



Viewing TULP1_sm_291-536-FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.01	99 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	1.88%	Goal: <1%
	Ramachandran outliers	2	0.82%	Goal: <0.05%
	Ramachandran favored	229	93.85%	Goal: >98%
	MolProbity score [^]	1.41		97 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 2017	0.00%	Goal: 0%
	Bad backbone angles:	11 / 2727	0.40%	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: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 291	PRO	50	-	-	85% (Cg_exo) chi angles: 331	0.144Å	-	-
A 292	ARG	50	-	Favored (87.97%) General / -59.9,-46.9	54.4% (ttm-85) chi angles: 188.8,184.2,305.5,288.3	0.048Å	-	-
A 293	GLU	50	-	Favored (2.89%) General / -59.5,-61.1	2.6% (tm-20) chi angles: 156.4,279.5,330.8	0.134Å	-	-
A 294	PHE	50	-	Favored (55.31%) General / -50.5,-49.5	73.7% (t80) chi angles: 181.5,86.5	0.09Å	-	-

A 295	VAL	50	-	Favored (43.36%) Isoleucine or valine / -63.2,-27.6	26.7% (<i>m</i>) chi angles: 301.8	0.231Å	-	-
A 296	LEU	50	-	Favored (36.49%) General / -89.8,-13.5	97.8% (<i>mt</i>) chi angles: 293.6,173.1	0.082Å	-	-
A 297	ARG	50	-	Favored (41.8%) Pre-proline / -83.3,138.6	30.7% (<i>mmm180</i>) chi angles: 294,297.4,293.4,169.7	0.034Å	-	-
A 298	PRO	50	-	Favored (97.81%) Trans-proline / -59.7,145.6	98.4% (<i>Cg_exo</i>) chi angles: 329.4	0.095Å	-	-
A 299	ALA	50	-	Favored (42.39%) Pre-proline / -55.8,147.4	-	0.043Å	-	-
A 300	PRO	50	-	Favored (91%) Trans-proline / -63.9,146.1	49.4% (<i>Cg_exo</i>) chi angles: 326.6	0.084Å	-	-
A 301	GLN	50	-	Favored (11.57%) General / -49.3,139.4	6.1% (<i>tp-100</i>) chi angles: 184.1,61.6,272.9	0.062Å	-	-
A 302	GLY	50	-	Favored (29.18%) Glycine / 65.7,6.4	-	-	-	-
A 303	ARG	50	-	Favored (10.9%) General / -108.9,166.3	75.4% (<i>mmt-85</i>) chi angles: 295.2,293.6,168.8,279.7	0.041Å	-	-
A 304	THR	50	-	Favored (23.79%) General / -129.4,119.4	90.7% (<i>m</i>) chi angles: 302.3	0.079Å	-	-
A 305	VAL	50	-	Favored (22.11%) Isoleucine or valine / -91.4,110.1	59.5% (<i>t</i>) chi angles: 181	0.043Å	-	-
A 306	ARG	50	-	Favored (44.45%) General / -97.0,129.7	80% (<i>mtt85</i>) chi angles: 294.6,191.1,179.5,95.3	0.023Å	-	-
A	CYS	50	-	Favored (26.38%)	75.5% (<i>m</i>)	0.055Å	-	-

307					General / -130.0,163.5	chi angles: 298.7			
A 308	ARG	50	-		Favored (46.31%) General / -120.9,125.0	20% (<i>tpp85</i>) chi angles: 186.9,64.1,71.4,84.6	0.063Å	-	-
A 309	LEU	50	-		Favored (50.72%) General / -108.8,124.5	7.7% (<i>tt</i>) chi angles: 193.4,157.2	0.065Å	-	-
A 310	THR	50	-		Favored (25.79%) General / -121.9,160.0	73.9% (<i>p</i>) chi angles: 60	0.063Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 311	ARG	50	-		Favored (32.98%) General / -133.7,162.1	40.4% (<i>ptt180</i>) chi angles: 61.9,183.1,180.9,186.1	0.043Å	-	-
A 312	ASP	50	-		Favored (41.67%) General / -61.4,129.5	33.7% (<i>m-20</i>) chi angles: 303.2,349.8	0.179Å	-	OUTLIER(S) worst is CA-CB- CG: 8.73 σ
A 313	LYS	99.99	-		Favored (25.89%) General / -54.8,143.3	64.7% (<i>tttp</i>) chi angles: 186,177.8,177.7,64.5	0.061Å	-	-
A 314	LYS	99.99	0.455Å HD2 with A 320 MET SD		Favored (44.1%) General / -143.9,155.5	46.8% (<i>mmtm</i>) chi angles: 298.8,299.2,176.8,290.9	0.07Å	-	-
A 315	GLY	99.99	-		Favored (46.9%) Glycine / -84.7,-170.3	-	-	-	-
A 316	MET	99.99	-		Allowed (1.94%) General / -98.9,72.8	18.5% (<i>tpt</i>) chi angles: 180.9,64.4,186.8	0.057Å	-	-
A 317	ASP	99.99	-		Favored (32.17%) General / -154.0,166.7	28.7% (<i>p-10</i>) chi angles: 63.2,334.6	0.052Å	-	-
					Favored				

A 318	ARG	99.99	-	(57.98%) General / -65.1,137.9	31.8% (<i>ptt-85</i>) chi angles: 57.5,184.4,176.2,267.5	0.043Å	-	-
A 319	GLY	99.99	-	Favored (2.96%) Glycine / -176.9,-138.5	-	-	-	OUTLIER(S) worst is C-N- CA: 5.292 σ
A 320	MET	50	0.455Å SD with A 314 LYS HD2	Favored (3.31%) General / -156.7,-170.4	2.4% (<i>ttn</i>) chi angles: 236.3,164.3,289	0.075Å	-	-
A 321	TYR	50	-	Favored (19.65%) Pre-proline / -142.8,69.8	55% (<i>m-85</i>) chi angles: 307.6,274.6	0.048Å	-	-
A 322	PRO	50	-	Favored (23.32%) Trans-proline / -79.7,154.1	40% (<i>Cg_endo</i>) chi angles: 36.5	0.06Å	-	-
A 323	SER	50	-	Favored (26.48%) General / -82.2,152.3	58.5% (<i>m</i>) chi angles: 290.9	0.038Å	-	-
A 324	TYR	50	-	Favored (51.87%) General / -126.1,141.6	86.5% (<i>m-85</i>) chi angles: 299,84.7	0.092Å	-	-
A 325	PHE	50	-	Favored (51.63%) General / -131.2,144.9	55.2% (<i>m-85</i>) chi angles: 307.6,274.6	0.066Å	-	-
A 326	LEU	50	-	Favored (44.86%) General / -127.2,127.7	20.9% (<i>tp</i>) chi angles: 191.3,70.6	0.1Å	-	-
A 327	HIS	50	-	Favored (27.02%) General / -123.3,160.2	65.1% (<i>m80</i>) chi angles: 294.5,72.2	0.122Å	-	-
A 328	LEU	50	-	Favored (55.81%) General / -68.4,140.4	70% (<i>mt</i>) chi angles: 290.7,179.8	0.07Å	-	-
A 329	ASP	50	-	Favored (2.84%) General / -90.1,54.6	10.9% (<i>t0</i>) chi angles: 208.3,24.1	0.075Å	-	-

A 330	THR	50	-	Favored (19.75%) General / -114.4,159.9	52% (<i>p</i>) chi angles: 55.9	0.037Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 331	GLU	50	-	Favored (47.27%) General / -49.4,-46.2	14% (<i>tm-20</i>) chi angles: 179.7,281.2,332.3	0.114Å	-	-	
A 332	LYS	50	-	Favored (5.83%) General / -80.3,85.2	46.7% (<i>mmtm</i>) chi angles: 299.2,293.2,175.4,292	0.053Å	-	-	
A 333	LYS	50	-	Allowed (1.92%) General / -74.7,70.9	45.2% (<i>mttp</i>) chi angles: 298.9,163.9,190.3,63.7	0.036Å	-	-	
A 334	VAL	50	-	Favored (27.14%) Isoleucine or valine / -61.7,134.3	8.1% (<i>p</i>) chi angles: 70.2	0.12Å	-	-	
A 335	PHE	50	-	Favored (50.02%) General / -70.9,145.8	81.2% (<i>t80</i>) chi angles: 172.3,77.9	0.053Å	-	-	
A 336	LEU	50	-	Allowed (1.04%) General / -120.8,-66.6	86.1% (<i>mt</i>) chi angles: 300.1,179.9	0.049Å	-	-	
A 337	LEU	50	-	Favored (42.62%) General / -142.9,153.0	88.2% (<i>mt</i>) chi angles: 292.8,168.9	0.098Å	-	-	
A 338	ALA	50	-	Favored (52.53%) General / -132.0,149.0	-	0.041Å	-	-	
A 339	GLY	50	0.407Å HA2 with A 351 LEU O	Favored (21.93%) Glycine / -139.4,151.5	-	-	-	-	
A 340	ARG	50	-	Favored (15.46%) General /	34.3% (<i>ttt180</i>) chi angles: 187.1,171.9,175.8,225.8	0.03Å	-	-	

A 341	LYS	50	-	-156.1,139.2 Favored (39.34%) General / -72.7,129.9	86.4% (tttt) chi angles: 189.2,175.2,180.9,175.9	0.048Å	-	-
A 342	ARG	50	-	Favored (29.35%) General / -78.5,125.4	72.4% (mtp85) chi angles: 297.4,176.1,57.6,77.8	0.1Å	-	-
A 343	LYS	50	-	Favored (71.14%) General / -70.6,-33.6	87.2% (tttt) chi angles: 180.8,174.3,182.4,182.4	0.086Å	-	-
A 344	ARG	50	-	Allowed (1.09%) General / -95.0,44.3	83.8% (mtp180) chi angles: 291.4,181.1,65.1,185.3	0.058Å	-	-
A 345	SER	50	-	Favored (46%) General / -122.9,148.0	34.1% (t) chi angles: 183.2	0.073Å	-	-
A 346	LYS	50	-	Favored (70.64%) General / -71.5,-35.1	26.9% (tptp) chi angles: 183.8,65.6,187.4,65.6	0.037Å	-	-
A 347	THR	50	-	Favored (11.73%) General / -115.9,166.7	80.5% (p) chi angles: 61.4	0.049Å	-	-
A 348	ALA	50	-	Favored (49.75%) General / -60.4,131.1	-	0.014Å	-	-
A 349	ASN	50	-	Favored (2.84%) General / -150.4,100.1	58.4% (t-20) chi angles: 185.3,339.7	0.111Å	-	-
A 350	TYR	50	-	Favored (33.9%) General / -95.1,137.7	22.2% (m-85) chi angles: 294.7,69.9	0.081Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 351	LEU	50	0.423Å CD2 with A 361 ARG HD2	Favored (43.49%) General /	66.3% (mt) chi angles: 303.2,183.6	0.052Å	-	-

A 352	ILE	50	-	-101.0,134.8 Favored (72.93%) Isoleucine or valine / -117.5,130.1	64.7% (<i>mt</i>) chi angles: 305,171.4	0.077Å	-	-
A 353	SER	50	-	Favored (46.55%) General / -128.5,154.0	41% (<i>t</i>) chi angles: 177.2	0.128Å	-	-
A 354	ILE	50	-	Favored (9.04%) Isoleucine or valine / -97.0,5.2	43.5% (<i>pt</i>) chi angles: 57.1,171.6	0.179Å	-	-
A 355	ASP	50	-	Favored (29.67%) Pre-proline / -118.3,123.0	58.6% (<i>t0</i>) chi angles: 177.6,352.6	0.109Å	-	OUTLIER(S) worst is CA-CB- CG: 4.188 σ
A 356	PRO	50	-	Favored (17.48%) Trans-proline / -76.3,-16.3	41.2% (<i>Cg_endo</i>) chi angles: 36.3	0.053Å	-	-
A 357	THR	50	-	Favored (25.5%) General / -90.4,-18.4	91.8% (<i>m</i>) chi angles: 302.5	0.123Å	-	-
A 358	ASN	99.99	-	Favored (48.33%) General / -101.5,127.2	50.9% (<i>t30</i>) chi angles: 187.3,15.1	0.043Å	-	-
A 359	LEU	99.99	-	Favored (15.53%) General / -98.8,-23.1	91.7% (<i>mt</i>) chi angles: 297.4,172.1	0.058Å	-	-
A 360	SER	99.99	-	Favored (48.01%) General / -63.7,148.8	27.5% (<i>t</i>) chi angles: 185.4	0.017Å	-	-
A 361	ARG	99.99	0.423Å HD2 with A 351 LEU CD2	Allowed (0.86%) General / -119.7,70.4	9% (<i>ptm-85</i>) chi angles: 60.7,173,293.1,281.3	0.125Å	-	-
A 362	GLY	99.99	-	Favored (42.45%) Glycine / -172.7,-178.0	-	-	-	-
A	GLY	99.99	-	Favored (29.09%) Glycine /	-	-	-	OUTLIER(S) worst is C-N-

363				55.4,-123.2				CA: 5.955 σ	
A 364	GLU	99.99	-	Favored (87.96%) General / -60.6,-39.4	2.1% (<i>pm0</i>) chi angles: 60.1,305.2,330.3	0.139Å	-	OUTLIER(S) worst is CB- CG-CD: 5.637 σ	
A 365	ASN	50	-	Favored (2.39%) General / -139.0,6.5	72.7% (<i>m-80</i>) chi angles: 291.2,298.6	0.159Å	-	-	
A 366	PHE	50	-	Favored (49.58%) General / -64.2,132.2	12% (<i>t80</i>) chi angles: 181.6,39.1	0.096Å	-	-	
A 367	ILE	50	-	Allowed (1.23%) Isoleucine or valine / -128.1,-26.0	7.1% (<i>tp</i>) chi angles: 204.1,69.7	0.164Å	-	-	
A 368	GLY	50	-	Favored (45.99%) Glycine / -173.0,175.2	-	-	-	-	
A 369	LYS	50	-	Favored (29.57%) General / -145.4,142.7	34.2% (<i>ttpt</i>) chi angles: 171.2,165.8,56.9,183.6	0.084Å	-	-	
A 370	LEU	50	-	Favored (36.06%) General / -111.7,118.6	28.8% (<i>tp</i>) chi angles: 175.6,72.6	0.094Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 371	ARG	50	-	Favored (36.46%) General / -124.6,122.0	30.1% (<i>ttp180</i>) chi angles: 175.8,208.9,62,182.3	0.115Å	-	-	
A 372	SER	50	-	Favored (25.22%) General / -79.8,162.3	59.9% (<i>p</i>) chi angles: 72.6	0.084Å	-	-	
A 373	ASN	50	-	Favored (2.99%) General / -72.2,-179.7	35.5% (<i>p-10</i>) chi angles: 65.6,335.5	0.073Å	-	-	

A 374	LEU	50	-	Favored (86.78%) General / -65.0,-37.2	48% (<i>tp</i>) chi angles: 184.8,63.3	0.141Å	-	-
A 375	LEU	50	-	Favored (62.8%) General / -72.4,-28.2	74.5% (<i>mt</i>) chi angles: 301.4,172.4	0.086Å	-	-
A 376	GLY	50	-	Favored (67.95%) Glycine / 91.9,3.6	-	-	-	-
A 377	ASN	50	-	Favored (19.71%) General / -98.9,-14.1	31.7% (<i>p-10</i>) chi angles: 66,331.9	0.093Å	-	-
A 378	ARG	50	-	Favored (49.16%) General / -123.5,145.0	90.4% (<i>mtt180</i>) chi angles: 297.9,187,177.2,198.3	0.03Å	-	-
A 379	PHE	50	-	Favored (52.39%) General / -132.5,148.8	77.7% (<i>m-85</i>) chi angles: 296.9,80.7	0.089Å	-	-
A 380	THR	50	-	Favored (49.67%) General / -117.7,140.4	7.2% (<i>m</i>) chi angles: 314.8	0.079Å	-	-
A 381	VAL	50	-	Favored (62.88%) Isoleucine or valine / -106.9,126.1	38.8% (<i>t</i>) chi angles: 185.3	0.07Å	-	-
A 382	PHE	50	-	Favored (20.45%) General / -114.0,159.0	86.5% (<i>m-85</i>) chi angles: 302.5,281.7	0.103Å	-	-
A 383	ASP	50	-	OUTLIER (0.04%) General / -74.4,-154.1	49.8% (<i>p-10</i>) chi angles: 66.3,353.3	0.187Å	-	-
A 384	ASN	50	-	Favored (51.04%) General / -95.6,-1.1	43.3% (<i>p-10</i>) chi angles: 57.9,354.3	0.125Å	-	-
A 385	GLY	50	-	Favored (21.77%) Glycine / -66.3,174.7	-	-	-	-

A 386	GLN	50	-	Favored (34.49%) General / -79.3,144.2	14.5% (<i>tt0</i>) chi angles: 192.8,191.7,113.2	0.037Å	-	-	
A 387	ASN	50	-	Favored (89.21%) Pre-proline / -74.2,123.5	35.1% (<i>t30</i>) chi angles: 177.9,36.9	0.085Å	-	-	
A 388	PRO	50	-	Favored (93.52%) Trans-proline / -59.0,-30.5	53.1% (<i>Cg_exo</i>) chi angles: 334.8	0.08Å	-	-	
A 389	GLN	50	-	Favored (25.56%) General / -69.0,-6.0	98.1% (<i>mt-30</i>) chi angles: 295.6,179.2,329	0.059Å	-	-	
A 390	ARG	50	-	Favored (23.9%) General / -91.6,-18.5	42.4% (<i>tpt85</i>) chi angles: 187.2,61.3,195.3,82.2	0.127Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 391	GLY	50	-	Allowed (0.11%) Glycine / -176.2,96.7	-	-	-	-	-
A 392	TYR	50	-	Favored (69.55%) General / -66.1,-29.3	31.9% (<i>t80</i>) chi angles: 191.6,61.3	0.133Å	-	-	
A 393	SER	50	-	Favored (55.34%) General / -74.1,-8.2	6.4% (<i>m</i>) chi angles: 313.3	0.053Å	-	-	
A 394	THR	50	-	Favored (57.78%) General / -61.5,135.7	90.9% (<i>m</i>) chi angles: 300.6	0.049Å	-	-	
A 395	ASN	50	-	Favored (5.28%) General / -46.8,139.6	45.8% (<i>t30</i>) chi angles: 182,10.7	0.049Å	-	-	
A 396	VAL	50	-	Favored (87.25%) Isoleucine or valine	53% (<i>t</i>) chi angles: 182.2	0.09Å	-	-	

				/ -59.8,-41.9				
A 397	ALA	50	-	Favored (67.71%) General / -58.6,-31.0	-	0.073Å	-	-
A 398	SER	50	-	Favored (52.56%) General / -83.6,-14.2	22.4% (<i>m</i>) chi angles: 305.1	0.059Å	-	-
A 399	LEU	50	-	Favored (47.87%) General / -71.6,137.3	85.9% (<i>mt</i>) chi angles: 300.8,179.5	0.058Å	-	-
A 400	ARG	50	-	Favored (41.95%) General / -57.3,142.8	36.5% (<i>ptt180</i>) chi angles: 64.9,190.4,190.5,178.9	0.063Å	-	-
A 401	GLN	50	-	Favored (16.44%) General / -102.7,158.2	5.7% (<i>pt20</i>) chi angles: 77.5,193.2,260.3	0.063Å	-	-
A 402	GLU	50	-	Favored (31.75%) General / -102.3,116.0	52.2% (<i>mt-10</i>) chi angles: 292.5,202.6,357.9	0.035Å	-	-
A 403	LEU	50	-	Favored (16.71%) General / -94.3,-26.1	70.8% (<i>mt</i>) chi angles: 301.1,171.4	0.054Å	-	-
A 404	ALA	50	-	Favored (9.68%) General / -167.9,157.1	-	0.043Å	-	-
A 405	ALA	50	-	Favored (46.87%) General / -134.6,142.3	-	0.057Å	-	-
A 406	VAL	50	-	Favored (72.59%) Isoleucine or valine / -125.6,130.9	34.1% (<i>t</i>) chi angles: 185.8	0.047Å	-	-
A 407	ILE	50	-	Favored (63%) Isoleucine or valine / -119.7,120.3	5.4% (<i>mp</i>) chi angles: 302.4,90.3	0.038Å	-	-
A 408	TYR	50	-	Favored (42.95%) General / -102.1,135.8	85.5% (<i>m-85</i>) chi angles: 289.7,274.8	0.095Å	-	-

A 409	GLU	50	-	Favored (41.13%) General / -75.2,146.4	67.4% (<i>mt-10</i>) chi angles: 287.3,177.6,26.7	0.065Å	-	-	
A 410	THR	50	-	Favored (43.66%) General / -97.7,132.1	69.6% (<i>p</i>) chi angles: 59.2	0.038Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 411	ASN	50	-	Favored (18.23%) General / -86.5,162.1	60.4% (<i>m-20</i>) chi angles: 305.7,324.3	0.038Å	-	-	
A 412	VAL	99.99	-	Favored (37.26%) Isoleucine or valine / -136.0,156.5	12.9% (<i>p</i>) chi angles: 65.4	0.097Å	-	-	
A 413	LEU	99.99	-	Favored (32.58%) General / -52.5,136.3	9.9% (<i>tt</i>) chi angles: 186.8,155	0.058Å	-	-	
A 414	GLY	99.99	-	Favored (52.57%) Glycine / 93.4,-19.4	-	-	-	-	
A 415	PHE	99.99	-	Favored (43.1%) General / -110.9,142.3	80.5% (<i>t80</i>) chi angles: 184.2,76.7	0.088Å	-	-	
A 416	ARG	99.99	-	Favored (21.94%) General / -85.9,153.9	99.8% (<i>mtt180</i>) chi angles: 295.1,180,179.3,180	0.085Å	-	-	
A 417	GLY	99.99	-	Allowed (0.21%) Glycine / -176.6,106.1	-	-	-	-	
A 418	PRO	50	-	Allowed (0.17%) Trans-proline / -39.3,113.3	56.9% (<i>Cg_endo</i>) chi angles: 26.1	0.045Å	-	-	
A 419	ARG	50	-	Favored (53.38%) General /	90.3% (<i>mtm180</i>) chi angles: 291.1,177.6,296.4,173.4	0.067Å	-	-	

A 420	ARG	50	-	-69.5,143.5 Favored (53.56%) General / -69.7,140.3	98.2% (<i>mtt180</i>) chi angles: 296,183.3,187.8,169	0.045Å	-	-
A 421	MET	50	-	Favored (54.62%) General / -121.9,137.9	87.6% (<i>mtp</i>) chi angles: 300.1,176.6,62.9	0.11Å	-	-
A 422	THR	50	-	Favored (55.18%) General / -113.4,133.4	70.9% (<i>m</i>) chi angles: 296.7	0.04Å	-	-
A 423	VAL	50	-	Favored (75.19%) Isoleucine or valine / -122.2,127.2	95.9% (<i>t</i>) chi angles: 176.7	0.062Å	-	-
A 424	ILE	50	-	Favored (72.52%) Isoleucine or valine / -117.6,130.4	45% (<i>mm</i>) chi angles: 305.2,303.5	0.075Å	-	-
A 425	ILE	50	-	Favored (27.11%) Pre-proline / -128.7,166.1	35.5% (<i>pt</i>) chi angles: 58.1,176.9	0.084Å	-	-
A 426	PRO	50	-	Favored (89.13%) Trans-proline / -64.2,145.5	72.8% (<i>Cg_exo</i>) chi angles: 328	0.102Å	-	-
A 427	GLY	50	-	Favored (16.56%) Glycine / -61.3,165.5	-	-	-	-
A 428	MET	50	-	Favored (41.38%) General / -117.5,148.9	84.2% (<i>mmm</i>) chi angles: 307.9,303.7,285.8	0.097Å	-	-
A 429	SER	50	-	Favored (9.36%) General / -79.5,176.8	27.4% (<i>p</i>) chi angles: 51.7	0.057Å	-	-
A 430	ALA	50	-	Favored (67.3%) General / -67.5,-27.8	-	0.09Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

Avg: 54.27				Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 431	GLU	50	-		Favored (70.27%) General / -57.2,-36.0	84.6% (<i>tt0</i>) chi angles: 182.1,184.9,2.4	0.05Å	-	-
A 432	ASN	50	-		OUTLIER (0.01%) General / 93.2,25.5	70.3% (<i>m-80</i>) chi angles: 296.2,287.6	0.204Å	-	-
A 433	GLU	50	-		Favored (15.74%) General / -109.5,161.0	30.4% (<i>tp10</i>) chi angles: 188.9,51.4,29.6	0.058Å	-	-
A 434	ARG	50	-		Favored (57.15%) General / -66.2,143.6	74% (<i>mtm-85</i>) chi angles: 278.8,187.2,299.7,289.8	0.094Å	-	-
A 435	VAL	50	-		Allowed (0.84%) Pre-proline / -91.7,95.1	61.4% (<i>t</i>) chi angles: 181.3	0.105Å	-	-
A 436	PRO	50	-		Favored (71.83%) Trans-proline / -59.4,136.4	78.5% (<i>Cg_exo</i>) chi angles: 333.5	0.079Å	-	-
A 437	ILE	50	-		Favored (31.94%) Isoleucine or valine / -106.8,110.5	97.4% (<i>mt</i>) chi angles: 293.4,167.9	0.072Å	-	-
A 438	ARG	50	-		Favored (75.29%) Pre-proline / -127.8,78.3	33.9% (<i>ttm-85</i>) chi angles: 199.4,177.7,302.9,256.3	0.135Å	-	-
A 439	PRO	50	-		Favored (94.75%) Trans-proline / -57.3,141.8	95.7% (<i>Cg_exo</i>) chi angles: 329.7	0.09Å	-	-
A 440	ARG	50	-		Favored (27.77%) General / -86.0,-21.4	85.3% (<i>mtp180</i>) chi angles: 293.6,177.4,64.8,187	0.084Å	-	-
A 441	ASN	50	-		Favored (5.17%) General / -147.7,-176.2	55.1% (<i>t30</i>) chi angles: 184.1,33	0.124Å	-	-
A					Favored (4.12%)				

442	ALA	50	-	General / -86.6,17.1	-	0.024Å	-	-
A 443	SER	50	-	Favored (57.41%) General / -91.6,-1.6	72.8% (<i>p</i>) chi angles: 57.9	0.152Å	-	-
A 444	ASP	50	-	Favored (20.68%) General / -134.5,167.5	41.3% (<i>t0</i>) chi angles: 187.6,26	0.082Å	-	-
A 445	GLY	50	-	Favored (12.01%) Glycine / 138.4,171.0	-	-	-	-
A 446	LEU	50	-	Favored (88.46%) General / -58.3,-44.3	95.1% (<i>mt</i>) chi angles: 293.3,171.4	0.074Å	-	-
A 447	LEU	50	-	Favored (69.31%) General / -69.2,-31.0	90.7% (<i>mt</i>) chi angles: 294.2,170.6	0.127Å	-	-
A 448	VAL	50	-	Favored (50.21%) Isoleucine or valine / -68.7,-51.0	77.7% (<i>t</i>) chi angles: 172.7	0.075Å	-	-
A 449	ARG	50	-	Favored (73.71%) General / -66.1,-32.3	96.3% (<i>mtt180</i>) chi angles: 298.4,178.6,192.3,183.1	0.052Å	-	-
A 450	TRP	50	-	Favored (99.15%) General / -63.3,-42.7	52.4% (<i>t-105</i>) chi angles: 167.6,255.7	0.128Å	-	OUTLIER(S) worst is CE3- CD2-CG: 5.015 σ

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 451	GLN	50	-	Favored (38.07%) General / -80.6,-26.1	46.8% (<i>tp60</i>) chi angles: 185.8,58,73.4	0.117Å	-	-
A 452	ASN	50	-	Favored (52.28%) General / -82.0,-15.8	48% (<i>m-20</i>) chi angles: 300.9,351.3	0.092Å	-	-

A 453	LYS	50	-	Favored (5.95%) General / 67.1,32.9	32.4% (<i>mmmt</i>) chi angles: 294.1,295.6,291.9,178	0.16Å	-	-
A 454	THR	50	-	Allowed (1.81%) General / -102.5,79.3	80.3% (<i>p</i>) chi angles: 61.5	0.094Å	-	-
A 455	LEU	50	-	Favored (47.25%) General / -99.0,5.0	59.1% (<i>mt</i>) chi angles: 306.6,180.5	0.061Å	-	OUTLIER(S) worst is C-N- CA: 4.132 σ
A 456	GLU	50	-	Favored (77.92%) General / -56.9,-48.5	55.2% (<i>mp0</i>) chi angles: 300.3,78.2,2.5	0.038Å	-	OUTLIER(S) worst is CB- CG-CD: 4.123 σ
A 457	SER	50	-	Favored (3.63%) General / -86.6,17.9	74.9% (<i>p</i>) chi angles: 58.2	0.092Å	-	-
A 458	LEU	50	-	Favored (21.51%) General / -128.6,165.1	30% (<i>mt</i>) chi angles: 307.2,187.7	0.076Å	-	-
A 459	ILE	50	-	Favored (75.38%) Isoleucine or valine / -122.9,129.0	96.7% (<i>mt</i>) chi angles: 297.3,169.7	0.057Å	-	-
A 460	GLU	50	-	Favored (48.99%) General / -102.7,132.2	65.2% (<i>tt0</i>) chi angles: 181.8,175.5,333.4	0.068Å	-	-
A 461	LEU	50	-	Favored (47.04%) General / -135.8,157.4	55.5% (<i>mt</i>) chi angles: 305.4,173.1	0.09Å	-	-
A 462	HIS	50	-	Favored (21.78%) General / -136.7,167.2	79.9% (<i>m80</i>) chi angles: 292.9,89	0.051Å	-	-
A 463	ASN	50	-	Favored (51.88%) General / -70.4,143.2	5.7% (<i>p-10</i>) chi angles: 72.1,281.9	0.083Å	-	-
A 464	LYS	50	0.42Å NZ with A 500 ASP OD1	Favored (83.48%) Pre-proline / -72.0,134.2	79.8% (<i>tttt</i>) chi angles: 190.1,166.3,177.8,173.5	0.038Å	-	-
				Favored				

A 465	PRO	50	-	(37.58%) Trans-proline / -67.4,135.8	34.7% (Cg_exo) chi angles: 325.5	0.101Å	-	-	
A 466	PRO	50	-	Favored (89.87%) Trans-proline / -62.9,149.9	33.1% (Cg_exo) chi angles: 325.4	0.061Å	-	-	
A 467	VAL	50	-	Favored (15.91%) Isoleucine or valine / -117.9,162.4	34.9% (<i>m</i>) chi angles: 298.4	0.069Å	-	-	
A 468	TRP	50	-	Favored (35.71%) General / -72.8,128.5	71% (<i>t</i> -105) chi angles: 183.5,245.7	0.028Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.295 σ	
A 469	ASN	50	-	Favored (7.62%) General / -112.3,98.9	1% chi angles: 199,105.2	0.031Å	-	-	
A 470	ASP	50	-	Favored (95.41%) General / -62.4,-40.1	0.5% chi angles: 232.6,338.1	0.128Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 471	ASP	50	-	Favored (63.16%) General / -55.4,-33.1	33% (<i>t</i> 70) chi angles: 178.6,70.1	0.062Å	-	-	
A 472	SER	50	-	Favored (15.25%) General / -111.4,-3.4	92.7% (<i>p</i>) chi angles: 65.1	0.107Å	-	-	
A 473	GLY	50	-	Favored (91.67%) Glycine / 59.7,37.0	-	-	-	-	
A 474	SER	50	-	Favored (30.52%) General / -148.9,149.0	29% (<i>t</i>) chi angles: 185.1	0.078Å	-	-	
A 475	TYR	50	-	Favored (14.38%) General / -83.0,105.9	21.4% (<i>m</i> -85) chi angles: 274.4,276	0.049Å	-	-	

A 476	THR	50	-	Allowed (1.79%) General / -142.3,-164.3	13.9% (<i>t</i>) chi angles: 190	0.202Å	-	-
A 477	LEU	50	-	Favored (47.65%) General / -139.4,153.7	94.5% (<i>mt</i>) chi angles: 293.3,171.1	0.055Å	-	-
A 478	ASN	50	-	Favored (6.42%) General / -79.9,96.6	60.4% (<i>t-20</i>) chi angles: 187.9,341.5	0.052Å	-	-
A 479	PHE	50	-	Favored (58.06%) General / -82.5,-4.8	98.2% (<i>m-85</i>) chi angles: 296.9,279.1	0.106Å	-	-
A 480	GLN	50	-	Favored (5.63%) General / 65.3,38.7	96.3% (<i>mt-30</i>) chi angles: 293.9,180.3,341.2	0.097Å	-	-
A 481	GLY	50	-	Favored (50.7%) Glycine / 66.7,9.2	-	-	-	-
A 482	ARG	50	-	Favored (41.84%) General / -79.8,-23.8	28.5% (<i>mmm180</i>) chi angles: 299.6,292.5,295.6,150.2	0.056Å	-	-
A 483	VAL	50	-	Favored (61.13%) Isoleucine or valine / -128.0,123.7	96.1% (<i>t</i>) chi angles: 178.6	0.106Å	-	-
A 484	THR	50	-	Favored (9.91%) General / -118.3,-12.6	38.5% (<i>p</i>) chi angles: 53.2	0.075Å	-	-
A 485	GLN	50	-	Favored (47.72%) General / -131.4,136.1	70.2% (<i>mt-30</i>) chi angles: 302.4,191.6,330.3	0.085Å	-	-
A 486	ALA	50	-	Favored (40.88%) General / -55.2,139.8	-	0.044Å	-	-
A 487	SER	50	-	Favored (2.53%) General / -170.8,145.9	32.7% (<i>t</i>) chi angles: 184	0.092Å	-	-
				Favored				

A 488	VAL	50	-	(26.43%) Isoleucine or valine / -67.5,-20.4	32.9% (<i>m</i>) chi angles: 300.2	0.126Å	-	-
A 489	LYS	50	-	Favored (59.25%) General / -83.1,-9.4	29.7% (<i>mtmm</i>) chi angles: 290.5,172.7,277,295.8	0.051Å	-	-
A 490	ASN	50	-	Favored (26.49%) General / -71.7,125.2	79.7% (<i>m-20</i>) chi angles: 296,347.5	0.093Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 491	PHE	50	-	Favored (39.65%) General / -156.9,162.2	18.3% (<i>p90</i>) chi angles: 61.4,74.7	0.038Å	-	-
A 492	GLN	50	-	Favored (54.76%) General / -122.4,137.7	98.6% (<i>mt-30</i>) chi angles: 291.2,178.8,334.7	0.104Å	-	-
A 493	ILE	50	-	Favored (66.75%) Isoleucine or valine / -109.6,125.1	44% (<i>mm</i>) chi angles: 301.8,305.1	0.068Å	-	-
A 494	VAL	50	-	Favored (25.47%) Isoleucine or valine / -130.1,167.4	28% (<i>m</i>) chi angles: 296.6	0.062Å	-	-
A 495	HIS	50	-	Favored (18.47%) General / -98.1,153.4	45.8% (<i>t-80</i>) chi angles: 192,263.2	0.059Å	-	-
A 496	ALA	50	-	Favored (73.53%) General / -58.0,-37.0	-	0.083Å	-	-
A 497	ASP	50	-	Favored (64.16%) General / -69.0,-24.0	0.1% chi angles: 321.7,1.4	0.114Å	-	OUTLIER(S) worst is CA-CB- CG: 5.948 σ
A 498	ASP	50	-	Favored (3.93%) Pre-proline / -146.8,101.8	63.2% (<i>t0</i>) chi angles: 186.8,346.5	0.025Å	-	-

A 499	PRO	50	-	Favored (11.06%) Trans-proline / -79.6,-0.9	69.4% (<i>Cg_endo</i>) chi angles: 33.5	0.055Å	-	-
A 500	ASP	50	0.42Å OD1 with A 464 LYS NZ	Favored (14.42%) General / -111.1,-8.4	75.4% (<i>m-20</i>) chi angles: 298.8,330.8	0.169Å	-	-
A 501	TYR	50	-	Favored (6.01%) General / -81.0,90.6	36.7% (<i>t80</i>) chi angles: 192,274.1	0.051Å	-	-
A 502	ILE	50	-	Allowed (1.12%) Isoleucine or valine / -73.9,98.6	15.8% (<i>mm</i>) chi angles: 311.6,311.6	0.077Å	-	-
A 503	VAL	50	-	Favored (87.03%) Isoleucine or valine / -67.5,-42.4	53.6% (<i>t</i>) chi angles: 182.2	0.058Å	-	-
A 504	LEU	50	-	Favored (22.21%) General / -146.2,134.8	32.2% (<i>tp</i>) chi angles: 188.7,60.5	0.077Å	-	-
A 505	GLN	50	-	Favored (54.13%) General / -123.2,134.9	23.9% (<i>tt0</i>) chi angles: 189.6,171.7,257.5	0.095Å	-	-
A 506	PHE	50	-	Favored (37.38%) General / -139.5,142.1	33.1% (<i>t80</i>) chi angles: 185.7,55.7	0.077Å	-	-
A 507	GLY	50	-	Favored (26.27%) Glycine / 179.3,161.1	-	-	-	-
A 508	ARG	50	-	Favored (45.2%) General / -74.2,140.5	78.4% (<i>ttt180</i>) chi angles: 186.4,177.1,178.2,188.5	0.087Å	-	-
A 509	VAL	50	-	Favored (2.33%) Isoleucine or valine / -122.3,-25.1	28.9% (<i>m</i>) chi angles: 295.2	0.18Å	-	-
A 510	ALA	50	-	Favored (4.43%) General / -149.3,-173.6	-	0.038Å	-	-

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		Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 511	GLU	50	-	Favored (75.71%) General / -56.9,-40.1	18.2% (<i>pt</i> -20) chi angles: 60.1,180.3,335.6	0.105Å	-	-
A 512	ASP	50	-	Favored (3.61%) General / -134.8,23.5	65.2% (<i>m</i> -20) chi angles: 301.5,308.8	0.071Å	-	-
A 513	ALA	50	-	Favored (51.16%) General / -129.7,140.2	-	0.04Å	-	-
A 514	PHE	50	-	Favored (45.63%) General / -141.2,154.0	45.7% (<i>m</i> -85) chi angles: 306.1,81.7	0.176Å	-	-
A 515	THR	50	-	Favored (18.02%) General / -97.8,153.8	33% (<i>p</i>) chi angles: 51.8	0.036Å	-	-
A 516	LEU	50	-	Favored (3.68%) General / -147.8,105.3	50.3% (<i>tp</i>) chi angles: 181.5,67	0.058Å	-	-
A 517	ASP	50	-	Favored (36.93%) General / -118.6,120.3	47.3% (<i>m</i> -20) chi angles: 303.4,341.9	0.071Å	-	-
A 518	TYR	50	-	Favored (36.37%) General / -120.8,153.9	47.9% (<i>p90</i>) chi angles: 68.4,272.1	0.043Å	-	-
A 519	ARG	50	-	Favored (13.05%) General / -127.1,169.8	70.9% (<i>mtp</i> 180) chi angles: 300.5,194.8,68.3,193.3	0.061Å	-	-
A 520	TYR	50	-	Favored (73.37%) Pre-proline / -56.0,136.0	80.9% (<i>t80</i>) chi angles: 179,84.8	0.075Å	-	-
A	PRO	50	-	Favored (58.18%)	6.2% (<i>Cg_endo</i>)	0.044Å	-	-

521					Cis-proline / -93.3,7.0	chi angles: 41			
A 522	LEU	50	-		Favored (41.78%) General / -74.7,147.0	83% (<i>mt</i>) chi angles: 296.9,181.7	0.058Å	-	-
A 523	CYS	50	-		Favored (8.38%) General / -98.3,171.2	29.5% (<i>p</i>) chi angles: 66.1	0.044Å	-	-
A 524	ALA	50	-		Favored (83.97%) General / -62.1,-37.1	-	0.12Å	-	-
A 525	LEU	50	-		Favored (91.52%) General / -65.6,-42.5	44.6% (<i>tp</i>) chi angles: 180.6,56	0.115Å	-	-
A 526	GLN	50	-		Favored (64.89%) General / -62.4,-52.1	78.7% (<i>mt-30</i>) chi angles: 291.4,165.7,305	0.083Å	-	-
A 527	ALA	50	-		Favored (68.23%) General / -54.0,-49.7	-	0.023Å	-	-
A 528	PHE	50	-		Favored (94.68%) General / -62.6,-45.0	37.9% (<i>t80</i>) chi angles: 184.5,57.3	0.039Å	-	-
A 529	ALA	50	-		Favored (77.59%) General / -68.3,-35.3	-	0.071Å	-	-
A 530	ILE	50	-		Favored (93.19%) Isoleucine or valine / -65.2,-45.7	66.1% (<i>mt</i>) chi angles: 295.9,160.9	0.113Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 1.01	Outliers: 2 of 244	Poor rotamers: 4 of 213	Outliers: 0 of 229	Outliers: 0 of 246	Outliers: 11 of 246
A 531	ALA	50	-		Favored (85.7%) General / -60.1,-39.3	-	0.07Å	-	-

A 532	LEU	50	-	Favored (71.73%) General / -63.5,-30.6	73.7% (<i>mt</i>) chi angles: 290.2,178.6	0.135Å	-	-
A 533	SER	50	-	Favored (61.63%) General / -72.6,-17.9	51.8% (<i>p</i>) chi angles: 75.3	0.17Å	-	-
A 534	SER	50	-	Favored (41.33%) General / -83.5,-17.6	18.1% (<i>p</i>) chi angles: 81	0.143Å	-	-
A 535	PHE	50	-	Favored (27.27%) General / -80.6,154.7	94.3% (<i>m-85</i>) chi angles: 297.9,266.9	0.107Å	-	-
A 536	ASP	99.99	-	-	0% chi angles: 15.8,43.4	0.169Å	-	OUTLIER(S) worst is CA-CB- CG: 7.951 σ

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