

Viewing aipl1_sm_173-312_FFX1Hmulti.table

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All-Atom	Clashscore, all atoms:	0.42		99 th percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the numbe	r of serious	steric ove	erlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	3	2.40%	Goal: <1%		
	Ramachandran outliers	1	0.72%	Goal: <0.05%		
	Ramachandran favored	131	94.93%	Goal: >98%		
Protein Geometry	MolProbity score [^]	1.29		98 th percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	3	2.21%	Goal: 0		
	Bad backbone bonds:	0 / 1192	0.00%	Goal: 0%		
	Bad backbone angles:	12 / 1603	0.75%	Goal: <0.1%		

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

[^] 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: 52.14	Clashscore: 0.42	Outliers: 1 of 138	Poor rotamers: 3 of 125	Outliers: 3 of 136		Outliers: 12 of 140
A 173		GLU	50	-	-	4.9% (<i>tp10</i>) chi angles: 184,47.1,112.3	0.102Å	-	OUTLIER(S) worst is C-N- CA: 8.173 σ
A 174		LYS	50	-	OUTLIER (0.01%) General / 128.2,-25.1	13.6% (<i>mtpt</i>) chi angles: 290.8,194.7,89.5,209.5	0.243Å	-	OUTLIER(S) worst is N-CA- CB: 4.529 σ
A 175		MET	50	-	Favored (75.03%) General / -66.0,-33.1	24.7% (<i>ptp</i>) chi angles: 65.8,176.8,73.5	0.167Å	-	-
A 176		LYS	50	-	Favored (62.32%) General / -71.5,-25.5	83.9% (tttt) chi angles: 192.2,177.6,176.7,179.9	0.049Å	-	-

^{* 100&}lt;sup>th</sup> 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.

A 177	ALA	50	-	Favored (45.76%) General / -78.8,-30.6	-	0.069Å	-	-
A 178	VAL	50	-	Favored (29.05%) Pre-proline / -44.8,-48.7	16.1% (<i>t</i>) chi angles: 161.9	0.194Å	-	-
A 179	PRO	50	-	Favored (24.75%) Trans-proline / -63.3,-41.9	88.8% (<i>Cg_exo</i>) chi angles: 331.4	0.095Å	-	-
A 180	VAL	50	-	Favored (44.21%) Isoleucine or valine / -71.6,-31.9	1.3% (<i>p</i>) chi angles: 85.4	0.222Å	-	-
A 181	LEU	50	-	Favored (91.68%) General / -65.8,-40.1	39.5% (<i>mt</i>) chi angles: 296,162.6	0.056Å	-	-
A 182	HIS	50	-	Favored (97.53%) General / -63.9,-41.8	5.8% (<i>t-160</i>) chi angles: 199,161.5	0.086Å	-	-
A 183	GLY	50	-	Favored (93.54%) Glycine / -66.9,-40.0	-	-	-	-
A 184	GLU	50	-	Favored (95.61%) General / -64.0,-40.1	19% (<i>tp10</i>) chi angles: 165.7,53.6,1	0.079Å	-	-
A 185	GLY	50	-	Favored (99.43%) Glycine / -63.4,-41.3	-	-	-	-
A 186	ASN	50	-	Favored (95.3%) General / -61.4,-40.7	26.7% (<i>m-20</i>) chi angles: 305.7,347.7	0.113Å	-	-
A 187	ARG	50	-	Favored (22.26%) General / -56.4,-56.4	49.5% (ttt-85) chi angles: 165.3,177.4,166.7,260.6	0.082Å	-	-
A 188	LEU	50	-	Favored (77.84%) General /	43.7% (<i>mt</i>) chi angles: 295.7,187.5	0.154Å	-	-

A 189	PHE	50	-	-65.5,-34.2 Favored (92.3%) General / -60.7,-40.5	91.2% (<i>t80</i>) chi angles: 180.1,77.4	0.047Å	-	-
A 190	LYS	50	-	Favored (61.81%) General / -74.7,-31.1	2.9% (tpmp?) chi angles: 191.4,65.8,244.9,71.4	0.098Å	-	-
A 191	LEU	50	-	Favored (56.34%) General / -79.9,-16.0	94.1% (<i>mt</i>) chi angles: 299.1,176.9	0.131Å	-	-
A 192	GLY	50	-	Favored (32.46%) Glycine / 109.7,-10.1	-	-	-	-
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 0.42	Outliers: 1 of 138	Poor rotamers: 3 of 125		Outliers:	Outliers: 12 of 140
A 193	ARC	G 99.99	-	Favored (7.25%) General / -89.7,66.8	26.3% (<i>mmt85</i>) chi angles: 298.8,296.6,188.3,78.4	0.034Å	-	-
A 194	TYR	50	-	Favored (63.04%) General / -73.4,-30.0	53.1% (<i>p</i> 90) chi angles: 64.4,273	0.145Å	-	-
A 195	GLU	J 50	-	Favored (71.91%) General / -68.9,-45.0	61.9% (<i>mt-10</i>) chi angles: 303.7,191.4,11.4	0.057Å	-	-
A 196	GLU	J 50	-	Favored (82.51%) General / -58.1,-41.0	51.9% (<i>mt-10</i>) chi angles: 292.7,167.5,37.4	0.072Å	-	-
A 197	ALA	50	-	Favored (88.11%) General / -59.7,-40.5	-	0.063Å	-	-
A 198	SER	50	-	Favored (97.82%) General / -62.8,-40.6	0.1% chi angles: 228.5	0.116Å	-	-
Α	SER	50	-	Favored (99.3%)	24.8% (t)	0.071Å	-	-

199				General / -61.4,-42.8	chi angles: 186			
A 200	LYS	50	-	Favored (94.96%) General / -62.8,-39.6	29.7% (mmtp) chi angles: 300.6,287.7,171.6,51.1	0.093Å	-	-
A 201	TYR	50	-	Favored (96.41%) General / -64.3,-42.5	19.6% (<i>m-30</i>) chi angles: 303.1,323.1	0.128Å	-	-
A 202	GLN	50	-	Favored (78.92%) General / -67.2,-35.1	11.6% (<i>tp-100</i>) chi angles: 190,55.2,227.3	0.155Å	-	-
A 203	GLU	50	-	Favored (90.79%) General / -62.8,-45.8	3.4% (<i>tp10</i>) chi angles: 161,34.2,50.2	0.124Å	-	-
A 204	ALA	50	-	Favored (81.58%) General / -58.0,-40.7	-	0.067Å	-	-
A 205	ILE	50	-	Favored (96.9%) Isoleucine or valine / -64.5,-43.2	35.3% (<i>mt</i>) chi angles: 287.7,156	0.132Å	-	-
A 206	ILE	50	-	Favored (53.23%) Isoleucine or valine / -69.6,-32.6	1.1% (<i>pt</i>) chi angles: 61.6,123.4	0.286Å	-	-
A 207	CYS	50	-	Favored (56.94%) General / -50.9,-50.8	81.8% (<i>m</i>) chi angles: 295.9	0.1Å	-	-
A 208	LEU	50	-	Favored (63.1%) General / -73.9,-31.5	68.9% (<i>mt</i>) chi angles: 302.4,172.2	0.106Å	-	-
A 209	ARG	50	-	Favored (82.3%) General / -63.2,-47.5	61.6% (<i>mtp180</i>) chi angles: 286.8,159.4,60.8,180.9	0.099Å	-	-
A 210	ASN	50	-	Favored (66.86%) General / -70.4,-30.1	2.7% (<i>m120</i>) chi angles: 297.4,48.4	0.139Å	-	-

A 211	LEU	50	-	Favored (83.17%) General / -67.9,-38.6	52.4% (<i>mt</i>) chi angles: 295,164	0.104Å	-	-
A 212	GLN	50	-	Favored (62.09%) General / -72.0,-26.2	43.1% (<i>tt0</i>) chi angles: 198.7,184.3,30.5	0.079Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 0.42	Outliers: 1 of 138	Poor rotamers: 3 of 125		Outliers: 0 of 140	Outliers: 12 of 140
A 213	THR	50	-	Favored (56.21%) General / -73.5,-8.5	10.9% (<i>p</i>) chi angles: 44.5	0.131Å	-	-
A 214	LYS	50	-	Favored (53.55%) General / -87.7,-9.6	2.2% (ttpm?) chi angles: 206,213.9,96.2,304	0.049Å	-	-
A 215	GLU	50	-	Favored (34.21%) General / -109.7,146.8	22.1% (<i>mm-40</i>) chi angles: 311.1,318.4,318.9	0.043Å	-	-
A 216	LYS	50	-	Favored (89.38%) Pre-proline / -69.5,132.5	36% (<i>mtmm</i>) chi angles: 296.8,176.2,297,299.7	0.044Å	-	-
A 217	PRO	50	-	Favored (9.68%) Trans-proline / -45.8,127.0	0.1% chi angles: 316.8	0.046Å	-	-
A 218	TRP	50	-	Favored (4.04%) General / 71.6,1.9	2.5% (<i>m0</i>) chi angles: 315.4,308.1	0.161Å	-	-
A 219	GLU	50	-	Favored (15.17%) General / -70.5,169.0	5.1% (<i>pt-20</i>) chi angles: 91.5,175.2,306.6	0.165Å	-	-
A 220	VAL	50	-	Favored (42.42%) Isoleucine or valine / -55.3,-37.1	5.9% (p) chi angles: 75.1	0.198Å	-	-
A 221	GLN	99.99	-	Favored (42.57%) General /	24.3% (<i>tp60</i>) chi angles: 195.7,47.7,76.1	0.134Å	-	-

A 222	TRP	50	-	-79.4,-31.1 Favored (90.86%) General / -64.4,-44.6	52.3% (<i>t</i> 90) chi angles: 193.5,94.6	0.04Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.118 σ
A 223	LEU	50	-	Favored (78.05%) General / -69.4,-38.4	67.8% (<i>mt</i>) chi angles: 297.5,167.3	0.098Å	-	-
A 224	LYS	50	-	Favored (99.47%) General / -62.8,-41.8	52% (<i>mtmt</i>) chi angles: 291.3,177.7,294.7,173.9	0.115Å	-	-
A 225	LEU	50	-	Favored (79.16%) General / -68.4,-36.4	30.5% (<i>mt</i>) chi angles: 290.5,159	0.134Å	-	-
A 226	GLU	50	-	Favored (78.81%) General / -56.1,-44.4	13.4% (<i>tm-20</i>) chi angles: 188.9,284.7,321.2	0.053Å	-	-
A 227	, LYS	50	-	Favored (63.8%) General / -72.9,-30.3	25.4% (<i>mtpp</i>) chi angles: 297.5,182.7,59.4,52.9	0.149Å	-	-
A 228	MET	50	-	Favored (68.42%) General / -72.2,-34.6	9.9% (ttt) chi angles: 203.9,176.9,196.6	0.099Å	-	-
A 229) ILE	50	-	Favored (89.87%) Isoleucine or valine / -66.6,-44.4	48% (<i>mt</i>) chi angles: 290,157.8	0.074Å	-	-
A 230) ASN	50	-	Favored (29.49%) General / -47.7,-48.8	1.9% (<i>t-20</i>) chi angles: 180.6,202.3	0.065Å	-	OUTLIER(S) worst is CA-CB- CG: 8.759 σ
A 231	THR	50	-	Favored (82.89%) General / -63.3,-36.2	8.8% (<i>t</i>) chi angles: 179.9	0.239Å	-	-
A 232	LEU	50	-	Favored (50.82%) General / -77.2,-38.5	8.1% (<i>mt</i>) chi angles: 277.7,152.4	0.108Å	-	-
#	Alt Res	High B	Clash > 0.4Å R	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

		Avg: 52.14	Clashscore: 0.42	Outliers: 1 of 138	Poor rotamers: 3 of 125		Outliers: 0 of 140	Outliers: 12 of 140
A 233	ILE	50	-	Favored (16.04%) Isoleucine or valine / -76.3,-24.3	19.3% (<i>pt</i>) chi angles: 52.5,179.6	0.324Å	-	-
A 234	LEU	50	-	Favored (83.18%) General / -58.7,-40.2	26.2% (<i>mt</i>) chi angles: 283.1,160.2	0.101Å	-	-
A 235	ASN	50	-	Favored (30.51%) General / -82.7,-28.5	11.3% (<i>m120</i>) chi angles: 304,149.2	0.143Å	-	OUTLIER(S) worst is CA-CB- CG: 4.729 σ
A 236	TYR	50	-	Favored (65.97%) General / -65.4,-50.3	91.1% (<i>t80</i>) chi angles: 178.4,75.6	0.062Å	-	-
A 237	CYS	50	-	Favored (76.06%) General / -63.4,-33.7	80.6% (<i>m</i>) chi angles: 296	0.146Å	-	-
A 238	GLN	50	-	Favored (83.82%) General / -60.5,-38.3	7% (<i>tp60</i>) chi angles: 180.6,63.7,104	0.077Å	-	-
A 239	CYS	50	-	Favored (62.5%) General / -74.5,-32.6	97.9% (<i>m</i>) chi angles: 294.6	0.135Å	-	-
A 240	LEU	50	-	Favored (28.58%) General / -73.6,-3.5	29.2% (<i>mt</i>) chi angles: 303.6,190.4	0.162Å	-	-
A 241	LEU	50	-	Favored (59.58%) General / -77.5,-10.6	74.4% (<i>mt</i>) chi angles: 288.9,176.8	0.131Å	-	-
A 242	LYS	50	-	Favored (5.74%) General / -127.2,-12.3	6.5% (<i>tptp</i>) chi angles: 192.6,62.7,226.4,69.7	0.159Å	-	-
A 243	LYS	50	-	Favored (59.55%) General / -76.3,-17.2	11.2% (<i>tptp</i>) chi angles: 177.4,59.4,208.4,52.2	0.139Å	-	OUTLIER(S) worst is C-N- CA: 4.81 σ

A 244	GLU	50	-	Favored (6.76%) General / 66.1,34.6	22.5% (<i>mt-10</i>) chi angles: 298.7,201.4,51.3	0.221Å	-	-
A 245	GLU	50	-	Allowed (1.55%) General / -100.0,69.8	50.4% (<i>mt-10</i>) chi angles: 285.2,180.5,43.7	0.105Å	-	-
A 246	TYR	50	-	Favored (70.3%) General / -61.7,-29.7	60.6% (<i>m-85</i>) chi angles: 303.6,293.2	0.12Å	-	-
A 247	TYR	50	-	Favored (95.01%) General / -60.1,-44.4	45.5% (<i>p90</i>) chi angles: 67,95.7	0.114Å	-	-
A 248	GLU	50	-	Favored (89.93%) General / -65.9,-42.6	4.8% (<i>mt-10</i>) chi angles: 271.3,214.3,92.4	0.106Å	-	-
A 249	VAL	50	-	Favored (22.18%) Isoleucine or valine / -54.5,-54.4	94.9% (<i>t</i>) chi angles: 175.9	0.111Å	-	-
A 250	LEU	50	-	Favored (97.67%) General / -63.9,-41.7	94.3% (<i>mt</i>) chi angles: 295.3,172	0.081Å	-	-
A 251	GLU	50	-	Favored (5.72%) General / -59.8,-59.3	0% chi angles: 191.2,325.1,101.6	0.032Å	-	-
A 252	HIS	50	-	Favored (36.14%) General / -82.0,-23.2	2.6% (<i>m-70</i>) chi angles: 325.7,318.2	0.202Å	-	-
# A	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 0.42	Outliers: 1 of 138	Poor rotamers: 3 of 125		Outliers:	Outliers: 12 of 140
A 253	THR	50	-	Favored (80.31%) General / -65.2,-46.5	31.4% (<i>p</i>) chi angles: 51.5	0.13Å	-	-
Α				Favored (72.54%)	75.3% (m)			

254	SER	50	-	General / -56.3,-39.3	chi angles: 294.7	0.146Å	-	-
A 255	ASP	50	-	Favored (91.09%) General / -61.1,-46.3	32.8% (<i>t70</i>) chi angles: 188.4,51.1	0.123Å	-	-
A 256	ILE	50	-	Favored (21.05%) Isoleucine or valine / -72.4,-23.2	31% (<i>pt</i>) chi angles: 54.7,175.3	0.308Å	-	-
A 257	LEU	50	-	Favored (69.05%) General / -72.3,-36.7	92.6% (<i>mt</i>) chi angles: 296,171.8	0.112Å	-	-
A 258	ARG	50	-	Favored (75.47%) General / -60.4,-35.3	52.9% (<i>mtm-85</i>) chi angles: 291,181.6,295.8,246.9	0.126Å	-	-
A 259	HIS	50	-	Favored (26.88%) General / -85.4,-25.6	8.2% (<i>m170</i>) chi angles: 313.8,163.1	0.09Å	-	-
A 260	HIS	50	-	Favored (2.09%) Pre-proline / -156.6,98.8	5.2% (<i>m-70</i>) chi angles: 329.5,289	0.092Å	-	OUTLIER(S) worst is CA-CB-CG: 5.806σ
A 261	PRO	50	-	Favored (2.86%) Trans-proline / -82.5,12.5	94.3% (<i>Cg_endo</i>) chi angles: 32.2	0.039Å	-	-
A 262	GLY	50	-	Favored (32.55%) Glycine / -108.6,-0.0	-	-	-	-
A 263	ILE	50	-	Favored (3.84%) Isoleucine or valine / -84.2,95.2	38% (<i>pt</i>) chi angles: 58.4,166.6	0.22Å	-	OUTLIER(S) worst is C-N-CA: 4.135σ
A 264	VAL	50	0.472Å HG11 with A 294 GLU HB2	Allowed (0.31%) Isoleucine or valine / -37.4,-54.2	3.5% (<i>t</i>) chi angles: 196.8	0.06Å	-	-
A 265	LYS	50	-	Favored (61.12%) General /	39.3% (<i>mmtm</i>) chi angles: 298.2,285.3,184.7,275.7	0.131Å	-	-

A 266	ALA	50	-	Favored (67.38%) General / -72.9,-36.8	-	0.112Å	-	-
A 267	TYR	50	-	Favored (97.21%) General / -64.1,-41.5	83.6% (<i>m-85</i>) chi angles: 291.8,283.2	0.133Å	-	-
A 268	TYR	50	-	Favored (83.08%) General / -67.5,-42.3	47.2% (<i>t80</i>) chi angles: 190.1,67.3	0.121Å	-	-
A 269	VAL	50	-	Favored (80%) Isoleucine or valine / -67.4,-38.0	70.3% (<i>t</i>) chi angles: 173.6	0.151Å	-	-
A 270	ARG	50	-	Favored (81.96%) General / -66.9,-36.3	24.3% (ttp180) chi angles: 201.9,175.8,77.8,160.4	0.083Å	-	-
A 271	ALA	50	-	Favored (74.97%) General / -58.6,-50.1	-	0.059Å	-	-
A 272	ARG	99.99	-	Favored (60.5%) General / -75.2,-30.1	10.8% (<i>tpt180</i>) chi angles: 195.9,65.1,188.8,259	0.17Å	-	-
272	ARG t Res	⊔iah	- Clash > 0.4Å	(60.5%) General /	chi angles:	0.17Å Cβ deviation	- Bond lengths	- Bond angles
272				(60.5%) General / -75.2,-30.1 Ramachandran	chi angles: 195.9,65.1,188.8,259	Cβ deviation	lengths Outliers:	
272		High B Avg: 52.14	Clashscore:	(60.5%) General / -75.2,-30.1 Ramachandran Outliers: 1 of 138 Favored (98.01%) General / -63.8,-41.1	chi angles: 195.9,65.1,188.8,259 Rotamer Poor rotamers: 3 of	Cβ deviation Outliers:	lengths Outliers:	Outliers: 12
272 # Al	t Res	High B Avg: 52.14	Clashscore:	(60.5%) General / -75.2,-30.1 Ramachandran Outliers: 1 of 138 Favored (98.01%) General / -63.8,-41.1 Favored (96.98%) General / -62.8,-40.3	chi angles: 195.9,65.1,188.8,259 Rotamer Poor rotamers: 3 of	Cβ deviation Outliers: 3 of 136	lengths Outliers:	Outliers: 12
272 # Alt A 273	t Res	High B Avg: 52.14 50	Clashscore:	(60.5%) General / -75.2,-30.1 Ramachandran Outliers: 1 of 138 Favored (98.01%) General / -63.8,-41.1 Favored (96.98%) General /	chi angles: 195.9,65.1,188.8,259 Rotamer Poor rotamers: 3 of 125 - 15.3% (<i>m170</i>)	Cβ deviation Outliers: 3 of 136 0.076Å	lengths Outliers:	Outliers: 12

-73.7,-17.3

276	GLU	50	-	General / -82.5,-17.0	305.9,309.8,153.5	0.196Å	-	-
A 277	VAL	50	-	Favored (9.67%) Isoleucine or valine / -89.2,-2.8	18% (<i>m</i>) chi angles: 304.6	0.208Å	-	-
A 278	TRP	50	-	Allowed (0.42%) General / 80.3,22.8	62% (<i>m</i> 95) chi angles: 299.4,76.4	0.243Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.534 σ
A 279	ASN	50	-	Favored (5.55%) General / -90.3,62.9	8.9% (<i>m120</i>) chi angles: 308.3,146.8	0.031Å	-	OUTLIER(S) worst is CA-CB- CG: 6.194 σ
A 280	GLU	50	-	Favored (88.34%) General / -65.7,-38.1	4.4% (<i>tm-20</i>) chi angles: 191.7,278.1,6.3	0.124Å	-	-
A 281	ALA	50	-	Favored (92.61%) General / -65.0,-39.0	-	0.091Å	-	-
A 282	GLU	50	-	Favored (78.35%) General / -67.2,-34.8	32.9% (<i>mt-10</i>) chi angles: 290,194.9,269.2	0.123Å	-	-
A 283	ALA	50	-	Favored (95.86%) General / -62.8,-39.9	-	0.08Å	-	-
A 284	LYS	50	-	Favored (94.25%) General / -60.5,-45.3	51% (<i>mttt</i>) chi angles: 286.6,164.2,172.8,148.1	0.082Å	-	-
A 285	ALA	50	-	Favored (93.64%) General / -62.7,-45.2	-	0.072Å	-	-
A 286	ASP	50	-	Favored (97.07%) General / -64.1,-41.9	98.6% (<i>m-20</i>) chi angles: 289.1,344.2	0.093Å	-	-
A 287	LEU	50	-	Favored (81.92%) General / -64.5,-35.7	77.4% (<i>mt</i>) chi angles: 293.1,166.7	0.12Å	-	-
				Favored				

A 288	GLN	50	-	(93.78%) General / -65.4,-41.2	11.8% (<i>tp-100</i>) chi angles: 184.2,53.6,240.2	0.107Å	-	-
A 289	LYS	50	-	Favored (72.44%) General / -67.2,-31.8	68.9% (mmtt) chi angles: 286.5,302.8,192.8,182.4	0.159Å	-	-
A 290	VAL	50	-	Favored (97.39%) Isoleucine or valine / -61.4,-43.8	71.3% (<i>t</i>) chi angles: 173.3	0.101Å	-	-
A 291	LEU	50	-	Favored (88.73%) General / -65.5,-43.9	37.5% (<i>tp</i>) chi angles: 184.4,68.9	0.034Å	-	-
A 292	GLU	50	-	Favored (60.87%) General / -58.6,-53.2	33.4% (tt0) chi angles: 180.7,185.2,286.6	0.046Å	-	-
# Al	t Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 1 of	Poor rotamers: 3 of	Outliers:	Outliers:	Outliers: 12
		52.14	0.42	138	125	3 of 136	0 of 140	of 140
A 293	LEU	52.14 50	0.42 -	138 Favored (31.34%) General / -83.8,-23.4	125 9.6% (<i>mt</i>) chi angles: 304.6,153.9	3 of 136 0.124Å	0 of 140 -	of 140 -
	LEU		0.42 - 0.472Å HB2 with A 264 VAL HG11	Favored (31.34%) General /	9.6% (mt)		0 of 140 - -	of 140 - -
293 A	LEU	50	- 0.472Å HB2 with A	Favored (31.34%) General / -83.8,-23.4 Favored (11.34%) Pre-proline /	9.6% (<i>mt</i>) chi angles: 304.6,153.9 5.5% (<i>mt-10</i>) chi angles:	0.124Å	0 of 140 - -	of 140 - -
293 A 294	LEU GLU	50 99.99	- 0.472Å HB2 with A	Favored (31.34%) General / -83.8,-23.4 Favored (11.34%) Pre-proline / -138.5,93.1 Favored (43.1%) Trans-proline /	9.6% (<i>mt</i>) chi angles: 304.6,153.9 5.5% (<i>mt-10</i>) chi angles: 260.1,177.5,80.2	0.124Å 0.064Å	0 of 140 - -	of 140 - -
293 A 294 A 295	LEU GLU PRO SER	50 99.99 50	- 0.472Å HB2 with A	Favored (31.34%) General / -83.8,-23.4 Favored (11.34%) Pre-proline / -138.5,93.1 Favored (43.1%) Trans-proline / -66.6,-14.2 Favored (60.44%) General /	9.6% (<i>mt</i>) chi angles: 304.6,153.9 5.5% (<i>mt-10</i>) chi angles: 260.1,177.5,80.2 19.8% (<i>Cg_endo</i>) chi angles: 17.5	0.124Å 0.064Å 0.115Å	o of 140 - -	of 140 - -

				-43.0,-35.6	71.9,211.4,145			σ
A 299	LYS	50	-	Favored (61.17%) General / -73.2,-26.5	32.1% (mtmm) chi angles: 294,169.5,287.6,301.3	0.141Å	-	-
A 300	ALA	50	-	Favored (10.19%) General / -94.6,-39.8	-	0.045Å	-	-
A 301	VAL	50	-	Favored (80.48%) Isoleucine or valine / -61.4,-38.7	23.6% (t) chi angles: 163.4	0.131Å	-	-
A 302	ARG	50	-	Favored (79.26%) General / -63.4,-35.1	27.8% (<i>tpt85</i>) chi angles: 190.3,69.7,201.1,94.3	0.161Å	-	-
A 303	ARG	50	-	Favored (54.58%) General / -77.5,-33.4	42.7% (<i>tpt85</i>) chi angles: 187.6,63.9,193.9,92.5	0.163Å	-	-
A 304	GLU	50	-	Favored (79.84%) General / -68.1,-42.8	25.6% (<i>mm-40</i>) chi angles: 293.6,293.1,13	0.079Å	-	-
A 305	LEU	50	-	Favored (85.48%) General / -60.7,-38.6	76.2% (<i>mt</i>) chi angles: 290.1,167	0.096Å	-	-
A 306	ARG	50	-	Favored (60.28%) General / -74.8,-12.0	5.8% (tpm_?) chi angles: 188.9,57.6,255.9,187.6	0.088Å	-	-
A 307	LEU	50	-	Favored (25.56%) General / -83.4,-34.5	3.3% (<i>tt</i>) chi angles: 181.3,132.5	0.07Å	-	-
A 308	LEU	50	-	Favored (80.55%) General / -68.4,-37.8	26.2% (<i>mt</i>) chi angles: 310,186.5	0.112Å	-	-
A 309	GLU	50	-	Allowed (0.43%) General / -74.2,14.4	19.1% (<i>mt-10</i>) chi angles: 299.6,152.1,47.2	0.061Å	-	-
				Favored				

A 310	ASN 50	-	(4.83%) General / -130.6,29.2	6.2% (<i>m120</i>) chi angles: 274.8,87.2	0.078Å	-	-
A 311	ARG 50	-	Allowed (0.15%) General / -160.7,26.6	17.8% (ptp180) chi angles: 60.4,176.5,65.7,188.1	0.049Å	-	OUTLIER(S) worst is C-N- CA: 7.346 σ
A 312	MET 99.99	-	-	20.9% (ttt) chi angles: 196.1,182.5,182.3	0.106Å	-	-

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