

## Viewing dhdds\_mb\_62-287Hmulti.table

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All-Atom				0 <sup>th</sup> percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of serious	steric ove	rlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	8	3.90%	Goal: <1%		
	Ramachandran outliers	2	0.88%	Goal: <0.05%		
	Ramachandran favored	221	97.36%	Goal: >98%		
Protein Geometry	MolProbity score <sup>^</sup>	3.06		21 <sup>st</sup> percentile* (N=27675, 0Å - 99Å)		
geometry	Cβ deviations >0.25Å	2	0.92%	Goal: 0		
	Bad backbone bonds:	0 / 1906	0.00%	Goal: 0%		
	Bad backbone angles:	33 / 2575	1.28%	Goal: <0.1%		

In the two column results, the left column gives the raw count, right column gives the percentage.

<sup>^</sup> 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	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205	Outliers: 2 of 218		
20	ILE	23.64	0.653Å HD13 with 248 GLN HG2	-	87.9% ( <i>mt</i> ) chi angles: 299,168.2	0.087Å	-	-
21	LYS	50.69	0.799Å HB2 with 24 PRO HD2	Favored (49.3%) General / -64.5,149.0	60.3% ( <i>mtpt</i> ) chi angles: 295.8,165.7,66.4,179.3	0.081Å	-	-
22	ALA	. 19.75	0.91Å HA with 25 MET CE	Favored (95.54%) General / -61.6,-40.6	-	0.087Å	-	-
23	GLY	22.3	-	Favored (99.7%) Glycine / -62.5,-42.5	-	-	-	-

<sup>\* 100&</sup>lt;sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

24	PRO 125.66	0.799Å HD2 with 21 LYS HB2	Favored (31.74%) Trans-proline / -70.8,-19.0	87.6% ( <i>Cg_exo</i> ) chi angles: 331.3	0.189Å	-	-
25	MET 46.45	0.91Å CE with 22 ALA HA	Favored (90.77%) Pre-proline / -73.0,155.0	69.6% ( <i>mtm</i> ) chi angles: 298.2,175.5,291.4	0.109Å	-	-
26	PRO 86.37	0.586Å HD2 with 244 ILE HG23	Favored (20.4%) Trans-proline / -73.0,133.8	10.2% ( <i>Cg_endo</i> ) chi angles: 13.3	0.098Å	-	-
27	LYS 38.12	-	Favored (70%) General / -70.9,-42.3	81.7% (tttt) chi angles: 181.7,166,180,179.8	0.091Å	-	-
28	HIS 56.4	-	Favored (40.2%) General / -129.7,127.3	10.3% ( <i>t-160</i> ) chi angles: 187,171.3	0.094Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.417 σ
29	ILE 39.9	0.882Å HG12 with 202 ILE CG2	Favored (69.74%) Isoleucine or valine / -119.0,132.2	82.2% ( <i>mt</i> ) chi angles: 300.3,168.3	0.081Å	-	-
30	ALA 35.16	0.838Å HA with 74 THR HG22	Favored (51.92%) General / -111.8,135.8	-	0.115Å	-	-
31	PHE 57.83	0.702Å CE2 with 240 LEU HD13	Favored (52.2%) General / -123.2,130.0	83.1% ( <i>m</i> -85) chi angles: 299.2,83.2	0.161Å	-	OUTLIER(S) worst is CA- CB-CG: 4.51 σ
32	ILE 159.94	0.696Å HG23 with 205 ARG HG3	Favored (22.09%) Isoleucine or valine / -105.4,107.2	0% chi angles: 185.6,293.7	0.053Å	-	-
33	MET 80.72	0.759Å HE3 with 75 VAL HG11	Favored (30.09%) General / -77.3,125.9	63.3% ( <i>mtt</i> ) chi angles: 299.2,171.9,179.9	0.106Å	-	-
34	ASP 73.54	-	Favored (43.05%) General / -148.8,156.9	38% ( <i>t0</i> ) chi angles: 197,2.4	0.086Å	-	-
35	GLY 38.43	0.665Å HA2 with 38 ARG HD3	Favored (44.26%) Glycine/	-	-	-	-

36	ASN	43.14	-	104.3,3.8 Favored (97.94%) General / -61.7,-43.9	97.8% ( <i>m-20</i> ) chi angles: 291.7,339.2	0.121Å	-	-
37	ARG	94.09	-	Favored (84.45%) General / -64.8,-45.9	79.1% (ttt180) chi angles: 179.9,182.2,179.9,184	0.087Å	-	-
38	ARG	107.27	0.666Å NH1 with 207 SER HB2	Favored (92.64%) General / -63.8,-38.9	2% (mpt_?) chi angles: 300.1,72.3,171.6,272	0.131Å	-	-
39	TYR	37.54	0.469Å HD1 with 234 GLU OE2	Favored (96.71%) General / -61.1,-44.9	89.9% ( <i>t</i> 80) chi angles: 176.2,79.5	0.076Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205		Outliers:	Outliers: 31 of 229
40	ALA	27.59	-	Favored (96.07%) General / -64.7,-41.3	-	0.087Å	-	-
41	LYS	91.73	-	Favored (85.12%) General / -59.6,-39.7	58.9% (tttm) chi angles: 180,166.9,178.1,291	0.083Å	-	-
42	LYS	91.28	-	Favored (88.5%) General / -59.5,-40.9	31.1% ( <i>ttmt</i> ) chi angles: 180,167.4,277.7,180	0.101Å	-	-
43	CYS	58.04	0.523Å O with 44 GLN HB2	Favored (62.21%) General / -71.7,-17.7	71.6% ( <i>m</i> ) chi angles: 297.3	0.066Å	-	-
44	GLN	65.91	0.523Å HB2 with 43 CYS O	Favored (2.63%) General / 67.5,40.3	25% ( <i>mt-30</i> ) chi angles: 296.2,175.6,171.5	0.07Å	-	-
45	VAL	38.5	0.59Å HG12 with 46 GLU N	Favored (15.65%) Isoleucine or valine / -117.6,162.4	64% ( <i>t</i> ) chi angles: 179.9	0.071Å	-	-
			0.59Å	Favored	18.7% ( <i>pt-20</i> )			

46	GLU 78.33 N with 45 VAL HG12	(47.02%) General / -63.8,149.4	chi angles: 60.1,180.8,338.2	0.086Å	-	-
47	0.671Å ARG 185.53 HD2 with 89 GLU CD	Favored (69.57%) General / -65.5,-29.0	5% ( <i>ptp180</i> ) chi angles: 60.8,189,89.2,141.8	0.144Å	-	-
48	0.935Å GLN 47.19 HA with 51 HIS HD2	Favored (69.21%) General / -59.2,-31.6	89.4% ( <i>mt-30</i> ) chi angles: 296.3,180.1,353.3	0.125Å	-	-
49	0.544Å GLU 108.83 HG2 with 45 VAL HG11	Favored (92.56%) General / -62.5,-39.2	11.9% ( <i>tp10</i> ) chi angles: 192.7,71.6,61.4	0.074Å	-	-
50	GLY 21.77 -	Favored (96.17%) Glycine / -63.6,-38.4	-	-	-	-
51	0.935Å HIS 66.26 HD2 with 48 GLN HA	Favored (99.52%) General / -62.9,-41.7	81.9% ( <i>m-70</i> ) chi angles: 304,301.7	0.082Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.522 σ
52	0.461Å SER 73.09 O with 55 PHE HD2	Favored (78.84%) General / -61.0,-36.2	69.2% ( <i>m</i> ) chi angles: 296	0.078Å	-	-
53	0.835Å GLN 81.23 HG2 with 233 PRO HB3	Favored (70.76%) General / -64.8,-29.8	34.3% ( <i>tp60</i> ) chi angles: 180.2,75.2,8.8	0.083Å	-	-
54	GLY 44.78 -	Favored (73.58%) Glycine / -61.6,-30.0	-	-	-	-
55	0.461Å PHE 104.14 HD2 with 52 SER O	Favored (96.32%) General / -61.3,-45.0	11.9% ( <i>p90</i> ) chi angles: 79.3,84.6	0.144Å	-	-
56	0.46Å ASN 65.29 N with 55 PHE CG	Favored (90.02%) General / -61.9,-38.9	32.7% ( <i>t-20</i> ) chi angles: 191,309	0.082Å	-	OUTLIER(S) worst is CA- CB-CG: 4.048 σ
57	0.643Å LYS 132.64 NZ with 61 THR HB	Favored (97.43%) General / -62.2,-40.8 Favored	0.1% chi angles: 201.5,305.1,101.8,174.4	0.088Å	-	-
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58	LEU 46.79	0.783Å O with 61 THR HG22	(91.9%) General / -60.9,-46.1	61.6% ( <i>tp</i> ) chi angles: 180,63.8	0.088Å	-	-
59	ALA 31.08	-	Favored (96.02%) General / -64.0,-40.3	-	0.086Å	-	-
#	Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
	Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205	Outliers: 2 of 218		Outliers: 31 of 229
60	GLU 96.63	-	Favored (99.26%) General / -62.5,-42.0	23.4% ( <i>tp10</i> ) chi angles: 189.3,76.3,352.9	0.087Å	-	-
61	THR 99.88	0.783Å HG22 with 58 LEU O	Favored (83.24%) General / -67.4,-37.5	8.3% ( <i>t</i> ) chi angles: 193.3	0.074Å	-	-
62	LEU 92.65	0.743Å HD13 with 58 LEU O	Favored (96.68%) General / -60.5,-43.7	8.3% ( <i>mp</i> ) chi angles: 276.1,51.4	0.099Å	-	-
63	ARG 96.87	-	Favored (98.53%) General / -62.8,-43.5	59.1% ( <i>ttm-85</i> ) chi angles: 182.3,184.4,300,271.3	0.092Å	-	-
64	TRP 141.47	1.038Å HB2 with 237 PHE HB2	Favored (89.85%) General / -66.0,-39.0	76.6% ( <i>t-105</i> ) chi angles: 179.9,254.1	0.141Å	-	-
65	CYS 29.36	-	Favored (93.96%) General / -62.7,-39.4	76.6% (m) chi angles: 296.4	0.09Å	-	-
66	LEU 119.74	0.741Å HB2 with 114 HIS CE1	Favored (94.91%) General / -63.5,-44.2	55.8% ( <i>tp</i> ) chi angles: 179.8,66.1	0.122Å	-	-
67	ASN 93.22	0.65Å OD1 with 64 TRP HA	Favored (91.94%) General / -64.8,-38.7	1.5% ( <i>p-10</i> ) chi angles: 64.5,258.7	0.114Å	-	-
68	LEU 108.71	0.786Å O with 68 LEU HD23	Favored (72.7%) General / -68.4,-32.6	6.1% (tt) chi angles: 192.7,168.6	0.079Å	-	-

69	GLY 38.41	-	Favored (13.98%) Glycine / 102.0,19.9	-	-	-	-
70	ILE 126.46	0.814Å HD11 with 244 ILE HD13	Favored (33.22%) Isoleucine or valine / -70.0,128.4	34% ( <i>mm</i> ) chi angles: 300.8,292.9	0.14Å	-	-
71	LEU 69.62	0.55Å HB2 with 72 GLU OE1	Favored (49.05%) General / -75.3,-43.9	87.3% ( <i>mt</i> ) chi angles: 297.9,180.8	0.09Å	-	-
72	GLU 81.06	0.55Å OE1 with 71 LEU HB2	Favored (46.3%) General / -133.5,138.9	58.8% ( <i>mp0</i> ) chi angles: 288.6,79.2,4.5	0.095Å	-	-
73	VAL 45.43	0.632Å HB with 150 LEU CD2	Favored (36.69%) Isoleucine or valine / -139.1,131.4	98.3% (t) chi angles: 176.6	0.08Å	-	-
74	THR 109.79	1.111Å HG21 with 216 LEU HD11	Favored (56.25%) General / -118.5,131.8	15.1% ( <i>t</i> ) chi angles: 188.1	0.063Å	-	-
75	VAL 46.1	0.759Å HG11 with 33 MET HE3	Favored (42.45%) Isoleucine or valine / -117.1,139.8	78.5% (t) chi angles: 172.4	0.086Å	-	-
76	TYR 169.54	0.553Å CD1 with 215 PHE CD1	Favored (2.52%) General / -103.4,85.7	3.3% ( <i>t80</i> ) chi angles: 198.7,38	0.084Å	-	-
77	ALA 66.17	-	Favored (71.06%) General / -70.6,-42.4	-	0.059Å	-	-
78	PHE 112.99	0.799Å HB2 with 154 PHE CE2	Favored (12.86%) General / -158.9,139.8	43.5% ( <i>t80</i> ) chi angles: 191.5,89.3	0.118Å	-	-
79	SER 132.05	0.427Å HB3 with 76 TYR OH	Favored (15.34%) General / -107.3,160.8	3.1% ( <i>m</i> ) chi angles: 317.7	0.278Å	-	OUTLIER(S) worst is CB-CA-C: $5.039 \sigma$
		Clash >			Сβ	Bond	

#	Alt Res High B	<b>0.4</b> Å	Ramachandran	Rotamer	deviation	lengths	<b>Bond angles</b>
	Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205	Outliers: 2 of 218		
80	ILE 138.09	0.718Å HD13 with 157 THR CB	Favored (44.91%) Isoleucine or valine / -61.9,-28.7	2% ( <i>mp</i> ) chi angles: 286.1,67.7	0.146Å	-	-
81	GLU 170.75	-	Favored (88.69%) General / -65.1,-37.8	0.9% chi angles: 233.8,71.8,63.4	0.132Å	-	OUTLIER(S) worst is CB- CG-CD: 5.596 σ
82	ASN 216.87	-	Allowed (0.42%) General / -82.2,29.4	32.3% ( <i>p-10</i> ) chi angles: 54.2,352	0.275Å	-	-
83	PHE 181.42	-	Favored (64.03%) General / -71.5,-28.6	14.9% ( <i>t80</i> ) chi angles: 199.7,278.5	0.191Å	-	-
84	LYS 170.56	0.614Å HB2 with 84 LYS NZ	Favored (73.7%) General / -59.3,-35.4	0% chi angles: 204.4,77.5,65.1,289.6	0.126Å	-	-
85	ARG 171.09	0.934Å HH21 with 93 LEU HD11	Favored (3.46%) General / -64.5,171.0	27.5% (mtm180) chi angles: 292.2,211.3,287.4,158.1	0.134Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.556 σ
86	SER 85.67	-	Favored (16.63%) General / -58.5,153.2	50.7% ( <i>m</i> ) chi angles: 301.6	0.17Å	-	-
87	LYS 125.34	0.561Å HA with 90 VAL HG22	Favored (75.3%) General / -65.3,-33.1	9.8% ( <i>ptmt</i> ) chi angles: 67.3,172,315.6,160.1	0.086Å	-	-
88	SER 32.87	-	Favored (96.37%) General / -61.8,-44.7	74.1% (m) chi angles: 294	0.082Å	-	-
89	GLU 163.12	0.671Å CD with 47 ARG HD2	Favored (85.31%) General / -64.4,-46.0	76.8% ( <i>mm-40</i> ) chi angles: 292.5,293.5,313.4	0.21Å	-	-
90	VAL 104.43	0.561Å HG22 with 87 LYS HA	Favored (91.24%) Isoleucine or valine / -65.0,-41.1	33.5% ( <i>m</i> ) chi angles: 297.2	0.078Å	-	-

91	ASP	69.22	0.532Å N with 90 VAL HG23	Favored (98.04%) General / -61.5,-43.9	51.7% ( <i>t0</i> ) chi angles: 189.1,11.2	0.095Å	-	OUTLIER(S) worst is CA- CB-CG: 4.865 σ
92	GLY	22.82	0.623Å O with 96 LEU HG	Favored (97.94%) Glycine / -63.9,-43.1	-	-	-	-
93	LEU	66.25	0.934Å HD11 with 85 ARG HH21	Favored (95.26%) General / -64.0,-40.0	83.9% ( <i>mt</i> ) chi angles: 301.2,180	0.048Å	-	-
94	MET	109.79	0.794Å HB3 with 128 PRO HG3	Favored (82.04%) General / -67.3,-43.3	65.9% ( <i>mtt</i> ) chi angles: 294.7,180,177.3	0.132Å	-	OUTLIER(S) worst is CG- SD-CE: 4.327 σ
95	ASP	72.33	-	Favored (90.21%) General / -66.2,-40.2	62.4% ( <i>t0</i> ) chi angles: 187.3,1.9	0.1Å	-	-
96	LEU	135.95	0.623Å HG with 92 GLY O	Favored (95.48%) General / -63.7,-43.8	76.8% ( <i>mt</i> ) chi angles: 292.5,180.3	0.072Å	-	-
97	ALA	27.64	0.429Å HA with 101 PHE HB3	Favored (97.77%) General / -63.8,-42.5	-	0.084Å	-	-
98	ARG	98.95	0.983Å HG2 with 134 LEU HD12	Favored (78.68%) General / -63.5,-48.2	28.5% (ttp180) chi angles: 180,212.1,71.3,203.3	0.133Å	-	-
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99	GLN	110.6	0.548Å O with 105 MET HB3	Favored (88.32%) General / -63.5,-45.9	8.9% ( <i>tt0</i> ) chi angles: 186,175.2,185	0.059Å	-	OUTLIER(S) worst is C-N- CA: 5.634 σ
	GLN <b>Alt Res</b>		O with 105	Favored (88.32%) General /	chi angles:	0.059Å Cβ deviation	- Bond lengths	worst is C-N-
			O with 105 MET HB3	Favored (88.32%) General / -63.5,-45.9	chi angles: 186,175.2,185	Cβ deviation	<b>lengths</b> Outliers:	worst is C-N-CA: $5.634 \sigma$
	Alt Res	<b>High B</b> Avg:	O with 105 MET HB3  Clash > 0.4Å  Clashscore:	Favored (88.32%) General / -63.5,-45.9 Ramachandran Outliers: 2 of	chi angles: 186,175.2,185 <b>Rotamer</b> Poor rotamers: 8 of	Cβ deviation Outliers:	<b>lengths</b> Outliers:	worst is C-N-CA: $5.634 \sigma$ <b>Bond angles</b> Outliers: 31

			-51.4,-57.3				σ
102	SER 100.55	0.629Å HB2 with 152 VAL CG1	Favored (5.93%) General / -88.5,61.1	56.5% ( <i>p</i> ) chi angles: 55.4	0.056Å	-	-
103	ARG 318.05	0.797Å CD with 118 ILE HD13	Favored (2.06%) General / 49.9,26.7	0% chi angles: 55.3,68.2,79.3,208.5	0.061Å	-	OUTLIER(S) worst is C-N- CA: 6.093 σ
104	LEU 248.73	0.908Å HD21 with 135 ILE HD11	OUTLIER (0.01%) General / -68.0,-89.4	3.2% ( <i>mm</i> ?) chi angles: 268.8,284.8	0.154Å	-	-
105	MET 160.58	0.631Å HE2 with 134 LEU CD1	Favored (35.39%) General / -72.3,-49.3	58.3% ( <i>tpp</i> ) chi angles: 181.9,70.3,68.8	0.081Å	-	-
106	GLU 83.44	-	Favored (65.37%) General / -70.0,-46.3	32.5% ( <i>tp10</i> ) chi angles: 191.2,76.2,3.7	0.08Å	-	-
107	GLU 71.44	0.791Å HB2 with 103 ARG CA	Favored (58.02%) General / -75.8,-27.5	51.3% ( <i>mt-10</i> ) chi angles: 291.8,183.3,57.5	0.11Å	-	-
108	LYS 148.79	0.775Å HB3 with 103 ARG NH1	Favored (72.58%) General / -55.9,-40.2	5.7% ( <i>ptmm</i> ?) chi angles: 54.1,179.4,269.3,278.8	0.117Å	-	-
109	GLU 75.86	-	Favored (99.02%) General / -62.8,-43.4	89.4% ( <i>tt0</i> ) chi angles: 180.2,180,357.1	0.081Å	-	-
110	LYS 42.43	0.615Å O with 113 LYS HG2	Favored (88.94%) General / -66.3,-42.0	93.1% ( <i>mttt</i> ) chi angles: 290,168.9,179.9,180	0.067Å	-	-
111	LEU 98.76	0.704Å HD11 with 103 ARG HB2	Favored (89.36%) General / -62.1,-38.6	6.9% ( <i>mp</i> ) chi angles: 288.8,76.9	0.158Å	-	-
112	GLN 84.21	0.559Å HG3 with 108 LYS O	Favored (98.05%) General / -60.8,-42.7	76.1% ( <i>mt-30</i> ) chi angles: 298.4,176.8,43.6	0.079Å	-	-
113	LYS 101.02	0.615Å HG2 with 110	Favored (74.5%) General /	20.7% ( <i>ptmt</i> ) chi angles:	0.062Å	-	-

			LYS O	-65.4,-32.7	65.4,170.5,298.8,178.4			
114	HIS	100.14	0.741Å CE1 with 66 LEU HB2	Favored (66.46%) General / -67.0,-25.7	51.2% ( <i>t-80</i> ) chi angles: 180.2,278.1	0.064Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.504 σ
115	GLY	29.32	0.783Å HA2 with 145 TYR CD2	Favored (49.39%) Glycine / 98.3,11.2	-	-	-	-
116	VAL	54.56	0.648Å HG23 with 114 HIS ND1	Favored (14.76%) Isoleucine or valine / -80.1,141.8	77.1% ( <i>t</i> ) chi angles: 172.3	0.088Å	-	-
117	CYS	52.86	0.734Å HA with 142 THR OG1	Favored (32.25%) General / -107.2,116.6	52.5% ( <i>t</i> ) chi angles: 180.1	0.113Å	-	-
118	ILE	71.89	0.797Å HD13 with 103 ARG CD	Favored (36.42%) Isoleucine or valine / -129.3,145.0	14.3% ( <i>tt</i> ) chi angles: 195.1,160.2	0.05Å	-	-
119	ARG	174.03	0.97Å HD2 with 149 PHE CZ	Favored (38.34%) General / -157.8,163.1	0% chi angles: 63.1,332,108,78.2	0.112Å	-	-
# Alt	t Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205		Outliers:	Outliers: 31 of 229
120	VAL	99.09	1.048Å HB with 135 ILE HG21	Favored (14.9%) Isoleucine or valine / -82.5,141.5	14.2% ( <i>p</i> ) chi angles: 63.1	0.071Å	-	-
121			0.827Å	Favored	1 00/ /4 2\			
	LEU	115.08	HD12 with 156 TYR CD1	(31.05%) General / -129.8,123.5	1.8% ( <i>tm</i> ?) chi angles: 193.7,296.8	0.095Å	-	-
122	GLY	115.08 27	HD12 with	General /		0.095Å -	-	-

			-98.3,138.0				
124	LEU 101.71	0.675Å O with 124 LEU HD23	Favored (78.19%) General / -68.4,-43.0	4.1% (tt) chi angles: 190.5,177.2	0.032Å	-	-
125	HIS 85.86	0.514Å HB3 with 126 LEU CD2	Favored (55.74%) General / -62.5,134.0	96.3% ( <i>m-70</i> ) chi angles: 297.4,276.3	0.09Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.408 o
126	LEU 245.68	0.549Å N with 126 LEU HD22	Allowed (0.74%) General / 75.7,-14.8	2% (mm?) chi angles: 292.9,293.9	0.08Å	-	-
127	LEU 76.51	1.12Å HD12 with 128 PRO HD2	Favored (79.54%) Pre-proline / -74.5,143.6	56.7% ( <i>tp</i> ) chi angles: 180,59.2	0.068Å	-	-
128	PRO 88.69	1.12Å HD2 with 127 LEU HD12	Favored (45.64%) Trans-proline / -67.9,138.9	9.3% ( <i>Cg_endo</i> ) chi angles: 10.9	0.135Å	-	-
129	LEU 85.18	0.692Å O with 129 LEU HD23	Favored (86.51%) General / -63.1,-37.3	3.3% ( <i>tt</i> ) chi angles: 188.8,180	0.059Å	-	-
130	ASP 89.82	0.764Å OD2 with 98 ARG HD3	Favored (79.22%) General / -60.6,-36.6	26.1% ( <i>p-10</i> ) chi angles: 62.3,331.5	0.073Å	-	-
131	LEU 38.13	0.503Å HD23 with 127 LEU HD11	Favored (86.35%) General / -66.9,-42.0	59.4% ( <i>tp</i> ) chi angles: 180.2,64.5	0.082Å	-	-
132	GLN 43.97	0.525Å HE22 with 124 LEU HG	Favored (97.85%) General / -63.8,-41.4	87.6% ( <i>mt-30</i> ) chi angles: 295.7,179.9,0.5	0.115Å	-	-
133	GLU 69.96	-	Favored (94.95%) General / -62.8,-44.9	87.2% (tt0) chi angles: 182.5,180,7.4	0.07Å	-	-
134	LEU 53.28	0.983Å HD12 with 98 ARG HG2	Favored (86.85%) General / -66.5,-38.2	36.2% ( <i>mt</i> ) chi angles: 293.4,188.1	0.084Å	-	-
135	ILE 91.94	1.048Å HG21 with	Favored (83.14%)	34.4% ( <i>mm</i> )	0.097Å	-	-

			120 VAL HB	Isoleucine or valine / -63.7,-38.8	chi angles: 295,294.7			
136	ALA	24.6	-	Favored (97.16%) General / -60.9,-42.0	-	0.086Å	-	-
137	GLN	64.47	-	Favored (96.03%) General / -64.6,-41.7	81.8% ( <i>mm-40</i> ) chi angles: 292,289.2,328.7	0.093Å	-	-
138	ALA	37.75	0.549Å HB2 with 103 ARG HH12	Favored (95.77%) General / -62.4,-40.2	-	0.075Å	-	-
139	VAL	30.64	0.718Å O with 143 LYS HG3	Favored (98.34%) Isoleucine or valine / -63.8,-44.6	97.5% ( <i>t</i> ) chi angles: 176.2	0.071Å	-	-
# A	It Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205	Outliers: 2 of 218		Outliers: 31 of 229
140	GLN	89.19	0.591Å HA with 143 LYS HE2	Favored (86.72%) General / -65.4,-44.7	1.1% ( <i>tm0?</i> ) chi angles: 195.7,288.6,128	0.071Å	-	-
141	ALA	57.16	0.438Å HB1 with 112 GLN OE1	Favored (89.52%) General / -64.1,-38.0	-	0.081Å	-	OUTLIER(S) worst is C-N- CA: 4.198 σ
142	THR	160.99	0.734Å OG1 with 117 CYS HA	Favored (54.63%) General / -82.1,-15.1	6.1% ( <i>t</i> ) chi angles: 195.6	0.053Å	-	-
143	LYS	97.47	0.718Å HG3 with 139 VAL O	Favored (62.78%) General / -53.9,-36.5	49.1% (mtmt) chi angles: 295.4,170.4,292.9,180	0.083Å	-	-
144	ASN	52.24	-	Favored (82.31%)	81.4% ( <i>m-20</i> ) chi angles: 293.1,309.1	0.082Å	_	OUTLIER(S) worst is CA- CB-CG: 4.278
				General / -68.1,-38.4	o ag.co. <b>2</b> 557.75557.			σ

146	ASN 185.82	0.49Å H with 147 LYS NZ	Allowed (1.96%) General / -143.0,20.9	32% ( <i>t-20</i> ) chi angles: 198.8,358.4	0.072Å	-	OUTLIER(S) worst is CA- CB-CG: 4.917 σ
147	LYS 116.48	0.727Å HE3 with 147 LYS N	Favored (68.45%) General / -68.4,-47.0	0.9% chi angles: 289.9,67.1,271.2,177.7	0.086Å	-	-
148	CYS 78.16	-	Favored (31.16%) General / -153.6,152.7	52.1% (t) chi angles: 180	0.113Å	-	-
149	PHE 56.99	0.97Å CZ with 119 ARG HD2	Favored (55.98%) General / -113.5,127.1	41.6% ( <i>t80</i> ) chi angles: 193.5,82.7	0.127Å	-	-
150	LEU 54.8	0.7Å HD11 with 62 LEU HG	Favored (45.38%) General / -117.4,123.0	88.7% ( <i>mt</i> ) chi angles: 298.5,180.1	0.088Å	-	-
151	ASN 60.46	0.417Å OD1 with 149 PHE HE2	Favored (22.11%) General / -93.8,110.5	79.6% ( <i>m-20</i> ) chi angles: 301.5,317.5	0.142Å	-	OUTLIER(S) worst is CA- CB-CG: 4.161 σ
152	VAL 53.8	0.787Å CG2 with 118 ILE HD11	Favored (18.38%) Isoleucine or valine / -93.8,106.7	76.6% (t) chi angles: 174.2	0.096Å	-	-
153	CYS 52.84	-	Favored (23.99%) General / -96.9,112.1	80.1% ( <i>m</i> ) chi angles: 300.9	0.072Å	-	-
154	PHE 142.34	0.799Å CE2 with 78 PHE HB2	Favored (50.65%) General / -126.7,134.5	15.1% ( <i>t80</i> ) chi angles: 201.6,271	0.088Å	-	OUTLIER(S) worst is CA- CB-CG: 6.105 σ
155	ALA 51.37	0.518Å O with 80 ILE HD11	Favored (20.83%) General / 58.8,41.8	-	0.07Å	-	-
156	TYR 75.18	0.827Å CD1 with 121 LEU HD12	Favored (45.74%) General / -99.8,131.6	71.1% ( <i>t80</i> ) chi angles: 175.4,87.1	0.122Å	-	-
157	THR 67.95	0.718Å CB with 80 ILE HD13	Favored (28.86%) General /	37.5% ( <i>m</i> ) chi angles: 292.9	0.148Å	-	-

158	SER	84.63	0.784Å HB2 with 217 LEU HB3	-140.4,133.1 Favored (89.93%) General / -63.5,-45.6	94.9% (p) chi angles: 64.9	0.075Å	-	-
159	ARG	80.19	0.423Å HG2 with 157 THR CG2	Favored (94.36%) General / -65.1,-40.4	29.1% ( <i>ptt-85</i> ) chi angles: 60.8,174.4,184.2,264.6	0.067Å	-	-
# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205		Outliers: 0 of 229	Outliers: 31 of 229
160	HIS	69.86	-	Favored (92.77%) General / -65.5,-40.1	64.8% ( <i>m80</i> ) chi angles: 284.6,85.8	0.084Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.497 σ
161	GLU	40.66	0.438Å HG2 with 192 LEU HD22	Favored (98.81%) General / -63.4,-43.0	45% (tt0) chi angles: 180.2,179.7,53.4	0.074Å	-	-
162	ILE	114.64	0.421Å HG12 with 159 ARG O	Favored (80.46%) Isoleucine or valine / -65.7,-37.6	40.7% ( <i>pt</i> ) chi angles: 60,175.5	0.111Å	-	-
163	SER	25.6	0.789Å O with 166 VAL HG12	Favored (87.2%) General / -64.4,-37.4	66.7% ( <i>m</i> ) chi angles: 296.4	0.086Å	-	-
164	ASN	25.29	0.54Å HA with 167 ARG NE	Favored (96.88%) General / -64.2,-40.8	93.9% ( <i>m-20</i> ) chi angles: 292.7,344.4	0.085Å	-	OUTLIER(S) worst is CA- CB-CG: 4.641 σ
165	ALA	27.2	0.486Å HB2 with 192 LEU HD23	Favored (99.26%) General / -63.2,-41.9	-	0.082Å	-	-
166	VAL	77.38	0.789Å HG12 with 163 SER O	Favored (81.4%) Isoleucine or valine / -64.4,-38.0	9.8% ( <i>p</i> ) chi angles: 72.1	0.077Å	-	-
167	ARG	101.62	0.54Å NE with 164 ASN HA	Favored (95.29%) General / -61.7,-40.5	32.2% (mtm105) chi angles: 294.7,180,297.6,87.5	0.092Å	-	-
168	GLU	31.59	0.549Å OE1 with 191	Favored (96.82%)	43.4% ( <i>tt0</i> ) chi angles:	0.102Å	-	-

		CYS HA	General / -62.1,-44.4	183.4,179.9,62.8			
169	MET 27.87	0.535Å O with 173 VAL HG23	Favored (95.11%) General / -62.7,-39.8	98% ( <i>mtp</i> ) chi angles: 294.5,179.9,68.3	0.107Å	-	-
170	ALA 22.97	-	Favored (95.69%) General / -61.9,-40.5	-	0.086Å	-	-
171	TRP 32	0.403Å CD1 with 167 ARG O	Favored (95.57%) General / -62.1,-44.9	98.7% ( <i>m</i> 95) chi angles: 291.7,97.3	0.118Å	-	-
172	GLY 15.12	-	Favored (99.28%) Glycine / -62.2,-40.7	-	-	-	-
173	VAL 25.04	0.535Å HG23 with 169 MET O	Favored (94.81%) Isoleucine or valine / -61.7,-42.6	74.5% (t) chi angles: 174	0.076Å	-	-
174	GLU 58.08	-	Favored (91.56%) General / -62.6,-38.8	87.9% (tt0) chi angles: 185.1,176,358.5	0.071Å	-	-
175	GLN 74.23	0.44Å OE1 with 177 LEU HD11	Favored (77.99%) General / -64.9,-34.3	77.5% ( <i>mt-30</i> ) chi angles: 296.4,180,51.5	0.081Å	-	-
176	GLY 18.73	-	Favored (50.12%) Glycine / 102.4,-0.6	-	-	-	-
177	LEU 46.99	0.44Å HD11 with 175 GLN OE1	Favored (82.44%) General / -65.8,-36.1	82.4% ( <i>mt</i> ) chi angles: 295.7,180.9	0.087Å	-	-
178	LEU 56.54	-	Favored (43.06%) General / -116.3,145.6	59.2% ( <i>tp</i> ) chi angles: 179.8,60	0.059Å	-	-
179	ASP 44.92	-	Favored (32.59%) Pre-proline / -100.3,127.6	64.5% ( <i>t0</i> ) chi angles: 186,348.5	0.094Å	-	-
# /	Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	<b>Bond angles</b>

		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205		Outliers: 0 of 229	Outliers: 31 of 229
180	PRO	65.4	-	Favored (70.33%) Trans-proline / -63.5,-27.6	87.1% ( <i>Cg_exo</i> ) chi angles: 331.3	0.158Å	-	-
181	SER	67.26	-	Favored (67.06%) General / -69.4,-29.4	47.5% (t) chi angles: 180	0.086Å	-	-
182	ASP	51.31	-	Favored (67.4%) General / -68.9,-29.2	82.9% ( <i>m-20</i> ) chi angles: 292.1,353.1	0.081Å	-	OUTLIER(S) worst is CA- CB-CG: 4.489 σ
183	ILE	75.08	1.071Å HA with 187 LEU HD12	Favored (2.78%) Isoleucine or valine / -46.0,132.8	89.9% ( <i>mt</i> ) chi angles: 298.6,168.2	0.059Å	-	-
184	SER	79.03	-	Favored (13.58%) General / -137.0,172.1	43.2% ( <i>t</i> ) chi angles: 178.1	0.122Å	-	-
185	GLU	72.66	-	Favored (79.25%) General / -62.6,-35.4	25.8% ( <i>pt-20</i> ) chi angles: 61.2,180,4.3	0.071Å	-	-
186	SER	70.87	-	Favored (72.5%) General / -63.9,-31.4	97.5% ( <i>p</i> ) chi angles: 64	0.075Å	-	-
187	LEU	140.02	1.071Å HD12 with 183 ILE HA	Favored (93.52%) General / -63.7,-39.1	27.7% ( <i>mt</i> ) chi angles: 292,189.8	0.07Å	-	-
188	LEU	72.96	0.829Å HD22 with 218 TRP CH2	Favored (95.53%) General / -64.7,-42.1	5.5% ( <i>mp</i> ) chi angles: 293.8,64.6	0.079Å	-	-
189	ASP	35.81	-	Favored (94.02%) General / -60.4,-41.5	60% ( <i>m-20</i> ) chi angles: 287.6,313.1	0.113Å	-	-
190	LYS	68.33	-	Favored (78.96%) General / -64.2,-34.8	61.7% ( <i>mttm</i> ) chi angles: 297.9,166.2,185.8,295.5	0.074Å	-	-

191	CYS 75.51	0.549Å HA with 168 GLU OE1	Favored (60.92%) General / -73.0,-20.8	99.5% ( <i>m</i> ) chi angles: 294.5	0.08Å	-	-
192	LEU 55.65	0.486Å HD23 with 165 ALA HB2	Favored (14.84%) General / -62.5,159.8	86.8% ( <i>mt</i> ) chi angles: 295.9,180	0.066Å	-	-
193	TYR 45.28	-	Favored (83.16%) General / -58.0,-47.4	88% ( <i>t80</i> ) chi angles: 178.7,82.5	0.088Å	-	-
194	THR 135.08	0.652Å HG22 with 121 LEU CD2	Favored (5.54%) General / -117.5,96.7	9.4% (t) chi angles: 180.3	0.051Å	-	-
195	ASN 90.8	-	Favored (71.36%) General / -65.3,-30.5	18.5% ( <i>p-10</i> ) chi angles: 64.5,307.7	0.086Å	-	OUTLIER(S) worst is CA- CB-CG: 4.615
196	ARG 115.13	0.411Å O with 198 PRO HD3	Favored (71.95%) General / -64.1,-30.9	89% ( <i>mtm180</i> ) chi angles: 295.1,168.6,293.2,168.2	0.077Å	-	-
197	SER 90.23	0.44Å HA with 198 PRO HD2	Favored (71.63%) Pre-proline / -56.0,128.5	47.4% (t) chi angles: 180.1	0.081Å	-	-
198	PRO 72.55	0.44Å HD2 with 197	Favored (17.27%)	15.9% ( <i>Cg_endo</i> )	0.096Å	_	_
		SER HA	Trans-proline / -82.0,165.7	chi angles: 16.7	0.030/		
199	HIS 89.01	SER HA -		chi angles: 16.7  80% ( <i>m80</i> )  chi angles: 291.8,85.4	0.090Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.413 σ
	HIS 89.01	- Clash >	-82.0,165.7 Favored (96.43%) Pre-proline /	80% ( <i>m80</i> ) chi angles: 291.8,85.4		- Bond lengths	worst is CD2- NE2-CE1:
		- Clash >	-82.0,165.7 Favored (96.43%) Pre-proline / -67.5,142.5	80% ( <i>m80</i> ) chi angles: 291.8,85.4	0.082Å Cβ deviation	<b>lengths</b> Outliers:	worst is CD2- NE2-CE1: 4.413 σ
	t Res High B Avg:	- Clash > 0.4Å Clashscore: 104.16 0.793Å	-82.0,165.7 Favored (96.43%) Pre-proline / -67.5,142.5 <b>Ramachandran</b> Outliers: 2 of	80% ( <i>m80</i> ) chi angles: 291.8,85.4 <b>Rotamer</b> Poor rotamers: 8 of	0.082Å  Cβ deviation Outliers:	<b>lengths</b> Outliers:	worst is CD2- NE2-CE1: 4.413 σ <b>Bond angles</b> Outliers: 31

			-78.8,-46.2				σ
202	ILE 93.63	0.882Å CG2 with 29 ILE HG12	Favored (63.67%) Isoleucine or valine / -131.0,130.1	21.1% (tt) chi angles: 188.7,168.3	0.059Å	-	-
203	LEU 99.6	0.754Å CD1 with 212 LEU HD22	Favored (56.4%) General / -113.2,128.2	3.3% ( <i>tt</i> ) chi angles: 189.2,180.1	0.056Å	-	-
204	ILE 106.77	0.685Å N with 203 LEU HD23	Favored (38.5%) Isoleucine or valine / -117.6,141.0	33.6% ( <i>mm</i> ) chi angles: 309.5,298.6	0.188Å	-	-
205	ARG 93.68	0.696Å HG3 with 32 ILE HG23	Favored (30.33%) General / -140.2,133.8	26.2% (ttt180) chi angles: 180.1,164.3,182.3,140.1	0.123Å	-	-
206	THR 47.29	0.516Å HB with 230 VAL O	Favored (5.02%) General / -99.8,177.8	73.6% (p) chi angles: 61.8	0.065Å	-	-
207	SER 80.64	0.666Å HB2 with 38 ARG NH1	Favored (3.4%) General / 76.4,1.8	27.7% (p) chi angles: 77.8	0.128Å	-	-
208	GLY 29.06	-	Favored (78.97%) Glycine / 92.0,-5.4	-	-	-	-
209	GLU 85.58	0.492Å HB2 with 205 ARG HE	Favored (37.19%) General / -79.1,141.7	75% ( <i>mm-40</i> ) chi angles: 300.8,294.9,345	0.086Å	-	-
210	VAL 112.57	0.914Å HG23 with 227 PHE CZ	Favored (2.19%) Isoleucine or valine / -112.4,92.8	3.2% (p) chi angles: 51.4	0.037Å	-	-
211	ARG 177.53	-	Favored (9.42%) General / -162.3,141.7	62.4% ( <i>mtt180</i> ) chi angles: 307.8,171.1,185,141.1	0.235Å	-	-
212	LEU 66.55	0.754Å HD22 with 203 LEU CD1	Favored (61.77%) General / -75.1,-36.0	82.3% ( <i>mt</i> ) chi angles: 299.6,181.6	0.098Å	-	-
			Favored (22.69%)	75.8% (m)			

213	SER 66.43	-	General / 54.8,47.3	chi angles: 294.5	0.081Å	-	-
214	ASP 106.44	0.426Å O with 158 SER HB3	Favored (19.26%) General / 59.6,29.7	48.3% ( <i>m-20</i> ) chi angles: 284,317.4	0.106Å	-	-
215	PHE 80.77	0.745Å HE2 with 30 ALA HB1	Favored (48.72%) General / -102.0,130.8	61.8% ( <i>t80</i> ) chi angles: 180.1,64.5	0.045Å	-	OUTLIER(S) worst is CA- CB-CG: 4.439 σ
216	LEU 71.62	1.111Å HD11 with 74 THR HG21	Favored (21.92%) General / 49.2,47.6	75.8% ( <i>mt</i> ) chi angles: 295,182	0.082Å	-	-
217	LEU 74.59	0.784Å HB3 with 158 SER HB2	Favored (78.09%) General / -62.2,-48.9	60.5% ( <i>tp</i> ) chi angles: 180,60.7	0.144Å	-	-
218	TRP 68.25	0.829Å CH2 with 188 LEU HD22	Favored (81.67%) General / -66.0,-45.5	47.5% ( <i>t-105</i> ) chi angles: 187.7,272.8	0.056Å	-	-
219	GLN 101.42	0.793Å HB3 with 200 PRO CD	Favored (81.36%) General /	28.7% ( <i>mp0</i> ) chi angles: 295.6,82.6,358.1	0.034Å	-	-
			-67.2,-36.2				
# <b>A</b>	lt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
# <b>A</b>	It Res High B  Avg: 83.62			Rotamer Poor rotamers: 8 of 205	deviation	<b>lengths</b> Outliers:	Bond angles Outliers: 31 of 229
# <b>A</b> 220	Avg:	<b>0.4Å</b> Clashscore:	Ramachandran Outliers: 2 of	Poor rotamers: 8 of	<b>deviation</b> Outliers:	<b>lengths</b> Outliers:	Outliers: 31
	Avg: 83.62	0.4Å Clashscore: 104.16 0.738Å HG22 with	Ramachandran Outliers: 2 of 227 Allowed (1.73%) General /	Poor rotamers: 8 of 205 15.2% (t)	deviation Outliers: 2 of 218	<b>lengths</b> Outliers:	Outliers: 31
220	Avg: 83.62 THR 167.95	0.4Å Clashscore: 104.16 0.738Å HG22 with	Ramachandran Outliers: 2 of 227 Allowed (1.73%) General / -97.4,34.8 Favored (88.32%) General /	Poor rotamers: 8 of 205  15.2% (t) chi angles: 187.9  47.5% (t)	deviation Outliers: 2 of 218 0.077Å	<b>lengths</b> Outliers:	Outliers: 31

224	CYS 70.71	-	Favored (27.55%) General / -94.4,142.3	52.8% ( <i>t</i> ) chi angles: 180.2	0.107Å	-	-
225	LEU 83.49	0.715Å HD21 with 212 LEU HD21	Favored (50.24%) General / -112.1,137.4	3.4% ( <i>mp</i> ) chi angles: 299.2,64	0.107Å	-	-
226	VAL 99.51	0.596Å HG12 with 204 ILE HD13	Favored (66.09%) Isoleucine or valine / -129.9,129.7	14.1% ( <i>p</i> ) chi angles: 64.7	0.07Å	-	-
227	PHE 47.73	0.914Å CZ with 210 VAL HG23	Favored (55.09%) General / -111.1,131.4	84.6% ( <i>m-85</i> ) chi angles: 298.7,286.2	0.097Å	-	OUTLIER(S) worst is CA- CB-CG: 6.002 σ
228	GLN 50.74	-	Favored (23%) Pre-proline / -116.6,133.6	78% ( <i>mt-30</i> ) chi angles: 295.4,169.5,296.8	0.06Å	-	-
229	PRO 124.45	-	Favored (32.12%) Trans-proline / -70.6,-19.3	13.8% ( <i>Cg_endo</i> ) chi angles: 16	0.187Å	-	-
230	VAL 90.33	0.672Å CG2 with 234 GLU HB2	Favored (13.78%) Isoleucine or valine / -67.9,145.2	14.9% ( <i>p</i> ) chi angles: 63.7	0.063Å	-	-
231	LEU 99.8	0.686Å HB2 with 234 GLU OE1	Favored (30.27%) General / -78.4,154.9	5.3% ( <i>mp</i> ) chi angles: 296.2,71.7	0.099Å	-	-
232	TRP 71.59	0.71Å HB3 with 233 PRO HD3	Favored (95.2%) Pre-proline / -58.9,-42.6	76.9% ( <i>t-105</i> ) chi angles: 180.4,253.5	0.074Å	-	-
233	PRO 76.42	0.835Å HB3 with 53 GLN HG2	Favored (69.52%) Trans-proline / -63.6,-24.5	84.3% ( <i>Cg_exo</i> ) chi angles: 331	0.15Å	-	-
234	GLU 91.99	0.686Å OE1 with 231 LEU HB2	Favored (51.39%) General / -77.5,-26.7	54.3% ( <i>mp0</i> ) chi angles: 288.5,83.8,352.7	0.095Å	-	-
235	TYR 92.64	0.455Å HD2 with 57 LYS HD2	Favored (55.77%) General /	16.7% ( <i>t80</i> ) chi angles: 201.7,82.3	0.052Å	-	-

236	THR	48.68	-	-60.7,142.5 Favored (8.86%) General / -140.0,176.3	67.8% ( <i>p</i> ) chi angles: 63.1	0.084Å	-	-
237	РНЕ	154.88	1.038Å HB2 with 64 TRP HB2	Favored (72.74%) General / -60.6,-33.4	39.4% ( <i>p90</i> ) chi angles: 59.3,82.1	0.043Å	-	-
238	TRP	56.58	0.76Å HA with 241 PHE CD2	Favored (88.7%) General / -59.0,-41.9	87.1% ( <i>m</i> 95) chi angles: 295.1,86	0.192Å	-	-
239	ASN	33.61	-	Favored (92.45%) General / -64.2,-38.8	95.8% ( <i>m-20</i> ) chi angles: 290.9,332.8	0.068Å	-	OUTLIER(S) worst is CA- CB-CG: 4.86 σ
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	<b>Bond angles</b>
		Avg: 83.62	Clashscore: 104.16	Outliers: 2 of 227	Poor rotamers: 8 of 205		Outliers:	Outliers: 31 of 229
240	LEU	49.42	0.802Å HD23 with 64 TRP HD1	Favored (99.05%) General / -62.5,-43.3	45.3% ( <i>tp</i> ) chi angles: 171.1,60.7	0.116Å	-	-
241	РНЕ	166.79	0.825Å HB3 with 64 TRP CE2	Favored (90.31%) General / -65.5,-38.7	7.8% ( <i>p</i> 90) chi angles: 73.6,74.5	0.17Å	-	-
242	GLU	67.85	0.416Å N with 241 PHE CD1	Favored (90.12%) General / -58.6,-44.7	83.8% (tt0) chi angles: 180.1,179.9,346.7	0.07Å	-	-
243	ALA	28.23	-	Favored (96.19%) General / -64.4,-42.4	-	0.076Å	-	-
244	ILE	40.47	0.814Å HD13 with 70 ILE HD11	Favored (84.23%) Isoleucine or valine / -64.8,-39.0	95.6% ( <i>mt</i> ) chi angles: 296.4,168.4	0.051Å	-	-
245	LEU	39.09	0.617Å O with 245 LEU HD23	Favored (99.94%) General / -62.8,-43.0	3.3% ( <i>tt</i> ) chi angles: 189.1,179.9	0.07Å	-	-
				Favored	65.8% (tt0)			

246	GLN 60.03 -	(99.53%) General / -62.5,-42.5	chi angles: 180.2,179.9,356.4	0.09Å	-	-
247	0.536Å PHE 36.59 HB2 with 202 ILE HD12	Favored (79.4%) General / -63.1,-48.3	81.9% ( <i>t80</i> ) chi angles: 177.4,85	0.091Å	-	OUTLIER(S) worst is CA- CB-CG: 5.21 σ
248	0.653Å GLN 108.76 HG2 with 20 ILE HD13	-	0% chi angles: 63,95.8,180.6	0.053Å	-	-

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