -63.7,130.9	49% (<i>Cg_exo</i>) chi angles: 337	0.118Å	-	OUTLIER(S) worst is N-CA- C: 10.992 σ
137	GLU	143.41	0.598Å CG with 133 CYS HB3	Favored (49.11%) General / -70.3,135.6	3.3% (<i>mp0</i>) chi angles: 297.2,76,78	0.088Å	-	-
138	LEU	126.97	0.594Å HD12 with 140 LYS HG3	Favored (37.43%) General / -101.2,118.7	2.7% (<i>tm?</i>) chi angles: 182.7,293.6	0.135Å	-	-
139	VAL	62.8	0.722Å HG23 with 108 GLN NE2	Favored (25.6%) Isoleucine or valine /	65.7% (<i>t</i>) chi angles: 171.4	0.08Å	-	-

140	LYS	85.48	0.801Å HB2 with 82 MET SD	-86.3,135.2 Favored (44.37%) General / -131.0,131.5	52.8% (<i>mttm</i>) chi angles: 301.9,163.9,184.8,289.6	0.063Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
141	ILE	68.25	0.622Å HG12 with 131 LEU HD22	Favored (40.94%) Isoleucine or valine / -89.1,128.9	85.9% (<i>mt</i>) chi angles: 298.7,166.9	0.045Å	-	-
142	ALA	63.87	-	Favored (13.1%) General / -97.9,162.8	-	0.091Å	-	-
143	ASP	98.55	0.516Å HB2 with 130 ASN HD21	Favored (7.38%) General / 68.5,23.7	80.9% (<i>m-20</i>) chi angles: 294.8,349.7	0.074Å	-	OUTLIER(S) worst is CA- CB-CG: 5.101 σ
144	PHE	110.37	0.98Å HZ with 113 LEU HD13	Favored (58.31%) General / -63.6,138.0	5.4% (<i>m-85</i>) chi angles: 265,273.5	0.162Å	-	-
145	GLY	55.09	0.576Å O with 149 GLU HG2	Favored (55.22%) Glycine / 85.0,-13.2	-	-	-	-
146	LEU	75.28	0.523Å HD22 with 77 PHE CZ	Favored (78.34%) General / -69.2,-39.8	45.8% (<i>mt</i>) chi angles: 298.2,187.9	0.052Å	-	-
147	ALA	45.98	0.472Å CB with 160 VAL HG21	Favored (96.45%) General / -60.9,-44.9	-	0.075Å	-	-
148	ARG	46.63	-	Favored (80.89%) General / -66.5,-45.0	77.1% (<i>ttt-85</i>) chi angles: 185.4,180.1,180.1,279.2	0.073Å	-	-
149	GLU	95.79	0.576Å HG2 with 145 GLY O	Favored (93.57%) General / -65.5,-41.0	50.8% (<i>mm-40</i>) chi angles: 298.5,315.3,323.2	0.051Å	-	-
			0.873Å	Favored				

150	LEU	173.77	HD22 with 15 TYR CE1	(80.47%) General / -66.5,-35.5 Favored	54.8% (<i>tp</i>) chi angles: 178.2,67.5	0.135Å	-	-
151	ARG	227.42	-	(47.87%) General / -63.9,131.5 Favored	71.4% (<i>ttt180</i>) chi angles: 187.3,180,180.1,197.4	0.072Å	-	-
152	SER	183.61	0.533Å O with 153 GLN HB2	(12.19%) General / -161.4,175.5 OUTLIER	97.7% (<i>p</i>) chi angles: 64.1	0.111Å	-	-
153	GLN	195.99	0.633Å CG with 39 PHE HD1	(0.04%) Pre-proline / 69.2,-176.8 Favored	94.3% (<i>mt-30</i>) chi angles: 293.1,180,309.6	0.098Å	-	-
154	PRO	161.71	0.568Å HD2 with 153 GLN HB3	(39.78%) Trans-proline / -69.7,163.0 Favored	89.3% (<i>Cg_exo</i>) chi angles: 331.5	0.081Å	-	-
155	PRO	167.17	-	(73.08%) Trans-proline / -65.4,142.7 Favored	81% (<i>Cg_exo</i>) chi angles: 330.6	0.196Å	-	-
156	TYR	220.91	-	(4.63%) General / -137.7,-177.1 Favored	75.6% (<i>m-85</i>) chi angles: 291.2,81.1	0.173Å	-	-
157	THR	255.06	-	(41.82%) General / -63.6,151.3 Favored	14.9% (<i>t</i>) chi angles: 188.6	0.083Å	-	-
158	ASP	215.56	0.455Å CG with 161 SER HB2	(32.48%) General / -61.8,127.7 Favored	32.9% (<i>p-10</i>) chi angles: 58.8,340	0.058Å	-	-
159	TYR	94.05	0.685Å HB2 with 150 LEU HD23	(71.55%) General / -65.2,-48.9 Favored	84.7% (<i>m-85</i>) chi angles: 296.5,286.4	0.127Å	-	-
160	VAL	115.39	0.523Å O with 160 VAL HG23	(33.71%) Isoleucine or valine / -81.1,120.9 Favored	25.7% (<i>m</i>) chi angles: 293.7	0.048Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
Avg:				Clashscore:	Outliers: 3 of	Poor rotamers: 12 of	Outliers:	Outliers:	Outliers: 43
100.17				94.26	282	258	1 of 271	0 of 284	of 284

161	SER	372.88	0.455Å HB2 with 158 ASP CG	Favored (33.03%) General / -157.9,166.3	47.4% (<i>t</i>) chi angles: 180	0.087Å	-	OUTLIER(S) worst is C-N- CA: 8.748 σ
162	THR	249.19	0.427Å O with 162 THR HG23	OUTLIER (0%) General / 154.0,131.3	9.5% (<i>t</i>) chi angles: 180.4	0.097Å	-	OUTLIER(S) worst is N-CA- C: 4.653 σ
163	ARG	193.1	0.633Å H with 163 ARG NE	Favored (43.27%) General / -79.5,-23.0	0% chi angles: 55.9,272,97.8,163.9	0.09Å	-	-
164	TRP	98.45	0.485Å CD1 with 201 PRO HA	Favored (75.08%) General / -56.1,-41.4	51.6% (<i>m0</i>) chi angles: 298,350.4	0.07Å	-	-
165	TYR	130.24	0.533Å HD1 with 188 SER HG	Favored (43.03%) General / -80.1,-21.6	74.3% (<i>m-85</i>) chi angles: 305,278.7	0.063Å	-	OUTLIER(S) worst is CA- CB-CG: 7.339 σ
166	ARG	83.31	0.894Å HD3 with 170 VAL CG1	Favored (50.08%) General / -70.4,137.1	46.3% (<i>ttm-85</i>) chi angles: 193.8,160.8,300.8,279.4	0.047Å	-	-
167	ALA	53.73	0.816Å HB1 with 168 PRO HD2	Favored (73.02%) Pre-proline / -80.3,157.4	-	0.076Å	-	-
168	PRO	81.45	0.816Å HD2 with 167 ALA HB1	Favored (92.99%) Trans-proline / -58.8,-30.5	55.4% (<i>Cg_endo</i>) chi angles: 25.6	0.102Å	-	-
169	GLU	144.21	0.853Å HG2 with 269 PRO HG3	Favored (99.31%) General / -63.2,-42.0	1.7% (<i>mp0</i>) chi angles: 306,85.3,272.5	0.204Å	-	-
170	VAL	48.56	0.894Å CG1 with 166 ARG HD3	Favored (82.22%) Isoleucine or valine / -68.9,-42.0	92.6% (<i>t</i>) chi angles: 178	0.064Å	-	-
171	LEU	65.21	0.689Å HD11 with 208 GLU HG2	Favored (79.79%) General / -62.9,-35.4	68.9% (<i>mt</i>) chi angles: 290.6,179.9	0.073Å	-	-
172	LEU	98.07	0.712Å HD11 with 228 TYR CE1	Favored (61.15%) General / -69.0,-11.8	69.2% (<i>mt</i>) chi angles: 290.8,180	0.068Å	-	-

173	ARG	85.05	0.66Å HG3 with 233 SER HB2	Allowed (0.07%) General / 85.4,26.2 Favored (43.23%) General / -74.0,136.0 Favored (55.11%) General / -83.1,-13.7 Favored (40.98%) Isoleucine or valine / -88.6,128.2 Favored (48.88%) General / -106.0,124.0	95.6% (<i>mtt-85</i>) chi angles: 298.2,183.1,181.1,273.5 47.7% (<i>t</i>) chi angles: 179.9 73.2% (<i>m</i>) chi angles: 293.8 92.7% (<i>t</i>) chi angles: 178 87.1% (<i>m-85</i>) chi angles: 290,270	0.088Å 0.105Å 0.082Å 0.073Å 0.165Å	- - - -	- - -
174	SER	47.27	-					
175	SER	52.71	-					
176	VAL	49.45	-					
177	TYR	71.28	-					
178	SER	36.8	0.662Å O with 181 ILE HG22	Favored (8.85%) General / -118.3,170.5	89.5% (<i>p</i>) chi angles: 62.3	0.107Å	-	-
179	SER	54.02	0.703Å HB3 with 122 PHE HE2	Favored (2.31%) Pre-proline / -58.1,-25.9	87.7% (<i>p</i>) chi angles: 61.5	0.076Å	-	-
180	PRO	160.75	0.807Å O with 183 VAL HG12	Favored (60.15%) Trans-proline / -62.0,-18.2	69.1% (<i>Cg_exo</i>) chi angles: 327.8	0.199Å	-	-
<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: 100.17</div> <div>Clashscore: 94.26</div> <div>Outliers: 3 of 282</div> <div>Poor rotamers: 12 of 258</div> <div>Outliers: 1 of 271</div> <div>Outliers: 0 of 284</div> <div>Outliers: 43 of 284</div> </div>								
181	ILE	84.37	0.662Å HG22 with 178 SER O	Favored (91.73%) Isoleucine or valine / -61.9,-41.7	21.5% (<i>tt</i>) chi angles: 188.3,167.7	0.046Å	-	-
182	ASP	46.81	0.543Å N with 181 ILE HG23	Favored (80.19%) General / -67.6,-36.1	96.8% (<i>m-20</i>) chi angles: 289,340.5	0.093Å	-	OUTLIER(S) worst is CA-CB-CG: 4.225 σ
183	VAL	90	0.831Å O with 186	Favored (84.51%)	9.7% (<i>p</i>)	0.073Å	-	-

			VAL HG12	Isoleucine or valine / -64.2,-39.2	chi angles: 71.3			
184	TRP	68.1	0.635Å HE3 with 272 ARG HE	Favored (98.37%) General / -60.8,-43.1	53% (<i>t-105</i>) chi angles: 177.4,269.9	0.094Å	-	-
185	ALA	39.23	0.465Å CB with 126 MET HB2	Favored (95.45%) General / -62.9,-39.8	-	0.093Å	-	-
186	VAL	87.88	0.831Å HG12 with 183 VAL O	Favored (92.55%) Isoleucine or valine / -62.5,-41.6	6.3% (<i>p</i>) chi angles: 74.7	0.066Å	-	-
187	GLY	23.87	0.434Å N with 186 VAL HG13	Favored (98.99%) Glycine / -62.4,-40.4	-	-	-	-
188	SER	80.49	0.533Å HG with 165 TYR HD1	Favored (94.07%) General / -65.0,-39.9	85.1% (<i>p</i>) chi angles: 68.3	0.089Å	-	-
189	ILE	104.73	0.816Å HG22 with 186 VAL O	Favored (82.66%) Isoleucine or valine / -68.2,-40.3	9% (<i>tt</i>) chi angles: 205.5,164.1	0.053Å	-	-
190	MET	76.74	0.494Å HE2 with 106 MET SD	Favored (94.32%) General / -61.6,-45.4	20.4% (<i>ttm</i>) chi angles: 182.3,199.5,313.9	0.146Å	-	-
191	ALA	38.45	0.745Å HB1 with 195 MET CE	Favored (93.06%) General / -61.0,-40.3	-	0.081Å	-	-
192	GLU	81.18	0.977Å HG2 with 198 PRO HA	Favored (84.06%) General / -65.3,-36.5	53.4% (<i>mt-10</i>) chi angles: 288.2,180.1,299.5	0.095Å	-	-
193	LEU	100.82	1.107Å HD13 with 102 ILE HG23	Favored (97.56%) General / -63.9,-41.9	1.1% (<i>tt</i>) chi angles: 198.5,189.3	0.076Å	-	-
194	TYR	110.64	0.768Å HB3 with 252 ASN HD21	Favored (35.87%) General / -69.7,-51.2	81.2% (<i>m-85</i>) chi angles: 291,82.5	0.068Å	-	-
195	MET	100.32	0.778Å HG3 with 250	Favored (71.67%)	76.8% (<i>mtm</i>) chi angles:	0.065Å	-	-

			ILE HD12	General / -70.0,-33.1	294.7,180,287.6			
196	LEU	64.95	0.51Å HB2 with 195 MET O	Favored (4.1%) General / 73.8,14.6	88.6% (<i>mt</i>) chi angles: 296.7,180.1	0.084Å	-	-
197	ARG	159.65	-	Favored (47.35%) Pre-proline / -146.7,157.6	85.4% (<i>mtt85</i>) chi angles: 295.4,180,180,85.7	0.133Å	-	-
198	PRO	149.32	0.977Å HA with 192 GLU HG2	Favored (46.05%) Trans-proline / -70.9,143.7	4.8% (<i>Cg_endo</i>) chi angles: 7.4	0.17Å	-	-
199	LEU	63.87	0.575Å HD23 with 200 PHE CE2	Favored (73.66%) General / -64.7,-48.7	60.1% (<i>tp</i>) chi angles: 180,64.4	0.091Å	-	-
200	PHE	104.47	0.751Å CE1 with 212 ILE HA	Favored (64.78%) Pre-proline / -127.8,83.9	74.5% (<i>m-85</i>) chi angles: 300,289.6	0.151Å	-	-
<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:</div> <div>Clashscore:</div> <div>Outliers: 3 of</div> <div>Poor rotamers: 12 of</div> <div>Outliers:</div> <div>Outliers:</div> <div>Outliers:</div> </div> <div> <div>100.17</div> <div>94.26</div> <div>282</div> <div>258</div> <div>1 of 271</div> <div>0 of 284</div> <div>43 of 284</div> </div>								
201	PRO	120.22	0.485Å HA with 164 TRP CD1	Allowed (1.5%) Trans-proline / -81.0,103.9	13.2% (<i>Cg_endo</i>) chi angles: 15.8	0.102Å	-	-
202	GLY	58.57	0.484Å O with 163 ARG HD2	Favored (15.69%) Glycine / -106.8,142.5	-	-	-	-
203	THR	51.8	-	Favored (57.24%) General / -76.3,-37.7	71% (<i>p</i>) chi angles: 63.9	0.075Å	-	-
204	SER	40.49	-	Favored (8.54%) General / -143.3,177.3	87.7% (<i>p</i>) chi angles: 61.5	0.098Å	-	-
205	GLU	111.65	-	Favored (98.47%) General / -62.5,-43.6	0.9% chi angles: 49.3,270.2,313.2	0.09Å	-	-
206	VAL	87.48	0.622Å O with 210 PHE HD1	Favored (91.37%) Isoleucine or valine / -66.3,-42.8	10.3% (<i>p</i>) chi angles: 61	0.052Å	-	-

207	ASP	38.64	0.548Å N with 206 VAL HG13	Favored (83.96%) General / -63.6,-36.5	56.3% (<i>t0</i>) chi angles: 188.9,5	0.091Å	-	OUTLIER(S) worst is CA- CB-CG: 4.657 σ
208	GLU	73.5	0.689Å HG2 with 171 LEU HD11	Favored (97.78%) General / -63.7,-43.0	48.2% (<i>tp10</i>) chi angles: 180,74.6,14	0.075Å	-	-
209	ILE	100.7	0.662Å HD11 with 238 PHE CE1	Favored (87.19%) Isoleucine or valine / -64.9,-39.9	36.7% (<i>pt</i>) chi angles: 66.1,168.5	0.083Å	-	-
210	PHE	55.62	0.622Å HD1 with 206 VAL O	Favored (94.04%) General / -60.2,-42.0	33.2% (<i>m-85</i>) chi angles: 279.8,76.2	0.075Å	-	OUTLIER(S) worst is CA- CB-CG: 6.635 σ
211	LYS	121.96	-	Favored (97.97%) General / -60.8,-42.6	26.8% (<i>mmtpt</i>) chi angles: 289.1,294,167.6,50.1	0.079Å	-	-
212	ILE	51.7	0.751Å HA with 200 PHE CE1	Favored (84.9%) Isoleucine or valine / -66.9,-46.5	91.2% (<i>mt</i>) chi angles: 298.1,167.5	0.071Å	-	-
213	CYS	80.34	0.801Å SG with 241 CYS HB2	Favored (77.84%) General / -64.0,-34.4	47.9% (<i>t</i>) chi angles: 185.4	0.07Å	-	-
214	GLN	42.02	-	Favored (95.23%) General / -60.6,-45.1	63.9% (<i>tt0</i>) chi angles: 180.1,175.9,353.2	0.054Å	-	-
215	VAL	62.96	1.069Å HA with 244 ILE HG12	Favored (26.88%) Isoleucine or valine / -74.9,-50.0	95% (<i>t</i>) chi angles: 176.8	0.058Å	-	OUTLIER(S) worst is C-N- CA: 4.04 σ
216	LEU	143.05	0.856Å HB3 with 267 TRP HE1	Favored (45.96%) General / -78.7,-30.1	1.2% (<i>mm?</i>) chi angles: 293.2,288	0.04Å	-	-
217	GLY	34.22	0.522Å N with 243 PRO HB3	Favored (29.55%) Glycine / 98.9,159.6	-	-	-	-
218	THR	107.99	0.546Å HG21 with 240 GLN OE1	Favored (58.06%) Pre-proline /	13.2% (<i>t</i>) chi angles: 186.2	0.065Å	-	-

219	PRO	163.19	0.472Å HD3 with 217 GLY O	-80.4,132.7 Favored (40.8%) Trans-proline / -75.4,158.3	65.1% (Cg_exo) chi angles: 334.1	0.107Å	-	-	
220	LYS	87.02	0.746Å HE3 with 222 SER HB2	Favored (6.75%) General / -134.5,178.8	53% (pttt) chi angles: 53.3,175.3,171.6,180.5	0.056Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
221	LYS	64.24	-	-	Favored (83.55%) General / -63.0,-36.4	81% (tttt) chi angles: 188.5,165.9,180.1,176.5	0.079Å	-	-
222	SER	30.83	0.746Å HB2 with 220 LYS HE3	Favored (5.06%) General / -63.4,-59.2	70% (m) chi angles: 297.7	0.092Å	-	-	
223	ASP	54.76	0.634Å C with 225 PRO HD3	Favored (84.12%) General / -66.6,-37.1	3.2% (p30) chi angles: 61,56.5	0.124Å	-	-	
224	TRP	98.08	0.72Å HE1 with 226 GLU HG3	Favored (51.18%) Pre-proline / -123.1,87.5	2.3% (t90) chi angles: 181.6,336.3	0.079Å	-	-	
225	PRO	178.48	0.634Å HD3 with 223 ASP C	Favored (23.8%) Trans-proline / -73.3,-10.2	77.1% (Cg_exo) chi angles: 333.6	0.12Å	-	OUTLIER(S) worst is C-N- CA: 7.165 σ	
226	GLU	206.26	0.72Å HG3 with 224 TRP HE1	Favored (10.54%) General / -86.0,69.4	19.1% (pt-20) chi angles: 65.9,168.4,29	0.156Å	-	-	
227	GLY	59.86	0.44Å O with 230 LEU HB3	Favored (33.43%) Glycine / 51.3,52.2	-	-	-	-	
228	TYR	143.22	0.712Å CE1 with 172 LEU HD11	Favored (90.04%) General / -58.7,-45.2	56.7% (t80) chi angles: 168.1,82.7	0.093Å	-	-	
			0.605Å HA with 234	Favored (71.66%)	21.5% (tm0?) chi angles:				

229	GLN	117.14	MET HG3	General / -65.4,-30.8	186.9,280.8,341.6	0.065Å	-	-
230	LEU	137.99	HB3 with 227 GLY O	Favored (73.32%) General / -65.5,-32.0	60.5% (<i>tp</i>) chi angles: 179.9,64.3	0.087Å	-	-
231	ALA	46.68	-	Favored (9.6%) General / -53.4,148.0	-	0.075Å	-	-
232	SER	81.95	-	Favored (85.12%) General / -59.2,-47.5	47.6% (<i>t</i>) chi angles: 180	0.079Å	-	-
233	SER	101.41	HB2 with 173 ARG HG3	Favored (50.25%) General / -80.2,-3.7	47.4% (<i>t</i>) chi angles: 180.1	0.06Å	-	-
234	MET	83.15	HG3 with 229 GLN HA	Favored (58.52%) General / -63.0,138.3	1.1% (<i>tmt?</i>) chi angles: 186.9,286.1,179.9	0.062Å	-	-
235	ASN	51.51	H with 238 PHE HE2	Favored (54.8%) General / -122.0,133.7	24.9% (<i>m120</i>) chi angles: 293,96.4	0.097Å	-	OUTLIER(S) worst is CA- CB-CG: 4.673 σ
236	PHE	100.01	-	Favored (72.45%) General / -65.1,-31.3	78.3% (<i>t80</i>) chi angles: 174.3,83.9	0.113Å	-	OUTLIER(S) worst is CA- CB-CG: 6.171 σ
237	ARG	101.41	-	Favored (70%) General / -63.0,-28.3	67.6% (<i>ttt-85</i>) chi angles: 178.7,175,169.7,263	0.047Å	-	-
238	PHE	88.49	CE1 with 209 ILE HD11	Favored (6.84%) Pre-proline / -47.2,140.5	43.8% (<i>m-85</i>) chi angles: 293.2,302.3	0.145Å	-	OUTLIER(S) worst is CA- CB-CG: 4.394 σ
239	PRO	66.87	-	Favored (72.93%) Trans-proline / -67.0,145.2	87.2% (<i>Cg_exo</i>) chi angles: 331.3	0.125Å	-	-
240	GLN	82.84	OE1 with 218 THR HG21	Favored (7.07%) General / -81.5,83.0	51.7% (<i>mm-40</i>) chi angles: 296.4,290.4,352.9	0.101Å	-	-

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

Avg: Clashscore: Outliers: 3 of Poor rotamers: 12 of Outliers: Outliers: Outliers: 43

		100.17	94.26	282	258	1 of 271	0 of 284	of 284
241	CYS	64.35	0.801Å HB2 with 213 CYS SG	Favored (41.44%) General / -75.1,134.2	99.8% (<i>m</i>) chi angles: 294.5	0.087Å	-	-
242	VAL	187.58	0.7Å CG1 with 243 PRO HD2	Favored (33.51%) Pre-proline / -100.5,127.2	76.9% (<i>t</i>) chi angles: 174.2	0.133Å	-	OUTLIER(S) worst is N-CA- C: 4.153 σ
243	PRO	102.93	0.746Å HB3 with 216 LEU C	Favored (96.16%) Trans-proline / -58.5,140.8	97% (<i>Cg_endo</i>) chi angles: 30.6	0.059Å	-	-
244	ILE	124.9	1.069Å HG12 with 215 VAL HA	Favored (87.5%) Isoleucine or valine / -66.9,-41.4	44.2% (<i>pt</i>) chi angles: 61.6,167.5	0.055Å	-	-
245	ASN	248.96	0.668Å N with 244 ILE HG13	OUTLIER (0.01%) General / 103.0,143.9	6.3% (<i>t-20</i>) chi angles: 190.7,221.6	0.134Å	-	OUTLIER(S) worst is CA- CB-CG: 4.555 σ
246	LEU	79.61	0.798Å HD12 with 262 THR HG22	Favored (87.6%) General / -64.5,-37.5	90.4% (<i>mt</i>) chi angles: 297.8,180	0.087Å	-	-
247	LYS	52.67	-	Favored (91.33%) General / -59.1,-45.2	62.3% (<i>tttm</i>) chi angles: 182.8,169.2,180.8,297.8	0.102Å	-	-
248	THR	26.78	-	Favored (92.75%) General / -64.4,-43.9	91.4% (<i>m</i>) chi angles: 300.6	0.074Å	-	-
249	LEU	79.67	0.565Å HD23 with 199 LEU CD1	Favored (77.48%) General / -66.0,-46.6	49.6% (<i>tp</i>) chi angles: 182.8,58.4	0.09Å	-	-
250	ILE	280.92	0.778Å HD12 with 195 MET HG3	Favored (35.82%) Pre-proline / -127.5,95.3	20.9% (<i>tt</i>) chi angles: 186,167.3	0.066Å	-	-
251	PRO	185.18	-	Favored (23.73%) Trans-proline / -70.4,-8.5	75% (<i>Cg_exo</i>) chi angles: 333	0.145Å	-	-
252	ASN	177.34	0.768Å HD21 with	Favored (2.02%)	51.2% (<i>p30</i>)	0.105Å	-	-

			194 TYR HB3	General / -91.3,52.0	chi angles: 65.9,4.4			
253	ALA	39.08	0.412Å HB1 with 257 ALA HB3	Favored (32.93%) General / -145.7,148.4	-	0.111Å	-	-
254	SER	25.21	-	Favored (10.93%) General / -75.6,173.5	97.3% (<i>p</i>) chi angles: 64	0.092Å	-	-
255	ASN	23.95	0.809Å O with 258 ILE HG22	Favored (97.07%) General / -64.2,-41.3	80.8% (<i>m-20</i>) chi angles: 291.3,310.4	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 4.733 σ
256	GLU	60.99	0.497Å HA with 256 GLU OE1	Favored (98.56%) General / -63.5,-41.5	18.9% (<i>mm-40</i>) chi angles: 293.3,288.9,19.4	0.11Å	-	-
257	ALA	26.77	0.663Å HB2 with 283 TYR CE1	Favored (99.63%) General / -63.0,-41.7	-	0.089Å	-	-
258	ILE	129.94	0.809Å HG22 with 255 ASN O	Favored (83.64%) Isoleucine or valine / -65.0,-38.8	0.1% chi angles: 200.9,294.3	0.041Å	-	-
259	GLN	110.79	0.472Å HG2 with 255 ASN O	Favored (96.51%) General / -62.6,-44.4	36.8% (<i>mm-40</i>) chi angles: 298.7,292.5,4	0.102Å	-	-
260	LEU	50.38	0.607Å CD2 with 106 MET HE1	Favored (92.95%) General / -64.1,-44.3	58.7% (<i>tp</i>) chi angles: 178.5,58.9	0.06Å	-	-
<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:</div> <div>Clashscore:</div> <div>Outliers: 3 of</div> <div>Poor rotamers: 12 of</div> <div>Outliers:</div> <div>Outliers:</div> <div>Outliers:</div> </div> <div> <div>100.17</div> <div>94.26</div> <div>282</div> <div>258</div> <div>1 of 271</div> <div>0 of 284</div> <div>43 of 284</div> </div>								
261	MET	104.79	0.691Å HE2 with 246 LEU HD13	Favored (98.6%) General / -63.3,-40.9	28.8% (<i>ptm</i>) chi angles: 66.3,180,284.5	0.068Å	-	-
262	THR	108.82	0.798Å HG22 with 246 LEU HD12	Favored (91.39%) General / -63.4,-38.5 Favored	77.3% (<i>p</i>) chi angles: 58.6	0.062Å	-	-

263	GLU	43.24	0.726Å O with 273 PRO HD3	(99.48%) General / -62.5,-42.3	90.7% (<i>mt-10</i>) chi angles: 292.8,184,7.5	0.075Å	-	-
264	MET	86.39	0.579Å HA with 273 PRO CG	Favored (73.31%) General / -66.9,-32.2	38.3% (<i>mtt</i>) chi angles: 287.5,180,159.9	0.08Å	-	-
265	LEU	137.5	0.568Å HD12 with 246 LEU CD1	Favored (44.63%) General / -80.3,-2.3	31.9% (<i>mt</i>) chi angles: 287.5,185	0.191Å	-	-
266	ASN	49.24	-	Favored (32.94%) General / -52.1,134.1	97.1% (<i>m-20</i>) chi angles: 291.9,335.8	0.082Å	-	OUTLIER(S) worst is CA- CB-CG: 4.775 σ
267	TRP	125.97	0.856Å HE1 with 216 LEU HB3	Favored (70.41%) General / -66.9,-47.9	9.1% (<i>m-90</i>) chi angles: 309.6,270.1	0.245Å	-	OUTLIER(S) worst is CB- CA-C: 4.202 σ
268	ASP	68.42	0.494Å OD1 with 269 PRO HD2	Favored (61.53%) Pre-proline / -73.1,117.6	56.7% (<i>t0</i>) chi angles: 183.2,340.7	0.077Å	-	-
269	PRO	77.95	0.853Å HG3 with 169 GLU HG2	Favored (84.44%) Trans-proline / -56.3,-31.4	53.8% (<i>Cg_endo</i>) chi angles: 25.4	0.08Å	-	-
270	LYS	63.83	0.476Å HE2 with 226 GLU OE1	Favored (93.03%) General / -63.5,-38.9	61% (<i>mttm</i>) chi angles: 292.8,167,177.4,291.7	0.092Å	-	-
271	LYS	110.02	0.403Å HD3 with 268 ASP HB3	Favored (63.04%) General / -70.5,-25.2	13.2% (<i>mpptt</i>) chi angles: 280.3,62.9,185.8,178.2	0.069Å	-	-
272	ARG	196.37	0.647Å HB3 with 273 PRO HD2	Favored (95.04%) Pre-proline / -61.8,141.6	66.8% (<i>mtt85</i>) chi angles: 285.9,196.7,187.2,87.6	0.133Å	-	-
273	PRO	153.98	0.726Å HD3 with 263 GLU O	Favored (91.25%) Trans-proline / -64.2,148.0	39% (<i>Cg_endo</i>) chi angles: 36.6	0.102Å	-	-
274	THR	90.98	0.939Å HG23 with 277 GLN H	Favored (19.15%) General / -85.6,161.8	15.1% (<i>t</i>) chi angles: 187.4	0.08Å	-	-

275	ALA	29.72	0.931Å HA with 110 LEU HD11	Favored (87.77%) General / -62.0,-38.2	-	0.096Å	-	-	
276	SER	28.23	-	Favored (86.72%) General / -60.8,-47.4	71.2% (<i>m</i>) chi angles: 295.8	0.084Å	-	-	
277	GLN	81.85	0.939Å H with 274 THR HG23	Favored (84.88%) General / -66.5,-37.3	8.8% (<i>tt0</i>) chi angles: 182.2,176.8,184.2	0.07Å	-	-	
278	ALA	29.63	0.771Å HB3 with 110 LEU HD21	Favored (94.47%) General / -61.1,-40.6	-	0.068Å	-	-	
279	LEU	43.84	1.059Å HD23 with 110 LEU HD23	Favored (85.59%) General / -61.5,-38.0	65.2% (<i>mt</i>) chi angles: 289.9,179.9	0.097Å	-	-	
280	LYS	91.69	-	Favored (73.01%) General / -65.9,-31.8	71.6% (<i>mmtt</i>) chi angles: 286.4,296.2,180,174.9	0.088Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 100.17	Clashscore: 94.26	Outliers: 3 of 282	Poor rotamers: 12 of 258	Outliers: 1 of 271	Outliers: 0 of 284	Outliers: 43 of 284
281	HIS	59.56	-	-	Favored (3.18%) Pre-proline / -46.9,145.5	57.6% (<i>t-80</i>) chi angles: 193,275.3	0.062Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.446 σ
282	PRO	62.66	-	-	Favored (48.61%) Trans-proline / -63.1,-15.5	89.2% (<i>Cg_exo</i>) chi angles: 331.5	0.124Å	-	-
283	TYR	42.21	0.663Å CE1 with 257 ALA HB2	Favored (89.2%) General / -59.6,-40.9	91.1% (<i>t80</i>) chi angles: 179.3,78.7	0.096Å	-	-	-
284	PHE	29.26	0.737Å HA with 103 ARG HH21	-	96.3% (<i>m-85</i>) chi angles: 296.6,280.9	0.084Å	-	-	OUTLIER(S) worst is CA- CB-CG: 7.178 σ

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