



# Viewing RPGR\_SM\_6-369\_FFX1FH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0.73	99 <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	2.33%	Goal: <1%
	Ramachandran outliers	3	0.83%	Goal: <0.05%
	Ramachandran favored	320	88.40%	Goal: >98%
	MolProbity score <sup>^</sup>	1.60		92 <sup>nd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.31%	Goal: 0
	Bad backbone bonds:	0 / 2834	0.00%	Goal: 0%
	Bad backbone angles:	34 / 3839	0.89%	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: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 6	GLU	50	-	-	Favored (24.78%) General / -62.7,156.0	3.1% ( <i>pm0</i> ) chi angles: 80.4,309,8.1	0.13Å	-	OUTLIER(S) worst is CB-CG-CD: 5.529 σ
A 7	LEU	50	-	-	Favored (94.47%) Pre-proline / -62.6,146.2	48.9% ( <i>tp</i> ) chi angles: 184.5,61.4	0.065Å	-	-
A 8	MET	50	-	-	Favored (9.84%) Trans-proline / -83.9,142.0	75.8% ( <i>mtm</i> ) chi angles: 292,184.2,280.1	0.106Å	-	-
A 9	PRO	50	-	-	Favored (66.94%)	88.8% ( <i>Cg_endo</i> ) chi angles: 31.9	0.039Å	-	-
A	ASP	50	-	-	Favored (66.94%)	2.2% ( <i>m-20</i> )	0.119Å	-	-

10					General / -59.1,-28.9	chi angles: 309.9,70		
A 11	SER	50	-		Favored (48.1%) General / -53.5,-31.9	67.4% ( <i>p</i> ) chi angles: 57.2	0.083Å	-
A 12	GLY	50	-		Favored (14.05%) Glycine / 118.1,167.3	-	-	-
A 13	ALA	50	-		Favored (29.62%) General / -133.4,163.3	-	0.106Å	-
A 14	VAL	50	0.414Å O with A 29 LYS HA		Favored (12.48%) Isoleucine or valine / -100.6,144.6	48.3% ( <i>t</i> ) chi angles: 182.8	0.07Å	-
A 15	PHE	50	-		Favored (49.91%) General / -127.4,134.1	4% ( <i>m-85</i> ) chi angles: 306.5,67.1	0.071Å	-
A 16	THR	50	-		Favored (2.46%) General / -125.5,85.9	71.7% ( <i>p</i> ) chi angles: 63.8	0.053Å	-
A 17	PHE	50	-		Favored (26.25%) General / -80.3,158.1	83.4% ( <i>m-85</i> ) chi angles: 302.7,283	0.035Å	-
A 18	GLY	50	-		Favored (53.35%) Glycine / 68.7,-156.4	-	-	-
A 19	LYS	50	-		Favored (3.35%) General / -78.7,63.0	8.4% ( <i>ttpt</i> ) chi angles: 198.8,206.6,82.8,205.2	0.051Å	-
A 20	SER	50	-		Favored (57.77%) General / -89.9,-4.0	83.9% ( <i>p</i> ) chi angles: 68.7	0.047Å	-
A 21	LYS	50	-		Allowed (0.66%) General / 73.9,-48.1	20.7% ( <i>mmtp</i> ) chi angles: 315.1,296.5,157.3,55.6	0.254Å	-
A	PHE	50	-		Favored (44.54%)	48.1% ( <i>t80</i> ) chi angles: 186.8,62.9	0.055Å	-

22					General / -62.5,148.9				
A 23	ALA	50	-		Favored (10.44%) General / 54.9,28.4	-	0.091Å	-	-
A 24	GLU	50	-		Favored (31.97%) General / 53.6,42.0	0.4% chi angles: 281.5,60,278.5	0.208Å	-	OUTLIER(S) worst is C-N- CA: 4.112 σ
A 25	ASN	50	-		OUTLIER (0.01%) General / 87.1,42.2	60% ( <i>m</i> -80) chi angles: 302.5,285.8	0.15Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 26	ASN	50	-		Favored (16.89%) Pre-proline / -138.0,168.3	65.6% ( <i>m</i> -80) chi angles: 288.1,281.1	0.069Å	-	-
A 27	PRO	50	-		Allowed (0.93%) Trans-proline / -68.4,71.5	91.6% ( <i>Cg</i> _exo) chi angles: 329.9	0.057Å	-	-
A 28	GLY	50	-		Favored (50.6%) Glycine / -80.5,167.6	-	-	-	-
A 29	LYS	50	0.414Å HA with A 14 VAL O		Favored (50.52%) General / -134.6,149.0	35.3% ( <i>ttpt</i> ) chi angles: 175.8,162.3,58.1,177.4	0.054Å	-	-
A 30	PHE	50	-		Favored (20.3%) General / -155.3,171.2	47.4% ( <i>p90</i> ) chi angles: 68,89.1	0.037Å	-	-
A 31	TRP	50	-		Favored (6.6%) General / -157.0,-177.4	35.3% ( <i>p90</i> ) chi angles: 55.7,81.9	0.063Å	-	-
A 32	PHE	50	-		Favored (53.24%) General / -126.4,139.5	18.4% ( <i>m</i> -85) chi angles: 308.9,309	0.075Å	-	-
A 33	LYS	50	-		Favored (2.88%) General / -70.7,104.5 Allowed	49.3% ( <i>tttm</i> ) chi angles: 184.5,189.5,170.6,291.4	0.04Å	-	-

A 34	ASN	50	-	(0.67%) General / 73.5,37.9	29.7% ( <i>m120</i> ) chi angles: 305.7,110.3	0.139Å	-	-
A 35	ASP	50	-	Favored (9.2%) General / -155.7,130.4	41.1% ( <i>t0</i> ) chi angles: 195.7,5.1	0.023Å	-	-
A 36	VAL	50	-	Favored (30.34%) Pre-proline / -108.0,144.9	8.6% ( <i>p</i> ) chi angles: 68.5	0.073Å	-	-
A 37	PRO	50	-	Favored (48.77%) Trans-proline / -67.8,139.8	57% ( <i>Cg_exo</i> ) chi angles: 327	0.108Å	-	-
A 38	VAL	50	-	Favored (2.36%) Isoleucine or valine / -128.7,-16.1	18.7% ( <i>m</i> ) chi angles: 304.3	0.176Å	-	-
A 39	HIS	50	-	Favored (3.17%) General / -157.3,115.5	9.9% ( <i>t-80</i> ) chi angles: 204.7,306	0.051Å	-	-
A 40	LEU	50	-	Favored (11.66%) General / -84.8,172.2	54.2% ( <i>mt</i> ) chi angles: 307.3,175.7	0.04Å	-	-
A 41	SER	50	-	Favored (10.4%) General / -166.3,154.5	6.1% ( <i>t</i> ) chi angles: 197.9	0.061Å	-	-
A 42	CYS	50	-	Favored (22.22%) General / -152.3,142.3	81.5% ( <i>m</i> ) chi angles: 295.9	0.147Å	-	-
A 43	GLY	50	-	Favored (17.7%) Glycine / -108.3,-154.8	-	-	-	-
A 44	ASP	50	-	Favored (57.01%) General / -66.4,-51.5	38.9% ( <i>t70</i> ) chi angles: 185.2,62.4	0.117Å	-	OUTLIER(S) worst is CA- CB-CG: 4.632 σ
A 45	GLU	50	-	Favored (15.53%) General / -105.3,-13.9	9.3% ( <i>mm-40</i> ) chi angles: 282.8,294.5,263.6	0.05Å	-	-

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles

Avg: Clashscore: 50.27    0.73    Outliers: 3 of 362    Poor rotamers: 7 of 301    Outliers: 1 of 319    Outliers: 0 of 364    Outliers: 33 of 364

A 46	HIS	50	-	Favored (32.04%) General / -145.1,164.2	10.2% ( <i>p</i> -80) chi angles: 76.7,303.1	0.043Å	-	-
A 47	SER	50	-	Favored (42.82%) General / -143.6,159.2	67.6% ( <i>m</i> ) chi angles: 292.8	0.08Å	-	-
A 48	ALA	50	-	Favored (52.37%) General / -130.7,149.3	-	0.129Å	-	-
A 49	VAL	50	-	Favored (3.95%) Isoleucine or valine / -136.9,105.1	99.4% ( <i>t</i> ) chi angles: 176.5	0.069Å	-	-
A 50	VAL	50	-	Favored (15.75%) Isoleucine or valine / -84.3,140.7	99.5% ( <i>t</i> ) chi angles: 176.5	0.069Å	-	-
A 51	THR	50	-	Favored (9.29%) General / -116.9,169.6	68.2% ( <i>p</i> ) chi angles: 64.5	0.045Å	-	-
A 52	GLY	50	-	Favored (77.37%) Glycine / -76.1,-20.5	-	-	-	-
A 53	ASN	50	-	Favored (10.93%) General / -80.7,7.1	31% ( <i>m</i> -20) chi angles: 304.6,348.8	0.072Å	-	OUTLIER(S) worst is C-N- CA: 4.297 $\sigma$
A 54	ASN	50	-	Allowed (0.88%) General / 69.8,44.0	3% ( <i>m</i> 120) chi angles: 320.8,131.7	0.125Å	-	OUTLIER(S) worst is CA- CB-CG: 4.075 $\sigma$
A 55	LYS	50	-	Favored (2.66%) General / -121.8,-173.5	26.6% ( <i>mmtm</i> ) chi angles: 308.4,295.3,158,276.5	0.157Å	-	-
A 56	LEU	50	-	Favored (23.54%) General / -148.6,140.2	61.3% ( <i>tp</i> ) chi angles: 174.4,63	0.134Å	-	-

Favored

A 57	TYR	50	-	(50.5%) General / -124.1,143.4	27.2% ( <i>m-85</i> ) chi angles: 295.6,71.4	0.044Å	-	-
A 58	MET	50	-	Favored (44.68%) General / -126.5,153.8	93.4% ( <i>mmm</i> ) chi angles: 293.7,299.1,301	0.119Å	-	-
A 59	PHE	50	-	Favored (27.26%) General / -161.6,159.1	45.1% ( <i>p90</i> ) chi angles: 59.3,275.7	0.044Å	-	-
A 60	GLY	50	-	Favored (23.97%) Glycine / 137.6,-169.7	-	-	-	-
A 61	SER	50	-	Favored (55.69%) General / -64.8,145.8	28.8% ( <i>m</i> ) chi angles: 304.2	0.063Å	-	-
A 62	ASN	50	-	Favored (4.88%) General / -129.5,30.9	63.9% ( <i>t30</i> ) chi angles: 195.4,28	0.078Å	-	-
A 63	ASN	50	-	Favored (57.47%) General / -73.4,-8.8	20.9% ( <i>p-10</i> ) chi angles: 57.9,329.7	0.112Å	-	-
A 64	TRP	50	-	Favored (6.77%) General / -127.5,11.2	88.1% ( <i>m95</i> ) chi angles: 297.7,88	0.029Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.196 σ
A 65	GLY	50	-	Favored (67.7%) Glycine / 82.9,17.4	-	-	-	-

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A 66	GLN	50	-	Favored (16.93%) General / -71.3,-2.7	8.1% ( <i>pm0</i> ) chi angles: 64.9,266.3,63.4	0.212Å	-	-
A 67	LEU	50	-	Favored (23.35%) General / -96.1,-13.8	23% ( <i>mt</i> ) chi angles: 311.9,185.2	0.14Å	-	-
A				Favored				

68	GLY	50	-	(61.81%) Glycine / 72.1,33.9 Favored	-	-	-	-
A 69	LEU	50	-	(14.78%) General / -105.7,-16.1 Allowed	52.1% ( <i>mt</i> ) chi angles: 307.4,175.2	0.1Å	-	-
A 70	GLY	50	-	(0.74%) Glycine / 109.1,-50.9 Favored	-	-	-	-
A 71	SER	50	-	(16.93%) General / -78.5,170.3 Favored	88.6% ( <i>p</i> ) chi angles: 61.9	0.038Å	-	-
A 72	LYS	50	-	(21.53%) General / -111.2,15.3 Favored	45% ( <i>mtpt</i> ) chi angles: 297.8,189.7,60,165.9	0.085Å	-	-
A 73	SER	50	-	(18.51%) General / -70.4,121.8 Favored	31.9% ( <i>p</i> ) chi angles: 52.4	0.089Å	-	-
A 74	ALA	50	-	(46.21%) General / -56.2,139.9 Favored	-	0.073Å	-	-
A 75	ILE	50	-	(55.53%) Isoleucine or valine / -130.1,123.1 Favored	46.5% ( <i>mm</i> ) chi angles: 304.4,298.5	0.033Å	-	-
A 76	SER	50	-	(32.36%) General / -81.5,-32.8 Favored	63% ( <i>p</i> ) chi angles: 56.6	0.078Å	-	-
A 77	LYS	50	-	(36.66%) Pre-proline / -85.1,139.0 Allowed	64.1% ( <i>mmtt</i> ) chi angles: 313.4,310.5,179,188.7	0.037Å	-	-
A 78	PRO	50	-	(0.9%) Trans-proline / -54.8,112.0 Favored	0.5% chi angles: 320.4	0.054Å	-	-
A 79	THR	50	-	(34.9%) General / -102.2,117.5 Favored	93.6% ( <i>m</i> ) chi angles: 300.1	0.075Å	-	-
A	CYS	50	-	(47.99%) Favored	9.4% ( <i>t</i> )	0.027Å	-	-

80

General /  
-65.5,132.1

chi angles: 196.4

A  
81

VAL 50 -

Allowed  
(1.31%)  
Isoleucine or  
valine /  
-77.7,93.471.6% (*t*)  
chi angles: 173.8

0.106Å - -

A  
82

LYS 50 -

Allowed  
(0.91%)  
General /  
-38.1,-45.246.4% (*pttt*)  
chi angles:  
54.1,193.4,173.3,182.6

0.095Å - -

A  
83

ALA 50 -

Favored  
(59.94%)  
General /  
-76.8,-14.3

- 0.068Å - -

A  
84

LEU 50 -

Favored  
(10.98%)  
General /  
-121.1,11.972.3% (*mt*)  
chi angles: 304.1,180.3

0.069Å - -

A  
85

LYS 50 -

Allowed  
(0.41%)  
Pre-proline /  
-74.0,-20.630.5% (*mtpt*)  
chi angles:  
302.7,198.6,67.1,158.3

0.194Å - -

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 86	PRO	50	-		Favored (32.87%) Trans-proline / -69.1,-24.4	67.7% ( <i>Cg_exo</i> ) chi angles: 327.7	0.06Å	-	-
A 87	GLU	50	-		Favored (8.14%) General / -94.7,172.5	6.3% ( <i>tt0</i> ) chi angles: 217.9,161.9,316.8	0.075Å	-	-
A 88	LYS	50	-		Allowed (1.92%) General / -106.4,83.7	59.1% ( <i>mtpt</i> ) chi angles: 286.7,173.1,64.9,185.6	0.04Å	-	-
A 89	VAL	50	-		Favored (29.22%) Isoleucine or valine / -63.2,133.0	96.2% ( <i>t</i> ) chi angles: 178.3	0.042Å	-	-
A 90	LYS	50	-		Favored (6.34%) General / -115.2,-30.3	38.5% ( <i>ttpt</i> ) chi angles: 189.8,177.6,71.9,177.3	0.042Å	-	-



A 91	LEU	50	-	Favored (44.92%) General / -142.0,157.4	44.9% ( <i>mt</i> ) chi angles: 301.6,167	0.114Å	-	-
A 92	ALA	50	-	Favored (18.94%) General / -156.3,143.3	-	0.052Å	-	-
A 93	ALA	50	-	Favored (45.05%) General / -133.3,135.8	-	0.044Å	-	-
A 94	CYS	50	-	Favored (15.5%) General / -125.5,111.8	61% ( <i>m</i> ) chi angles: 286.1	0.088Å	-	-
A 95	GLY	50	-	Favored (34.96%) Glycine / -93.4,-160.0	-	-	-	-
A 96	ARG	50	-	Favored (2.27%) General / -46.8,-60.7	17.1% ( <i>ttp85</i> ) chi angles: 157.8,169.5,39.8,92.9	0.094Å	-	OUTLIER(S) worst is CD- NE-CZ: 5.031 σ
A 97	ASN	50	-	Favored (2.75%) General / -138.1,9.3	26.6% ( <i>p-10</i> ) chi angles: 60.1,333	0.047Å	-	-
A 98	HIS	50	-	Favored (15.76%) General / -123.2,166.1	27.7% ( <i>p-80</i> ) chi angles: 70.7,293.8	0.06Å	-	OUTLIER(S) worst is CA- CB-CG: 5.294 σ
A 99	THR	50	-	Favored (29.16%) General / -144.2,140.1	36.1% ( <i>m</i> ) chi angles: 306.2	0.109Å	-	-
A 100	LEU	50	-	Favored (49.27%) General / -125.4,147.2	25.2% ( <i>mt</i> ) chi angles: 312.4,174.6	0.085Å	-	-
A 101	VAL	50	-	Favored (27.24%) Isoleucine or valine / -138.1,146.3	57.4% ( <i>t</i> ) chi angles: 180.5	0.098Å	-	-
A 102	SER	50	-	Favored (21.13%) General / -144.5,168.0	45.2% ( <i>t</i> ) chi angles: 178.7	0.094Å	-	-
				Favored				

A 103	THR	50	-	(3.26%) General / -139.0,-172.2	13% ( <i>p</i> ) chi angles: 76.3	0.104Å	-	-	
A 104	GLU	50	-	Favored (51.4%) General / -77.8,-21.6	33.1% ( <i>tt0</i> ) chi angles: 194.5,181.7,75.2	0.029Å	-	-	
A 105	GLY	50	-	Favored (40.96%) Glycine / -69.9,-48.4	-	-	-	-	
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A 106	GLY	50	-	Favored (7.5%) Glycine / 117.8,-27.4	-	-	-	-	OUTLIER(S) worst is C-N- CA: 4.251 σ
A 107	ASN	50	-	Allowed (0.11%) General / -29.5,115.5	1.9% ( <i>m-20</i> ) chi angles: 300.1,32.2	0.136Å	-	-	
A 108	VAL	50	-	Favored (42.76%) Isoleucine or valine / -93.1,130.0	89.7% ( <i>t</i> ) chi angles: 175.3	0.043Å	-	-	
A 109	TYR	50	-	Favored (54.28%) General / -112.6,134.1	95.8% ( <i>m-85</i> ) chi angles: 299.8,277.4	0.041Å	-	-	
A 110	ALA	50	-	Favored (47.95%) General / -124.1,147.4	-	0.107Å	-	-	
A 111	THR	50	-	Favored (35.68%) General / -158.3,159.2	3.1% ( <i>t</i> ) chi angles: 200.5	0.1Å	-	-	
A 112	GLY	50	-	Favored (16.5%) Glycine / 102.9,-166.1	-	-	-	-	
A 113	GLY	50	-	Favored (50.68%) Glycine / -64.0,149.6	-	-	-	-	
A				Favored	62.2% ( <i>t30</i> )			OUTLIER(S) worst is CA-	

114	ASN	50	-	(3.52%) General / -135.1,27.4	chi angles: 187,31.6	0.112Å	-	CB-CG: 4.033 σ
A 115	ASN	50	-	Favored (68.88%) General / -60.3,-29.5	3.1% ( <i>m120</i> ) chi angles: 322,102.8	0.108Å	-	OUTLIER(S) worst is C-N- CA: 4.925 σ
A 116	GLU	50	-	Favored (21.53%) General / -106.1,-3.4	12.2% ( <i>mp0</i> ) chi angles: 316.4,72.4,7.2	0.074Å	-	-
A 117	GLY	50	-	Favored (65.26%) Glycine / 92.1,6.1	-	-	-	-
A 118	GLN	50	-	Favored (10.71%) General / -69.0,-2.7	23.5% ( <i>pt20</i> ) chi angles: 68,185.3,353.7	0.137Å	-	-
A 119	LEU	50	-	Favored (25.54%) General / -89.1,-19.4	21.5% ( <i>mt</i> ) chi angles: 297.2,193.2	0.172Å	-	-
A 120	GLY	50	-	Favored (50.53%) Glycine / 77.1,31.9	-	-	-	-
A 121	LEU	50	-	Favored (13.05%) General / -118.2,10.8	81.7% ( <i>mt</i> ) chi angles: 302.9,176.9	0.091Å	-	-
A 122	GLY	50	-	Allowed (1.49%) Glycine / 96.0,-58.2	-	-	-	-
A 123	ASP	50	-	Favored (2.57%) General / -74.0,-176.6	7.2% ( <i>p-10</i> ) chi angles: 62.3,100.5	0.11Å	-	-
A 124	THR	50	-	Favored (10.98%) General / -121.7,20.4	47.8% ( <i>p</i> ) chi angles: 55.5	0.062Å	-	-
A 125	GLU	50	-	Favored (28.57%) General / -140.7,165.0	4.3% ( <i>tp10</i> ) chi angles: 196.6,45.3,286.3	0.158Å	-	OUTLIER(S) worst is C-N- CA: 5.589 σ

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:			Clashscore:	Outliers: 3 of	Poor rotamers: 7 of	Outliers: 1 of	Outliers: 0 of	Outliers: 33 of	
50.27			0.73	362	301	319	364	364	

A 126	GLU	50	-	OUTLIER (0.03%) General / -51.1,171.4	7.4% ( <i>pt</i> -20) chi angles: 82.1,178.4,232.3	0.1Å	-	-
A 127	ARG	50	-	Favored (45.64%) General / -133.5,137.4	85.4% ( <i>mm</i> t-85) chi angles: 299.4,299.7,187.3,273.4	0.032Å	-	-
A 128	ASN	50	-	Favored (48.48%) General / -82.1,-16.9	44.5% ( <i>p</i> -10) chi angles: 65,342.7	0.052Å	-	-
A 129	THR	50	-	Favored (48%) General / -137.0,150.2	4.4% ( <i>p</i> ) chi angles: 41.2	0.088Å	-	-
A 130	PHE	50	-	Favored (56.87%) General / -60.0,134.2	57.9% ( <i>m</i> -85) chi angles: 284.6,281.1	0.028Å	-	-
A 131	HIS	50	-	Favored (49.13%) General / -130.6,136.7	43.4% ( <i>m</i> 80) chi angles: 285.5,67.8	0.099Å	-	-
A 132	VAL	50	-	Favored (13.01%) Isoleucine or valine / -69.8,145.5	3.3% ( <i>p</i> ) chi angles: 79.8	0.088Å	-	-
A 133	ILE	50	-	Favored (36.73%) Isoleucine or valine / -90.1,119.1	98.8% ( <i>mt</i> ) chi angles: 296.5,172.3	0.067Å	-	-
A 134	SER	50	-	Favored (71.32%) General / -58.7,-34.5	58.5% ( <i>p</i> ) chi angles: 55.8	0.114Å	-	-
A 135	PHE	50	-	Favored (81.21%) General / -61.6,-36.6	84.2% ( <i>t</i> 80) chi angles: 178.9,83.7	0.066Å	-	-
A 136	PHE	50	-	Favored (8.75%) General / -87.1,79.1	52.6% ( <i>m</i> -85) chi angles: 293.5,299.2	0.091Å	-	-
A 137	THR	50	-	Allowed (0.35%) General / -63.5,-179.4	68.5% ( <i>p</i> ) chi angles: 62	0.043Å	-	-

A 138	SER	50	-	Favored (37.03%) General / -75.2,-4.2	42.7% ( <i>p</i> ) chi angles: 53.9	0.108Å	-	-
A 139	GLU	50	-	Favored (19.81%) General / -89.3,-28.5	0% chi angles: 144.8,290.1,306.3	0.157Å	-	-
A 140	HIS	50	-	Favored (4.49%) General / -78.0,78.7	27.9% ( <i>m80</i> ) chi angles: 279.2,66.2	0.049Å	-	-
A 141	LYS	50	-	Favored (3.84%) General / -73.2,103.1	73.2% ( <i>mm</i> ) chi angles: 303.8,306.4,186.1,186.1	0.037Å	-	-
A 142	ILE	50	-	Favored (38.46%) Isoleucine or valine / -79.2,125.4	24.6% ( <i>mm</i> ) chi angles: 304.1,311.7	0.041Å	-	OUTLIER(S) worst is C-N- CA: 4.331 σ
A 143	LYS	50	0.414Å HB2 with A 157 GLU HA	Favored (24.15%) General / -74.4,-49.1	71.7% ( <i>tttt</i> ) chi angles: 199.7,186.3,178.1,190.3	0.094Å	-	-
A 144	GLN	50	-	Favored (21.36%) General / -151.2,140.5	7.6% ( <i>tt0</i> ) chi angles: 193.4,212.7,343.3	0.128Å	-	-
A 145	LEU	50	-	Favored (29.67%) General / -108.4,148.8	79.8% ( <i>mt</i> ) chi angles: 288.1,173.3	0.098Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364

A 146	SER	50	-	Favored (46.34%) General / -140.8,154.6	48.2% ( <i>t</i> ) chi angles: 179.7	0.06Å	-	-
A 147	ALA	50	-	Allowed (0.56%) General / -168.3,109.9	-	0.068Å	-	-
A 148	GLY	50	-	Favored (13.2%) Glycine / -107.1,-146.7	-	-	-	-

A 149	SER	50	0.488Å HB3 with A 199 TYR O	Favored (34.44%) General / -86.3,130.6	22.7% ( <i>t</i> ) chi angles: 186.6	0.025Å	-	-
A 150	ASN	50	-	Allowed (0.05%) General / 85.5,-41.7	0% chi angles: 333.4,354.9	0.223Å	-	OUTLIER(S) worst is CA- CB-CG: 9.792 σ
A 151	THR	50	-	Favored (7.9%) General / -116.5,171.4	74.2% ( <i>p</i> ) chi angles: 58.1	0.092Å	-	OUTLIER(S) worst is C-N- CA: 4.621 σ
A 152	SER	50	-	Favored (40.12%) General / -145.4,161.2	38.8% ( <i>m</i> ) chi angles: 288.2	0.172Å	-	-
A 153	ALA	50	-	Favored (23.61%) General / -160.4,154.8	-	0.034Å	-	-
A 154	ALA	50	-	Favored (4.58%) General / -148.3,110.4	-	0.053Å	-	-
A 155	LEU	50	-	Favored (42.88%) General / -97.0,127.3	50.5% ( <i>tp</i> ) chi angles: 171.4,62.1	0.162Å	-	-
A 156	THR	50	-	Favored (26.02%) General / -79.9,160.3	6.7% ( <i>p</i> ) chi angles: 42.6	0.138Å	-	-
A 157	GLU	50	0.414Å HA with A 143 LYS HB2	Favored (63.94%) General / -53.3,-39.4	8.7% ( <i>mm-40</i> ) chi angles: 326.2,296.8,314	0.179Å	-	OUTLIER(S) worst is CB- CG-CD: 4.781 σ
A 158	ASP	50	-	Favored (74%) General / -65.1,-32.3	18.1% ( <i>p30</i> ) chi angles: 50.1,16.7	0.106Å	-	-
A 159	GLY	50	-	Favored (6.67%) Glycine / 128.4,-3.9	-	-	-	-
A 160	ARG	50	-	Favored (6.18%) General / -76.1,103.6	67.9% ( <i>mtm180</i> ) chi angles: 299.2,173.2,284.7,150.7	0.065Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.312 σ
A 161	LEU	50	-	Favored (36.13%) General /	46.5% ( <i>tp</i> ) chi angles: 170.8,63.7	0.047Å	-	-

A 162	PHE	50	-	-80.4,135.2 Favored (52.38%) General / -125.8,132.2	66% ( <i>m-85</i> ) chi angles: 306.3,279.9	0.057Å	-	-	
A 163	MET	50	-	Favored (40.88%) General / -126.2,156.1	28.1% ( <i>mtp</i> ) chi angles: 291.7,206.9,82.1	0.074Å	-	-	
A 164	TRP	50	-	Favored (26.73%) General / -161.8,166.2	38.2% ( <i>p90</i> ) chi angles: 62.8,98	0.103Å	-	-	
A 165	GLY	50	-	Favored (17.75%) Glycine / 103.5,-151.1	-	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 166	ASP	50	-	Favored (22.14%) General / -55.9,146.4	27.7% ( <i>t0</i> ) chi angles: 186.6,35.8	0.083Å	-	-	
A 167	ASN	50	-	Favored (2.69%) General / -138.7,19.7	16.2% ( <i>t30</i> ) chi angles: 199.8,66.7	0.062Å	-	OUTLIER(S) worst is C-N- CA: 4.193 σ	
A 168	SER	50	-	Allowed (0.23%) General / -32.4,-62.4	78.2% ( <i>p</i> ) chi angles: 59	0.08Å	-	OUTLIER(S) worst is C-N- CA: 4.298 σ	
A 169	GLU	50	-	Favored (5.69%) General / -117.4,33.3	2.7% ( <i>mm-40</i> ) chi angles: 256.4,281.4,274.6	0.121Å	-	-	
A 170	GLY	50	-	Favored (33.7%) Glycine / 91.3,21.9	-	-	-	-	
A 171	GLN	50	-	Favored (47.8%) General / -72.0,-7.3	47.4% ( <i>tt0</i> ) chi angles: 198.2,180.8,7.4	0.129Å	-	-	
A 172	ILE	50	-	Favored (6.8%) Isoleucine or valine / -118.7,7.5	32.1% ( <i>pt</i> ) chi angles: 56.3,176.9	0.223Å	-	-	

A 173	GLY	50	-	Favored (78.98%) Glycine / 84.1,11.2	-	-	-	-
A 174	LEU	50	-	Allowed (1.7%) General / -95.9,33.3	80.2% ( <i>mt</i> ) chi angles: 301.2,181.5	0.104Å	-	-
A 175	LYS	50	-	Allowed (0.6%) General / 56.6,-111.2	49.2% ( <i>mttp</i> ) chi angles: 285.1,173.8,165,54	0.233Å	-	-
A 176	ASN	50	-	Favored (51.31%) General / -95.0,-2.0	21.8% ( <i>p-10</i> ) chi angles: 63.2,316	0.07Å	-	-
A 177	VAL	50	-	Favored (8.46%) Isoleucine or valine / -55.6,143.6	37.3% ( <i>t</i> ) chi angles: 165.6	0.082Å	-	-
A 178	SER	50	-	Favored (37.05%) General / -75.2,-46.0	73% ( <i>p</i> ) chi angles: 58	0.069Å	-	-
A 179	ASN	50	-	Allowed (0.83%) General / 178.4,166.8	15.3% ( <i>p-10</i> ) chi angles: 64,298.3	0.083Å	-	-
A 180	VAL	50	-	Favored (45.4%) Isoleucine or valine / -134.4,140.7	25% ( <i>m</i> ) chi angles: 302.1	0.089Å	-	-
A 181	CYS	50	-	Favored (45.05%) General / -100.0,5.0	6.5% ( <i>m</i> ) chi angles: 317.1	0.117Å	-	-
A 182	VAL	50	-	Favored (50.81%) Pre-proline / -131.3,163.2	30.8% ( <i>m</i> ) chi angles: 294.7	0.052Å	-	-
A 183	PRO	50	-	Favored (13.46%) Trans-proline / -72.9,128.7	60.2% ( <i>Cg_exo</i> ) chi angles: 334.3	0.05Å	-	-
A 184	GLN	50	-	Favored (50.32%) General /	45% ( <i>tp60</i> ) chi angles: 174.6,60.1,72.8	0.101Å	-	-



-109.3,135.5

A 185	GLN	50	-	Favored (30.94%) General / -72.6,126.9	14.9% ( <i>tt0</i> ) chi angles: 199,173.1,250.7	0.033Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 186	VAL	50	-	Favored (53.34%) Isoleucine or valine / -128.9,138.9	56.6% ( <i>t</i> ) chi angles: 170.8	0.077Å	-	-	
A 187	THR	50	-	Allowed (0.25%) General / 174.6,170.3	5.8% ( <i>t</i> ) chi angles: 177.2	0.126Å	-	-	
A 188	ILE	50	-	Favored (11.12%) Isoleucine or valine / -81.6,-19.4	2.4% ( <i>pp</i> ) chi angles: 60.9,98.8	0.138Å	-	-	
A 189	GLY	50	-	Allowed (1.96%) Glycine / 144.9,-22.9	-	-	-	-	
A 190	LYS	50	-	Favored (45.6%) Pre-proline / -86.0,162.8	55.3% ( <i>mtpt</i> ) chi angles: 294.2,182.7,69.2,168.5	0.069Å	-	-	
A 191	PRO	50	-	Favored (18.52%) Trans-proline / -77.0,138.7	67.2% ( <i>Cg_endo</i> ) chi angles: 27.9	0.027Å	-	-	
A 192	VAL	50	-	Favored (16.49%) Isoleucine or valine / -96.2,140.8	74.8% ( <i>t</i> ) chi angles: 173	0.105Å	-	-	
A 193	SER	50	-	Favored (10.27%) General / -105.5,-29.3	7.3% ( <i>t</i> ) chi angles: 196.6	0.099Å	-	-	
A 194	TRP	50	-	Favored (37.74%) General / -157.1,159.2	20.3% ( <i>t-105</i> ) chi angles: 168.9,274.5	0.109Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.201 σ	

A 195	ILE	99.99	-	(8.27%) Isoleucine or valine / -149.4,155.4	18.9% ( <i>tt</i> ) chi angles: 188.9,163.4	0.082Å	-	-
A 196	SER	50	-	Favored (48.47%) General / -133.9,143.8	9.4% ( <i>t</i> ) chi angles: 192.8	0.079Å	-	-
A 197	CYS	50	-	Favored (22.09%) General / -117.4,113.4	37.4% ( <i>m</i> ) chi angles: 308.1	0.069Å	-	-
A 198	GLY	50	-	Favored (9.55%) Glycine / -79.2,-155.7	-	-	-	-
A 199	TYR	50	0.488Å O with A 149 SER HB3	Favored (42.11%) General / -76.6,-42.6	5.2% ( <i>m-30</i> ) chi angles: 288.8,16.4	0.21Å	-	-
A 200	TYR	50	-	Allowed (1.91%) General / -136.8,-6.6	6.6% ( <i>m-85</i> ) chi angles: 322.5,291.8	0.073Å	-	-
A 201	HIS	50	-	Favored (19.55%) General / -131.6,167.4	53.4% ( <i>p-80</i> ) chi angles: 66,283.9	0.023Å	-	-
A 202	SER	50	-	Favored (8.48%) General / -139.2,176.7	20.3% ( <i>m</i> ) chi angles: 305.6	0.042Å	-	-
A 203	ALA	50	-	Favored (2.7%) General / -170.4,145.8	-	0.102Å	-	-
A 204	PHE	50	-	Favored (27.49%) General / -128.5,162.3	14% ( <i>p90</i> ) chi angles: 65.2,73.9	0.084Å	-	OUTLIER(S) worst is CA- CB-CG: 4.312 σ
A 205	VAL	50	-	Favored (73.21%) Isoleucine or valine / -124.9,130.8	74.8% ( <i>t</i> ) chi angles: 179.3	0.125Å	-	-

# Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles  
 Avg: Clashscore: Outliers: 3 of Poor rotamers: 7 of Outliers: Outliers: Outliers: 33

		50.27	0.73	362	301	1 of 319	0 of 364	of 364
A 206	THR	50	-	Favored (4.83%) General / -75.2,179.9	80.6% ( <i>p</i> ) chi angles: 61.4	0.083Å	-	-
A 207	THR	50	-	Favored (69.68%) General / -56.9,-36.1	3.3% ( <i>p</i> ) chi angles: 40.5	0.068Å	-	-
A 208	ASP	50	-	Favored (5.09%) General / -111.1,32.7	4.2% ( <i>p-10</i> ) chi angles: 42.9,322.8	0.177Å	-	OUTLIER(S) worst is CA- CB-CG: 6.433 σ
A 209	GLY	50	-	Favored (76.89%) Glycine / 74.6,22.7	-	-	-	-
A 210	GLU	50	-	Favored (35.19%) General / -92.7,122.5	13.8% ( <i>mt-10</i> ) chi angles: 304.4,154.7,305.8	0.056Å	-	-
A 211	LEU	50	-	Favored (41.06%) General / -95.6,126.7	57.1% ( <i>tp</i> ) chi angles: 174.6,60.5	0.073Å	-	-
A 212	TYR	50	-	Favored (38.45%) General / -120.6,121.5	90.1% ( <i>m-85</i> ) chi angles: 293.4,84.6	0.024Å	-	-
A 213	VAL	50	-	Favored (10.89%) Isoleucine or valine / -109.5,154.7	24% ( <i>m</i> ) chi angles: 293.4	0.042Å	-	-
A 214	PHE	50	-	Favored (6.89%) General / -171.4,163.1	14.2% ( <i>p90</i> ) chi angles: 46.9,275.7	0.028Å	-	-
A 215	GLY	50	-	Favored (19.61%) Glycine / 99.8,-164.2	-	-	-	-
A 216	GLU	50	-	Favored (82.58%) Pre-proline / -58.2,128.9	34.1% ( <i>tt0</i> ) chi angles: 189.1,180.3,104.6	0.094Å	-	-
A 217	PRO	50	-	Allowed (0.29%) Trans-proline /	11.3% ( <i>Cg_endo</i> ) chi angles: 40	0.034Å	-	-

-98.9,-13.1

A 218	GLU	50	-	Favored (2.33%) General / -43.2,121.9	0.6% chi angles: 317.7,321.6,261.1	0.095Å	-	OUTLIER(S) worst is C-N- CA: 4.12 $\sigma$
A 219	ASN	50	-	Allowed (0.08%) General / 87.2,17.7	61.8% ( <i>m-80</i> ) chi angles: 304.6,295.4	0.148Å	-	-
A 220	GLY	50	-	Favored (69.67%) Glycine / 77.9,22.1	-	-	-	-
A 221	LYS	50	-	Favored (5.87%) General / -81.8,10.6	10.2% ( <i>pttt</i> ) chi angles: 65.7,200.4,173,220.8	0.192Å	-	-
A 222	LEU	50	-	Favored (14.34%) General / -102.0,-22.2	51.8% ( <i>mt</i> ) chi angles: 304.7,185	0.141Å	-	-
A 223	GLY	50	-	Favored (7.02%) Glycine / 72.4,55.1	-	-	-	-
A 224	LEU	50	-	Favored (28.07%) Pre-proline / -140.1,165.8	83% ( <i>mt</i> ) chi angles: 291.1,177.6	0.083Å	-	-
A 225	PRO	50	-	Favored (11.52%) Trans-proline / -85.1,164.2	38.3% ( <i>Cg_endo</i> ) chi angles: 36.6	0.042Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 226	ASN	50	-	-	Favored (63.56%) General / -53.6,-37.9	24.1% ( <i>p-10</i> ) chi angles: 68.6,322.4	0.128Å	-	-
A 227	GLN	50	-	-	Favored (93.69%) General / -64.6,-39.4	27.9% ( <i>mm100</i> ) chi angles: 304.7,305.2,126.8	0.1Å	-	-
A 228	LEU	50	-	-	Favored (41.63%) General /	52.2% ( <i>mt</i> ) chi angles: 306.9,182.9	0.149Å	-	-

				-79.9,-23.6				
				Favored				
A	LEU	50	-	(71.82%)	91.1% ( <i>mt</i> )	0.156Å	-	-
229				General /	chi angles: 297.3,172			
				-66.3,-31.2				
				Favored				
A	GLY	50	-	(79.1%)	-	-	-	-
230				Glycine /				
				-67.2,-45.7				
				Allowed				
A	ASN	50	-	(0.82%)	33.2% ( <i>t30</i> )	0.088Å	-	-
231				General /	chi angles: 177.4,39.9			
				-89.2,36.5				
				Favored				
A	HIS	50	-	(59.16%)	15.9% ( <i>p80</i> )	0.094Å	-	-
232				General /	chi angles: 76.9,75.4			
				-73.2,-9.8				
				Favored				
A	ARG	50	-	(56.85%)	43.5% ( <i>mtt-85</i> )	0.084Å	-	-
233				General /	chi angles:			
				-85.9,-9.5	298.9,170.1,159.4,254.1			
				Favored				
A	THR	50	-	(34.56%)	86.5% ( <i>m</i> )	0.093Å	-	-
234				Pre-proline /	chi angles: 301.7			
				-93.3,147.9				
				Favored				
A	PRO	50	-	(6.77%)	76.8% ( <i>Cg_exo</i> )	0.046Å	-	-
235				Trans-proline /	chi angles: 332.2			
				-69.5,119.9				
				Favored				
A	GLN	50	-	(50.41%)	23.3% ( <i>mt-30</i> )	0.118Å	-	-
236				General /	chi angles:			
				-125.0,144.4	297,162,117.8			
				Favored				
A	LEU	50	-	(56.8%)	22.2% ( <i>tp</i> )	0.065Å	-	-
237				General /	chi angles: 187,73.6			
				-64.0,135.8				
				Favored				
A	VAL	50	-	(13.92%)	79.8% ( <i>t</i> )	0.049Å	-	-
238				Isoleucine or	chi angles: 172.5			
				valine /				
				-76.4,112.2				
				Favored				
A	SER	50	-	(58.56%)	7.4% ( <i>p</i> )	0.087Å	-	-
239				General /	chi angles: 44.9			
				-75.3,-26.1				
				Favored				
A	GLU	50	-	(59.68%)	3.1% ( <i>mp0</i> )	0.059Å	-	-
240				General /	chi angles:			
					310,91.7,294.1			

-81.8,-8.3

Favored

A 241	ILE	50	-	(47.71%) Pre-proline / -114.1,98.3	57.4% ( <i>mt</i> ) chi angles: 299.3,181.5	0.042Å	-	-
A 242	PRO	50	-	Allowed (1.54%) Trans-proline / -83.7,-27.9	36.6% ( <i>Cg_endo</i> ) chi angles: 36.8	0.055Å	-	-
A 243	GLU	50	-	Favored (20.18%) General / -86.6,156.0	10.8% ( <i>pm0</i> ) chi angles: 84.4,292.6,359.2	0.117Å	-	OUTLIER(S) worst is CB- CG-CD: 4.2 $\sigma$
A 244	LYS	50	-	Favored (17.04%) General / -59.3,123.5	68% ( <i>mmtt</i> ) chi angles: 297.6,305.9,194.4,170.3	0.053Å	-	-
A 245	VAL	50	-	Favored (39.78%) Isoleucine or valine / -81.2,126.5	71.9% ( <i>t</i> ) chi angles: 171.9	0.055Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 246	ILE	50	-		Favored (12.1%) Isoleucine or valine / -96.9,-42.7	74.6% ( <i>mt</i> ) chi angles: 297.3,178.2	0.119Å	-	-
A 247	GLN	50	-		Favored (45.66%) General / -141.5,154.6	62.2% ( <i>mt-30</i> ) chi angles: 290.2,164.3,32.8	0.092Å	-	-
A 248	VAL	50	-		Favored (47.63%) Isoleucine or valine / -132.8,140.3	12.5% ( <i>p</i> ) chi angles: 65.7	0.096Å	-	-
A 249	ALA	50	-		Favored (6.64%) General / -130.5,103.4	-	0.05Å	-	-
A 250	CYS	50	-		Favored (32.47%) General / -91.4,120.7	85.6% ( <i>m</i> ) chi angles: 300.4	0.032Å	-	-

A 251	GLY	50	-	Favored (9.36%) Glycine / -92.4,-140.1	-	-	-	-
A 252	GLY	50	-	Allowed (0.39%) Glycine / -79.2,-91.4	-	-	-	-
A 253	GLU	50	-	Favored (53.24%) General / -92.7,4.7	10.6% ( <i>mm</i> -40) chi angles: 307.2,324.8,295.8	0.102Å	-	-
A 254	HIS	50	-	Favored (17.35%) General / -143.4,169.6	11.9% ( <i>p</i> -80) chi angles: 80.7,295.2	0.037Å	-	-
A 255	THR	50	-	Favored (47.02%) General / -134.5,157.2	11.7% ( <i>m</i> ) chi angles: 312.6	0.122Å	-	-
A 256	VAL	50	0.51Å HG22 with A 265 THR HG22	Favored (28.97%) Isoleucine or valine / -136.1,146.6	85.2% ( <i>t</i> ) chi angles: 174.9	0.082Å	-	-
A 257	VAL	50	-	Favored (46.11%) Isoleucine or valine / -132.3,141.1	40.8% ( <i>t</i> ) chi angles: 166.7	0.144Å	-	-
A 258	LEU	50	-	Favored (57.06%) General / -115.5,131.0	60.6% ( <i>tp</i> ) chi angles: 179,64.9	0.114Å	-	-
A 259	THR	50	-	Allowed (1.45%) General / -116.5,-168.4	17.3% ( <i>p</i> ) chi angles: 74.7	0.116Å	-	-
A 260	GLU	50	-	Favored (77.74%) General / -61.1,-35.7	6.1% ( <i>pt</i> -20) chi angles: 46.8,168.9,290.4	0.085Å	-	-
A 261	ASN	50	-	Allowed (1.37%) General / -143.9,6.1	58% ( <i>m</i> -80) chi angles: 283.6,285.7	0.066Å	-	-
A 262	ALA	50	-	Favored (10.62%) General / -148.4,176.0	-	0.057Å	-	-

A 263	VAL	50	-	Favored (50.52%) Isoleucine or valine / -123.5,139.3	49.6% ( <i>t</i> ) chi angles: 168.5	0.074Å	-	-
A 264	TYR	50	-	Favored (50.4%) General / -127.7,148.9	5.4% ( <i>m-85</i> ) chi angles: 265.9,103.9	0.097Å	-	-
A 265	THR	50	0.51Å HG22 with A 256 VAL HG22	Favored (42.08%) General / -140.6,159.5	41.8% ( <i>p</i> ) chi angles: 67.6	0.053Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 50.27</div> <div>Clashscore: 0.73</div> <div>Outliers: 3 of 362</div> <div>Poor rotamers: 7 of 301</div> <div>Outliers: 1 of 319</div> <div>Outliers: 0 of 364</div> <div>Outliers: 33 of 364</div> </div>								
A 266	PHE	50	-	Favored (21.97%) General / -161.4,155.2	6.8% ( <i>p90</i> ) chi angles: 40.3,269.6	0.072Å	-	-
A 267	GLY	50	-	Favored (15.66%) Glycine / 106.0,-158.3	-	-	-	-
A 268	LEU	50	-	Favored (58.1%) General / -61.3,136.6	22.8% ( <i>tp</i> ) chi angles: 192.1,66.8	0.05Å	-	OUTLIER(S) worst is C-N- CA: 4.85 σ
A 269	GLY	50	-	Favored (5.37%) Glycine / -130.5,-0.5	-	-	-	OUTLIER(S) worst is C-N- CA: 4.04 σ
A 270	GLN	50	-	Allowed (0.14%) General / -45.5,-22.4	80.5% ( <i>mt-30</i> ) chi angles: 288.1,179.4,19.2	0.086Å	-	-
A 271	PHE	50	-	Favored (16.94%) General / -114.1,8.1	19.3% ( <i>m-30</i> ) chi angles: 301.5,331.7	0.088Å	-	-
A 272	GLY	50	-	Favored (58.25%) Glycine / 97.0,5.8	-	-	-	-
A 273	GLN	50	-	Favored (52.92%) General /	18.6% ( <i>pm0</i> ) chi angles: 71.8,277.3,29.9	0.226Å	-	-



-75.9,-6.9

Favored

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 274	LEU	50	-	-	Favored (34.61%) General / -81.3,-28.3	87.6% (mt) chi angles: 290.7,174.8	0.083Å	-	-

Favored

A 275	GLY	50	-	-	Favored (71.63%) Glycine / 70.7,27.9	-	-	-	-
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Favored

A 276	LEU	50	-	-	Favored (10.73%) General / -120.4,1.7	87% (mt) chi angles: 292.2,168.5	0.036Å	-	-
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Favored

A 277	GLY	50	-	-	Favored (12.57%) Glycine / 127.9,169.0	-	-	-	-
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Favored

A 278	THR	50	-	-	Favored (59.06%) General / -77.8,-15.4	10.4% (p) chi angles: 44.4	0.123Å	-	-
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Favored

A 279	PHE	50	-	-	Favored (12.31%) General / -115.8,-2.7	17% (m-85) chi angles: 312.7,125	0.09Å	-	-
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Favored (7.5%)

A 280	LEU	50	-	-	Favored (7.5%) General / -88.7,88.2	29% (tp) chi angles: 187.3,69.7	0.05Å	-	-
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Favored

A 281	PHE	50	-	-	Favored (62.22%) General / -72.4,-27.3	17.9% (m-30) chi angles: 306.9,313.8	0.133Å	-	-
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Favored

A 282	GLU	50	-	-	Favored (23.8%) General / -163.3,165.9	1.6% (pm0) chi angles: 39.4,284.4,309.8	0.079Å	-	-
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Favored

A 283	THR	50	-	-	Favored (7.08%) General / -154.3,125.0	13.7% (t) chi angles: 190.3	0.09Å	-	-
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Favored

A 284	SER	50	-	-	Favored (32.4%) General / -81.3,-33.7	75.7% (m) chi angles: 294.5	0.133Å	-	-
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Favored

A 285	GLU	50	-	-	Favored (26.49%) Pre-proline / -102.8,160.3	0.7% chi angles: 98,311.1,340.9	0.109Å	-	-
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#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg: Clashscore: 50.27 0.73 Outliers: 3 of 362 Poor rotamers: 7 of 301 Outliers: 1 of 319 Outliers: 0 of 364 Outliers: 33 of 364

A 286	PRO	50	-	Favored (29.73%) Trans-proline / -72.6,138.6	21.4% (Cg_exo) chi angles: 344.3	0.083Å	-	-
A 287	LYS	50	-	Favored (49.51%) General / -125.4,146.6	55.5% (mttp) chi angles: 285.3,172.2,170.7,67	0.064Å	-	-
A 288	VAL	50	-	Favored (28.23%) Isoleucine or valine / -82.5,133.8	77.7% (t) chi angles: 172.3	0.051Å	-	-
A 289	ILE	50	-	Favored (3.64%) Isoleucine or valine / -85.0,93.6	42.8% (mt) chi angles: 296.7,184.3	0.089Å	-	-
A 290	GLU	50	-	Favored (59.91%) General / -77.2,-13.6	73.2% (mm-40) chi angles: 285.3,301.3,317.1	0.065Å	-	-
A 291	ASN	50	-	Allowed (0.1%) General / -73.0,18.7	2.3% (m120) chi angles: 311.4,166.4	0.076Å	-	OUTLIER(S) worst is CA- CB-CG: 9.084 σ
A 292	ILE	50	-	OUTLIER (0.02%) Isoleucine or valine / -158.3,46.6	1.4% (pp) chi angles: 32.9,64.7	0.239Å	-	-
A 293	ARG	50	-	Favored (7.01%) General / -70.7,0.5	1.5% (mpt_?) chi angles: 251.4,57,170.6,95.1	0.148Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.395 σ
A 294	ASP	50	-	Favored (41.02%) General / -83.2,-17.9	18.1% (p-10) chi angles: 60.8,312.5	0.056Å	-	-
A 295	GLN	50	-	Favored (19.43%) General / -108.6,108.5	33% (mm-40) chi angles: 294.7,304.4,273.3	0.046Å	-	-
A 296	THR	50	-	Allowed (1.67%) General / -74.0,77.9	22.5% (m) chi angles: 309.7	0.022Å	-	-

A 297	ILE	50	-	Favored (32.94%) Isoleucine or valine / -68.4,129.5	32.8% ( <i>mm</i> ) chi angles: 297.8,307.1	0.068Å	-	-
A 298	SER	50	-	Favored (9.59%) General / -120.9,-5.3	57.9% ( <i>p</i> ) chi angles: 55.6	0.124Å	-	-
A 299	TYR	50	-	Favored (6.83%) General / -156.4,127.3	4.7% ( <i>t80</i> ) chi angles: 177.8,111.5	0.083Å	-	-
A 300	ILE	50	-	Favored (5.5%) Isoleucine or valine / -114.4,169.5	44.8% ( <i>pt</i> ) chi angles: 60.6,168.8	0.111Å	-	-
A 301	SER	50	-	Favored (2.89%) General / -167.5,137.8	17.7% ( <i>t</i> ) chi angles: 169.3	0.108Å	-	-
A 302	CYS	50	-	Favored (35.78%) General / -137.1,161.6	53.2% ( <i>m</i> ) chi angles: 284.1	0.074Å	-	-
A 303	GLY	50	-	Allowed (1.11%) Glycine / 177.8,127.9	-	-	-	-
A 304	GLU	50	-	Favored (2.27%) General / 53.8,-129.4	0.3% chi angles: 182.8,234.6,248.5	0.216Å	-	OUTLIER(S) worst is C- CA-CB: 4.827 σ
A 305	ASN	50	-	Allowed (0.97%) General / -120.0,56.1	94.5% ( <i>m-20</i> ) chi angles: 291,330.1	0.128Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 50.27</div> <div>Clashscore: 0.73</div> <div>Outliers: 3 of 362</div> <div>Poor rotamers: 7 of 301</div> <div>Outliers: 1 of 319</div> <div>Outliers: 0 of 364</div> <div>Outliers: 33 of 364</div> </div>								
A 306	HIS	50	-	Favored (26.1%) General / -151.8,168.1	13.5% ( <i>p-80</i> ) chi angles: 82.2,289.3	0.058Å	-	-
A 307	THR	50	-	Favored (28.03%) General / -134.4,164.2	27.4% ( <i>m</i> ) chi angles: 308	0.138Å	-	-

A 308	ALA	50	-	Favored (20.84%) General / -147.8,135.3	-	0.089Å	-	-
A 309	LEU	50	-	Favored (54.86%) General / -121.6,137.2	8.6% ( <i>mt</i> ) chi angles: 321.9,173.7	0.073Å	-	-
A 310	ILE	50	-	Favored (56%) Isoleucine or valine / -118.7,136.4	14.5% ( <i>mt</i> ) chi angles: 280.1,180	0.14Å	-	-
A 311	THR	50	-	Favored (11.95%) General / -85.6,171.1	56.7% ( <i>p</i> ) chi angles: 65.3	0.121Å	-	OUTLIER(S) worst is C-N- CA: 4.776 $\sigma$
A 312	ASP	50	-	Favored (7.55%) General / -48.6,-56.8	20.5% ( <i>p-10</i> ) chi angles: 49,358	0.048Å	-	OUTLIER(S) worst is CA- CB-CG: 5.524 $\sigma$
A 313	ILE	50	-	Favored (15.78%) Isoleucine or valine / -75.8,-21.4	48.7% ( <i>pt</i> ) chi angles: 61.9,170.8	0.179Å	-	-
A 314	GLY	50	-	Favored (4.64%) Glycine / 116.0,22.3	-	-	-	-
A 315	LEU	50	-	Favored (20%) General / -85.5,159.1	55.4% ( <i>mt</i> ) chi angles: 307.1,175.7	0.025Å	-	-
A 316	MET	50	-	Favored (31.09%) General / -141.8,136.8	54.9% ( <i>ttp</i> ) chi angles: 191.9,177.5,73.8	0.041Å	-	-
A 317	TYR	50	-	Favored (50.36%) General / -122.7,142.8	4.3% ( <i>m-85</i> ) chi angles: 280.3,49	0.067Å	-	-
A 318	THR	50	-	Favored (41.02%) General / -134.0,159.3	54.1% ( <i>p</i> ) chi angles: 65.4	0.086Å	-	-
A 319	PHE	50	-	Favored (36.83%) General / -158.9,162.1	17.2% ( <i>p90</i> ) chi angles: 49.8,278.9	0.048Å	-	OUTLIER(S) worst is CA- CB-CG: 4.062 $\sigma$
				Favored				

A 320	GLY	50	-	(16.14%) Glycine / 107.3,-155.9	-	-	-	-	
A 321	ASP	50	-	Favored (18.34%) General / -58.2,124.1	49.3% ( <i>t0</i> ) chi angles: 185.4,17.8	0.027Å	-	-	
A 322	GLY	50	-	Favored (42.14%) Glycine / -104.8,0.2	-	-	-	-	
A 323	ARG	50	-	Allowed (0.48%) General / -51.0,111.0	55.7% ( <i>mtt85</i> ) chi angles: 289.9,161.6,179,107.4	0.038Å	-	-	
A 324	HIS	50	-	Allowed (1.05%) General / 69.5,43.1	85.5% ( <i>m-70</i> ) chi angles: 302.5,302	0.209Å	-	-	
A 325	GLY	50	-	Favored (72.17%) Glycine / 66.8,22.8	-	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 326	LYS	50	-	Favored (60.28%) General / -75.9,-14.4	53% ( <i>pttt</i> ) chi angles: 53.3,177.3,176.7,171.7	0.189Å	-	-	
A 327	LEU	50	-	Favored (56.91%) General / -75.5,-24.2	96.8% ( <i>mt</i> ) chi angles: 294.2,173.7	0.093Å	-	-	
A 328	GLY	50	-	Favored (84.03%) Glycine / 57.9,37.2	-	-	-	-	
A 329	LEU	50	-	Favored (59.74%) General / -74.6,-26.2	30.3% ( <i>mt</i> ) chi angles: 295.3,160	0.055Å	-	-	
A 330	GLY	50	-	Favored (2.24%) Glycine / 117.3,-40.8	-	-	-	-	
A				Favored					

331	LEU	50	-	(27.89%) General / -68.6,125.9	28.8% ( <i>mt</i> ) chi angles: 312.1,179.4	0.081Å	-	-
A 332	GLU	50	-	Favored (18.5%) General / -89.4,-30.2	11% ( <i>tm-20</i> ) chi angles: 185.2,292.5,329.5	0.056Å	-	-
A 333	ASN	50	-	Allowed (0.1%) General / -29.5,128.8	24.6% ( <i>t-20</i> ) chi angles: 183.2,277.5	0.059Å	-	-
A 334	PHE	50	-	Favored (26.71%) General / -69.8,-5.6	2.8% ( <i>m-30</i> ) chi angles: 311.7,346.1	0.081Å	-	OUTLIER(S) worst is CA- CB-CG: 4.48 σ
A 335	THR	50	-	Favored (30.32%) General / -64.6,156.4	2.8% ( <i>t</i> ) chi angles: 201.1	0.135Å	-	-
A 336	ASN	50	-	Favored (17.86%) General / -89.2,158.4	99.4% ( <i>m-20</i> ) chi angles: 288.5,341.6	0.049Å	-	-
A 337	HIS	50	-	Favored (7.41%) General / -128.7,104.0	74.3% ( <i>m-70</i> ) chi angles: 284.7,268.4	0.091Å	-	-
A 338	PHE	50	-	Favored (36.17%) General / -84.8,-18.1	54.8% ( <i>m-85</i> ) chi angles: 288.4,77.2	0.173Å	-	-
A 339	ILE	50	-	Favored (44.52%) Pre-proline / -117.1,158.3	42.3% ( <i>pt</i> ) chi angles: 58.9,168.4	0.068Å	-	-
A 340	PRO	50	-	Favored (9.81%) Trans-proline / -63.1,121.8	42.2% ( <i>Cg_exo</i> ) chi angles: 337.7	0.032Å	-	-
A 341	THR	50	-	Favored (48.84%) General / -105.5,134.3	62.6% ( <i>m</i> ) chi angles: 303.7	0.08Å	-	-
A 342	LEU	50	-	Favored (30.69%) General / -56.1,127.5	41.8% ( <i>tp</i> ) chi angles: 171.7,58.5	0.071Å	-	-
A				Favored	72.2% ( <i>m</i> )			

343	CYS	50	-	(6.06%) General / -81.3,88.7 Favored (70.3%) General / -59.3,-32.7 Favored (69.39%) General / -57.0,-35.6	chi angles: 297.2	0.065Å	-	-	
A 344	SER	50	-		88.6% ( <i>p</i> ) chi angles: 61.9	0.146Å	-	-	
A 345	ASN	50	-		37.3% ( <i>p</i> -10) chi angles: 60.4,341.4	0.102Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 346	PHE	50	-		Favored (58.11%) General / -87.0,-1.8	46% ( <i>m</i> -85) chi angles: 284.4,294	0.145Å	-	-
A 347	LEU	50	-		Favored (68.74%) General / -56.7,-35.7	41.6% ( <i>mt</i> ) chi angles: 291,161.2	0.072Å	-	-
A 348	ARG	50	-		Favored (3.99%) General / -86.2,16.9	94.9% ( <i>mtt</i> -85) chi angles: 293.4,183.3,177.8,279.6	0.124Å	-	-
A 349	PHE	50	-		Favored (5.21%) General / -137.9,-178.3	94.1% ( <i>m</i> -85) chi angles: 298.4,88.4	0.07Å	-	-
A 350	ILE	50	-		Favored (2.19%) Isoleucine or valine / -128.9,93.7	81.7% ( <i>mt</i> ) chi angles: 299.1,175.5	0.043Å	-	-
A 351	VAL	50	-		Favored (33.69%) Isoleucine or valine / -81.8,120.6	39.7% ( <i>t</i> ) chi angles: 185	0.05Å	-	-
A 352	LYS	50	-		Favored (6.55%) General / -126.8,-3.1	30.5% ( <i>mmmt</i> ) chi angles: 296.3,304.5,303.7,186.8	0.165Å	-	-
A 353	LEU	50	-		Favored (35.25%) General / -140.2,138.7 Favored	84.6% ( <i>mt</i> ) chi angles: 298,171.2	0.066Å	-	-

A 354	VAL	50	-	(24.13%) Isoleucine or valine / -144.4,140.2	11.9% ( <i>p</i> ) chi angles: 62	0.085Å	-	-
A 355	ALA	50	-	Favored (7.33%) General / -128.1,103.6	-	0.026Å	-	-
A 356	CYS	50	-	Favored (36.89%) General / -62.7,128.6	67.9% ( <i>m</i> ) chi angles: 287.9	0.073Å	-	-
A 357	GLY	50	-	Favored (33.66%) Glycine / -93.4,-157.9	-	-	-	-
A 358	GLY	50	-	Allowed (1.1%) Glycine / -89.2,-94.1	-	-	-	-
A 359	CYS	50	-	Allowed (0.1%) General / -62.6,6.0	29.5% ( <i>p</i> ) chi angles: 66.1	0.063Å	-	-
A 360	HIS	50	-	Favored (6.21%) General / -157.8,-176.9	20.2% ( <i>p</i> -80) chi angles: 78.4,289.6	0.064Å	-	-
A 361	MET	50	-	Favored (4.53%) General / -165.4,138.8	26.2% ( <i>ttp</i> ) chi angles: 174.7,153.2,74.7	0.087Å	-	-
A 362	VAL	50	-	Favored (38.1%) Isoleucine or valine / -115.9,140.3	99.2% ( <i>t</i> ) chi angles: 178.5	0.092Å	-	-
A 363	VAL	50	-	Favored (39.92%) Isoleucine or valine / -128.3,155.5	46.3% ( <i>t</i> ) chi angles: 183.4	0.103Å	-	-
A 364	PHE	50	-	Favored (44.23%) General / -133.3,134.8	8.7% ( <i>t</i> 80) chi angles: 156.3,80.6	0.025Å	-	-
A 365	ALA	50	-	Favored (24.28%) General /	-	0.122Å	-	-



-154.7,147.4

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 50.27	Clashscore: 0.73	Outliers: 3 of 362	Poor rotamers: 7 of 301	Outliers: 1 of 319	Outliers: 0 of 364	Outliers: 33 of 364
A 366	ALA	50	-	Favored (66%) Pre-proline / -82.2,151.2	-	0.014Å	-	-
A 367	PRO	50	-	Favored (4.09%) Trans-proline / -89.4,141.7	7.6% ( <i>Cg_endo</i> ) chi angles: 40.7	0.076Å	-	-
A 368	HIS	50	-	Favored (62.18%) General / -72.0,-26.3	70.8% ( <i>m-70</i> ) chi angles: 285.2,301.1	0.207Å	-	-
A 369	ARG	99.99	-	-	4.7% ( <i>tpt85</i> ) chi angles: 198.8,70.9,216.3,97	0.082Å	-	-

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