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All-Atom	Clashscore, all atoms:	26.19		19 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	1	0.80%	Goal: <1%		
	Ramachandran outliers	0	0.00%	Goal: <0.05%		
	Ramachandran favored	136	98.55%	Goal: >98%		
Protein Geometry	MolProbity score [^]	1.91		80 th percentile* (N=27675, 0Å - 99Å)		
Geometry	Cβ deviations >0.25Å	1	0.74%	Goal: 0		
	Bad backbone bonds:	11 / 1192	0.92%	Goal: 0%		
	Bad backbone angles:	6 / 1603	0.37%	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 Re	es	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.14		Outliers: 0 of 138	Poor rotamers: 1 of 125	Outliers: 1 of 136	Outliers: 6 of 140	Outliers: 6 of 140
A 173	GL	LU	50	-	-	5.4% (<i>mp0</i>) chi angles: 322.6,72.8,22.8	0.089Å	-	-
A 174	LY	/S	50	-	Favored (41.62%) General / -99.4,10.3	6.6% (<i>mtpm?</i>) chi angles: 306.3,194.9,83,295.8	0.024Å	-	-
A 175	MI	ET	50	-	Favored (67.06%) General / -66.2,-25.7	25.8% (<i>ptp</i>) chi angles: 62.6,180.3,67.2	0.034Å	-	-
A 176	LY	/S	50	-	Favored (56.3%) General / -76.8,-30.4	74.5% (tttt) chi angles: 181.6,161.6,181.7,166.7	0.056Å	-	-

^{* 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	0.509Å O with A 180 VAL HG12	Favored (67.21%) General / -70.0,-30.0	-	0.027Å	-	-
A 178	VAL	50	0.517Å HB with A 179 PRO HD3	Favored (81.51%) Pre-proline / -55.2,-51.2	67.9% (<i>t</i>) chi angles: 179.5	0.108Å	-	-
A 179	PRO	50	0.517Å HD3 with A 178 VAL HB	Favored (90.71%) Trans-proline / -56.9,-39.5	99.6% (<i>Cg_exo</i>) chi angles: 329.5	0.056Å	-	-
A 180	VAL	50	0.509Å HG12 with A 177 ALA O	Favored (77.11%) Isoleucine or valine / -70.0,-39.2	9.1% (p) chi angles: 68.2	0.157Å	-	-
A 181	LEU	50	-	Favored (89.54%) General / -66.5,-40.9	95.7% (<i>mt</i>) chi angles: 294.9,175.6	0.023Å	-	-
A 182	HIS	50	-	Favored (87.49%) General / -59.1,-46.8	8.3% (<i>t-160</i>) chi angles: 185.2,168.2	0.075Å	OUTLIER(S) worst is CG ND1: 4.559 σ	-
A 183	GLY	50	-	Favored (99.44%) Glycine / -63.3,-41.9	-	-	-	-
A 184	GLU	50	-	Favored (80.16%) General / -68.6,-37.9	36.5% (<i>tp10</i>) chi angles: 183.2,52.7,25.6	0.029Å	-	-
A 185	GLY	50	-	Favored (99.69%) Glycine / -60.9,-42.6	-	-	-	-
A 186	ASN	50	-	Favored (89.1%) General / -66.4,-39.4	41.8% (<i>m-20</i>) chi angles: 288,6.1	0.013Å	-	-
A 187	ARG	50	0.605Å HG2 with A 187 ARG HH11	Favored (77.64%) General / -63.2,-48.6	0% chi angles: 193.4,180.7,88.9,359.6	0.022Å	-	OUTLIER(S) worst is CD- NE-CZ: 5.079 σ
A 188	LEU	50	-	Favored (95.02%) General /	93.7% (<i>mt</i>) chi angles: 293.4,171	0.027Å	-	-

					-61.3,-40.7				
A 189	F	PHE	50	-	Favored (73.9%) General / -63.6,-49.3	82.8% (<i>t80</i>) chi angles: 182.4,81.5	0.017Å	-	-
A 190	I	YS.	50	-	Favored (68.53%) General / -69.5,-30.6	65.4% (<i>mttp</i>) chi angles: 294,182.9,179.2,64.4	0.021Å	-	-
A 191	L	.EU	50	0.441Å HG with A 187 ARG O	Favored (64.54%) General / -68.5,-22.5	83.3% (<i>mt</i>) chi angles: 292.4,178.9	0.064Å	-	-
A 192	(GLY	50	-	Favored (28.1%) Glycine / 111.6,-11.2	-	-	-	-
#	Alt I	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 1 of	Outliers:	Outliers: 6	Outliers: 6
			52.14	26.19	138	125	1 of 136	of 140	of 140
A 193	A	ιRG	99.99	-	Favored (4.81%) General / -78.3,71.5	99.3% (<i>mtt180</i>) chi angles: 297.8,180.6,178.3,180.9	0.033Å	-	-
A 194	Т	YR	50	0.557Å CE2 with A 195 GLU HG3	Favored (79.93%) General / -68.5,-41.5	54.5% (<i>p90</i>) chi angles: 63.5,270.2	0.067Å	-	-
A 195	(SLU	50	0.557Å HG3 with A 194 TYR CE2	Favored (97.31%) General / -61.2,-44.4	56.4% (<i>mt-10</i>) chi angles: 293.9,181.1,298.7	0.051Å	-	-
A 196	C	GLU	50	-	Favored (88.46%) General / -66.6,-39.4	50.4% (<i>mt-10</i>) chi angles: 291.8,178.3,63.2	0.011Å	-	-
A 197	A	ΛLA	50	-	Favored (90.55%) General / -61.3,-39.5	-	0.038Å	-	-
A 198	S	SER	50	-	Favored (94.81%) General / -62.5,-39.9	30.8% (<i>t</i>) chi angles: 184.7	0.028Å	-	-
A	S	SER	50	-	Favored (97.72%)	33.3% (t)	0.009Å	-	-

199				General / -63.8,-40.9	chi angles: 183.6			
A 200	LYS	50	-	Favored (73.63%) General / -62.9,-49.7	31% (<i>mmtp</i>) chi angles: 289.1,295.8,170.4,64.1	0.049Å	-	-
A 201	TYR	50	-	Favored (86.5%) General / -58.9,-41.1	22.5% (<i>m-30</i>) chi angles: 295.8,319.8	0.029Å	-	-
A 202	GLN	50	0.54Å O with A 206 ILE HG23	Favored (96.35%) General / -60.6,-42.1	53% (<i>tt0</i>) chi angles: 185.3,181,58.9	0.018Å	-	-
A 203	GLU	50	0.585Å O with A 206 ILE HG12	Favored (76.66%) General / -69.6,-37.0	54.3% (<i>mt-10</i>) chi angles: 298,181.6,296.8	0.03Å	-	-
A 204	ALA	50	-	Favored (92.34%) General / -65.4,-42.8	-	0.04Å	-	-
A 205	ILE	50	0.505Å HD13 with A 233 ILE HG22	Favored (91.57%) Isoleucine or valine / -65.2,-41.5	62.3% (<i>mt</i>) chi angles: 300.9,162.9	0.042Å	-	-
A 206	ILE	50	0.585Å HG12 with A 203 GLU O	Favored (77.34%) Isoleucine or valine / -61.9,-37.1	25.4% (<i>pt</i>) chi angles: 69.2,176.8	0.131Å	-	-
A 207	CYS	50	-	Favored (80.63%) General / -62.6,-48.2	92.1% (<i>m</i>) chi angles: 293.5	0.037Å	-	-
A 208	LEU	50	-	Favored (80.24%) General / -66.2,-35.4	97.2% (<i>mt</i>) chi angles: 297.7,178.1	0.019Å	-	-
A 209	ARG	50	0.498Å O with A 213 THR HG23	Favored (83.31%) General / -67.9,-38.8	83.2% (<i>mtp180</i>) chi angles: 291.1,180.8,66.4,184.9	0.028Å	-	-
A 210	ASN	50	-	Favored (85.9%) General / -65.4,-37.1	94.4% (<i>m-20</i>) chi angles: 290.4,330.5	0.024Å	-	-

A 211	LEU	50	-	Favored (78.69%) General / -69.2,-38.2	85.4% (<i>mt</i>) chi angles: 291.4,177.4	0.014Å	-	-
A 212	GLN	50	-	Favored (69.55%) General / -69.2,-31.1	44.9% (tt0) chi angles: 196.8,182.7,40	0.032Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 26.19	Outliers: 0 of 138	Poor rotamers: 1 of 125	Outliers: 1 of 136	Outliers: 6 of 140	Outliers: 6 of 140
A 213	THR	50	0.498Å HG23 with A 209 ARG O	Favored (68.44%) General / -64.2,-26.3	62.9% (p) chi angles: 62.8	0.032Å	-	-
A 214	LYS	50	-	Favored (59.68%) General / -78.0,-14.0	86.3% (tttt) chi angles: 188.4,180.8,177.4,177.7	0.046Å	-	-
A 215	GLU	50	0.459Å HB3 with A 219 GLU OE2	Favored (32.58%) General / -100.0,141.6	71% (mm-40) chi angles: 300.9,305.8,330.7	0.164Å	-	-
A 216	LYS	50	0.526Å N with A 219 GLU OE2	Favored (88.69%) Pre-proline / -61.0,128.0	38.7% (ttpt) chi angles: 188.7,177.7,66.9,180.7	0.126Å	-	-
A 217	PRO	50	-	Favored (59.8%) Trans-proline / -56.3,133.7	96% (<i>Cg_exo</i>) chi angles: 329.3	0.094Å	-	-
A 218	TRP	50	-	Allowed (0.54%) General / 88.2,-5.8	29.7% (<i>m0</i>) chi angles: 308.4,340.1	0.144Å	-	-
A 219	GLU	50	0.526Å OE2 with A 216 LYS N	Favored (26.82%) General / -76.2,163.7	10.1% (<i>pt-20</i>) chi angles: 77.7,174.5,289.4	0.068Å	OUTLIER(S) worst is CD OE1: 4.867 σ	-
A 220	VAL	50	-	Favored (70.19%) Isoleucine or valine / -54.5,-45.4	10.7% (<i>p</i>) chi angles: 61.3	0.098Å	-	-
A	O	~~ ~~		Favored (77.97%)	94% (<i>mt-30</i>) chi angles:	~ ~~ · °		

221	I GLN	99.99) -	General / -69.3,-38.0	294.3,183./,330./	0.026A	-	-
A 222	TRP	50	0.512Å H with A 219 GLU HG3	Favored (95.26%) General / -63.4,-44.2	76.1% (<i>t90</i>) chi angles: 185.6,94.8	0.061Å	-	-
A 223	3 LEU	50	-	Favored (87.07%) General / -66.3,-38.1	96.2% (<i>mt</i>) chi angles: 294.8,174.1	0.014Å	-	-
A 224	4 LYS	50	-	Favored (86%) General / -65.9,-44.2	38.9% (<i>ttpt</i>) chi angles: 184.6,182.6,64.1,181.5	0.025Å	-	-
A 225	LEU	50	-	Favored (84.94%) General / -65.2,-36.7	79.2% (<i>mt</i>) chi angles: 289.6,167.9	0.019Å	-	-
A 226	GLU	50	-	Favored (87.36%) General / -63.6,-37.4	12% (<i>tm-20</i>) chi angles: 183.6,288.5,324.9	0.071Å	-	-
A 227	₇ LYS	50	-	Favored (62.04%) General / -74.8,-32.7	30.6% (<i>mtpp</i>) chi angles: 294.1,183.1,66.3,63.3	0.008Å	-	-
A 228	₃ Met	50	-	Favored (69.16%) General / -68.7,-30.5	27.3% (ttt) chi angles: 188.7,179.3,180	0.031Å	-	-
A 229	e ILE	50	0.728Å HG22 with A 233 ILE HD13	Favored (58.85%) Isoleucine or valine / -71.8,-36.5	72% (<i>mt</i>) chi angles: 291.3,176.3	0.087Å	-	-
A 230) ASN	50	0.513Å HA with A 233 ILE HD11	Favored (8.95%) General / -50.5,-57.1	25.6% (<i>t-20</i>) chi angles: 187.1,298.8	0.05Å	-	-
A 231	1 THR	50	-	Favored (76.63%) General / -66.2,-33.8	73.7% (p) chi angles: 61.8	0.058Å	-	-
A 232	2 LEU	50	-	Favored (90.52%) General / -65.9,-42.2	51% (<i>mt</i>) chi angles: 284.1,174.1	0.025Å	-	-
#	Alt Res	High	Clash >	Ramachandran	Rotamer	Сβ	Bond	Bond
		-	-				•	

		В	U.4A			deviation	lengths	angles
		Avg: 52.14	Clashscore: 26.19	Outliers: 0 of 138	Poor rotamers: 1 of 125	Outliers: 1 of 136	Outliers: 6 of 140	Outliers: 6 of 140
A 233	ILE	50	0.728Å HD13 with A 229 ILE HG22	Favored (53.02%) Isoleucine or valine / -69.6,-32.6	5.6% (<i>pt</i>) chi angles: 53.5,191	0.162Å	-	-
A 234	LEU	50	-	Favored (76.96%) General / -69.5,-37.0	77.2% (<i>mt</i>) chi angles: 290,177.6	0.054Å	-	-
A 235	ASN	50	-	Favored (96.2%) General / -64.3,-43.0	63.3% (<i>m-20</i>) chi angles: 285.3,359.8	0.048Å	-	-
A 236	TYR	50	0.511Å CE2 with A 240 LEU HD11	Favored (96.83%) General / -61.0,-41.7	90.9% (<i>t80</i>) chi angles: 178.3,80.4	0.048Å	-	-
A 237	CYS	50	-	Favored (78.26%) General / -67.1,-34.7	99.4% (<i>m</i>) chi angles: 290.5	0.035Å	-	-
A 238	GLN	50	-	Favored (96.88%) General / -62.8,-40.3	58% (<i>tp60</i>) chi angles: 180.3,55.1,36.7	0.014Å	-	-
A 239	CYS	50	-	Favored (90.28%) General / -65.4,-38.5	88.6% (<i>m</i>) chi angles: 295.3	0.032Å	-	-
A 240	LEU	50	0.511Å HD11 with A 236 TYR CE2	Favored (78.18%) General / -66.3,-34.5	95.4% (<i>mt</i>) chi angles: 294.9,176.3	0.028Å	-	-
A 241	LEU	50	0.78Å HD11 with A 269 VAL HG23	Favored (96.79%) General / -64.2,-41.8	66.8% (<i>mt</i>) chi angles: 287.6,177.3	0.047Å	-	-
A 242	LYS	50	-	Favored (98.94%) General / -63.3,-41.3	27.8% (<i>tptp</i>) chi angles: 185.6,62.1,183.2,66.2	0.022Å	-	-
A 243	LYS	50	0.419Å HD3 with A 194 TYR HE2	Favored (31.89%) General / -86.6,6.3	25.1% (<i>tptp</i>) chi angles: 189.4,55.6,184,71.3	0.067Å	-	-

A 244	GLU	50	-	Favored (12.23%) General / 61.6,41.6	41% (<i>mt-10</i>) chi angles: 305.4,180.4,45.9	0.062Å	-	-
A 245	GLU	50	-	Favored (12.45%) General / -113.4,104.6	77.7% (<i>mt-10</i>) chi angles: 288.9,177.2,20.9	0.039Å	-	-
A 246	TYR	50	0.957Å CZ with A 276 GLU HG2	Favored (13.86%) General / -98.2,-28.1	53.1% (<i>m-85</i>) chi angles: 304.4,295.8	0.043Å	-	-
A 247	TYR	50	-	Favored (81.58%) General / -59.1,-39.2	32.7% (<i>p90</i>) chi angles: 51.2,89.2	0.119Å	-	-
A 248	GLU	50	-	Favored (58.81%) General / -76.3,-32.7	20.8% (mt-10) chi angles: 275,198.2,29.6	0.108Å	-	-
A 249	VAL	50	0.429Å HG13 with A 269 VAL HG22	Favored (81.53%) Isoleucine or valine / -59.3,-50.0	97% (<i>t</i>) chi angles: 176.2	0.027Å	-	-
A 250	LEU	50	-	Favored (84.82%) General / -58.0,-42.2	96.6% (<i>mt</i>) chi angles: 296.1,176.3	0.013Å	-	-
A 251	GLU	50	-	Favored (61.47%) General / -72.5,-45.0	53.6% (<i>mt-10</i>) chi angles: 295.3,183.5,296	0.034Å	-	-
A 252	HIS	50	-	Favored (73.72%) General / -70.4,-40.9	16.7% (<i>m-70</i>) chi angles: 290.4,326.6	0.042Å	OUTLIER(S) worst is CG ND1: 4.331 σ	-
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 26.19	Outliers: 0 of 138	Poor rotamers: 1 of 125		•	Outliers: 6 of 140
A 253	THR	50	0.479Å HG21 with A 269 VAL HG13	Favored (91.21%) General / -65.1,-38.6	67.7% (p) chi angles: 59.6	0.017Å	-	-
A				Favored	58.1% (<i>m</i>)			
				(80.53%)	30.1 /6 (111)			

2 34	SEK	ΣU	-	-68.1,-36.9	Cili aligico. 271.1	U.USSA	-	-
A 255	ASP	50	-	Favored (85.51%) General / -66.5,-43.3	35.7% (<i>t70</i>) chi angles: 184.5,54.7	0.016Å	-	-
A 256	ILE	50	0.912Å HG22 with A 263 ILE HD12	Favored (80.78%) Isoleucine or valine / -63.0,-50.1	89% (<i>mt</i>) chi angles: 298.2,174.4	0.076Å	-	-
A 257	LEU	50	0.415Å HA with A 263 ILE HD11	Favored (72.69%) General / -64.9,-31.4	76.3% (<i>mt</i>) chi angles: 289.2,167.3	0.022Å	-	-
A 258	ARG	50	-	Favored (66.11%) General / -66.6,-21.8	61.8% (ttm-85) chi angles: 186.4,178.9,290.4,275.4	0.037Å	-	-
A 259	HIS	50	-	Favored (5.61%) General / -104.4,-41.9	62.2% (<i>m170</i>) chi angles: 296.8,162.4	0.023Å	OUTLIER(S) worst is CG-ND1: 4.607σ	-
A 260	HIS	50	0.47Å O with A 263 ILE HD13	Favored (45.69%) Pre-proline / -122.3,82.2	99.2% (<i>m-70</i>) chi angles: 297.1,283.8	0.079Å	OUTLIER(S) worst is CG ND1: 4.483 σ	OUTLIER(S) worst is CB- CG-CD2: 4.097 σ
A 261	PRO	50	-	Allowed (0.8%) Trans-proline / -73.6,13.0	59.9% (<i>Cg_endo</i>) chi angles: 34.5	0.034Å	-	-
A 262	GLY	50	-	Favored (9.15%) Glycine / -120.2,20.2	-	-	-	-
A 263	ILE	50	0.912Å HD12 with A 256 ILE HG22	Favored (16.51%) Isoleucine or valine / -95.8,105.0	2.2% (<i>pt</i>) chi angles: 58.1,200.3	0.083Å	-	-
A 264	VAL	50	0.662Å HG21 with A 294 GLU HG3	Favored (97.63%) Isoleucine or valine / -61.3,-45.9	86.7% (<i>t</i>) chi angles: 177.3	0.082Å	-	-
A 265	LYS	50	0.588Å O with A 269 VAL HG12	Favored (75.21%)	61.8% (<i>mttp</i>) chi angles:	0.04Å	-	-

			V/\L \U 4	-60.0,-35.5	494,101.9,101,00.1			
A 266	ALA	50	0.688Å HB3 with A 263 ILE HG13	Favored (74.27%) General / -70.5,-38.7	-	0.07Å	-	-
A 267	TYR	50	0.415Å CZ with A 257 LEU HD22	Favored (95.17%) General / -63.9,-39.9	39.9% (<i>m</i> -85) chi angles: 281.7,293	0.049Å	-	-
A 268	TYR	50	0.579Å O with A 271 ALA HB3	Favored (51.72%) General / -68.4,-50.6	84.9% (<i>t80</i>) chi angles: 182.4,79.9	0.027Å	-	-
A 269	VAL	50	0.78Å HG23 with A 241 LEU HD11	Favored (92.51%) Isoleucine or valine / -61.4,-42.1	7.4% (p) chi angles: 57.5	0.15Å	-	-
A 270	ARG	50	-	Favored (81.56%) General / -67.2,-36.4	54.8% (ttp180) chi angles: 189.7,171,68.8,184.7	0.031Å	-	-
A	ALA	50	0.861Å HB1 with A	Favored (85.59%)	-	0.263Å	-	OUTLIER(S) worst is N-CA-
271			287 LEU HD12	General / -61.5,-47.5				CB: 5.981 σ
271 A 272		99.99			86.5% (<i>mtm180</i>) chi angles: 292.6,182.9,286.4,178.7	0.067Å	-	CB: 5.981 σ -
A 272			HD12 0.636Å HE with A	-61.5,-47.5 Favored (81.63%) General /	chi angles: 292.6,182.9,286.4,178.7	0.067Å Cβ deviation	- Bond lengths	CB: 5.981 σ - Bond angles
A 272	ARG	99.99 High B	HD12 0.636Å HE with A 269 VAL HA Clash > 0.4Å Clashscore:	-61.5,-47.5 Favored (81.63%) General / -60.0,-38.1 Ramachandran	chi angles: 292.6,182.9,286.4,178.7	Cβ deviation	lengths	- Bond
A 272	ARG	99.99 High B Avg: 52.14	HD12 0.636Å HE with A 269 VAL HA Clash > 0.4Å Clashscore:	-61.5,-47.5 Favored (81.63%) General / -60.0,-38.1 Ramachandran Outliers: 0 of	chi angles: 292.6,182.9,286.4,178.7 Rotamer Poor rotamers: 1 of	C β deviation Outliers:	lengths Outliers: 6	Bond angles Outliers: 6
A 272 # A	ARG Alt Res ALA	99.99 High B Avg: 52.14	HD12 0.636Å HE with A 269 VAL HA Clash > 0.4Å Clashscore:	-61.5,-47.5 Favored (81.63%) General / -60.0,-38.1 Ramachandran Outliers: 0 of 138 Favored (68.54%) General / -71.6,-41.7 Favored (98.68%) General / -62.1,-41.9	chi angles: 292.6,182.9,286.4,178.7 Rotamer Poor rotamers: 1 of	Cβ deviation Outliers: 1 of 136	lengths Outliers: 6	Bond angles Outliers: 6
A 272 # A 273	ARG Alt Res ALA HIS	99.99 High B Avg: 52.14 50	HD12 0.636Å HE with A 269 VAL HA Clash > 0.4Å Clashscore: 26.19 - 0.548Å HD2 with A 279 ASN	-61.5,-47.5 Favored (81.63%) General / -60.0,-38.1 Ramachandran Outliers: 0 of 138 Favored (68.54%) General / -71.6,-41.7 Favored (98.68%) General /	chi angles: 292.6,182.9,286.4,178.7 Rotamer Poor rotamers: 1 of 125 - 16.7% (<i>m170</i>)	C β deviation Outliers: 1 of 136 0.035Å	lengths Outliers: 6 of 140 - OUTLIER(S) worst is CG	Bond angles Outliers: 6 of 140 - OUTLIER(S) worst is CB-CG-CD2:

A 276	GLU	50	HG2 with A 246 TYR CZ	(65.06%) General / -72.0,-30.3	53.0 /0 (φ10) chi angles: 187.7,74.7,1.9	0.052Å	-	worst is CA-CB-CG: 4.436
A 277	VAL	50	-	Favored (2.82%) Isoleucine or valine / -97.6,16.5	29.9% (<i>m</i>) chi angles: 296.8	0.082Å	-	-
A 278	TRP	50	0.511Å CZ3 with A 311 ARG NH1	Favored (10.07%) General / 65.1,32.7	41% (<i>m</i> 95) chi angles: 314.2,112.5	0.036Å	-	-
A 279	ASN	50	0.548Å HD22 with A 274 HIS HD2	Favored (2.4%) General / -96.9,69.4	90.6% (<i>m-20</i>) chi angles: 294.8,329.4	0.033Å	-	-
A 280	GLU	50	-	Favored (76.7%) General / -57.2,-40.1	11% (<i>pt-20</i>) chi angles: 58.5,175.4,70.2	0.062Å	-	-
A 281	ALA	50	-	Favored (79.28%) General / -67.8,-43.7	-	0.018Å	-	-
A 282	GLU	50	-	Favored (71.87%) General / -70.4,-33.9	25.2% (<i>mp0</i>) chi angles: 289.8,65.4,34.6	0.022Å	-	-
A 283	ALA	50	-	Favored (72.26%) General / -65.0,-48.9	-	0.018Å	-	-
A 284	LYS	50	-	Favored (78.48%) General / -59.9,-37.1	30.8% (<i>mtpp</i>) chi angles: 295,181.4,66.2,63.7	0.04Å	-	-
A 285	ALA	50	0.743Å O with A 288 GLN HG2	Favored (87.41%) General / -66.0,-43.6	-	0.021Å	-	-
A 286	ASP	50	-	Favored (77.75%) General / -69.5,-38.6	93.1% (<i>m-20</i>) chi angles: 288,337.5	0.073Å	-	-
A 287	LEU	50	0.861Å HD12 with A 271 ALA HB1	Favored (75.29%) General / -66.0,-33.2	7.7% (mp) chi angles: 275.5,75.6	0.063Å	-	OUTLIER(S) worst is CD1- CG-CD2: 4.995 σ
Δ	CINI	E O	0 743 Å	Favored	9 7% (nt20)	0 070 Å		
-			, ,			, J A		

288	ULIN	ЭU	6.7 - 3.7. HG2 with A 285 ALA O	General / -68.1,-36.0	chi angles: 79.3,187.8,39.4	U.U/ 0/\	-	-
A 289	LYS	50	-	Favored (78.11%) General / -67.8,-35.1	21.1% (mmtt) chi angles: 257.9,292.4,185.6,178	0.022Å	-	-
A 290	VAL	50	-	Favored (84.79%) Isoleucine or valine / -64.0,-48.7	86.2% (<i>t</i>) chi angles: 177.6	0.006Å	-	-
A 291	LEU	50	0.404Å HG with A 301 VAL HG11	Favored (77.29%) General / -56.0,-43.0	2% (<i>mt</i>) chi angles: 247.8,188.6	0.056Å	-	-
A 292	GLU	50	-	Favored (98.52%) General / -63.5,-41.2	40.1% (<i>tt0</i>) chi angles: 183,194.9,326.8	0.053Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 52.14	Clashscore: 26.19	Outliers: 0 of 138	Poor rotamers: 1 of 125	Outliers: 1 of 136	Outliers: 6 of 140	Outliers: 6 of 140
A 293	LEU	50	-	Favored (17.13%) General / -89.1,-33.4	90.9% (<i>mt</i>) chi angles: 292.8,169.8	0.065Å	-	-
		50 99.99	- 0.662Å HG3 with A 264 VAL HG21	(17.13%) General /	, ,	0.065Å 0.044Å	-	-
293 A		99.99	HG3 with A 264 VAL	(17.13%) General / -89.1,-33.4 Favored (11.33%) Pre-proline /	chi angles: 292.8,169.8 99.5% (<i>mt-10</i>) chi angles:		-	-
293 A 294 A	GLU	99.99	HG3 with A 264 VAL	(17.13%) General / -89.1,-33.4 Favored (11.33%) Pre-proline / -139.7,90.0 Favored (76.78%) Trans-proline /	chi angles: 292.8,169.8 99.5% (<i>mt-10</i>) chi angles: 291.4,178.3,354 71.9% (<i>Cg_endo</i>)	0.044Å	-	-
293 A 294 A 295	GLU PRO SER	99.99 50	HG3 with A 264 VAL	(17.13%) General / -89.1,-33.4 Favored (11.33%) Pre-proline / -139.7,90.0 Favored (76.78%) Trans-proline / -61.6,-23.7 Favored (63.3%) General /	chi angles: 292.8,169.8 99.5% (<i>mt-10</i>) chi angles: 291.4,178.3,354 71.9% (<i>Cg_endo</i>) chi angles: 29.4	0.044Å 0.064Å	-	-
293 A 294 A 295 A	GLU PRO SER	99.99 50 50 99.99	HG3 with A 264 VAL	(17.13%) General / -89.1,-33.4 Favored (11.33%) Pre-proline / -139.7,90.0 Favored (76.78%) Trans-proline / -61.6,-23.7 Favored (63.3%) General / -60.3,-22.6 Favored (8.25%) General /	chi angles: 292.8,169.8 99.5% (<i>mt-10</i>) chi angles: 291.4,178.3,354 71.9% (<i>Cg_endo</i>) chi angles: 29.4 27.8% (<i>t</i>) chi angles: 185.4 97.8% (<i>mmm</i>) chi angles:	0.044Å 0.064Å 0.014Å	-	-

				,				
A 299	LYS	50	-	Favored (82.91%) General / -57.6,-47.2	32.7% (mmmt) chi angles: 293.8,295.7,295.1,180.8	0.028Å	-	-
A 300	ALA	50	-	Favored (79.46%) General / -67.5,-44.0	-	0.018Å	-	-
A 301	VAL	50	0.431Å O with A 305 LEU HG	Favored (97.11%) Isoleucine or valine / -64.4,-43.8	91% (<i>t</i>) chi angles: 177.9	0.053Å	-	-
A 302	ARG	50	0.441Å HG3 with A 298 GLN O	Favored (82.2%) General / -58.5,-40.3	77.4% (<i>mtp85</i>) chi angles: 292.3,177.7,67.5,82.4	0.063Å	-	-
A 303	ARG	50	-	Favored (69.19%) General / -63.5,-50.5	42.8% (ttm105) chi angles: 185.7,172.4,299.4,106.9	0.049Å	-	-
A 304	GLU	50	0.581Å HB3 with A 287 LEU HD21	Favored (78.09%) General / -60.4,-36.4	80.2% (<i>mm-40</i>) chi angles: 291.7,299.7,334.9	0.056Å	-	-
A 305	LEU	50	0.431Å HG with A 301 VAL O	Favored (72.26%) General / -69.9,-43.2	95.7% (<i>mt</i>) chi angles: 295.3,176.5	0.02Å	-	-
A 306	ARG	50	0.406Å HG3 with A 302 ARG O	Favored (84.45%) General / -63.0,-36.7	78.3% (<i>mtp85</i>) chi angles: 292.3,178.3,66.8,83.2	0.045Å	-	-
A 307	LEU	50	0.443Å HD21 with A 311 ARG HH21	Favored (76.12%) General / -69.9,-37.8	9.6% (tt) chi angles: 188.9,154.1	0.083Å	-	-
A 308	LEU	50	0.46Å O with A 311 ARG HG2	Favored (89.35%) General / -64.3,-45.1	60.4% (<i>mt</i>) chi angles: 285.5,174.3	0.065Å	-	-
A 309	GLU	50	-	Favored (77.01%) General / -64.4,-33.9 Favored	11.5% (<i>tm-20</i>) chi angles: 182.1,288.9,326.5	0.087Å	-	-
Α				(80.58%)				
310	ASN	50	-	General /	21.5% (<i>t-20</i>)	0.03Å	-	-

J			-61.7,-36.3	chi angles: 188.3,294			
A 311	ARG 50		General /	17.8% (<i>ptp180</i>) chi angles: 66.6,178.6,58.6,190.2	0.042Å	-	-
A 312	MET 99.99	-	-	58.7% (ttp) chi angles: 186.7,183.3,66.4	0.039Å	-	-

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