



# Viewing TIMP3\_mb\_24-199-FFX1FH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0	100 <sup>th</sup> percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	7	3.29%	Goal: <1%
	Ramachandran outliers	4	1.64%	Goal: <0.05%
	Ramachandran favored	210	86.07%	Goal: >98%
	MolProbity score <sup>^</sup>	1.53		94 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	0.87%	Goal: 0
	Bad backbone bonds:	0 / 2017	0.00%	Goal: 0%
	Bad backbone angles:	20 / 2727	0.73%	Goal: <0.1%

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

\* 100<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.

<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	Bond angles
		Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 291	PRO	50	-	-	54.2% (Cg_exo) chi angles: 334.6	0.118Å	-	-
A 292	ARG	50	-	Favored (98.21%) General / -62.1,-41.4	58.6% (ttm-85) chi angles: 187.8,186,299.5,272	0.051Å	-	-
A 293	GLU	50	-	Favored (97.39%) General / -60.8,-44.0	0% chi angles: 66.6,314.9,302.6	0.135Å	-	-
A 294	PHE	50	-	Favored (72.57%) General / -58.6,-35.6	80.5% (t80) chi angles: 183.3,81.1	0.052Å	-	-
A 295	VAL	50	-	Favored (16.57%) Isoleucine or valine /	5.6% (m) chi angles: 310.3	0.26Å	-	-

-75.2,-22.0

A 296	LEU	50	-	Favored (13.77%) General / -93.6,-33.2	54.4% ( <i>mt</i> ) chi angles: 308,178.8	0.101Å	-	-
A 297	ARG	50	-	Favored (86.52%) Pre-proline / -73.3,146.4	31.6% ( <i>mmm180</i> ) chi angles: 295.1,299.2,293.1,162.8	0.065Å	-	-
A 298	PRO	50	-	Favored (38.46%) Trans-proline / -65.6,161.5	62.9% ( <i>Cg_exo</i> ) chi angles: 327.4	0.12Å	-	-
A 299	ALA	50	-	Favored (84.23%) Pre-proline / -58.1,133.3	-	0.08Å	-	-
A 300	PRO	50	-	Favored (45.48%) Trans-proline / -51.2,135.2	0.1% chi angles: 317.3	0.054Å	-	-
A 301	GLN	50	-	Favored (23.44%) General / -50.2,133.4	6.8% ( <i>tp-100</i> ) chi angles: 180.6,61.6,267.3	0.055Å	-	-
A 302	GLY	50	-	Favored (74.66%) Glycine / 71.1,15.9	-	-	-	-
A 303	ARG	50	-	Allowed (1.84%) General / -129.6,-167.7	37.6% ( <i>mmt-85</i> ) chi angles: 312,295.8,174.7,242.8	0.107Å	-	-
A 304	THR	50	-	Favored (30.25%) General / -154.2,152.4	51.2% ( <i>m</i> ) chi angles: 304.8	0.124Å	-	-
A 305	VAL	50	-	Favored (62.88%) Isoleucine or valine / -121.0,134.9	64.4% ( <i>t</i> ) chi angles: 179.8	0.074Å	-	-
A 306	ARG	50	-	Favored (41.47%) General / -125.3,124.4	4.6% ( <i>mtp180</i> ) chi angles: 314.7,203.9,87,139	0.05Å	-	-
A 307	CYS	50	-	Favored (13.07%) General / -128.6,170.6	30% ( <i>m</i> ) chi angles: 310.2	0.062Å	-	-

A 308	ARG	50	-	Favored (43.95%) General / -132.9,133.9	10.2% ( <i>tpp85</i> ) chi angles: 196,77.4,68.1,107.8	0.105Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.759 σ
A 309	LEU	50	-	Favored (54.22%) General / -115.4,135.3	9.4% ( <i>tt</i> ) chi angles: 181.1,146.7	0.111Å	-	-
A 310	THR	50	-	Favored (46.95%) General / -123.6,126.6	31.4% ( <i>p</i> ) chi angles: 51.4	0.072Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 311	ARG	50	-	Favored (19.17%) General / -84.5,163.9	38.7% ( <i>ptt180</i> ) chi angles: 65.4,173.5,185.2,176.7	0.058Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.677 σ
A 312	ASP	50	-	Favored (11.03%) General / -63.8,120.0	0.9% chi angles: 297.4,45.1	0.116Å	-	-
A 313	LYS	99.99	-	Favored (3.26%) General / -47.6,144.2	53.5% ( <i>tttp</i> ) chi angles: 180.6,172.2,158.6,59.6	0.054Å	-	-
A 314	LYS	99.99	-	Favored (6.2%) General / -138.8,179.9	34.8% ( <i>mmtm</i> ) chi angles: 298.3,294.3,160.6,294	0.043Å	-	-
A 315	GLY	99.99	-	Favored (4.57%) Glycine / -123.5,-135.6	-	-	-	-
A 316	MET	99.99	-	Allowed (1.07%) General / -100.0,43.3	15.6% ( <i>tpt</i> ) chi angles: 192.4,67.3,186.9	0.059Å	-	-
A 317	ASP	99.99	-	Favored (41.43%) General / -73.3,151.3	6.5% ( <i>p-10</i> ) chi angles: 50.4,297.7	0.083Å	-	OUTLIER(S) worst is CA- CB-CG: 4.042 σ
A 318	ARG	99.99	-	Favored (10.69%) General / -85.0,68.8	6% ( <i>ptt-85</i> ) chi angles: 25.7,182.5,175.6,272.2	0.195Å	-	-
A	GLY	99.99	-	Favored (4.34%)	-	-	-	OUTLIER(S) worst is C-N-

319

Glycine /  
-164.7,-145.3A  
320

MET 50 -

Allowed  
(0.26%)  
General /  
-141.4,-149.24.7% (*ttm*)  
chi angles:  
214.6,210,277.4

0.147Å - -

A  
321

TYR 50 -

Favored  
(63.47%)  
Pre-proline /  
-135.8,71.861.5% (*m-85*)  
chi angles: 306,272.1

0.043Å - -

A  
322

PRO 50 -

Favored  
(12.71%)  
Trans-proline /  
-83.6,168.617.9% (*Cg\_endo*)  
chi angles: 38.9

0.1Å - -

A  
323

SER 50 -

Favored (7.3%)  
General /  
-103.0,171.622.8% (*t*)  
chi angles: 186.7

0.032Å - -

A  
324

TYR 50 -

Favored  
(38.38%)  
General /  
-140.3,146.328.8% (*m-85*)  
chi angles: 311.7,91.6

0.074Å - -

A  
325

PHE 50 -

Favored  
(22.11%)  
General /  
-138.0,125.544.6% (*m-85*)  
chi angles: 307.8,266.9

0.045Å - -

A  
326

LEU 50 -

Favored  
(21.58%)  
General /  
-96.8,149.718% (*tp*)  
chi angles: 195.8,65.4

0.071Å - -

A  
327

HIS 50 -

Favored  
(44.06%)  
General /  
-145.4,156.96.5% (*m80*)  
chi angles: 316.6,72.6

0.138Å - -

A  
328

LEU 50 -

Favored  
(50.94%)  
General /  
-71.0,141.954.3% (*mt*)  
chi angles: 286.4,178.5

0.066Å - -

A  
329

ASP 50 -

Allowed  
(1.21%)  
General /  
-96.3,51.51.8% (*t0*)  
chi angles: 225.5,342.6

0.057Å - -

A  
330

THR 50 -

Allowed  
(0.64%)  
General /  
-110.5,-158.320.6% (*p*)  
chi angles: 48.5

0.182Å - -

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			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246

A 331	GLU	50	-	Allowed (0.99%) General / -72.2,-64.2	3.7% ( <i>tm-20</i> ) chi angles: 182.3,280.9,294.8	0.113Å	-	-
A 332	LYS	50	-	Favored (18.68%) General / -79.2,115.1	46.9% ( <i>mmtm</i> ) chi angles: 298.7,297.3,177.5,289	0.043Å	-	-
A 333	LYS	50	-	Allowed (1.32%) General / -98.1,58.5	46.2% ( <i>mttp</i> ) chi angles: 295.7,161.7,185,68.4	0.099Å	-	-
A 334	VAL	50	-	Favored (5.29%) Isoleucine or valine / -54.5,144.7	5.7% ( <i>p</i> ) chi angles: 75.4	0.082Å	-	-
A 335	PHE	50	-	Favored (45.96%) General / -67.1,152.3	61.4% ( <i>t80</i> ) chi angles: 169.6,72.6	0.049Å	-	-
A 336	LEU	50	-	Allowed (0.89%) General / -132.3,-60.5	87% ( <i>mt</i> ) chi angles: 299.7,174.4	0.054Å	-	-
A 337	LEU	50	-	Favored (42.43%) General / -145.1,154.4	22.6% ( <i>mt</i> ) chi angles: 282.7,159.1	0.093Å	-	-
A 338	ALA	50	-	Favored (30.01%) General / -134.2,163.3	-	0.074Å	-	-
A 339	GLY	50	-	Favored (4.26%) Glycine / -178.3,139.7	-	-	-	-
A 340	ARG	50	-	Favored (46.66%) General / -121.6,146.8	7.6% ( <i>ttt85</i> ) chi angles: 197.4,160.8,202.8,113.2	0.04Å	-	-
A 341	LYS	50	-	Favored (16.57%) General / -70.8,120.6	83.2% ( <i>tttt</i> ) chi angles: 193.6,175.9,180.3,177	0.056Å	-	-
A 342	ARG	50	-	Favored (6.48%) General / -74.3,107.4	43.5% ( <i>mtp85</i> ) chi angles: 288.7,201.8,57.7,76.2	0.061Å	-	-

A 343	LYS	50	-	Favored (84.93%) General / -65.2,-36.7	81.1% ( <i>tttt</i> ) chi angles: 191.5,168.8,183.9,177.9	0.13Å	-	-
A 344	ARG	50	-	Favored (4.77%) General / -94.2,85.8	58.6% ( <i>mtp180</i> ) chi angles: 294.3,187.6,79,170.3	0.136Å	-	-
A 345	SER	50	-	Favored (21.12%) General / -156.8,171.0	46.2% ( <i>t</i> ) chi angles: 178.9	0.035Å	-	-
A 346	LYS	50	-	Favored (11.1%) General / -108.4,-25.2	8.5% ( <i>tptp</i> ) chi angles: 181,66.9,221.7,75.5	0.074Å	-	-
A 347	THR	50	-	Favored (7.53%) General / -124.6,174.9	70% ( <i>p</i> ) chi angles: 64.1	0.074Å	-	-
A 348	ALA	50	-	Favored (37.31%) General / -65.7,128.8	-	0.02Å	-	-
A 349	ASN	50	-	Favored (3.36%) General / -162.3,127.6	51.9% ( <i>t-20</i> ) chi angles: 185.8,332.1	0.139Å	-	OUTLIER(S) worst is CA- CB-CG: 4.018 σ
A 350	TYR	50	-	Favored (34.05%) General / -138.3,134.3	17.4% ( <i>m-85</i> ) chi angles: 306,73.4	0.047Å	-	-

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A 351	LEU	50	-	-	Favored (42.65%) General / -100.1,122.2	30.2% ( <i>mt</i> ) chi angles: 300,190.9	0.035Å	-	-
A 352	ILE	50	-	-	Favored (19.45%) Isoleucine or valine / -113.3,145.2	95.8% ( <i>mt</i> ) chi angles: 294.4,167.3	0.105Å	-	-
A 353	SER	50	-	-	Favored (44.41%) General / -148.7,159.1	23.3% ( <i>t</i> ) chi angles: 170.2	0.162Å	-	-

A 354	ILE	50	-	Favored (10.91%) Isoleucine or valine / -85.3,-14.8	30% ( <i>pt</i> ) chi angles: 65,164.3	0.147Å	-	OUTLIER(S) worst is C-N- CA: 4.506 $\sigma$
A 355	ASP	50	-	Favored (23.91%) Pre-proline / -107.5,129.7	4.9% ( <i>t0</i> ) chi angles: 163.3,353.5	0.149Å	-	OUTLIER(S) worst is CA- CB-CG: 8.65 $\sigma$
A 356	PRO	50	-	Favored (15.8%) Trans-proline / -74.9,-21.8	16.4% ( <i>Cg_endo</i> ) chi angles: 39.1	0.059Å	-	-
A 357	THR	50	-	Favored (13.77%) General / -89.8,-38.4	9% ( <i>m</i> ) chi angles: 313.7	0.047Å	-	-
A 358	ASN	99.99	-	Favored (4.1%) General / -72.9,104.6	59.6% ( <i>t-20</i> ) chi angles: 189.4,345.8	0.037Å	-	-
A 359	LEU	99.99	-	Favored (13.13%) General / -119.1,18.2	23.1% ( <i>mt</i> ) chi angles: 311.1,169.9	0.096Å	-	-
A 360	SER	99.99	-	Favored (5.35%) General / -93.4,179.6	14.1% ( <i>t</i> ) chi angles: 190.3	0.067Å	-	-
A 361	ARG	99.99	-	Allowed (1.2%) General / -101.5,68.8	14% ( <i>tpt180</i> ) chi angles: 174,52.6,185.3,124.6	0.08Å	-	-
A 362	GLY	99.99	-	Favored (6.79%) Glycine / -98.5,-130.3	-	-	-	-
A 363	GLY	99.99	-	OUTLIER (0.03%) Glycine / -173.2,-29.7	-	-	-	-
A 364	GLU	99.99	-	Allowed (1.24%) General / -38.1,-55.7	0% chi angles: 60.9,316.3,281.6	0.132Å	-	-
A 365	ASN	50	-	Favored (3.52%) General / -128.9,-20.1	78.6% ( <i>m-20</i> ) chi angles: 299.8,330.5	0.071Å	-	-
Favored								

A 366	PHE	50	-	(17.25%) General / -62.6,123.0	51.4% ( <i>t80</i> ) chi angles: 166.7,75.8	0.033Å	-	-
A 367	ILE	50	-	(1.43%) Isoleucine or valine / -129.0,-22.5	1.6% ( <i>tp</i> ) chi angles: 211.9,85.6	0.152Å	-	-
A 368	GLY	50	-	Favored (11.33%) Glycine / -137.9,140.6	-	-	-	-
A 369	LYS	50	-	Favored (5.24%) General / -128.1,98.8	4.3% ( <i>ttpm?</i> ) chi angles: 186.5,160.9,51.7,268.6	0.138Å	-	-
A 370	LEU	50	-	Favored (48.25%) General / -101.8,130.2	53% ( <i>tp</i> ) chi angles: 176.1,57.7	0.085Å	-	-

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A 371	ARG	50	-		Favored (25.22%) General / -146.2,138.4	10.9% ( <i>ttp85</i> ) chi angles: 172.9,210.2,50.2,58.5	0.146Å	-	-
A 372	SER	50	-		Favored (5.22%) General / -101.8,176.4	23.2% ( <i>p</i> ) chi angles: 79.7	0.058Å	-	-
A 373	ASN	50	-		Favored (4.76%) General / -74.3,179.0	33.1% ( <i>p-10</i> ) chi angles: 66.1,333.2	0.065Å	-	-
A 374	LEU	50	-		Favored (75.53%) General / -63.3,-33.4	34.1% ( <i>tp</i> ) chi angles: 184.4,54.8	0.108Å	-	-
A 375	LEU	50	-		Favored (64.32%) General / -73.7,-33.1	19.7% ( <i>mt</i> ) chi angles: 315,181.3	0.116Å	-	-
A 376	GLY	50	-		Favored (56.37%) Glycine / 97.0,9.2	-	-	-	-
Favored									



A 377	ASN	50	-	(13.51%) General / -107.8,-19.5	17.5% ( <i>p</i> -10) chi angles: 71.7,318.3	0.076Å	-	-
A 378	ARG	50	-	Favored (31.61%) General / -113.4,117.4	94% ( <i>mtt</i> 180) chi angles: 286.9,192.8,175.4,181.4	0.031Å	-	-
A 379	PHE	50	-	Favored (19.92%) General / -117.9,161.3	75.7% ( <i>m</i> -85) chi angles: 295.5,80.4	0.071Å	-	-
A 380	THR	50	-	Favored (46.56%) General / -135.1,143.5	2% ( <i>m</i> ) chi angles: 322.7	0.055Å	-	-
A 381	VAL	50	-	Favored (59.82%) Isoleucine or valine / -105.5,128.2	32.3% ( <i>t</i> ) chi angles: 186	0.103Å	-	-
A 382	PHE	50	-	Favored (7.48%) General / -119.0,172.5	10.6% ( <i>m</i> -85) chi angles: 319.4,287.5	0.053Å	-	-
A 383	ASP	50	-	Allowed (0.06%) General / -76.3,-155.2	53.9% ( <i>p</i> -10) chi angles: 66.5,359.1	0.157Å	-	OUTLIER(S) worst is C-N- CA: 4.017 σ
A 384	ASN	50	-	Favored (56.41%) General / -93.3,2.8	37.3% ( <i>p</i> -10) chi angles: 55.6,359.2	0.078Å	-	-
A 385	GLY	50	-	Favored (54.03%) Glycine / -73.2,167.9	-	-	-	-
A 386	GLN	50	-	Favored (39.04%) General / -76.3,146.2	8.3% ( <i>tt</i> 0) chi angles: 193.6,201.6,116	0.085Å	-	-
A 387	ASN	50	-	Favored (75.29%) Pre-proline / -71.4,119.7	38.2% ( <i>t</i> 30) chi angles: 178.5,28.8	0.066Å	-	-
A 388	PRO	50	-	Favored (8.52%) Trans-proline / -51.5,-20.4	89.6% ( <i>Cg</i> _exo) chi angles: 329	0.076Å	-	-
A				Favored (61.03%)	57.6% ( <i>mt</i> -30)			

389	GLN	50	-	General / -73.7,-13.7	chi angles: 309.2,179.1,293.1	0.086Å	-	-	
A 390	ARG	50	-	Favored (34.49%) General / -81.6,-26.8	47.5% ( <i>tpt85</i> ) chi angles: 181.5,59.6,189,94.5	0.163Å	-	-	
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A 391	GLY	50	-	Allowed (0.26%) Glycine / -162.5,105.4	-	-	-	-	-
A 392	TYR	50	-	Favored (80.34%) General / -56.9,-42.7	84.1% ( <i>t80</i> ) chi angles: 174.7,82.1	0.09Å	-	-	-
A 393	SER	50	-	Allowed (1.7%) General / -79.2,13.9	23.7% ( <i>m</i> ) chi angles: 304.9	0.057Å	-	-	-
A 394	THR	50	-	Favored (58.89%) General / -64.4,141.1	76.2% ( <i>m</i> ) chi angles: 297	0.043Å	-	-	-
A 395	ASN	50	-	Favored (4.72%) General / -43.3,131.1	18.8% ( <i>t-20</i> ) chi angles: 177.8,284	0.063Å	-	-	-
A 396	VAL	50	-	Favored (59.93%) Isoleucine or valine / -63.8,-33.1	53.6% ( <i>t</i> ) chi angles: 170.3	0.167Å	-	-	-
A 397	ALA	50	-	Favored (59.77%) General / -75.3,-28.7	-	0.085Å	-	-	-
A 398	SER	50	-	Favored (58.59%) General / -75.0,-25.1	13.9% ( <i>m</i> ) chi angles: 309.8	0.1Å	-	-	-
A 399	LEU	50	-	Favored (5.67%) General / -61.4,164.3	65% ( <i>mt</i> ) chi angles: 292.5,182.6	0.043Å	-	-	-
A				Favored	7.6% ( <i>ptt-85</i> )				OUTLIER(S)

400	ARG	50	-	(45.58%) General / -69.4,151.9	chi angles: 84,182.5,209.9,255.8	0.044Å	-	worst is CD- NE-CZ: 5.118 σ
A 401	GLN	50	-	Favored (33.02%) General / -120.2,155.5	6.5% ( <i>pt20</i> ) chi angles: 83.7,201.1,355.5	0.043Å	-	-
A 402	GLU	50	-	Favored (29.77%) General / -85.2,141.9	8.2% ( <i>mm-40</i> ) chi angles: 300.9,305.2,265.7	0.081Å	-	-
A 403	LEU	50	-	Favored (3.06%) General / -125.7,-30.4	96.3% ( <i>mt</i> ) chi angles: 296.1,175.3	0.105Å	-	-
A 404	ALA	50	-	Favored (3.36%) General / -171.1,152.1	-	0.072Å	-	-
A 405	ALA	50	-	Favored (45.76%) General / -115.3,143.1	-	0.053Å	-	-
A 406	VAL	50	-	Favored (63.42%) Isoleucine or valine / -130.2,133.9	23.1% ( <i>t</i> ) chi angles: 187.3	0.037Å	-	-
A 407	ILE	50	-	Favored (26.8%) Isoleucine or valine / -127.9,112.2	4.7% ( <i>mp</i> ) chi angles: 302.2,95.8	0.039Å	-	-
A 408	TYR	50	-	Favored (22.41%) General / -93.1,148.0	96.9% ( <i>m-85</i> ) chi angles: 293.5,273	0.1Å	-	-
A 409	GLU	50	-	Favored (50.53%) General / -64.3,148.4	81.9% ( <i>mt-10</i> ) chi angles: 290.4,175.9,323.9	0.099Å	-	-
A 410	THR	50	-	Favored (5.16%) General / -109.8,94.7	30.3% ( <i>p</i> ) chi angles: 51.3	0.036Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
Allowed						

A 411	ASN	50	-	(1.1%) General / -46.2,147.3	3.7% ( <i>m120</i> ) chi angles: 296,53	0.124Å	-	-
A 412	VAL	99.99	-	Favored (6.58%) Isoleucine or valine / -106.7,159.2	8.5% ( <i>p</i> ) chi angles: 73.4	0.099Å	-	-
A 413	LEU	99.99	-	Favored (46.09%) General / -54.7,136.3	7.6% ( <i>tt</i> ) chi angles: 188.7,142.6	0.049Å	-	-
A 414	GLY	99.99	-	Favored (30.41%) Glycine / 83.0,-15.8	-	-	-	-
A 415	PHE	99.99	-	Favored (31.42%) General / -69.0,127.0	6.5% ( <i>t80</i> ) chi angles: 171.1,37.3	0.042Å	-	-
A 416	ARG	99.99	-	Favored (2.39%) General / -75.3,73.3	98.5% ( <i>mtt180</i> ) chi angles: 300.6,179.8,186.5,177.1	0.059Å	-	-
A 417	GLY	99.99	-	Allowed (0.54%) Glycine / -116.0,91.2	-	-	-	-
A 418	PRO	50	-	Allowed (1.19%) Trans-proline / -80.6,90.9	74.2% ( <i>Cg_endo</i> ) chi angles: 33.3	0.045Å	-	-
A 419	ARG	50	-	Allowed (0.06%) General / -26.7,115.2	16.7% ( <i>mtm180</i> ) chi angles: 310.6,191.1,299.5,226.2	0.079Å	-	-
A 420	ARG	50	-	Favored (39.26%) General / -65.9,154.4	81.1% ( <i>mtt85</i> ) chi angles: 299,181.6,182.9,95.3	0.111Å	-	-
A 421	MET	50	-	Favored (48.43%) General / -130.3,135.8	88.4% ( <i>mtp</i> ) chi angles: 291,165.1,70.2	0.095Å	-	-
A 422	THR	50	-	Favored (46.84%) General / -102.9,134.2	88.2% ( <i>m</i> ) chi angles: 297.7	0.05Å	-	-
				Favored				

A 423	VAL	50	-	(48.15%) Isoleucine or valine / -128.3,118.5	94.1% ( <i>t</i> ) chi angles: 175.8	0.058Å	-	-
A 424	ILE	50	-	Favored (53.86%) Isoleucine or valine / -114.0,135.4	37.6% ( <i>mm</i> ) chi angles: 307.1,305.4	0.045Å	-	-
A 425	ILE	50	-	Allowed (1.33%) Pre-proline / -129.6,179.3	21.2% ( <i>pt</i> ) chi angles: 72.1,170.8	0.147Å	-	-
A 426	PRO	50	-	Favored (32.51%) Trans-proline / -77.4,159.7	78.5% ( <i>Cg_exo</i> ) chi angles: 333.5	0.08Å	-	-
A 427	GLY	50	-	Favored (6.06%) Glycine / -60.2,171.9	-	-	-	-
A 428	MET	50	-	Favored (20.32%) General / -108.8,155.8	87.2% ( <i>mmm</i> ) chi angles: 299.7,310.9,286.7	0.094Å	-	-
A 429	SER	50	-	Favored (17.6%) General / -84.0,166.7	98.9% ( <i>p</i> ) chi angles: 64.3	0.032Å	-	-
A 430	ALA	50	-	Favored (68.78%) General / -67.7,-29.5	-	0.081Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 431	GLU	50	-	-	Favored (73.27%) General / -61.6,-33.1	1.7% ( <i>tm-20</i> ) chi angles: 158.4,288.9,312	0.171Å	-	OUTLIER(S) worst is C-N- CA: 4.386 σ
A 432	ASN	50	-	-	OUTLIER (0%) General / 102.4,35.5	69.2% ( <i>m-80</i> ) chi angles: 293.1,282.6	0.229Å	-	-
A 433	GLU	50	-	-	Favored (13.61%) General / -112.0,164.0	2.6% ( <i>tp10</i> ) chi angles: 200.4,34.2,91.9	0.056Å	-	-
						Favored 22.5% ( <i>mtm-85</i> )			

A 434	ARG	50	-	(33.58%) General / -81.7,141.5	chi angles: 295.7,170.4,308,303.1	0.039Å	-	-
A 435	VAL	50	-	Favored (66.16%) Pre-proline / -62.4,121.3	79.4% ( <i>t</i> ) chi angles: 174.5	0.052Å	-	-
A 436	PRO	50	-	Favored (2.41%) Trans-proline / -72.6,76.2	88% ( <i>Cg_exo</i> ) chi angles: 331.4	0.05Å	-	-
A 437	ILE	50	-	Favored (2.23%) Isoleucine or valine / -64.7,114.1	62.9% ( <i>mt</i> ) chi angles: 290.4,177.8	0.072Å	-	-
A 438	ARG	50	-	Favored (50.62%) Pre-proline / -123.8,90.4	64.1% ( <i>mtt-85</i> ) chi angles: 286.8,161.3,171.5,281.2	0.077Å	-	-
A 439	PRO	50	-	Favored (87.09%) Trans-proline / -60.5,149.3	20.8% ( <i>Cg_exo</i> ) chi angles: 324.2	0.079Å	-	-
A 440	ARG	50	-	Favored (58.66%) General / -80.7,-13.8	76.9% ( <i>mtp180</i> ) chi angles: 290.8,165.4,69.3,194.1	0.092Å	-	-
A 441	ASN	50	-	Favored (8.91%) General / -145.8,177.4	47.3% ( <i>t30</i> ) chi angles: 194.6,14.4	0.091Å	-	-
A 442	ALA	50	-	Favored (56.97%) General / -83.1,-12.6	-	0.111Å	-	-
A 443	SER	50	-	Favored (85.42%) General / -65.8,-37.1	58.9% ( <i>p</i> ) chi angles: 55.9	0.107Å	-	-
A 444	ASP	50	-	Favored (18.88%) General / -93.3,152.9	44.5% ( <i>t0</i> ) chi angles: 188.5,22.7	0.045Å	-	-
A 445	GLY	50	-	Favored (8.73%) Glycine / 154.8,158.5	-	-	-	-

A 446	LEU	50	-	Favored (69.55%) General / -57.0,-35.8	89.2% ( <i>mt</i> ) chi angles: 297.4,171.6	0.159Å	-	-
A 447	LEU	50	-	Favored (83.75%) General / -66.1,-36.6	17.4% ( <i>mt</i> ) chi angles: 275.2,174.8	0.142Å	-	-
A 448	VAL	50	-	Favored (63.8%) Isoleucine or valine / -72.0,-45.4	38.6% ( <i>t</i> ) chi angles: 166	0.102Å	-	-
A 449	ARG	50	-	Favored (74.15%) General / -58.6,-36.6	94.4% ( <i>mtt180</i> ) chi angles: 295.6,187.6,185.1,195.2	0.095Å	-	-
A 450	TRP	50	-	Favored (92.96%) General / -59.6,-42.6	56% ( <i>t-105</i> ) chi angles: 170,258.9	0.125Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.509 $\sigma$

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 451	GLN	50	-	-	Favored (59.94%) General / -75.0,-19.7	15.1% ( <i>tp60</i> ) chi angles: 194.5,50.1,87.2	0.135Å	-	-
A 452	ASN	50	-	-	Favored (27.41%) General / -85.4,-24.9	2.4% ( <i>m-20</i> ) chi angles: 321.6,331.2	0.121Å	-	OUTLIER(S) worst is CA- CB-CG: 5.527 $\sigma$
A 453	LYS	50	-	-	Favored (9.47%) General / 67.0,24.9	26.7% ( <i>mmmt</i> ) chi angles: 286.7,293.8,305.4,192.2	0.158Å	-	-
A 454	THR	50	-	-	Favored (7.41%) General / -92.0,90.5	36.2% ( <i>p</i> ) chi angles: 52.6	0.032Å	-	-
A 455	LEU	50	-	-	Favored (11.75%) General / -120.4,21.1	16.4% ( <i>mt</i> ) chi angles: 316.7,179.6	0.067Å	-	-
A 456	GLU	50	-	-	Favored (69.02%) General / -68.6,-30.3	10.8% ( <i>mp0</i> ) chi angles: 304,59.3,49.1	0.08Å	-	-

A 457	SER	50	-	Favored (22.68%) General / -109.1,16.2	10.5% ( <i>p</i> ) chi angles: 46.4	0.091Å	-	-
A 458	LEU	50	-	Favored (2.69%) General / -119.2,-174.3	15.8% ( <i>mt</i> ) chi angles: 313,188.6	0.043Å	-	-
A 459	ILE	50	-	Favored (42.3%) Isoleucine or valine / -137.8,131.1	10.3% ( <i>mt</i> ) chi angles: 275.7,160.8	0.095Å	-	-
A 460	GLU	50	-	Favored (46.06%) General / -100.0,129.8	62.8% ( <i>tt0</i> ) chi angles: 179.1,161.7,8.2	0.053Å	-	-
A 461	LEU	50	-	Favored (49.98%) General / -134.2,155.6	47% ( <i>mt</i> ) chi angles: 306.9,173	0.101Å	-	-
A 462	HIS	50	-	Favored (32.89%) General / -141.7,163.4	51.2% ( <i>m80</i> ) chi angles: 282,90.9	0.083Å	-	-
A 463	ASN	50	-	Favored (42.54%) General / -71.1,153.5	7.6% ( <i>p-10</i> ) chi angles: 69.4,284.4	0.067Å	-	-
A 464	LYS	50	-	Favored (90.92%) Pre-proline / -72.5,126.4	76.9% ( <i>tttt</i> ) chi angles: 179.2,167.8,177.4,164.1	0.027Å	-	-
A 465	PRO	50	-	Favored (27.67%) Trans-proline / -62.0,129.5	15.6% ( <i>Cg_exo</i> ) chi angles: 323.6	0.086Å	-	-
A 466	PRO	50	-	Favored (90.98%) Trans-proline / -57.9,139.6	0.1% chi angles: 318.4	0.091Å	-	-
A 467	VAL	50	-	Allowed (0.25%) Isoleucine or valine / -131.7,-160.1	35.5% ( <i>m</i> ) chi angles: 297.9	0.17Å	-	-
A 468	TRP	50	-	Favored (52.98%) General /	56.9% ( <i>t-105</i> ) chi angles: 171.6,262	0.025Å	-	OUTLIER(S) worst is CE3- CD2-CG:



-69.6,144.3

4.399  $\sigma$ 

A 469	ASN	50	-	Favored (2.85%) General / -149.2,98.7	11.3% ( <i>t</i> 30) chi angles: 198.1,75.7	0.082Å	-	OUTLIER(S) worst is C-N- CA: 4.236 $\sigma$
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A 470	ASP	50	-	Favored (79.74%) General / -67.5,-35.8	21.1% ( <i>p</i> -10) chi angles: 50.7,349.1	0.08Å	-	-
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#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 471	ASP	50	-	OUTLIER (0.02%) General / -41.1,-22.7	1.1% ( <i>t</i> 70) chi angles: 162.5,93.6	0.111Å	-	OUTLIER(S) worst is CA- CB-CG: 5.137 $\sigma$	
A 472	SER	50	-	Favored (3.61%) General / -131.9,-3.2	79.3% ( <i>p</i> ) chi angles: 59.7	0.02Å	-	-	
A 473	GLY	50	-	Favored (60.27%) Glycine / 55.6,34.2	-	-	-	-	
A 474	SER	50	-	Favored (2.87%) General / -148.1,-167.7	7.1% ( <i>t</i> ) chi angles: 196.8	0.107Å	-	-	
A 475	TYR	50	-	Favored (2.83%) General / -116.2,88.2	75.8% ( <i>m</i> -85) chi angles: 296.8,260.4	0.042Å	-	-	
A 476	THR	50	-	Allowed (0.14%) General / -158.1,-145.6	13.2% ( <i>t</i> ) chi angles: 186.2	0.278Å	-	OUTLIER(S) worst is C- CA-CB: 4.43 $\sigma$	
A 477	LEU	50	-	Favored (24.9%) General / -146.6,138.9	55.5% ( <i>mt</i> ) chi angles: 302.2,169.6	0.15Å	-	-	
A 478	ASN	50	-	Favored (22.46%) General / -54.9,144.6	17.4% ( <i>t</i> -20) chi angles: 168.7,264.2	0.036Å	-	-	
A 479	PHE	50	-	Favored (13.23%) General / -119.1,17.7	74.8% ( <i>m</i> -85) chi angles: 298.8,290.3	0.076Å	-	-	

A 480	GLN	50	-	Favored (10.94%) General / 63.2,37.7	86% ( <i>mt-30</i> ) chi angles: 300.1,177.2,353.9	0.102Å	-	-
A 481	GLY	50	-	Favored (69.05%) Glycine / 67.1,18.4	-	-	-	-
A 482	ARG	50	-	Favored (15.02%) General / -96.0,-27.7	20.1% ( <i>mmm180</i> ) chi angles: 297.7,289.1,297.8,135.7	0.056Å	-	-
A 483	VAL	50	-	Favored (68.93%) Isoleucine or valine / -118.2,132.1	75% ( <i>t</i> ) chi angles: 172.9	0.125Å	-	-
A 484	THR	50	-	Favored (5.13%) General / -128.6,-7.6	62% ( <i>p</i> ) chi angles: 56.7	0.102Å	-	-
A 485	GLN	50	-	Favored (43.68%) General / -139.4,149.0	84.8% ( <i>mt-30</i> ) chi angles: 293.1,187.1,349.6	0.029Å	-	-
A 486	ALA	50	-	Favored (37.81%) General / -53.3,131.7	-	0.036Å	-	-
A 487	SER	50	-	Allowed (0.64%) General / -176.4,146.8	2.9% ( <i>t</i> ) chi angles: 157.1	0.072Å	-	-
A 488	VAL	50	-	Favored (10.17%) Isoleucine or valine / -83.6,-18.4	35.9% ( <i>m</i> ) chi angles: 297.6	0.178Å	-	-
A 489	LYS	50	-	Favored (3.8%) General / -92.9,63.2	64.5% ( <i>mttm</i> ) chi angles: 303.6,177.9,189.2,297.2	0.052Å	-	-
A 490	ASN	50	-	Favored (4.1%) General / -143.8,103.9	27.2% ( <i>m-20</i> ) chi angles: 284.5,11	0.133Å	-	OUTLIER(S) worst is CA- CB-CG: 4.975 σ

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles  
 Avg: Clashscore: Outliers: 4 of Poor rotamers: 7 of Outliers: Outliers: Outliers: 20

54.27 0				244	213	2 of 229	0 of 246	of 246
A 491	PHE	50	-	Favored (32.64%) General / -156.7,166.7	41.1% ( <i>p90</i> ) chi angles: 56.3,84.1	0.046Å	-	-
A 492	GLN	50	-	Favored (53.77%) General / -120.6,138.7	90.1% ( <i>mt-30</i> ) chi angles: 290.7,168.7,344.8	0.156Å	-	-
A 493	ILE	50	-	Favored (64.64%) Isoleucine or valine / -111.8,130.8	39.4% ( <i>mm</i> ) chi angles: 306,305.3	0.046Å	-	OUTLIER(S) worst is C-N- CA: 4.606 $\sigma$
A 494	VAL	50	-	Allowed (0.19%) Isoleucine or valine / -134.9,-158.8	28.6% ( <i>m</i> ) chi angles: 296.7	0.158Å	-	-
A 495	HIS	50	-	Allowed (0.1%) General / -77.7,-157.7	10.4% ( <i>t-160</i> ) chi angles: 202,190.3	0.135Å	-	OUTLIER(S) worst is CA- CB-CG: 5.921 $\sigma$
A 496	ALA	50	-	Favored (9.57%) General / -99.5,-36.4	-	0.022Å	-	OUTLIER(S) worst is C-N- CA: 5.861 $\sigma$
A 497	ASP	50	-	Allowed (0.5%) General / -95.7,-76.5	1.9% ( <i>p-10</i> ) chi angles: 43,293.1	0.106Å	-	-
A 498	ASP	50	-	Favored (8.25%) Pre-proline / -47.7,121.6	0% chi angles: 143.2,58.7	0.069Å	-	-
A 499	PRO	50	-	Allowed (0.42%) Trans-proline / -101.3,-3.6	1.1% ( <i>Cg_endo</i> ) chi angles: 42.3	0.015Å	-	-
A 500	ASP	50	-	Favored (2.34%) General / -138.4,3.4	9.8% ( <i>m-20</i> ) chi angles: 287.4,275.4	0.179Å	-	-
A 501	TYR	50	-	Allowed (1.44%) General / -72.5,91.9	7.8% ( <i>t80</i> ) chi angles: 194.7,290.6	0.049Å	-	-
A				OUTLIER (0.08%)	39.4% ( <i>mm</i> )			

502	ILE	50	-	Isoleucine or valine / -66.5,82.0	chi angles: 302.6,307	0.088Å	-	-
A 503	VAL	50	-	Favored (83.13%) Isoleucine or valine / -64.8,-38.6	76% ( <i>t</i> ) chi angles: 172.2	0.135Å	-	-
A 504	LEU	50	-	Favored (45.77%) General / -141.0,157.1	16.8% ( <i>tp</i> ) chi angles: 197.2,62.7	0.076Å	-	-
A 505	GLN	50	-	Favored (17.42%) General / -150.4,135.1	20% ( <i>tt0</i> ) chi angles: 191,175.9,249.1	0.079Å	-	-
A 506	PHE	50	-	Favored (36.18%) General / -141.8,146.7	59.6% ( <i>t80</i> ) chi angles: 181.5,63.7	0.08Å	-	-
A 507	GLY	50	-	Favored (30.84%) Glycine / 177.6,164.3	-	-	-	-
A 508	ARG	50	-	Favored (53.36%) General / -69.2,137.6	60.8% ( <i>ttt180</i> ) chi angles: 185.5,190.7,165.4,189.7	0.098Å	-	-
A 509	VAL	50	-	Allowed (1.44%) Isoleucine or valine / -121.9,-31.1	19.5% ( <i>m</i> ) chi angles: 292.4	0.23Å	-	-
A 510	ALA	50	-	Allowed (0.33%) General / -134.6,-148.7	-	0.141Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 511	GLU	50	-	-	Favored (18.76%) General / -87.4,-34.3	1.6% ( <i>pt-20</i> ) chi angles: 58.2,146.9,320.5	0.136Å	-	-
A 512	ASP	50	-	-	Favored (12.56%) General /	17.5% ( <i>m-20</i> ) chi angles: 312.6,316.2	0.058Å	-	-

A 513	ALA	50	-	-113.7,-14.9	-	0.033Å	-	-
				Favored (48.28%) General / -104.4,134.0				
A 514	PHE	50	-	Favored (40.2%) General / -131.3,158.6	43.2% ( <i>m</i> -85) chi angles: 303.6,77.9	0.087Å	-	-
A 515	THR	50	-	Favored (26.1%) General / -106.8,150.7	4.9% ( <i>p</i> ) chi angles: 41.5	0.046Å	-	-
A 516	LEU	50	-	Favored (3.53%) General / -151.6,108.5	62.2% ( <i>tp</i> ) chi angles: 180.8,63	0.06Å	-	-
A 517	ASP	50	-	Favored (39.72%) General / -118.0,150.2	29.7% ( <i>m</i> -20) chi angles: 306.6,338.4	0.075Å	-	-
A 518	TYR	50	-	Favored (43.85%) General / -146.2,157.9	46.2% ( <i>p</i> 90) chi angles: 68.6,273.4	0.047Å	-	-
A 519	ARG	50	-	Favored (12.95%) General / -133.5,172.3	43.5% ( <i>mtp</i> 180) chi angles: 302.9,185.8,70.9,236.9	0.037Å	-	-
A 520	TYR	50	-	Favored (47.24%) Pre-proline / -52.9,135.7	55.7% ( <i>t</i> 80) chi angles: 181.9,93.2	0.098Å	-	-
A 521	PRO	50	-	Favored (43.58%) Cis-proline / -96.1,7.8	0.5% chi angles: 42.7	0.079Å	-	-
A 522	LEU	50	-	Favored (41.63%) General / -74.3,148.1	71.8% ( <i>mt</i> ) chi angles: 294.4,182.5	0.08Å	-	-
A 523	CYS	50	-	Favored (9.13%) General / -98.1,170.1	30.3% ( <i>p</i> ) chi angles: 63.2	0.035Å	-	-
A 524	ALA	50	-	Favored (82.07%) General / -64.2,-35.8	-	0.138Å	-	-

A 525	LEU	50	-	Favored (98.61%) General / -62.0,-43.5	22.2% ( <i>tp</i> ) chi angles: 179.5,49.9	0.097Å	-	-
A 526	GLN	50	-	Favored (75.52%) General / -64.4,-48.4	68.1% ( <i>mt-30</i> ) chi angles: 293.2,165.9,290.6	0.113Å	-	-
A 527	ALA	50	-	Favored (64.63%) General / -53.6,-51.0	-	0.03Å	-	-
A 528	PHE	50	-	Favored (95.82%) General / -63.8,-43.6	84.4% ( <i>t80</i> ) chi angles: 182.4,73.5	0.046Å	-	-
A 529	ALA	50	-	Favored (82.47%) General / -65.9,-36.1	-	0.076Å	-	-
A 530	ILE	50	-	Favored (80.34%) Isoleucine or valine / -68.8,-39.6	65% ( <i>mt</i> ) chi angles: 294.5,160.4	0.119Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 0	Outliers: 4 of 244	Poor rotamers: 7 of 213	Outliers: 2 of 229	Outliers: 0 of 246	Outliers: 20 of 246
A 531	ALA	50	-	-	Favored (87.98%) General / -60.0,-40.1	-	0.069Å	-	-
A 532	LEU	50	-	-	Favored (72.88%) General / -66.4,-31.9	2.9% ( <i>mt</i> ) chi angles: 303.7,212.5	0.171Å	-	-
A 533	SER	50	-	-	Favored (63.26%) General / -71.0,-26.7	14.6% ( <i>p</i> ) chi angles: 82	0.136Å	-	-
A 534	SER	50	-	-	Favored (68.63%) General / -72.2,-39.3	10.4% ( <i>p</i> ) chi angles: 83.6	0.16Å	-	-
A 535	PHE	50	-	-	Allowed (1.56%) General /	62.4% ( <i>m-85</i> ) chi angles: 288.6,290.1	0.035Å	-	-

-57.5,165.5

A  
536

ASP 99.99

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10.7% (*m*-20)  
chi angles: 315.6,131.2

0.06Å

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