



Viewing RDH12_mb_33-610H-multi.table

When finished, you should [close this window](#).

Hint: Use File | Save As... to save a copy of this page.

All-Atom Contacts	Clashscore, all atoms:	146.96	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	11	4.70%	Goal: <1%
	Ramachandran outliers	14	5.07%	Goal: <0.05%
	Ramachandran favored	248	89.86%	Goal: >98%
	MolProbity score [^]	3.69		6 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	9	3.47%	Goal: 0
	Bad backbone bonds:	10 / 2208	0.45%	Goal: 0%
	Bad backbone angles:	74 / 2985	2.48%	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	C β deviation	Bond lengths	Bond angles
Avg: Clashscore: 124.27 146.96 Outliers: 14 of 276 Poor rotamers: 11 of 234 Outliers: 9 of 259 Outliers: 8 of 278 Outliers: 60 of 278								
33	THR	101.21	0.768Å HB with 258 ALA HB2	-	14.6% (t) chi angles: 187	0.072Å	-	-
34	ASN	126.06	-	Favored (70.82%) General / -65.1,-29.9	4.4% (p30) chi angles: 65.1,101.5	0.103Å	-	OUTLIER(S) worst is CA- CB-CG: 4.621 σ
35	VAL	63.88	0.441Å H with 33 THR HG23	Favored (47.69%) Isoleucine or valine / -57.8,-34.3	94.8% (t) chi angles: 175.9	0.06Å	-	-
36	GLN	169.63	0.608Å HA with 36 GLN HE21	Favored (70.91%) General / -63.9,-29.8	1% chi angles: 177.5,70.5,172.2	0.08Å	-	-

37	LEU	112.63	0.589Å CD2 with 271 ALA HB2	Favored (6.22%) Pre-proline / -47.5,142.6	90.4% (<i>mt</i>) chi angles: 297.3,180	0.106Å	-	-
38	PRO	117.63	1.136Å HG2 with 119 LEU HD21	Allowed (0.62%) Trans-proline / -93.0,-176.6	37.7% (<i>Cg_endo</i>) chi angles: 23.2	0.083Å	-	-
39	GLY	107.62	0.775Å O with 119 LEU HD13	Favored (36.28%) Glycine / -94.7,178.2	-	-	OUTLIER(S) worst is C--N: 5.744 σ	-
40	LYS	241.57	1.135Å HD3 with 42 VAL HG23	OUTLIER (0%) General / 153.0,177.1	0.1% chi angles: 41.6,55.4,181.4,63.7	0.097Å	-	-
41	VAL	174.29	1.1Å HG23 with 65 ARG HB2	Favored (8%) Isoleucine or valine / -120.5,99.7	13.3% (<i>p</i>) chi angles: 62.8	0.156Å	-	-
42	VAL	86.48	1.135Å HG23 with 40 LYS HD3	Favored (23.12%) Isoleucine or valine / -108.2,141.6	87.7% (<i>t</i>) chi angles: 175.1	0.069Å	-	-
43	VAL	127.51	0.751Å HG23 with 122 LEU HD12	Favored (48.2%) Isoleucine or valine / -99.6,130.7	5.7% (<i>m</i>) chi angles: 285.4	0.094Å	-	-
44	ILE	72.86	0.522Å HG12 with 123 ILE HD12	Favored (64.29%) Isoleucine or valine / -129.6,127.2	82% (<i>mt</i>) chi angles: 300.9,170.6	0.091Å	-	-
45	THR	49.61	0.435Å O with 125 ASN HB3	Favored (31.09%) General / -82.5,143.5	67.6% (<i>p</i>) chi angles: 63.1	0.07Å	-	-
46	GLY	57.86	-	Favored (20.32%) Glycine / -140.9,148.7	-	-	-	OUTLIER(S) worst is C-N- CA: 6.545 σ
47	ALA	112.55	0.476Å O with 48 ASN HB2	Favored (55.17%) General / -81.0,-15.8	-	0.063Å	-	-
48	ASN	89.79	0.476Å HB2 with 47 ALA O	Allowed (1.46%) General / -10.0,10.0	56.1% (<i>m-20</i>) chi angles: 275.4,330	0.112Å	-	-

				ALA	General / 70.2,38.4				
49	THR	58.21	0.62Å	HG22 with 50 GLY N	Favored (12.09%) General / -123.1,168.7	59.2% (<i>m</i>) chi angles: 304.1	0.055Å	-	-
50	GLY	55.63	0.62Å	N with 49 THR HG22	Favored (97.65%) Glycine / -62.1,-39.4	-	-	-	-
51	ILE	170.53	0.686Å	O with 51 ILE HD13	Favored (99.45%) Isoleucine or valine / -61.6,-44.9	0% chi angles: 193.7,294.1	0.044Å	-	-
52	GLY	48.34	0.534Å	N with 51 ILE HG23	Favored (97.06%) Glycine / -65.2,-40.9	-	-	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:				Clashscore:	Outliers: 14 of	Poor rotamers: 11 of	Outliers:	Outliers: 8	Outliers: 60
124.27				146.96	276	234	9 of 259	of 278	of 278
53	LYS	111.57	0.784Å	HG3 with 88 LYS CE	Favored (90.34%) General / -63.4,-45.6	25% (<i>ttpt</i>) chi angles: 186.8,165.5,98.3,175	0.087Å	-	-
54	GLU	129.58	0.762Å	HA with 57 ARG HG2	Favored (92.34%) General / -65.7,-40.3	10% (<i>mm-40</i>) chi angles: 284.3,262.5,340.7	0.106Å	-	-
55	THR	165.86	0.446Å	O with 59 LEU HG	Favored (99.22%) General / -61.0,-43.1	41.6% (<i>p</i>) chi angles: 54.4	0.101Å	-	-
56	ALA	60.53	-	-	Favored (97.95%) General / -63.7,-42.1	-	0.078Å	-	-
57	ARG	159.86	0.762Å	HG2 with 54 GLU HA	Favored (92.61%) General / -64.0,-44.5	12.9% (<i>ptm180</i>) chi angles: 60.2,172.8,294.5,198.5	0.081Å	-	-
58	GLU	154.28	0.53Å	HG2 with 266 LEU HD13	Favored (90.29%) General / -66.2,-40.6	20.8% (<i>tp10</i>) chi angles: 171.5,53.5,42.8	0.078Å	-	-
			0.493Å		Favored (91.50%)	86.6% (<i>mt</i>)	0		

59	LEU	93.02	HD12 with 44 ILE HD11	(91.5%) General / -65.7,-42.1	chi angles: 299.3,180.3	0.042Å	-	-
60	ALA	57.5	1.105Å HB1 with 90 SER HB2	Favored (91.38%) General / -60.4,-40.6	-	0.076Å	-	-
61	SER	52.86	-	Favored (67.83%) General / -59.7,-29.1	67.1% (<i>m</i>) chi angles: 296.3	0.084Å	-	-
62	ARG	141.07	-	Favored (64.03%) General / -69.1,-23.7	26.2% (<i>mmm180</i>) chi angles: 293,310.4,297.3,159.3	0.07Å	-	-
63	GLY	49.05	-	Favored (18.45%) Glycine / 110.6,11.8	-	-	-	-
64	ALA	67.18	-	Favored (38.13%) General / -75.7,149.0	-	0.088Å	-	-
65	ARG	127.01	1.1Å HB2 with 41 VAL HG23	Favored (23.96%) General / -90.6,112.3	85.1% (<i>mtp180</i>) chi angles: 294,178.4,65.8,187.8	0.129Å	-	-
66	VAL	63.89	-	Favored (49.57%) Isoleucine or valine / -106.4,133.9	83.5% (<i>t</i>) chi angles: 174.8	0.077Å	-	-
67	TYR	197.65	0.936Å HE2 with 69 ALA HB2	Favored (26.96%) General / -111.9,114.2	26% (<i>t80</i>) chi angles: 161.6,72.2	0.143Å	-	OUTLIER(S) worst is CA- CB-CG: 6.959 σ
68	ILE	59.25	0.451Å CD1 with 92 VAL CG1	Favored (54.74%) Isoleucine or valine / -101.4,123.8	91% (<i>mt</i>) chi angles: 296.7,174.3	0.097Å	-	-
69	ALA	63.09	0.936Å HB2 with 67 TYR HE2	Favored (32.26%) General / -106.6,116.6	-	0.123Å	-	-
70	CYS	85.61	-	Favored (42.33%) General / -143.2,159.4	42.8% (<i>t</i>) chi angles: 184.5	0.085Å	-	-

71	ARG	92.77	-	Favored (70.41%) General / -69.2,-45.2	24.9% (<i>ttm-85</i>) chi angles: 180.1,194.6,288.8,251	0.096Å	-	-
72	ASP	52.25	-	Favored (7.21%) General / -103.4,97.1	39.5% (<i>t0</i>) chi angles: 192.2,328.5	0.08Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
Avg: 124.27				Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278
73	VAL	43.52	0.555Å HG13 with 94 VAL CG1	Favored (72.59%) Isoleucine or valine / -68.4,-35.9	92% (<i>t</i>) chi angles: 177	0.059Å	-	-
74	LEU	120.77	0.528Å C with 74 LEU HD13	Favored (89.81%) General / -61.2,-46.6	3.1% (<i>tm?</i>) chi angles: 184.8,290.2	0.06Å	-	-
75	LYS	92.14	-	Favored (93.44%) General / -63.8,-44.4	1.9% (<i>ttmp?</i>) chi angles: 178.7,169.7,273.1,55	0.12Å	-	-
76	GLY	28.71	-	Favored (99.77%) Glycine / -62.9,-42.0	-	-	-	-
77	GLU	73.29	-	Favored (96.89%) General / -64.2,-41.8	3.6% (<i>tp10</i>) chi angles: 189.9,79.2,298.3	0.08Å	-	-
78	SER	28.67	-	Favored (81.94%) General / -59.7,-48.4	95.5% (<i>p</i>) chi angles: 63.6	0.085Å	-	-
79	ALA	36.58	-	Favored (90.66%) General / -65.4,-43.5	-	0.085Å	-	-
80	ALA	66.25	0.487Å HA with 88 LYS HD2	Favored (75.08%) General / -70.2,-39.5	-	0.072Å	-	-
81	SER	105.76	-	Favored (79.97%) General / -65.4,-43.5	96.4% (<i>p</i>) chi angles: 189.9,79.2,298.3	0.087Å	-	-

81	SER	193.70	-	General / -95.9,172.5	chi angles: 64.8	0.097 Å	-	-
82	GLU	265.7	1.015 Å HB3 with 86 ASP HA	Favored (50.72%) General / -107.2,134.2	1.9% (<i>pp20?</i>) chi angles: 64.9,87.7,48.1	0.106 Å	-	-
83	ILE	88.92	0.447 Å O with 83 ILE HG22	Allowed (0.75%) Isoleucine or valine / -109.2,84.9	96.1% (<i>mt</i>) chi angles: 295.5,168.4	0.128 Å	-	-
84	ARG	198.75	-	Favored (2.46%) General / 65.0,4.3	60.9% (<i>mtt180</i>) chi angles: 291.7,190.6,180,217.8	0.075 Å	-	-
85	VAL	77.25	0.596 Å C with 82 GLU HB2	Favored (2.67%) Isoleucine or valine / -155.4,133.4	73.5% (<i>t</i>) chi angles: 173.9	0.106 Å	-	-
86	ASP	128.54	1.015 Å HA with 82 GLU HB3	Favored (10.61%) General / -77.4,108.6	52.6% (<i>m-20</i>) chi angles: 293.1,1.8	0.105 Å	-	OUTLIER(S) worst is CA- CB-CG: 4.792 σ
87	THR	87.12	-	Favored (82.61%) General / -64.9,-46.2	74.1% (<i>p</i>) chi angles: 58.1	0.066 Å	-	-
88	LYS	69.92	0.784 Å CE with 53 LYS HG3	Favored (36.27%) General / -109.5,118.3	96.9% (<i>mttt</i>) chi angles: 285.6,176.7,176.2,180.6	0.12 Å	-	-
89	ASN	57.49	-	Favored (46.14%) General / -73.3,145.3	89.3% (<i>m-20</i>) chi angles: 286.7,328.1	0.072 Å	-	OUTLIER(S) worst is CA- CB-CG: 5.24 σ
90	SER	164.78	1.105 Å HB2 with 60 ALA HB1	OUTLIER (0%) General / 95.0,-165.2	16.2% (<i>m</i>) chi angles: 307.8	0.096 Å	-	-
91	GLN	82.79	-	Favored (21.34%) General / -106.9,109.4	71.5% (<i>mt-30</i>) chi angles: 292.6,188.7,57.1	0.13 Å	-	-
92	VAL	61.77	0.451 Å CG1 with 68 ILE CD1	Favored (39.91%) Isoleucine or valine / -121.7,113.6	79.7% (<i>t</i>) chi angles: 174.5	0.103 Å	-	-

Alt Res High R Clash > Ramachandran Rotamer Cβ Bond Bond

Residues High β		0.4Å	ramaChandran	rotamer	deviation	lengths	angles
Avg: 124.27		Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278	Outliers: 60 of 278
93	LEU 148.87	0.572Å N with 93 LEU HD22	Favored (24.2%) General / -104.9,151.2	1.9% (<i>mm?</i>) chi angles: 295.6,296.3	0.086Å	-	-
94	VAL 116.56	0.555Å CG1 with 73 VAL HG13	Favored (62.69%) Isoleucine or valine / -121.5,135.1	1% chi angles: 86.8	0.037Å	-	-
95	ARG 134.86	0.68Å HB2 with 67 TYR CE1	Favored (33.29%) General / -134.7,162.1	44.3% (<i>mtm180</i>) chi angles: 301.6,202.1,301.3,185.6	0.185Å	-	OUTLIER(S) worst is N-CA- CB: 4.407 σ
96	LYS 110.69	0.721Å NZ with 98 ASP HB2	Favored (34.37%) General / -84.7,134.0	5.7% (<i>tmtt?</i>) chi angles: 197.2,290.9,182.5,158	0.034Å	-	-
97	LEU 74.49	0.65Å N with 96 LYS HD3	Favored (11.91%) General / -151.2,129.4	62.2% (<i>tp</i>) chi angles: 175.3,61.6	0.094Å	-	-
98	ASP 63.07	0.721Å HB2 with 96 LYS NZ	Favored (11.04%) General / -117.7,104.5	66.2% (<i>t0</i>) chi angles: 186,356.3	0.113Å	-	-
99	LEU 81.38	-	Favored (68.16%) General / -64.1,-25.6	68.6% (<i>mt</i>) chi angles: 290.5,179.9	0.061Å	-	-
100	SER 66.61	-	Favored (36.54%) General / -76.8,-3.1	71.2% (<i>m</i>) chi angles: 295.8	0.079Å	-	-
101	ASP 64.01	-	Favored (13.85%) General / -132.2,113.9	60.4% (<i>t0</i>) chi angles: 187.9,344.2	0.084Å	-	-
102	THR 107.33	0.825Å O with 105 ILE HG22	Favored (78.85%) General / -62.5,-35.2	15% (<i>t</i>) chi angles: 188.3	0.073Å	-	-
103	LYS 66.57	0.496Å N with 102 THR HG23	Favored (97.36%) General / -63.0,-40.3	74.1% (<i>tttt</i>) chi angles: 191.6,162.8,181,169.4	0.078Å	-	-

104	SER	88.71	-	Favored (74.45%) General / -68.4,-33.6	78.4% (<i>p</i>) chi angles: 59.2	0.098Å	-	-
105	ILE	131.35	0.856Å HD11 with 154 LEU HA	Favored (90.59%) Isoleucine or valine / -62.8,-41.0	0.1% chi angles: 198.4,292.5	0.061Å	-	-
106	ARG	134.57	0.425Å N with 105 ILE CG2	Favored (93.73%) General / -63.0,-45.2	13.4% (<i>mmm</i> 180) chi angles: 288.4,271.4,304.4,139.5	0.1Å	-	-
107	ALA	23.77	-	Favored (99.75%) General / -63.1,-42.9	-	0.089Å	-	-
108	PHE	63.38	0.553Å CZ with 112 PHE CD1	Favored (91.25%) General / -63.9,-45.0	37% (<i>t80</i>) chi angles: 164.2,72.5	0.084Å	-	OUTLIER(S) worst is CA- CB-CG: 8.957 σ
109	ALA	42.58	-	Favored (90.45%) General / -61.9,-39.0	-	0.084Å	-	-
110	GLU	80.26	-	Favored (72.86%) General / -60.7,-33.5	40.6% (<i>tt0</i>) chi angles: 180.6,178.4,304.3	0.066Å	-	-
111	GLY	36.4	0.493Å C with 95 ARG HH22	Favored (93.48%) Glycine / -64.0,-36.6	-	-	-	-
112	PHE	80.44	0.648Å O with 161 ARG HD3	Favored (20.78%) General / -80.8,116.3	8.8% (<i>m-85</i>) chi angles: 267.9,89.6	0.175Å	-	OUTLIER(S) worst is CA- CB-CG: 8.593 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:		Clashscore:	Outliers: 14 of	Poor rotamers: 11 of	Outliers: 9 of 259	Outliers: 8 of 278	Outliers: 60 of 278	
124.27		146.96	276	234				
113	LEU	134.77	0.848Å HD22 with 114 ALA N	Favored (85.29%) General / -67.5,-40.5	0% chi angles: 52.4,301.6	0.073Å	-	-
114	ALA	51.84	0.848Å N with 113 LEU HD22	Favored (2.09%) General /	-	0.098Å	-	-

			LEU 119.54	-175.7,157.9				
115	GLU	119.5	HB2 with 121 ILE CG1	0.91Å Favored (54.03%) General / -121.6,131.3	0.3% chi angles: 25.7,265,11.6	0.066Å	-	OUTLIER(S) worst is CB- CG-CD: 4.01 σ
116	GLU	175.54	CG with 41 VAL HG12	0.833Å Favored (70.34%) General / -57.1,-51.2	8.5% (<i>mm-40</i>) chi angles: 278.7,268.3,20	0.139Å	-	-
117	LYS	262.06	HB3 with 167 PRO HA	1.052Å Favored (12.25%) General / 61.5,41.8	23.8% (<i>tttt</i>) chi angles: 215.1,161.7,170.4,197.8	0.089Å	-	-
118	GLN	130.36	-	Favored (90.52%) General / -63.3,-38.3	7.9% (<i>tt0</i>) chi angles: 179.9,182.2,180.6	0.159Å	-	-
119	LEU	232.59	HD21 with 38 PRO HG2	1.136Å Allowed (1.7%) General / -107.3,-170.4	8% (<i>mp</i>) chi angles: 280.7,53.1	0.079Å	-	-
120	HIS	212.87	CG with 171 VAL HG23	0.679Å Favored (49.02%) General / -57.6,131.1	22.8% (<i>m-70</i>) chi angles: 287.7,242.5	0.191Å	-	OUTLIER(S) worst is C-N- CA: 4.467 σ
121	ILE	246.39	HD12 with 42 VAL HG22	1.089Å Favored (11.18%) Isoleucine or valine / -108.7,-9.1	4.8% (<i>tp</i>) chi angles: 206,54.1	0.136Å	-	-
122	LEU	69.93	HD12 with 43 VAL HG23	0.751Å Favored (44.57%) General / -119.8,123.8	65.6% (<i>tp</i>) chi angles: 175.9,62.8	0.111Å	-	-
123	ILE	63.03	HD12 with 44 ILE HG12	0.522Å Favored (44.82%) Isoleucine or valine / -116.1,114.0	99.2% (<i>mt</i>) chi angles: 297.5,171.8	0.086Å	-	-
124	ASN	77.78	HD22 with 172 ASN ND2	0.55Å Favored (5.85%) General / -91.1,78.9	86.8% (<i>m-20</i>) chi angles: 292.6,315.9	0.098Å	-	OUTLIER(S) worst is CA- CB-CG: 4.505 σ
125	ASN	107.01	HB3 with 45 THR O	0.435Å Favored (17.51%) General / -87.2,-37.1	31.4% (<i>t30</i>) chi angles: 179.9,71.4	0.073Å	-	OUTLIER(S) worst is CA- CB-CG: 4.449 σ
126	ASN	107.01	HB3 with 45 THR O	0.435Å Favored (17.51%) General / -87.2,-37.1	31.4% (<i>t30</i>) chi angles: 179.9,71.4	0.073Å	-	OUTLIER(S) worst is CA- CB-CG: 4.449 σ

126	ALA	52.42	-	(55.58%) General / -62.4,144.8	-	0.081Å	-	-
127	GLY	42.59	0.497Å HA2 with 147 ASN OD1	Favored (24.09%) Glycine / -163.8,153.6	-	-	-	-
128	VAL	123.43	0.806Å HG12 with 146 VAL HG21	Favored (19.15%) Isoleucine or valine / -117.3,152.3	9% (<i>p</i>) chi angles: 60.3	0.095Å	-	-
129	MET	125.09	0.453Å HE2 with 200 TYR CZ	Favored (22.78%) General / -142.7,131.5	40.7% (<i>t</i> _{tm}) chi angles: 192.3,179.9,304	0.094Å	-	-
130	MET	139.48	0.506Å HG2 with 130 MET O	Favored (20.07%) General / 51.9,49.8	55.3% (<i>t</i> _{tm}) chi angles: 188.6,181.4,294.7	0.071Å	-	-
131	CYS	40.41	0.647Å H with 143 HIS CE1	Allowed (1.59%) Pre-proline / -100.2,177.2	87.9% (<i>m</i>) chi angles: 293	0.096Å	-	-
132	PRO	63.86	0.438Å HD2 with 131 CYS HB3	Favored (37.31%) Trans-proline / -71.4,164.0	71.9% (<i>Cg_exo</i>) chi angles: 332.6	0.092Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:			Clashscore:	Outliers: 14 of	Poor rotamers: 11 of	Outliers:	Outliers: 8	Outliers: 60
124.27			146.96	276	234	9 of 259	of 278	of 278
133	TYR	139.16	-	Favored (26.89%) General / -71.5,125.4	74.7% (<i>t</i> ₈₀) chi angles: 177.3,87.3	0.049Å	-	-
134	SER	54.02	0.757Å O with 142 THR HG23	Favored (37.16%) General / -158.5,160.9	44.9% (<i>p</i>) chi angles: 54.1	0.062Å	-	-
135	LYS	72.92	-	Favored (28.21%) General / -116.1,155.4	53.8% (<i>mtmt</i>) chi angles: 290.5,177.3,291.4,178.9	0.115Å	-	-
136	THR	33.03	-	Favored (6.19%) General / -86.7,-177.7	59.2% (<i>p</i>) chi angles: 62.4	0.089Å	-	-

137	ALA	34.67	-	Favored (88.57%) General / -61.2,-39.0	-	0.098Å	-	-
138	ASP	77.41	0.454Å CB with 140 PHE CE2	Favored (62.47%) General / -70.9,-21.0	62.2% (<i>m-20</i>) chi angles: 291.4,0.6	0.065Å	-	OUTLIER(S) worst is CA- CB-CG: 5.106 σ
139	GLY	39.01	-	Favored (35.41%) Glycine / 99.7,14.2	-	-	-	-
140	PHE	102.17	0.578Å HD1 with 189 GLN OE1	Favored (20.24%) General / -89.9,154.0	28.6% (<i>m-85</i>) chi angles: 308.8,302.2	0.18Å	-	-
141	GLU	147.02	0.513Å OE2 with 143 HIS HB2	Favored (55.59%) General / -66.2,145.6	1.1% (<i>pp20?</i>) chi angles: 80.1,92.9,351.3	0.086Å	-	-
142	THR	128.56	0.757Å HG23 with 134 SER O	Favored (99.58%) General / -62.1,-42.8	66.9% (<i>p</i>) chi angles: 59.5	0.081Å	-	-
143	HIS	88.83	0.647Å CE1 with 131 CYS H	Favored (65.21%) General / -68.1,-48.5	75.3% (<i>m80</i>) chi angles: 295.1,78.2	0.048Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.418 σ
144	LEU	96.48	0.963Å HD22 with 188 LEU HG	Favored (96.82%) General / -64.0,-40.6	21.3% (<i>tp</i>) chi angles: 175.4,75.6	0.165Å	-	-
145	GLY	44.64	-	Favored (90.89%) Glycine / -64.0,-46.6	-	-	-	-
146	VAL	115.9	0.806Å HG21 with 128 VAL HG12	Favored (22%) Isoleucine or valine / -74.3,-51.8	30.4% (<i>m</i>) chi angles: 294.3	0.052Å	-	-
147	ASN	82.24	0.606Å N with 146 VAL HG23	Favored (38.02%) General / -70.4,-50.5	91.6% (<i>m-20</i>) chi angles: 294.3,331.1	0.075Å	-	OUTLIER(S) worst is CA- CB-CG: 4.899 σ
148	HIS	107.98	0.531Å HD2 with 149 LEU HD22	Favored (2.18%) General / -91.0,-59.4	86.3% (<i>t60</i>) chi angles: 180.7,69	0.075Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.464 σ

149	LEU	124.52	0.857Å HD23 with 144 LEU HG	Favored (90.17%) General / -63.8,-45.3	2.1% (<i>mm?</i>) chi angles: 283.5,283.4	0.079Å	-	-
150	GLY	29.97	-	Favored (98.4%) Glycine / -63.8,-40.4	-	-	-	-
151	HIS	65.7	-	Favored (80.49%) General / -67.6,-36.3	29.3% (<i>m170</i>) chi angles: 284.2,146.9	0.055Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.458 σ
152	PHE	59.27	-	Favored (81.4%) General / -60.1,-48.5	79.8% (<i>t80</i>) chi angles: 180.1,84.7	0.094Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 124.27				Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278
153	LEU	98.03	-	Favored (92.18%) General / -65.3,-43.1	81.8% (<i>mt</i>) chi angles: 297.8,182.4	0.09Å	-	-
154	LEU	52.29	0.856Å HA with 105 ILE HD11	Favored (98.36%) General / -61.9,-43.7	63.1% (<i>tp</i>) chi angles: 179.7,63.5	0.096Å	-	-
155	THR	47.6	0.601Å O with 159 LEU HG	Favored (91.19%) General / -65.2,-43.6	86.6% (<i>m</i>) chi angles: 301.2	0.046Å	-	-
156	TYR	104.02	-	Favored (96.35%) General / -60.2,-43.2	24.8% (<i>t80</i>) chi angles: 161,76.4	0.123Å	-	OUTLIER(S) worst is CA- CB-CG: 4.68 σ
157	LEU	59.98	-	Favored (94.6%) General / -65.0,-42.3	83.8% (<i>mt</i>) chi angles: 294.7,180	0.076Å	-	-
158	LEU	83.5	0.624Å O with 162 LEU HD13	Favored (62.63%) General / -73.9,-30.5	81.5% (<i>mt</i>) chi angles: 294.4,180.3	0.081Å	-	-
159	LEU	77.13	0.601Å HG with 155 THR O	Favored (67.83%) General / -53.7,-42.2	55.6% (<i>mt</i>) chi angles: 288.2,180.1	0.1Å	-	-

160	GLU	71.75	-	0.648Å HD3 with 112 PHE O	Favored (98.92%) General / -62.3,-41.9	62.6% (<i>mm-40</i>) chi angles: 291.1,289,303.7	0.073Å	-	-
161	ARG	90.56		0.925Å HD23 with 117 LYS HD2	Favored (98.56%) General / -62.1,-41.8	82.5% (<i>mtt-85</i>) chi angles: 308,179.3,194.3,275.1	0.154Å	-	-
162	LEU	151.09		0.595Å N with 167 PRO HG2	Favored (5.79%) General / -79.3,77.2	5% (<i>mp</i>) chi angles: 291.5,56.3	0.112Å	-	-
163	LYS	231.57		0.601Å HG13 with 165 SER N	Favored (5.98%) General / -54.0,152.2	0.1% chi angles: 179.7,160.6,254.4,52.9	0.081Å	-	-
164	VAL	160.06		0.601Å N with 164 VAL HG13	Favored (90.19%) Isoleucine or valine / -58.7,-46.9	6.3% (<i>p</i>) chi angles: 55.3	0.049Å	-	-
165	SER	51.06		0.903Å HB3 with 167 PRO HD3	OUTLIER (0.04%) General / -60.9,-78.1	79.9% (<i>p</i>) chi angles: 59.9	0.079Å	-	-
166	ALA	54.33		1.052Å HA with 117 LYS HB3	Favored (41%) Pre-proline / -67.7,-48.9	-	0.092Å	-	-
167	PRO	228.32		0.867Å HB1 with 169 ARG HD2	Favored (6.49%) Trans-proline / -72.3,120.0	84.3% (<i>Cg_exo</i>) chi angles: 331	0.288Å	-	-
168	ALA	103.41		0.867Å HD2 with 168 ALA HB1	Favored (6.89%) General / -72.0,-55.7	-	0.089Å	-	-
169	ARG	235.77			Favored (11.99%) General / -166.3,171.6	8.5% (<i>mpt_?</i>) chi angles: 292,85.7,171.5,159.8	0.14Å	-	-
170	VAL	75.62			Favored (69.94%) Isoleucine or valine / -121.7,132.8	79.8% (<i>t</i>) chi angles: 174.5	0.125Å	-	-
171	VAL	90.06			Favored (73.91%) Isoleucine or valine / -121.7,132.8	77.7% (<i>t</i>) chi angles: 172.3	0.208Å	-	-

			120 HIS CG	valine / -116.8,125.8				
172	ASN	74.14	0.55Å ND2 with 124 ASN HD22	Favored (55.8%) General / -113.8,132.6	8.8% (<i>m120</i>) chi angles: 286.1,75.9	0.127Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: Clashscore: Outliers: 14 of Poor rotamers: 11 of Outliers: Outliers: 8 Outliers: 60 124.27 146.96 276 234 9 of 259 of 278 of 278								
173	VAL	77.62	-	Favored (46.1%) Isoleucine or valine / -94.6,128.1	78.1% (<i>t</i>) chi angles: 179.2	0.058Å	-	-
174	SER	143.26	0.633Å O with 229 HIS HB2	Allowed (0.5%) General / -115.7,-152.4	60.3% (<i>p</i>) chi angles: 72.2	0.104Å	-	-
175	SER	107.93	0.512Å OG with 234 ARG HB3	Favored (25.23%) General / -162.2,166.6	41.6% (<i>t</i>) chi angles: 177.5	0.114Å	-	-
176	VAL	169.83	0.429Å HG13 with 177 ALA N	Favored (40.89%) Isoleucine or valine / -63.2,-26.4	14.5% (<i>p</i>) chi angles: 63.3	0.109Å	-	-
177	ALA	104.75	0.429Å N with 176 VAL HG13	Favored (62.14%) General / -58.4,-25.4	-	0.079Å	-	-
178	HIS	136.37	0.714Å NE2 with 291 SER HB3	Favored (67.33%) General / -64.5,-23.6	4% (<i>p-80</i>) chi angles: 69.4,240.8	0.17Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.372 σ
179	HIS	105.73	-	Favored (71.76%) General / -56.1,-50.2	58.3% (<i>t-80</i>) chi angles: 197.3,286.1	0.067Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.44 σ
180	ILE	157.37	0.432Å CG2 with 201 CYS SG	Favored (36.62%) Isoleucine or valine / -69.2,-27.9	11.2% (<i>tp</i>) chi angles: 192.1,66.6	0.075Å	-	-
181	GLY	63.94	-	Favored (33.76%) Glycine / -60.3,154.3	-	-	-	-

182	LYS	87.5	-	0.602Å HD13 with 202 HIS CD2	Favored (36.11%) General / -142.2,147.2	53.6% (<i>mttm</i>) chi angles: 290.5,167.8,168.5,291.3	0.138Å	-	-
183	ILE	138.76	-	0.602Å HD13 with 202 HIS CD2	Favored (65.37%) Pre-proline / -98.4,114.5	43.9% (<i>mm</i>) chi angles: 303.1,296	0.097Å	-	-
184	PRO	120.69	-	0.632Å HD2 with 202 HIS CE1	Allowed (1.94%) Trans-proline / -84.3,115.3	12.5% (<i>Cg_endo</i>) chi angles: 15.5	0.121Å	-	-
185	PHE	115.05	-	-	Favored (66.6%) General / -70.7,-44.5	46.3% (<i>m-85</i>) chi angles: 308.8,273	0.14Å	-	OUTLIER(S) worst is CA- CB-CG: 5.928 σ
186	HIS	90.21	-	-	Favored (64.62%) General / -64.0,-51.4	71.8% (<i>m80</i>) chi angles: 298.1,77.6	0.075Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.457 σ
187	ASP	180.94	-	0.78Å HB3 with 190 SER HB3	Allowed (1.21%) General / -123.7,73.6	75.5% (<i>m-20</i>) chi angles: 290.5,323.4	0.15Å	-	-
188	LEU	97.32	-	0.963Å HG with 144 LEU HD22	Favored (72.35%) General / -63.4,-49.8	27.4% (<i>tp</i>) chi angles: 190.5,65	0.121Å	-	OUTLIER(S) worst is C-N- CA: 4.289 σ
189	GLN	140.17	-	0.578Å OE1 with 140 PHE HD1	Favored (17.86%) General / -90.2,-30.0	22.5% (<i>mt-30</i>) chi angles: 300.8,172.8,188.9	0.136Å	-	OUTLIER(S) worst is C-N- CA: 6.985 σ
190	SER	196.77	-	0.78Å HB3 with 187 ASP HB3	OUTLIER (0.03%) General / -66.0,-165.3	2.1% (<i>t</i>) chi angles: 205.1	0.14Å	-	OUTLIER(S) worst is C-N- CA: 7.645 σ
191	GLU	141.52	-	-	Favored (67.06%) General / -56.1,-35.5	13.3% (<i>pt-20</i>) chi angles: 64.1,180.1,54	0.109Å	-	-
192	LYS	115.39	-	0.421Å NZ with 184 PRO HG3	Favored (3.74%) General / -56.3,159.1	19% (<i>pttm</i>) chi angles: 61.6,164.9,174.3,283.6	0.086Å	-	-

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

Avg: Clashscore: Outliers: 14 of Poor rotamers: 11 of Outliers: Outliers: 8 Outliers: 60

		124.27	146.96	276	234	9 of 259	of 278	of 278
193	ARG	112.01	-	Favored (9.18%) General / -53.9,149.1	17.4% (<i>ptm180</i>) chi angles: 62.6,186,293.3,171.5	0.107Å	-	-
194	TYR	91.21	-	Favored (44.79%) General / -102.6,135.2	79.5% (<i>t80</i>) chi angles: 184.4,78.2	0.07Å	-	-
195	SER	100.86	0.773Å OG with 198 PHE HB2	Favored (46.81%) General / -127.6,129.2	93.6% (<i>p</i>) chi angles: 66.9	0.107Å	-	-
196	ARG	107.71	0.628Å HG2 with 131 CYS O	Favored (92.61%) General / -61.6,-45.8	77.2% (<i>mtm180</i>) chi angles: 293.4,173.3,290,153.4	0.075Å	-	-
197	GLY	51.63	-	Favored (77.77%) Glycine / -67.9,-44.9	-	-	-	-
198	PHE	72.95	0.773Å HB2 with 195 SER OG	Favored (75.89%) General / -67.8,-34.0	34.7% (<i>m-85</i>) chi angles: 278.5,80.8	0.159Å	-	-
199	ALA	42.08	-	Favored (95.4%) General / -62.5,-40.0	-	0.086Å	-	-
200	TYR	78.18	0.552Å OH with 204 LYS HE3	Favored (93.75%) General / -64.0,-44.1	66.5% (<i>t80</i>) chi angles: 183.2,66.6	0.036Å	-	-
201	CYS	60.18	0.432Å SG with 180 ILE CG2	Favored (91.47%) General / -63.2,-38.5	68.8% (<i>m</i>) chi angles: 301.8	0.036Å	-	-
202	HIS	75.92	0.828Å CE1 with 188 LEU HD12	Favored (98.19%) General / -61.4,-42.1	5.1% (<i>t-160</i>) chi angles: 180,163.1	0.102Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.56 σ
203	SER	101.46	-	Favored (92.16%) General / -65.7,-41.5	17.8% (<i>m</i>) chi angles: 307.1	0.173Å	-	-
204	LYS	143.54	0.552Å HE3 with 200	Favored (77.38%)	37.3% (<i>mmtt</i>) chi angles:	0.109Å	-	-

205	LEU	132.3	0.772Å O with 208 VAL HG22	Favored (92.78%) General / -65.4,-40.0	1% chi angles: 192.5,304.9	0.142Å	-	-	
206	ALA	49.87	-	Favored (82.9%) General / -61.2,-37.4	-	0.086Å	-	-	
207	ASN	81.16	-	Favored (85.55%) General / -59.3,-40.3	25.6% (<i>m120</i>) chi angles: 292,132.1	0.142Å	-	-	
208	VAL	152.71	0.782Å HG11 with 248 TRP CZ3	Favored (61.22%) Isoleucine or valine / -72.8,-41.7	20.8% (<i>m</i>) chi angles: 303.3	0.113Å	-	-	
209	LEU	71.19	0.569Å HG with 205 LEU CD1	Favored (82.63%) General / -62.1,-36.7	79.3% (<i>mt</i>) chi angles: 292.8,179.9	0.09Å	-	-	
210	PHE	78.7	-	Favored (88.79%) General / -59.5,-46.5	61.1% (<i>t80</i>) chi angles: 168.6,79.9	0.094Å	-	-	
211	THR	69.96	0.51Å HG23 with 225 THR HG23	Favored (95.3%) General / -64.7,-40.4	92.2% (<i>m</i>) chi angles: 300.4	0.051Å	-	-	
212	ARG	182.06	0.613Å HB2 with 212 ARG NH1	Favored (78.47%) General / -65.1,-47.1	12.7% (<i>ttm105</i>) chi angles: 168.4,172,277.8,84.9	0.083Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:				Clashscore:	Outliers: 14 of	Poor rotamers: 11 of	Outliers:	Outliers: 8	Outliers: 60
124.27				146.96	276	234	9 of 259	of 278	of 278
213	GLU	102.08	0.525Å HG3 with 217 ARG HE	Favored (85.1%) General / -67.5,-40.3	19.1% (<i>tp10</i>) chi angles: 178.1,65.9,345.5	0.066Å	-	-	
214	LEU	144.29	0.99Å HD13 with 218 LEU HD13	Favored (91.76%) General / -59.0,-44.9	1.8% (<i>tm?</i>) chi angles: 186.1,299.8	0.135Å	-	-	

215	ALA	61.08	-	(91.1%) General / -64.3,-38.5	-	0.074Å	-	-
216	LYS	146.29	0.62Å C with 216 LYS HD2	Favored (97.12%) General / -61.8,-44.3	3.6% (<i>tmmm?</i>) chi angles: 179.7,286.7,286.6,294.8	0.014Å	-	-
217	ARG	70.09	0.525Å HE with 213 GLU HG3	Favored (94.7%) General / -65.2,-41.2	86.3% (<i>mtt-85</i>) chi angles: 298.2,171.5,185.7,261.7	0.019Å	-	-
218	LEU	139	1.07Å HD23 with 223 VAL HG23	Favored (64.71%) General / -68.3,-22.1	10.1% (<i>mp</i>) chi angles: 278,56.2	0.104Å	-	-
219	GLN	89.88	-	Favored (68.41%) General / -56.3,-36.2	64.6% (<i>tt0</i>) chi angles: 179.9,181.4,359.2	0.133Å	-	-
220	GLY	45.97	-	Favored (71.64%) Glycine / -64.8,-48.5	-	-	-	-
221	THR	130.17	0.903Å HG22 with 218 LEU HA	Favored (49.24%) General / -69.6,-49.9	7.1% (<i>t</i>) chi angles: 194.1	0.108Å	-	-
222	GLY	54.18	0.582Å N with 221 THR HG23	Favored (4.08%) Glycine / 121.6,-34.0	-	-	-	-
223	VAL	132.42	1.07Å HG23 with 218 LEU HD23	Favored (5.29%) Isoleucine or valine / -77.3,157.4	27.8% (<i>m</i>) chi angles: 295.5	0.07Å	-	-
224	THR	155.12	0.646Å HG23 with 169 ARG HG2	Favored (30.6%) General / -128.5,161.0	10.1% (<i>t</i>) chi angles: 181.3	0.172Å	-	-
225	THR	133.18	0.602Å HB with 214 LEU HD12	Favored (55.21%) General / -121.2,133.9	14.8% (<i>t</i>) chi angles: 188.7	0.057Å	-	-
226	TYR	124.84	0.893Å CG with 274 LEU HB2	Favored (10.91%) General / -133.0,173.9	0.9% chi angles: 314.7,352.2	0.265Å	-	OUTLIER(S) worst is N-CA- CB: 4.747 σ

227	ALA	85.56	1.021Å HB3 with 277 LEU HG	Favored (22.82%) General / -142.2,167.1	-	0.088Å	-	-
228	VAL	158.02	0.779Å HG21 with 264 THR C	Favored (3.54%) Isoleucine or valine / -154.4,158.7	13.4% (<i>p</i>) chi angles: 62.8	0.155Å	-	-
229	HIS	152.9	0.877Å NE2 with 247 LEU HB3	Favored (29.58%) Pre-proline / -149.7,149.9	0.9% chi angles: 90.4,69.1	0.324Å	-	OUTLIER(S) worst is CA- CB-CG: 6.445 σ
230	PRO	164.25	0.967Å HB2 with 244 LEU HD22	Favored (26.59%) Trans-proline / -72.9,-13.3	23.5% (<i>Cg_endo</i>) chi angles: 19.9	0.172Å	-	OUTLIER(S) worst is C-N- CA: 4.702 σ
231	GLY	98.78	0.748Å HA3 with 245 CYS C	Favored (19.11%) Glycine / 100.0,-151.0	-	-	-	-
232	VAL	157.39	0.759Å HG13 with 284 ASP O	Favored (32.85%) Isoleucine or valine / -56.0,-32.3	34.5% (<i>m</i>) chi angles: 298.7	0.085Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 124.27			Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278	Outliers: 60 of 278
233	VAL	181.19	1.194Å HG21 with 240 HIS HB3	Favored (28.86%) Isoleucine or valine / -69.9,-25.8	86.7% (<i>t</i>) chi angles: 177.7	0.339Å	-	OUTLIER(S) worst is CA- CB-CG2: 5.339 σ
234	ARG	269.11	0.803Å HG2 with 230 PRO HG2	Favored (21.11%) General / -77.8,1.2	15.8% (<i>mmt85</i>) chi angles: 275.9,304.5,178.4,91.2	0.145Å	-	-
235	SER	136.67	-	Allowed (0.16%) General / -88.2,-148.8	96.4% (<i>p</i>) chi angles: 66.4	0.161Å	-	OUTLIER(S) worst is N-CA- C: 4.003 σ
236	GLU	224.8	0.548Å HG2 with 236 GLU O	Favored (62.37%) General / -59.1,-23.7	38.1% (<i>tt0</i>) chi angles: 180.1,191.9,43.9	0.085Å	OUTLIER(S) worst is C--N: 4.235 σ	OUTLIER(S) worst is C-N- CA: 5.005 σ

237	LEU 328.28	0.636Å N with 237 LEU HD12	(0.11%) General / -83.9,-150.4	4% (<i>mp</i>) chi angles: 299.3,69	0.135Å	OUTLIER(S) worst is C--N: 7.431 σ	OUTLIER(S) worst is C-N- CA: 6.299 σ
238	VAL 361.18	0.664Å HG12 with 239 ARG N	OUTLIER (0%) Isoleucine or valine / -161.2,-125.8	39.6% (<i>t</i>) chi angles: 185.1	0.04Å	-	OUTLIER(S) worst is C-N- CA: 5.731 σ
239	ARG 374.78	0.664Å N with 238 VAL HG12	OUTLIER (0%) General / -0.7,63.3	50.3% (<i>mtm180</i>) chi angles: 293.8,196.5,298.1,148.7	0.093Å	-	-
240	HIS 277.74	1.194Å HB3 with 233 VAL HG21	Allowed (1.95%) General / -138.7,-0.2	15% (<i>p-80</i>) chi angles: 45.1,273.9	0.604Å	OUTLIER(S) worst is CA-- C: 5.154 σ	OUTLIER(S) worst is CB- CA-C: 9.31 σ
241	SER 148.65	0.64Å HA with 240 HIS CD2	Favored (9.62%) General / -49.9,-56.7	5.5% (<i>t</i>) chi angles: 198.9	0.081Å	-	-
242	SER 133.54	0.603Å O with 260 GLU HB3	Favored (4.99%) General / -70.5,-57.2	47.3% (<i>t</i>) chi angles: 180.1	0.09Å	-	-
243	LEU 201.95	0.49Å HA with 260 GLU HA	Favored (59.3%) General / -69.4,-49.0	62.7% (<i>tp</i>) chi angles: 179.9,63.5	0.119Å	-	OUTLIER(S) worst is C-N- CA: 4.324 σ
244	LEU 277.91	1.105Å HD23 with 233 VAL HB	OUTLIER (0.01%) General / -2.5,115.6	2.3% (<i>mp</i>) chi angles: 313.1,93.4	0.212Å	-	OUTLIER(S) worst is N-CA- CB: 4.214 σ
245	CYS 110.49	1.1Å HB3 with 285 CYS HA	Favored (8.14%) General / -92.9,93.0	96.3% (<i>m</i>) chi angles: 294.8	0.126Å	-	OUTLIER(S) worst is C-N- CA: 9.838 σ
246	LEU 264.8	1.048Å HD11 with 261 GLY HA2	OUTLIER (0%) General / -28.3,176.4	0.1% chi angles: 319.5,311.4	0.155Å	-	-
247	LEU 344.54	0.877Å HB3 with 229 HIS NE2	Favored (2.35%) General / -161.2,119.0	61.7% (<i>tp</i>) chi angles: 174.9,61.8	0.122Å	-	-
248	TRP 450.74	1.028Å CG with 277 LEU HB2	OUTLIER (0%) General / 152.2,145.8	1.9% (<i>t-105</i>) chi angles: 201.7,299	0.272Å	-	OUTLIER(S) worst is N-CA- CB: 4.192 σ
249	ARG 426.24	0.779Å HB3 with 288 THR C	OUTLIER (0%) General / 146.7,173.1	2.3% (<i>tpm_?</i>) chi angles: 189.1,67.5,264.7,265.7	0.14Å	-	-
		0.619Å	Favored (0.000%)	50.0% (<i>tp</i>)	0.000Å	-	-

250	LEU	311.48	N with 249 ARG HG3	(0.99%) General / -96.2,170.8	55.5% (<i>ψ</i>) chi angles: 180,60.4	0.101Å	-	-
251	PHE	250.74	0.568Å N with 250 LEU HG	Favored (36.45%) General / -77.0,129.7	87.4% (<i>m</i> -85) chi angles: 291.5,280.3	0.116Å	-	OUTLIER(S) worst is CA- CB-CG: 6.175 σ
252	SER	163.36	-	Favored (31.17%) Pre-proline / -116.5,122.9	66.8% (<i>m</i>) chi angles: 292.7	0.101Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 124.27				Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278
253	PRO	153.91	-	Favored (54.64%) Trans-proline / -57.4,-23.3	91.3% (<i>Cg_endo</i>) chi angles: 30.2	0.054Å	-	-
254	PHE	183.36	-	Favored (51.82%) General / -66.1,148.4	82.2% (<i>m</i> -85) chi angles: 301.6,88.3	0.054Å	-	OUTLIER(S) worst is CA- CB-CG: 8.788 σ
255	VAL	139.98	0.774Å HG12 with 287 ARG NH2	Allowed (0.87%) Isoleucine or valine / -127.8,-172.6	35.1% (<i>m</i>) chi angles: 298.3	0.087Å	-	-
256	LYS	305.67	0.524Å HG3 with 256 LYS O	Favored (12.94%) General / 58.1,48.5	13.1% (<i>tppt?</i>) chi angles: 187.3,62.6,48.9,181.9	0.089Å	-	-
257	THR	276.04	-	Favored (33.11%) General / -79.4,145.9	59.8% (<i>p</i>) chi angles: 62.4	0.068Å	-	-
258	ALA	210.82	0.768Å HB2 with 33 THR HB	Favored (16.98%) General / -80.4,170.0	-	0.104Å	-	-
259	ARG	213.72	0.919Å HG2 with 280 LYS HZ1	Favored (23.26%) General / -118.5,114.7	73.8% (<i>mtt</i> -85) chi angles: 305.8,186.9,201.3,275.2	0.189Å	-	-
260	GLU	247.55	1.112Å HB2 with 263 GLN HB2	Favored (15.85%) General / -154.8,138.2	6% (<i>mp0</i>) chi angles: 292.9,94.2,49	0.159Å	-	-

261	GLY	105.41	1.048Å HA2 with 246 LEU HD11	Favored (86.94%) Glycine / -65.9,-45.6	-	-	-	-
262	ALA	78.65	0.577Å O with 266 LEU HG	Favored (72.21%) General / -63.8,-31.1	-	0.105Å	-	-
263	GLN	161.92	1.112Å HB2 with 260 GLU HB2	Favored (98.29%) General / -60.9,-43.5	53.8% (<i>tt0</i>) chi angles: 179.9,176.8,329.4	0.302Å	-	OUTLIER(S) worst is C-N- CA: 6.135 σ
264	THR	202.67	0.983Å HG21 with 279 GLY HA2	Favored (80.91%) General / -65.8,-35.5	23.1% (<i>p</i>) chi angles: 49.6	0.352Å	-	OUTLIER(S) worst is N-CA- CB: 6.274 σ
265	SER	84.86	0.617Å HA with 228 VAL HG11	Favored (93.97%) General / -61.5,-40.2	69.4% (<i>m</i>) chi angles: 296	0.11Å	-	-
266	LEU	87.95	0.577Å HG with 262 ALA O	Favored (96.14%) General / -63.9,-40.3	82.6% (<i>mt</i>) chi angles: 294.2,179.9	0.057Å	-	-
267	HIS	94.4	0.661Å O with 272 GLU HG2	Favored (94.8%) General / -64.6,-43.1	9.5% (<i>t-160</i>) chi angles: 198.9,174.6	0.085Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.401 σ
268	CYS	116.65	0.795Å SG with 226 TYR HB2	Favored (65.81%) General / -68.6,-27.2	42.8% (<i>t</i>) chi angles: 178.3	0.09Å	-	-
269	ALA	131.85	0.5Å O with 120 HIS HB2	Favored (27.38%) General / -51.4,-32.8	-	0.083Å	-	-
270	LEU	308.31	0.948Å CD2 with 119 LEU HA	OUTLIER (0%) General / 143.4,18.3	47.9% (<i>tp</i>) chi angles: 183.5,65.8	0.203Å	-	OUTLIER(S) worst is N-CA- CB: 5.959 σ
271	ALA	133.76	0.589Å HB2 with 37 LEU CD2	Favored (75.74%) General / -59.7,-36.0	-	0.149Å	-	OUTLIER(S) worst is N-CA- C: 4.054 σ
272	GLU	143.4	0.756Å HG3 with 274 LEU HD11	Favored (2.12%) General / -130.8,-169.2	22.3% (<i>pt-20</i>) chi angles: 61.1,180,351.7	0.089Å	-	-

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

		Average		Clashscore		Outliers: 14 of 276		Poor rotamers: 11 of 234		Outliers: 9 of 259		Outliers: 8 of 278		Outliers: 60 of 278	
		Avg: 124.27		Clashscore: 146.96		Outliers: 14 of 276		Poor rotamers: 11 of 234		Outliers: 9 of 259		Outliers: 8 of 278		Outliers: 60 of 278	
273	GLY	71.24	0.766Å	C with 274	LEU HD12	Favored (18.9%)	Glycine / -116.8,147.6	-	-	-	-	-	-	-	-
274	LEU	210.77	0.893Å	HB2 with 226	TYR CG	Allowed (0.15%)	General / -166.5,-153.1	5.7% (<i>mp</i>)	chi angles: 295.7,78.3	0.17Å	OUTLIER(S) worst is C--N: 4.372 σ	OUTLIER(S) worst is C-N-CA: 10.582 σ			
275	GLU	359.39	0.744Å	HB3 with 276	PRO HD3	OUTLIER (0%)	Pre-proline / 146.8,-33.6	65.7% (<i>tt0</i>)	chi angles: 180,179.9,28.6	0.185Å	-	OUTLIER(S) worst is N-CA-C: 5.65 σ			
276	PRO	211.07	0.744Å	HD3 with 275	GLU HB3	Favored (8.5%)	Trans-proline / -66.3,172.7	32.9% (<i>Cg_exo</i>)	chi angles: 325.4	0.167Å	-	-			
277	LEU	186.18	1.028Å	HB2 with 248	TRP CG	Favored (5.31%)	General / -115.3,175.9	0.6%	chi angles: 304.4,54.3	0.114Å	-	-			
278	SER	125.06	0.474Å	HA with 248	TRP O	Favored (40.31%)	General / -122.8,152.9	47.4% (<i>t</i>)	chi angles: 180	0.107Å	-	-			
279	GLY	95.24	0.983Å	HA2 with 264	THR HG21	Favored (5.11%)	Glycine / 150.0,149.8	-	-	-	-	OUTLIER(S) worst is C-N-CA: 4.273 σ			
280	LYS	167.75	0.936Å	HD2 with 245	CYS HB3	Favored (27.83%)	General / -54.4,142.2	42.2% (<i>mttm</i>)	chi angles: 304,193.7,162.2,298.3	0.117Å	-	OUTLIER(S) worst is C-N-CA: 4.381 σ			
281	TYR	159.78	0.739Å	HB3 with 286	LYS HB3	Favored (86.39%)	General / -65.7,-44.3	82.5% (<i>t80</i>)	chi angles: 178.9,84.3	0.072Å	-	-			
282	PHE	226.87	0.745Å	H with 286	LYS HB2	Favored (63.34%)	General / -69.9,-20.6	34.3% (<i>t80</i>)	chi angles: 195.2,87.1	0.085Å	-	OUTLIER(S) worst is CA-CB-CG: 9.749 σ			
283	SER	265	0.708Å	OG with 247	LEU HD22	OUTLIER (0.02%)	General / 90.7,-43.2	47.9% (<i>t</i>)	chi angles: 179.8	0.088Å	-	-			
284	ASP	112.42	0.759Å	O with 232		Favored (61.54%)		70.2% (<i>m-20</i>)		0.107Å	-	OUTLIER(S) worst is CA-CB-CG: 4.465 σ			

		VAL HG13	General / -75.2,-34.6	cni angles: 293.9,355.5			CD-CC: 4.405 σ
285	CYS 124.36	1.1Å HA with 245 CYS HB3	Favored (30.21%) General / -158.2,167.3	25.6% (<i>p</i>) chi angles: 57.8	0.09Å	-	-
286	LYS 198.14	0.803Å H with 280 LYS HD3	OUTLIER (0%) General / 125.9,-161.4	29.6% (<i>mmmt</i>) chi angles: 283.7,297.5,296.8,180.9	0.218Å	-	OUTLIER(S) worst is N-CA- CB: 4.087 σ
287	ARG 169.79	0.774Å NH2 with 255 VAL HG12	Favored (17.23%) General / -94.4,154.9	7.2% (<i>ptp180</i>) chi angles: 62.3,161.3,78.1,171.5	0.144Å	-	-
288	THR 258.81	0.831Å HA with 279 GLY O	Favored (47.82%) General / -59.5,130.6	70% (<i>p</i>) chi angles: 63.3	0.086Å	OUTLIER(S) worst is C--N: 5.808 σ	OUTLIER(S) worst is C-N- CA: 4.42 σ
289	TRP 288.47	0.687Å HA with 249 ARG O	Favored (2.7%) General / -170.2,145.2	16.4% (<i>t-105</i>) chi angles: 163.3,268.1	0.105Å	OUTLIER(S) worst is C--N: 5.71 σ	OUTLIER(S) worst is C-N- CA: 10.755 σ
290	VAL 243.63	1.033Å HG11 with 295 ARG HH21	Allowed (1.64%) Isoleucine or valine / -72.4,169.2	9.2% (<i>p</i>) chi angles: 71	0.053Å	OUTLIER(S) worst is C--N: 8.205 σ	OUTLIER(S) worst is C-N- CA: 5.873 σ
291	SER 177.14	0.714Å HB3 with 178 HIS NE2	Favored (31.47%) Pre-proline / -118.9,142.2	60% (<i>p</i>) chi angles: 71.9	0.178Å	-	-
292	PRO 130.67	0.605Å O with 295 ARG HB2	Favored (3.86%) Trans-proline / -66.9,-45.8	12.4% (<i>Cg_endo</i>) chi angles: 15.5	0.292Å	-	OUTLIER(S) worst is N-CA- C: 5.189 σ

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 124.27	Clashscore: 146.96	Outliers: 14 of 276	Poor rotamers: 11 of 234	Outliers: 9 of 259	Outliers: 8 of 278	Outliers: 60 of 278
293	ARG 189.56	-	-	Favored (69.29%) General / -65.5,-28.6	61.1% (<i>ttt85</i>) chi angles: 185.6,181.2,184.8,84.7	0.111Å	-	-
294	ALA 74.64	0.612Å CB with 208 VAL HG21	-	Favored (69.4%) General / -62.2,-28.0	-	0.065Å	-	-
295	ARG 114.88	1.033Å HH21 with	-	Favored (64.26%)	52% (<i>mtt180</i>) chi angles:	0.09Å	-	-

			290 VAL HG11	General / -68.8,-22.8	292.3,191.4,179.3,224.7			
296	ASN	64.72	0.758Å O with 299 THR HG22	Favored (3.84%) General / -66.2,112.2	21.4% (<i>t</i> -20) chi angles: 194.3,302.1	0.061Å	-	OUTLIER(S) worst is CA- CB-CG: 4.39 σ
297	ASN	84.45	-	Favored (80.64%) General / -68.7,-39.6	20.5% (<i>p</i> -10) chi angles: 63.9,313.5	0.09Å	-	OUTLIER(S) worst is CA- CB-CG: 4.372 σ
298	LYS	89.34	0.652Å O with 301 GLU HG2	Favored (99.7%) General / -62.8,-42.4	35.6% (<i>ttmt</i>) chi angles: 183,167,288.2,179.7	0.085Å	-	-
299	THR	103.53	0.758Å HG22 with 296 ASN O	Favored (89.59%) General / -65.3,-38.2	12.2% (<i>t</i>) chi angles: 191.4	0.061Å	-	-
300	ALA	40.25	0.473Å N with 299 THR HG23	Favored (99.6%) General / -61.6,-43.0	-	0.08Å	-	-
301	GLU	86.77	0.652Å HG2 with 298 LYS O	Favored (85.32%) General / -67.5,-40.5	22.4% (<i>pt</i> -20) chi angles: 59,187.9,354.5	0.057Å	-	-
302	ARG	72.72	-	Favored (91.51%) General / -65.9,-40.5	15.7% (<i>mtp</i> -105) chi angles: 298.5,193.7,94.2,247.5	0.067Å	-	-
303	LEU	56.07	0.711Å O with 306 VAL HG12	Favored (83.88%) General / -64.2,-36.4	62% (<i>tp</i>) chi angles: 179.3,60.8	0.072Å	-	-
304	TRP	70.38	-	Favored (99.72%) General / -62.4,-42.8	40.5% (<i>t</i> -105) chi angles: 186.5,275.5	0.096Å	-	-
305	ASN	69.55	-	Favored (97.75%) General / -61.8,-44.0	26.4% (<i>t</i> -20) chi angles: 180.6,254.3	0.074Å	-	OUTLIER(S) worst is CA- CB-CG: 4.157 σ
306	VAL	85.59	0.711Å HG12 with 303 LEU O	Favored (84.54%) Isoleucine or valine / -65.2,-39.1	7.5% (<i>p</i>) chi angles: 69.2	0.068Å	-	-
307	ASP	40.07	0.49Å	Favored (95.27%)	74.2% (<i>m</i>)	0.070Å	-	-

307	SEK	48.57	N with 306 VAL HG13	(99.27%) General / -64.8,-40.5 Favored (84.31%) General / -66.4,-37.0 Favored (97.12%) General / -64.1,-42.1	chi angles: 294.1	0.078Å	-	-
308	CYS	77.9	-	(84.31%) General / -66.4,-37.0 Favored (97.12%) General / -64.1,-42.1	7.2% (<i>p</i>) chi angles: 49.4	0.09Å	-	-
309	GLU	23.43	-	(97.12%) General / -64.1,-42.1	98% (<i>mt-10</i>) chi angles: 292.9,177.6,359.4	0.059Å	-	-
310	LEU	34.93	0.797Å HD12 with 149 LEU HD11	-	79.5% (<i>mt</i>) chi angles: 293.5,180.3	0.065Å	-	-

About [MolProbity](#) | Website for [the Richardson Lab](#) | Using ecloud x-H | Internal reference 4.1-537