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All-Atom Contacts	Clashscore, all atoms:	124.27		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	8	6.90%	Goal: <1%
	Ramachandran outliers	6	4.62%	Goal: <0.05%
	Ramachandran favored	103	79.23%	Goal: >98%
	MolProbity score^	3.94		3 rd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	7	5.65%	Goal: 0
	Bad backbone bonds:	23 / 1053	2.18%	Goal: 0%
	Bad backbone angles:	50 / 1435	3.48%	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	Cβ deviation	Bond lengths	Bond angles
		Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 105	ASN	50	0.968Å ND2 with A 224 ALA HB1	-	60.5% (t30) chi angles: 187,27.3	0.095Å	OUTLIER(S) worst is N--CA: 9.574 σ	OUTLIER(S) worst is CA-CB-CG: 5.805 σ
A 106	LEU	50	0.792Å HD22 with A 120 LEU HD11	Favored (81.11%) General / -68.4,-40.9	93.3% (mt) chi angles: 298.1,174.4	0.061Å	-	-
A 107	TYR	99.99	0.873Å CD1 with A 133 GLU HB2	Favored (76.71%) General / -65.6,-33.8	16.2% (p90) chi angles: 71.9,286.8	0.03Å	-	OUTLIER(S) worst is CD1-CE1-CZ: 8.567 σ
A 108	GLU	50	-	Favored (71.51%) General / -59.5,-33.5	2.3% (mt-10) chi angles: 267.6,224,283.1	0.092Å	-	-
A 109	THR	50	0.68Å HG21 with A 116 THR OG1	Favored (69.36%) General / -60.2,-51.5	55% (m) chi angles: 294.6	0.113Å	-	-

A 110	LEU	99.99	0.809Å HD23 with A 124 ARG CZ	Favored (2.7%) General / -44.2,-36.4	61.3% (<i>tp</i>) chi angles: 179.3,60.4	0.05Å	-	OUTLIER(S) worst is CD1- CG-CD2: 6.519 σ
A 111	GLY	50	0.589Å HA2 with A 124 ARG HH21	Favored (94.92%) Glycine / -58.1,-44.1	-	-	-	-
A 112	VAL	50	0.633Å HG13 with A 113 VAL H	Allowed (0.44%) Isoleucine or valine / -107.2,-77.1	7.3% (<i>p</i>) chi angles: 57.6	0.163Å	-	-
A 113	VAL	99.99	0.972Å HG11 with A 121 TYR HB2	OUTLIER (0.05%) Isoleucine or valine / 68.1,86.6	0.1% chi angles: 270.3	0.243Å	-	OUTLIER(S) worst is CA- CB-CG1: 10.025 σ
A 114	GLY	50	-	Favored (3.89%) Glycine / -108.3,-30.4	-	-	-	-
A 115	SER	50	-	Favored (6.03%) General / -124.9,-16.8	51.7% (<i>m</i>) chi angles: 300.1	0.024Å	-	-
A 116	THR	99.99	0.68Å OG1 with A 109 THR HG21	Allowed (1.88%) General / -139.1,48.3	38.1% (<i>p</i>) chi angles: 53.1	0.075Å	-	OUTLIER(S) worst is CA- CB-CG2: 4.147 σ
A 117	THR	50	0.598Å HA with A 113 VAL HG11	Favored (64.51%) General / -68.5,-23.1	6.8% (<i>t</i>) chi angles: 194.4	0.093Å	-	-
A 118	THR	50	0.483Å HG21 with A 148 TRP CD1	Favored (29.73%) General / -83.9,-25.9	12% (<i>t</i>) chi angles: 185.3	0.088Å	-	-
A 119	GLN	50	0.627Å HB2 with A 148 TRP CZ2	Allowed (0.36%) General / -141.8,-46.0	53.1% (<i>tt0</i>) chi angles: 185.2,181.8,57.2	0.061Å	-	-
A 120	LEU	50	0.805Å HG with A 123 ASP OD2	Favored (56.38%) General / -77.0,-31.4	0.3% chi angles: 212.8,102.4	0.046Å	-	-
A 121	TYR	99.99	0.972Å HB2 with A 113 VAL HG11	Favored (50.12%) General / -51.2,-51.9	18% (<i>t80</i>) chi angles: 195.3,57.7	0.237Å	OUTLIER(S) worst is CG-- CD1: 4.078 σ	OUTLIER(S) worst is CB- CG-CD1: 6.259 σ
A			0.536Å HG21 with A	Favored (62.52%)	68.1% (<i>p</i>)			

122	THR	50	165 ILE HG21	General / -65.6,-15.2	chi angles: 63.2	0.106Å	-	-
A 123	ASP	50	0.805Å OD2 with A 120 LEU HG	Favored (2.51%) General / -48.6,-60.7	79.6% (<i>m</i> -20) chi angles: 292.7,324.6	0.071Å	-	-
A 124	ARG	99.99	1.124Å HG3 with A 129 ARG HB2	Favored (60.12%) General / -74.8,-27.0	54.9% (<i>ttp85</i>) chi angles: 173.1,177.1,79.8,82.9	0.159Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 125	THR	99.99	0.714Å OG1 with A 110 LEU HD11	Favored (40.03%) General / -80.9,-0.6	1.1% (<i>m</i>) chi angles: 270.5	0.154Å	-	OUTLIER(S) worst is CA- CB-CG2: 7.517 σ
A 126	GLU	50	0.501Å HG2 with A 126 GLU O	Favored (14.61%) General / -112.2,22.6	77.8% (<i>tt0</i>) chi angles: 187.8,186.8,350.3	0.053Å	-	-
A 127	LYS	50	0.472Å HB3 with A 126 GLU O	Favored (5.43%) General / 67.2,33.5	28.4% (<i>tptp</i>) chi angles: 181.6,65.5,182.1,66.1	0.094Å	-	-
A 128	LEU	50	0.727Å HD12 with A 123 ASP HA	Favored (17.32%) General / -109.4,-3.1	9% (<i>mt</i>) chi angles: 321.6,177.1	0.067Å	-	-
A 129	ARG	99.99	1.124Å HB2 with A 124 ARG HG3	Favored (5.33%) Pre-proline / -50.4,-60.4	67.2% (<i>ttp85</i>) chi angles: 176.6,179.8,71.9,83.2	0.026Å	-	-
A 130	PRO	99.99	0.864Å HD3 with A 129 ARG HB3	Favored (67.22%) Trans-proline / -64.3,-20.9	88% (<i>Cg_exo</i>) chi angles: 331.4	0.071Å	-	OUTLIER(S) worst is CA- N-CD: 4.096 σ
A 131	GLU	50	0.642Å HG2 with A 128 LEU O	Favored (6.53%) General / -87.6,-50.4	8.4% (<i>pt</i> -20) chi angles: 81.9,184.2,46.8	0.139Å	-	-
A 132	MET	50	0.708Å SD with A 123 ASP HB3	Favored (28.95%) General / -71.5,-50.7	57.3% (<i>mtt</i>) chi angles: 290.9,187.3,174.5	0.041Å	-	-
A 133	GLU	99.99	0.873Å HB2 with A 107 TYR CD1	Allowed (1.38%) General / -100.3,39.1	48.7% (<i>tp10</i>) chi angles: 186.3,69.4,8.3	0.248Å	-	OUTLIER(S) worst is C- CA-CB: 4.242 σ

A 134	GLY	50	-	OUTLIER (0.01%) Glycine / -56.6,-97.7	-	-	-	-
A 135	PRO	50	-	OUTLIER (0%) Trans-proline / -143.4,87.6	29.3% (<i>Cg_endo</i>) chi angles: 37.4	0.12Å	-	-
A 136	GLY	50	-	Favored (7.77%) Glycine / 151.7,157.2	-	-	-	-
A 137	SER	50	0.449Å HA with A 226 ASN O	Allowed (1.81%) General / -59.8,112.4	99% (<i>p</i>) chi angles: 64.3	0.03Å	-	-
A 138	PHE	50	-	Favored (56.09%) General / -115.9,128.8	10.7% (<i>m-85</i>) chi angles: 270.7,293.7	0.035Å	-	-
A 139	THR	50	0.729Å HG21 with A 179 ARG HD2	Favored (38.67%) General / -96.2,122.1	4.7% (<i>t</i>) chi angles: 175.2	0.054Å	-	-
A 140	ILE	50	0.655Å HG21 with A 106 LEU CD2	Favored (40.13%) Isoleucine or valine / -132.6,119.9	7.6% (<i>tp</i>) chi angles: 185.5,72.8	0.077Å	-	OUTLIER(S) worst is CB- CG1-CD1: 4.039 σ
A 141	PHE	50	0.666Å HB2 with A 236 ILE CD1	Favored (7.47%) General / -84.5,89.6	0.4% chi angles: 326,75.2	0.104Å	OUTLIER(S) worst is C--N: 4.271 σ	OUTLIER(S) worst is CB- CG-CD2: 4.913 σ
A 142	ALA	50	0.673Å HB3 with A 231 LEU HD22	Favored (37.01%) Pre-proline / -97.9,106.9	-	0.06Å	-	-
A 143	PRO	50	0.621Å HB3 with A 232 ILE HG13	Favored (15.37%) Trans-proline / -56.5,158.6	58.1% (<i>Cg_endo</i>) chi angles: 26.5	0.029Å	-	-
A 144	SER	50	-	Favored (42.34%) General / -70.0,154.1	46.4% (<i>t</i>) chi angles: 180.5	0.028Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
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A	Favored (35.5%)	53.1% (<i>t30</i>)
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145	ASN	50	-	General / -53.8,-28.5	chi angles: 184.9,56.5	0.032Å	-	-
A 146	GLU	50	-	Favored (72.27%) General / -70.6,-34.5	12.5% (<i>pt-20</i>) chi angles: 63.9,178.8,64.5	0.034Å	-	-
A 147	ALA	50	-	Favored (99.34%) General / -62.7,-41.9	-	0.047Å	-	-
A 148	TRP	99.99	0.74Å CE3 with A 159 LEU HD13	Favored (96.1%) General / -64.4,-42.4	93% (<i>m95</i>) chi angles: 298,95.4	0.063Å	OUTLIER(S) worst is NE1-- CE2: 6.227 σ	OUTLIER(S) worst is CZ2- CH2-CZ3: 4.461 σ
A 149	ALA	50	0.842Å HA with A 156 LEU HD12	Favored (67.07%) General / -68.5,-28.5	-	0.118Å	-	-
A 150	SER	50	-	Favored (80.91%) General / -68.3,-37.9	35.8% (<i>t</i>) chi angles: 182.6	0.034Å	-	-
A 151	LEU	50	0.725Å HB3 with A 155 VAL HG21	Favored (31.17%) Pre-proline / -56.8,119.6	21% (<i>mt</i>) chi angles: 299.7,193.3	0.144Å	-	-
A 152	PRO	50	0.793Å O with A 155 VAL HG22	Allowed (0.26%) Trans-proline / -72.6,-166.1	93% (<i>Cg_endo</i>) chi angles: 32.7	0.016Å	-	-
A 153	ALA	50	-	Allowed (0.14%) General / 52.4,-157.7	-	0.074Å	-	-
A 154	GLU	50	-	Favored (3.55%) General / -93.5,25.2	11.9% (<i>pt-20</i>) chi angles: 63.7,176.8,61.5	0.033Å	-	-
A 155	VAL	50	0.793Å HG22 with A 152 PRO O	Favored (36.17%) Isoleucine or valine / -73.5,-32.5	19% (<i>m</i>) chi angles: 304.1	0.042Å	-	-
A 156	LEU	50	0.842Å HD12 with A 149 ALA HA	Favored (72.8%) General / -71.0,-37.5	6.2% (<i>tt</i>) chi angles: 183.5,166.4	0.055Å	-	-
A 157	ASP	50	0.733Å O with A 160 VAL HG12	Favored (84.49%) General / -66.9,-37.5	38.7% (<i>t70</i>) chi angles: 186.4,57.2	0.019Å	-	-

A 158	SER	50	-	Favored (71.85%) General / -71.0,-34.9	69.8% (<i>m</i>) chi angles: 297.8	0.028Å	-	-	
A 159	LEU	50	0.74Å HD13 with A 148 TRP CE3	Favored (61.05%) General / -74.1,-15.2	58% (<i>mt</i>) chi angles: 285.2,174.3	0.138Å	-	-	
A 160	VAL	50	0.733Å HG12 with A 157 ASP O	Favored (7.2%) Isoleucine or valine / -84.1,-28.2	8.9% (<i>p</i>) chi angles: 73.1	0.144Å	-	-	
A 161	SER	50	-	Favored (43.43%) General / -74.8,144.6	68.6% (<i>m</i>) chi angles: 296.1	0.041Å	-	-	
A 162	ASN	50	0.828Å O with A 165 ILE HG12	Favored (63.36%) General / -64.7,-16.8	32.6% (<i>m120</i>) chi angles: 292.2,115.5	0.02Å	-	-	
A 163	VAL	50	-	Favored (57.87%) Isoleucine or valine / -61.3,-33.7	14.8% (<i>p</i>) chi angles: 63.8	0.069Å	-	-	
A 164	ASN	50	-	Favored (71.86%) General / -59.5,-33.9	7.2% (<i>p30</i>) chi angles: 77.6,62.5	0.017Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 165	ILE	50	0.828Å HG12 with A 162 ASN O	Favored (45.89%) Isoleucine or valine / -70.5,-31.3	18.2% (<i>pt</i>) chi angles: 70.1,180.7	0.061Å	-	-	
A 166	GLU	50	-	Favored (77.79%) General / -64.5,-34.2	2.7% (<i>mt-10</i>) chi angles: 274.1,132,47.9	0.03Å	-	-	
A 167	LEU	99.99	0.703Å O with A 167 LEU HD23	Favored (43.05%) General / -98.7,9.6	7.2% (<i>tt</i>) chi angles: 187.9,163.2	0.053Å	-	OUTLIER(S) worst is CD1- CG-CD2: 4.202 σ	
A 168	LEU	99.99	0.435Å C with A 168 LEU HD23	Favored (81.72%) General /	5.9% (<i>tt</i>) chi angles: 179.6,164.8	0.103Å	-	-	

A 169	ASN	99.99	0.799Å HA with A 171 LEU N	-68.1,-38.0 Favored (48.97%) General / -102.2,130.9	1.5% (<i>p30</i>) chi angles: 89,20.1	0.149Å	-	OUTLIER(S) worst is CA- CB-CG: 6.641 σ
A 170	ALA	50	0.748Å C with A 169 ASN HA	OUTLIER (0.01%) General / 31.3,36.3	-	0.193Å	OUTLIER(S) worst is C--N: 8.665 σ	OUTLIER(S) worst is C-N- CA: 5.369 σ
A 171	LEU	50	0.799Å N with A 169 ASN HA	Favored (72.44%) General / -70.2,-34.0	0.5% chi angles: 57.7,182.4	0.288Å	-	OUTLIER(S) worst is N- CA-CB: 7.196 σ
A 172	ARG	50	0.753Å HA with A 175 MET HG2	Favored (66.38%) General / -53.0,-43.1	58.3% (<i>mmm-85</i>) chi angles: 296.5,295.9,297.3,275.7	0.025Å	-	-
A 173	TYR	50	0.529Å OH with A 194 MET HB2	Favored (70.96%) General / -65.0,-30.0	21.1% (<i>t80</i>) chi angles: 200,80.8	0.05Å	-	-
A 174	HIS	50	0.579Å CE1 with A 236 ILE HD11	Favored (22.66%) General / -90.4,-20.6	0.3% chi angles: 212.2,359.4	0.067Å	OUTLIER(S) worst is CG-- ND1: 4.416 σ	OUTLIER(S) worst is CB- CG-CD2: 4.342 σ
A 175	MET	50	0.753Å HG2 with A 172 ARG HA	Favored (49.17%) General / -105.2,133.9	27.3% (<i>ptm</i>) chi angles: 64.7,180.9,281	0.024Å	-	-
A 176	VAL	50	0.798Å HG11 with A 179 ARG NH2	Allowed (0.56%) Isoleucine or valine / -151.1,114.4	24% (<i>t</i>) chi angles: 187.1	0.015Å	-	OUTLIER(S) worst is CA- CB-CG1: 4.113 σ
A 177	GLY	50	0.441Å O with A 178 ARG HG2	Favored (25.37%) Glycine / -74.9,139.5	-	-	-	-
A 178	ARG	50	0.441Å HG2 with A 177 GLY O	Allowed (0.5%) General / 56.0,72.4	33.9% (<i>ptt-85</i>) chi angles: 66,179.7,176.4,273.2	0.128Å	-	-
A 179	ARG	50	0.929Å HH22 with A 192 THR HB	Favored (5.61%) General / -129.0,100.3	61.5% (<i>ttm-85</i>) chi angles: 181.9,182.6,299,276.7	0.025Å	-	-
A 180	VAL	50	0.417Å HG21 with A 184 GLU HG3	Favored (6.33%) Isoleucine or valine / -89.6,146.3	13% (<i>p</i>) chi angles: 65.4	0.139Å	-	-

A 181	LEU	50	0.737Å HD23 with A 183 ASP H	Favored (54.19%) General / -62.0,145.0	7% (<i>tt</i>) chi angles: 192.5,162.3	0.088Å	-	OUTLIER(S) worst is CD1- CG-CD2: 4.788 σ
A 182	THR	50	0.814Å HG22 with A 189 MET HG2	Favored (77.69%) General / -56.0,-43.3	41% (<i>p</i>) chi angles: 54.1	0.188Å	-	OUTLIER(S) worst is CA- CB-CG2: 4.973 σ
A 183	ASP	50	0.737Å H with A 181 LEU HD23	Favored (49.2%) General / -54.9,-28.3	34.5% (<i>t70</i>) chi angles: 179.4,64.4	0.033Å	-	-
A 184	GLU	50	0.417Å HG3 with A 180 VAL HG21	Favored (72.94%) General / -60.9,-33.3	14.7% (<i>tm-20</i>) chi angles: 182.7,283.6,331.6	0.069Å	-	-

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			Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 185	LEU	50	0.479Å HG with A 186 LYS H	Allowed (0.58%) General / -114.4,-87.1		0.2% chi angles: 41.2,155.8	0.103Å	-	-
A 186	LYS	50	0.479Å H with A 185 LEU HG	Favored (46.49%) General / -129.5,155.0		27.3% (<i>tptp</i>) chi angles: 187.8,61,182.5,64.7	0.067Å	-	-
A 187	HIS	50	0.525Å CD2 with A 202 ILE HG21	Favored (22%) General / -87.2,112.5		65.4% (<i>m170</i>) chi angles: 294.8,168.6	0.065Å	OUTLIER(S) worst is CD2- -NE2: 4.992 σ	-
A 188	GLY	50	-	Allowed (0.69%) Glycine / 111.7,73.8		-	-	-	-
A 189	MET	50	0.814Å HG2 with A 182 THR HG22	Allowed (1.11%) General / -129.0,-161.4		15.6% (<i>ptt?</i>) chi angles: 79.3,178.3,195.6	0.166Å	-	OUTLIER(S) worst is C-N- CA: 5.383 σ
A 190	THR	50	1.079Å HA with A 198 SER HB3	Favored (34.83%) General / -114.4,150.3		75.7% (<i>p</i>) chi angles: 58.3	0.335Å	OUTLIER(S) worst is CB-- OG1: 5.107 σ	OUTLIER(S) worst is CA- CB-CG2: 10.663 σ
A 191	LEU	50	0.842Å HD13 with A 200 ILE HB	Favored (5.05%) General / -120.7,96.3		8.6% (<i>mp</i>) chi angles: 266.8,63.3	0.057Å	-	-
			0.929Å	Favored					OUTLIER(S)

A 192	THR	99.99	HB with A 179 ARG HH22	(2.03%) General / 58.2,12.7	14% (<i>t</i>) chi angles: 189.9	0.092Å	-	worst is CA- CB-CG2: 4.836 σ
A 193	SER	99.99	-	Allowed (1.37%) General / 45.8,64.7	38.4% (<i>t</i>) chi angles: 181.9	0.074Å	-	-
A 194	MET	99.99	0.529Å HB2 with A 173 TYR OH	Favored (10.74%) General / -70.6,116.3	24.3% (<i>ptp</i>) chi angles: 64.5,177.9,64.7	0.043Å	-	-
A 195	TYR	99.99	0.491Å CD2 with A 195 TYR O	Favored (14.57%) General / 62.3,36.4	87.8% (<i>t80</i>) chi angles: 180.1,80.5	0.056Å	-	-
A 196	GLN	99.99	0.535Å HG2 with A 196 GLN O	Favored (16.62%) General / 61.7,27.1	51.4% (<i>tt0</i>) chi angles: 182,185.4,60.7	0.054Å	-	-
A 197	ASN	99.99	0.822Å HD21 with A 213 ASN HD22	Favored (46.72%) General / -130.4,155.2	50.3% (<i>t30</i>) chi angles: 182.8,27	0.104Å	-	-
A 198	SER	99.99	1.079Å HB3 with A 190 THR HA	OUTLIER (0.02%) General / -56.8,-79.8	0.9% chi angles: 338.8	0.272Å	-	OUTLIER(S) worst is CA- CB-OG: 8.916 σ
A 199	ASN	99.99	1.061Å HB3 with A 213 ASN ND2	Favored (8.91%) General / -116.3,101.7	11.5% (<i>t-20</i>) chi angles: 200.5,302.8	0.779Å	OUTLIER(S) worst is CA-- C: 4.122 σ	OUTLIER(S) worst is CA- CB-CG: 10.844 σ
A 200	ILE	50	0.842Å HB with A 191 LEU HD13	Favored (16.69%) Isoleucine or valine / -97.8,105.0	10.1% (<i>tp</i>) chi angles: 188.7,68.3	0.116Å	-	-
A 201	GLN	50	0.637Å NE2 with A 208 GLY H	Favored (45.76%) General / -113.2,142.5	19.4% (<i>pt20</i>) chi angles: 59,177.8,70.2	0.038Å	-	-
A 202	ILE	50	0.641Å HG23 with A 203 HIS H	Allowed (1.17%) Isoleucine or valine / -122.0,-66.5	7.6% (<i>tp</i>) chi angles: 181,66.4	0.125Å	-	-
A 203	HIS	50	0.641Å H with A 202 ILE HG23	Favored (47.53%) General / -63.5,148.9	20.8% (<i>t-160</i>) chi angles: 182.8,204.2	0.069Å	OUTLIER(S) worst is CD2- -NE2: 4.883 σ	-
A	HIS	50	0.467Å C with A 205	Favored (26.3%)	14.2% (<i>t-160</i>)	0.038Å	OUTLIER(S) worst is CG--	-

204

TYR CD1

General /
56.5,35.6

chi angles: 178.7,212.4

ND1: 4.382 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	
				Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 205		TYR	50	0.467Å CD1 with A 204 HIS C	OUTLIER (0%) Pre-proline / 109.2,104.0	0.7% chi angles: 305.8,12.4	0.215Å	-	OUTLIER(S) worst is N- CA-CB: 4.398 σ	
A 206		PRO	50	0.637Å HB3 with A 202 ILE HD12	Favored (14.82%) Trans-proline / -66.9,126.2	74.1% (Cg_endo) chi angles: 28.6	0.034Å	-	-	-
A 207		ASN	99.99	0.758Å HB3 with A 215 ALA O	Favored (29.69%) General / 53.5,39.2	32.7% (m120) chi angles: 292.3,116.1	0.087Å	-	-	-
A 208		GLY	99.99	0.637Å H with A 201 GLN NE2	Favored (24.9%) Glycine / -76.6,-167.0	-	-	-	-	-
A 209		ILE	99.99	0.533Å HG22 with A 214 CYS SG	Favored (5.47%) Isoleucine or valine / -122.9,14.3	41.4% (pt) chi angles: 64.1,174.6	0.039Å	-	-	-
A 210		VAL	99.99	-	Favored (53.61%) Isoleucine or valine / -57.0,-37.2	11.1% (p) chi angles: 61.4	0.066Å	-	-	-
A 211		THR	99.99	0.688Å HB with A 213 ASN OD1	Favored (11.54%) General / -119.3,22.9	76.2% (m) chi angles: 303.1	0.086Å	-	-	-
A 212		VAL	99.99	0.403Å O with A 212 VAL HG12	Allowed (0.28%) Isoleucine or valine / 60.1,51.7	87.9% (t) chi angles: 178.9	0.084Å	-	-	-
A 213		ASN	99.99	1.061Å ND2 with A 199 ASN HB3	Favored (27.23%) General / -92.2,-15.6	16% (m120) chi angles: 292.2,144.9	0.302Å	-	OUTLIER(S) worst is C-N- CA: 6.467 σ	
A 214		CYS	50	0.533Å SG with A 209 ILE HG22	Allowed (1.16%) General / -141.0,-5.0	12.6% (t) chi angles: 169	0.116Å	-	-	-
A				0.758Å	Favored (50.42%)					

215	ALA	50	O with A 207 ASN HB3	General / -113.1,138.1	-	0.109Å	-	-
A 216	ARG	50	0.743Å HA with A 207 ASN CB	Favored (33.58%) General / -87.4,124.6	31.6% (<i>ptt-85</i>) chi angles: 62.4,175,180.8,279.8	0.107Å	-	-
A 217	LEU	50	0.618Å HD13 with A 230 HIS HB3	Allowed (0.75%) General / -71.4,76.3	93% (<i>mt</i>) chi angles: 297.6,172.8	0.025Å	-	-
A 218	LEU	99.99	0.604Å HD22 with A 233 ASP OD1	Allowed (0.28%) General / -31.8,-57.7	51.7% (<i>tp</i>) chi angles: 183.5,64.1	0.012Å	-	-
A 219	LYS	50	-	Favored (2.49%) General / -122.5,85.9	39% (<i>ttpt</i>) chi angles: 184.4,183.5,64.5,180.8	0.081Å	-	-
A 220	ALA	50	-	Favored (3.68%) General / -72.0,104.8	-	0.021Å	-	-
A 221	ASP	50	0.735Å HB3 with A 229 VAL HG13	Favored (30.63%) General / -80.2,-38.8	46.1% (<i>t0</i>) chi angles: 183.6,333.4	0.047Å	-	-
A 222	HIS	50	0.578Å O with A 228 VAL HG13	Allowed (0.59%) General / 69.1,-52.2	18.1% (<i>t-160</i>) chi angles: 177.1,204.8	0.089Å	OUTLIER(S) worst is CG-- ND1: 4.775 σ	-
A 223	HIS	50	-	Favored (23.2%) General / -105.2,110.7	81% (<i>t60</i>) chi angles: 184.6,61.8	0.02Å	OUTLIER(S) worst is CG-- ND1: 4.471 σ	-
A 224	ALA	50	0.968Å HB1 with A 105 ASN ND2	Favored (7.57%) General / -87.8,176.0	-	0.263Å	OUTLIER(S) worst is N- CA-CB: 6.329 σ	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 62.12	Clashscore: 124.27	Outliers: 6 of 130	Poor rotamers: 8 of 116	Outliers: 7 of 124	Outliers: 14 of 132	Outliers: 31 of 132
A 225	THR	50	0.616Å HB with A 105 ASN HA	Favored (66.05%) General / -68.8,-27.7	90.4% (<i>m</i>) chi angles: 302.3	0.054Å	-	-
A 226	ASN	50	0.46Å ND2 with A 133 GLU CD	Favored (2.74%) General / -138.4,17.8	50.3% (<i>t30</i>) chi angles: 182,57.1	0.133Å	-	-

A 227	GLY	50	0.611Å C with A 224 ALA HB3	Allowed (0.63%) Glycine / -178.4,-120.0	-	-	-	-
A 228	VAL	50	0.578Å HG13 with A 222 HIS O	Favored (43.24%) Isoleucine or valine / -130.4,142.6	95.8% (<i>t</i>) chi angles: 176	0.069Å	-	-
A 229	VAL	50	0.735Å HG13 with A 221 ASP HB3	Favored (33.04%) Isoleucine or valine / -140.8,134.8	11.3% (<i>p</i>) chi angles: 61.6	0.11Å	-	-
A 230	HIS	50	0.735Å O with A 231 LEU HD23	Favored (32.22%) General / -141.9,138.6	37.2% (<i>m80</i>) chi angles: 291.2,120	0.29Å	OUTLIER(S) worst is CG-- ND1: 5.034 σ	OUTLIER(S) worst is CB- CG-CD2: 4.275 σ
A 231	LEU	99.99	0.735Å HD23 with A 230 HIS O	Favored (52.58%) General / -124.1,130.5	15.3% (<i>mt</i>) chi angles: 306.4,194.7	0.213Å	-	OUTLIER(S) worst is C- CA-CB: 4.145 σ
A 232	ILE	50	0.651Å HD13 with A 236 ILE HG12	Favored (13.32%) Isoleucine or valine / -90.7,142.2	16.7% (<i>pt</i>) chi angles: 48.7,168.6	0.077Å	-	-
A 233	ASP	50	0.604Å OD1 with A 218 LEU HD22	Favored (62.49%) General / -71.2,-16.6	22.2% (<i>t0</i>) chi angles: 201.8,25.7	0.037Å	-	-
A 234	LYS	50	0.81Å HG3 with A 235 VAL H	Allowed (0.31%) General / -122.7,-138.6	24.2% (<i>tptp</i>) chi angles: 188.2,59.1,183.7,78.3	0.127Å	-	-
A 235	VAL	50	0.81Å H with A 234 LYS HG3	Favored (31.43%) Isoleucine or valine / -125.1,146.0	21.6% (<i>t</i>) chi angles: 188	0.069Å	-	-
A 236	ILE	99.99	0.666Å CD1 with A 141 PHE HB2	-	6.6% (<i>pt</i>) chi angles: 62.1,149.4	0.049Å	-	OUTLIER(S) worst is CB- CG1-CD1: 4.78 σ