Viewing RPGR_sm_6-369H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	5.12		93rd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	8	2.66%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	351	96.96%	Goal: >98%
	MolProbity score$^{\wedge}$	1.77		87th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	24 / 2834	0.85%	Goal: 0%
	Bad backbone angles:	8 / 3839	0.21%	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.

$^{\wedge}$ 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: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 6		GLU	50	-	-	8.3% (*mt-10*) chi angles: 284.6,211.7,35	0.087Å	-	-
A 7		LEU	50	0.433Å HD23 with A 8 MET O	Favored (42.54%) General / -71.4,130.9	7% (*tt*) chi angles: 196.1,153.3	0.1Å	-	-
A 8		MET	50	0.433Å O with A 7 LEU HD23	Favored (25.2%) Pre-proline / -55.5,119.5	33.7% (*ttm*) chi angles: 185.5,200,299.8	0.063Å	-	-
A 9		PRO	50	-	Favored (41.91%) Trans-proline / -58.6,154.6	60.2% (*Cg_endo*) chi angles: 27.1	0.041Å	-	-
A 10		ASP	50	-	Favored (65.92%) General / -58.1,-30.1	83.7% (*m-20*) chi angles: 295.4,332.9	0.037Å	-	-
					Favored				

A 11	SER	50	-	(66.02%) General / -66.4,-20.2	57% (*p*) chi angles: 55.5	0.088Å	-	-
A 12	GLY	50	-	Favored (13.47%) Glycine / 112.8,-159.8	-	-	-	-
A 13	ALA	50	-	Favored (42.98%) General / -152.9,159.6	-	0.052Å	-	-
A 14	VAL	50	-	Favored (43.66%) Isoleucine or valine / -91.0,126.5	45.3% (*t*) chi angles: 183.7	0.066Å	-	-
A 15	PHE	50	-	Favored (52.84%) General / -110.8,134.1	68.6% (*m-85*) chi angles: 300.6,81	0.078Å	-	-
A 16	THR	50	-	Favored (51.84%) General / -116.4,137.8	81.4% (*p*) chi angles: 61.1	0.01Å	-	-
A 17	PHE	50	0.438Å CD1 with A 328 GLY HA2	Favored (47.8%) General / -129.7,153.8	98.1% (*m-85*) chi angles: 296.8,271.3	0.042Å	-	-
A 18	GLY	50	0.532Å HA2 with A 324 HIS O	Favored (46.07%) Glycine / 75.6,-154.8	-	-	-	-
A 19	LYS	50	-	Favored (7.08%) General / -90.2,74.1	25.1% (*mtpt*) chi angles: 300.8,184,69.6,207.5	0.047Å	-	-
A 20	SER	50	0.451Å O with A 21 LYS HB2	Favored (58.5%) General / -82.7,-11.2	93.8% (*p*) chi angles: 63.3	0.037Å	-	-
A 21	LYS	50	0.55Å HB2 with A 60 GLY HA2	Favored (3.53%) General / 75.7,9.3	0.5% chi angles: 259.1,48.5,154.5,42.1	0.071Å	-	-
A 22	PHE	50	-	Favored (53.5%) General / -112.8,135.5	40.6% (*t80*) chi angles: 176.1,58.2	0.059Å	-	-
A 23	ALA	50	-	Favored (28.64%) General /	-	0.067Å	-	-

56.3,37.2

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 24		GLU	50	-	Favored (21.27%) General / 57.6,32.0	11.3% (*mt-10*) chi angles: 290.6,150.1,89	0.049Å	-	-
A 25		ASN	50	-	Favored (13.52%) General / 63.4,23.0	65% (*m-20*) chi angles: 303.7,329.1	0.079Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 26		ASN	50	-	Favored (51.27%) Pre-proline / -88.3,156.5	63.3% (*m-80*) chi angles: 302.5,289.1	0.087Å	-	-
A 27		PRO	50	-	Allowed (0.22%) Trans-proline / -50.4,108.4	81.8% (*Cg_exo*) chi angles: 328.6	0.046Å	-	-
A 28		GLY	50	-	Favored (15.69%) Glycine / -104.6,160.2	-	-	-	-
A 29		LYS	50	-	Favored (22.55%) General / -147.9,137.6	34.8% (*ttpt*) chi angles: 176.2,177.9,54.3,166.6	0.124Å	-	-
A 30		PHE	50	-	Favored (25.39%) General / -160.5,156.1	31.5% (*p90*) chi angles: 73.5,87.8	0.012Å	-	-
A 31		TRP	50	-	Favored (3.44%) General / -142.2,-171.7	49.2% (*p90*) chi angles: 58.8,90.6	0.081Å	-	-
A 32		PHE	50	-	Favored (45.15%) General / -119.9,147.1	89.3% (*m-85*) chi angles: 301.9,275.5	0.038Å	-	-
A 33		LYS	50	-	Favored (7.35%) General / -70.2,113.5	37.4% (*tttp*) chi angles: 183.2,200.9,182.1,71.1	0.1Å	-	-
A 34		ASN	50	-	Favored (19.15%) General / 55.5,32.5	24.8% (*m120*) chi angles: 303.6,129.8	0.016Å	-	-

Favored

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 35		ASP	50	-	(44.56%) General / -150.9,158.8	20.2% (*t0*) chi angles: 204.4,356.9	0.065Å	-	-
A 36		VAL	50	-	Favored (43.84%) Pre-proline / -137.2,144.0	7.4% (*p*) chi angles: 69.3	0.118Å	-	-
A 37		PRO	50	-	Favored (83.16%) Trans-proline / -63.4,142.0	53% (*Cg_exo*) chi angles: 334.8	0.134Å	-	-
A 38		VAL	50	-	Favored (3.12%) Isoleucine or valine / -125.8,-18.5	30.7% (*m*) chi angles: 294.8	0.141Å	-	-
A 39		HIS	50	-	Favored (7.85%) General / -156.3,129.2	57.8% (*t-80*) chi angles: 188.4,269.2	0.079Å	OUTLIER(S) worst is CG--ND1: 4.523 σ	OUTLIER(S) worst is CB-CG-CD2: 4.03 σ
A 40		LEU	50	-	Favored (40.84%) General / -115.8,147.6	66.3% (*mt*) chi angles: 305.3,180.1	0.085Å	-	-
A 41		SER	50	-	Favored (14.98%) General / -155.3,137.7	91.1% (*p*) chi angles: 62.7	0.029Å	-	-
A 42		CYS	50	-	Favored (51.74%) General / -125.7,142.0	83.1% (*m*) chi angles: 300.7	0.028Å	-	-
A 43		GLY	50	-	Favored (24.03%) Glycine / -103.4,-154.1	-	-	-	-
A 44		ASP	50	-	Favored (74.86%) General / -67.3,-46.0	35.6% (*t70*) chi angles: 186.9,66.7	0.047Å	-	-
A 45		GLU	50	-	Favored (2.42%) General / -139.8,23.9	94.4% (*mt-10*) chi angles: 291.9,183.3,3.3	0.026Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A		HIS	50	-	Favored (40.01%)	32.5% (*p-80*)	0.079Å	OUTLIER(S) worst is CD2-	OUTLIER(S) worst is CB-

46				General / -149.5,162.5	chi angles: 72.3,290.3		-NE2: 4.551 σ	CG-CD2: 5.561 σ
A 47	SER	50	-	Favored (47.14%) General / -137.6,150.0	48.7% (*m*) chi angles: 300.5	0.063Å	-	-
A 48	ALA	50	-	Favored (48.8%) General / -131.3,137.5	-	0.07Å	-	-
A 49	VAL	50	-	Favored (72.68%) Isoleucine or valine / -125.1,128.1	46.9% (*t*) chi angles: 183.2	0.022Å	-	-
A 50	VAL	50	-	Favored (42.51%) Isoleucine or valine / -104.8,135.5	61.2% (*t*) chi angles: 181.3	0.039Å	-	-
A 51	THR	50	-	Favored (14.33%) General / -104.1,161.1	43.8% (*p*) chi angles: 67.1	0.021Å	-	-
A 52	GLY	50	-	Favored (46.4%) Glycine / -54.6,-28.8	-	-	-	-
A 53	ASN	50	-	Favored (10.39%) General / -89.6,14.9	95.3% (*m-20*) chi angles: 293.1,335.7	0.04Å	-	-
A 54	ASN	50	-	Favored (10.52%) General / 62.8,39.6	48.2% (*m-80*) chi angles: 308.6,296	0.051Å	-	-
A 55	LYS	50	-	Favored (17.88%) General / -107.6,157.7	97.7% (*mttt*) chi angles: 295.5,176,183.6,172.3	0.044Å	-	-
A 56	LEU	50	-	Favored (56.76%) General / -115.6,130.1	52.8% (*tp*) chi angles: 181.7,65.9	0.061Å	-	-
A 57	TYR	50	-	Favored (54.22%) General / -120.8,131.0	59% (*m-85*) chi angles: 290.1,77.7	0.027Å	-	-
A 58	MET	50	-	Favored (46.91%) General /	96.8% (*mmm*) chi angles: 299.7,299.8,296.9	0.094Å	-	-

-121.5,146.4

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 59		PHE	50	-	Favored (19.2%) General / -163.0,155.9	47.5% (*p90*) chi angles: 61.9,276	0.06Å	-	-
A 60		GLY	50	0.55Å HA2 with A 21 LYS HB2	Favored (15.72%) Glycine / 121.0,-159.0	-	-	-	-
A 61		SER	50	-	Favored (30.13%) General / -60.3,150.6	71% (*m*) chi angles: 297.5	0.044Å	-	-
A 62		ASN	50	-	Allowed (0.86%) General / -150.1,21.6	67.1% (*t30*) chi angles: 192.3,36.1	0.085Å	-	-
A 63		ASN	50	-	Favored (67.34%) General / -63.9,-23.4	19% (*p-10*) chi angles: 58,313.6	0.089Å	-	-
A 64		TRP	50	-	Favored (36.96%) General / -103.6,6.0	90.2% (*m95*) chi angles: 285,100.5	0.008Å	-	-
A 65		GLY	50	-	Favored (72.32%) Glycine / 69.0,30.2	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 66		GLN	50	-	Favored (66.15%) General / -66.6,-22.3	7.2% (*pm0*) chi angles: 57.5,262.7,64.1	0.119Å	-	-
A 67		LEU	50	-	Favored (64.19%) General / -70.1,-27.0	41.5% (*mt*) chi angles: 302.1,188.3	0.098Å	-	-
A 68		GLY	50	-	Favored (71.55%) Glycine / 69.3,30.4	-	-	-	-
A 69		LEU	50	-	Favored (40.86%) General / -101.2,10.3	96.5% (*mt*) chi angles: 293.2,174.2	0.055Å	-	-

A 70	GLY	50	-	Favored (54.87%) Glycine / 73.9,35.1	-	-	-	-
A 71	SER	50	-	Favored (5.78%) General / -157.2,-176.1	5.8% (*p*) chi angles: 86.7	0.023Å	-	-
A 72	LYS	50	-	Favored (5.5%) General / -129.1,26.1	56.3% (*mtpt*) chi angles: 298.9,172.2,73.2,181	0.08Å	-	-
A 73	SER	50	-	Favored (49.57%) General / -106.7,134.7	50.2% (*p*) chi angles: 54.5	0.014Å	-	-
A 74	ALA	50	-	Favored (9.2%) General / -54.0,149.3	-	0.03Å	-	-
A 75	ILE	50	-	Favored (57.5%) Isoleucine or valine / -123.2,119.4	19.7% (*mm*) chi angles: 298.7,286.5	0.067Å	-	-
A 76	SER	50	0.452Å HA with A 21 LYS O	Favored (76.03%) General / -69.7,-36.6	16.2% (*p*) chi angles: 49.2	0.014Å	-	-
A 77	LYS	50	-	Favored (25.56%) Pre-proline / -107.2,142.7	33.2% (*tttm*) chi angles: 202,181.1,207.8,287.1	0.19Å	-	-
A 78	PRO	50	-	Favored (2.44%) Trans-proline / -56.5,115.4	97.1% (*Cg_exo*) chi angles: 329.4	0.064Å	-	-
A 79	THR	50	-	Favored (55.38%) General / -118.0,129.1	89% (*m*) chi angles: 300.9	0.044Å	-	-
A 80	CYS	50	-	Favored (48.3%) General / -67.3,132.7	41.5% (*t*) chi angles: 177.9	0.01Å	-	-
A 81	VAL	50	-	Allowed (1.87%) Isoleucine or valine / -82.5,86.9	47.8% (*t*) chi angles: 182.9	0.063Å	-	-
A 82	LYS	50	-	Favored (65.88%) General /	33.3% (*mttp*) chi angles: 286.3,170.1,149.4,56	0.026Å	-	-

-57.7,-30.9

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 83		ALA	50	-	Favored (63.12%) General / -57.8,-27.4	-	0.021Å	-	-
A 84		LEU	50	-	Favored (38.01%) General / -100.3,-0.6	96.6% (*mt*) chi angles: 295.9,176.8	0.015Å	-	-
A 85		LYS	50	-	Favored (36.79%) Pre-proline / -54.6,-35.8	55.5% (*mtpt*) chi angles: 289.4,175.6,66,188.6	0.063Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 86		PRO	50	-	Favored (78%) Trans-proline / -58.2,-26.8	78.7% (*Cg_exo*) chi angles: 328.5	0.068Å	-	-
A 87		GLU	50	-	Favored (13.78%) General / -104.5,161.8	40.8% (*mt-10*) chi angles: 288,174.1,272.4	0.02Å	-	-
A 88		LYS	50	-	Favored (4.46%) General / -97.2,88.5	60.3% (*mttm*) chi angles: 302.9,190.5,185.5,306.7	0.064Å	-	-
A 89		VAL	50	-	Favored (25.61%) Isoleucine or valine / -60.2,133.8	89.4% (*t*) chi angles: 177.8	0.048Å	-	-
A 90		LYS	50	-	Favored (2.85%) General / -119.0,-40.3	72.3% (*mmtt*) chi angles: 288.8,292.5,178.8,176.8	0.007Å	-	-
A 91		LEU	50	-	Favored (43.13%) General / -139.8,149.2	65.2% (*mt*) chi angles: 301.3,170.6	0.069Å	-	-
A 92		ALA	50	-	Favored (35.76%) General / -142.1,146.8	-	0.029Å	-	-
A 93		ALA	50	-	Favored (50.23%) General / -130.8,140.1	-	0.049Å	-	-

Favored

A 94	CYS	50	-	(44.06%) General / -118.6,123.0	79.7% (*m*) chi angles: 299.5	0.067Å	-	-
A 95	GLY	50	-	Favored (30.86%) Glycine / -97.3,-158.4	-	-	-	-
A 96	ARG	50	-	Favored (67.79%) General / -60.9,-51.8	64.3% (*ttp85*) chi angles: 185.2,182.2,60.5,95.2	0.061Å	-	-
A 97	ASN	50	-	Favored (2.7%) General / -137.8,27.7	46.3% (*p30*) chi angles: 69.1,0.9	0.055Å	-	-
A 98	HIS	50	-	Favored (43.72%) General / -151.8,160.1	21.4% (*p-80*) chi angles: 73.8,294.9	0.04Å	OUTLIER(S) worst is CD2--NE2: 4.193 σ	OUTLIER(S) worst is CB-CG-CD2: 4.866 σ
A 99	THR	50	-	Favored (50.59%) General / -130.1,142.6	81.8% (*m*) chi angles: 302.9	0.057Å	-	-
A 100	LEU	50	-	Favored (49.18%) General / -115.6,140.4	70.3% (*mt*) chi angles: 304.6,176.2	0.1Å	-	-
A 101	VAL	50	-	Favored (47.4%) Isoleucine or valine / -133.1,140.3	44% (*t*) chi angles: 184	0.035Å	-	-
A 102	SER	50	-	Favored (54.28%) General / -120.3,137.4	47.3% (*t*) chi angles: 180.1	0.078Å	-	-
A 103	THR	50	-	Favored (37.07%) General / -117.2,151.3	42.8% (*p*) chi angles: 67.5	0.028Å	-	-
A 104	GLU	50	-	Favored (69.46%) General / -60.9,-29.3	35.4% (*tt0*) chi angles: 191.9,174.3,84	0.043Å	-	-
A 105	GLY	50	-	Favored (60.46%) Glycine / -56.6,-31.5	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 8 of	Outliers:	Outliers: 13	Outliers: 8

		50.27	5.12	362	301	0 of 319	of 364	of 364
A 106	GLY	50	-	Favored (4.47%) Glycine / 112.4,25.9	-	-	-	-
A 107	ASN	50	-	Favored (42.38%) General / -111.4,143.3	81.8% (*m-20*) chi angles: 289.7,314.5	0.063Å	-	-
A 108	VAL	50	-	Favored (70.91%) Isoleucine or valine / -121.6,132.4	58.8% (*t*) chi angles: 180.4	0.056Å	-	-
A 109	TYR	50	-	Favored (29.41%) General / -121.4,157.9	80.3% (*m-85*) chi angles: 301.6,266.8	0.041Å	-	-
A 110	ALA	50	-	Favored (37.51%) General / -147.7,152.2	-	0.045Å	-	-
A 111	THR	50	-	Favored (37.07%) General / -153.2,155.7	13.9% (*t*) chi angles: 190.1	0.049Å	-	-
A 112	GLY	50	-	Favored (18.63%) Glycine / 115.5,-150.7	-	-	-	-
A 113	GLY	50	-	Favored (40.29%) Glycine / -61.0,152.4	-	-	-	-
A 114	ASN	50	-	Allowed (0.37%) General / -156.0,26.6	63.7% (*t30*) chi angles: 195.6,27.8	0.074Å	-	-
A 115	ASN	50	-	Favored (71.65%) General / -61.6,-31.6	5.7% (*m-20*) chi angles: 279.3,29.8	0.051Å	-	-
A 116	GLU	50	-	Favored (26.68%) General / -108.8,10.0	68.3% (*mm-40*) chi angles: 303.6,304.3,318	0.039Å	-	-
A 117	GLY	50	-	Favored (61.27%) Glycine / 76.5,27.5	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 118		GLN	50	-	Favored (67.22%) General / -62.9,-23.1	15.8% (*pm0*) chi angles: 57,267.6,42.3	0.117Å	-	-
A 119		LEU	50	-	Favored (63.48%) General / -69.8,-20.9	47.5% (*mt*) chi angles: 299.5,187.4	0.102Å	-	-
A 120		GLY	50	-	Favored (91.72%) Glycine / 65.1,35.4	-	-	-	-
A 121		LEU	50	-	Favored (20.38%) General / -98.2,-14.4	88.9% (*mt*) chi angles: 300.7,178.3	0.067Å	-	-
A 122		GLY	50	-	Favored (54.49%) Glycine / 101.1,1.0	-	-	-	-
A 123		ASP	50	-	Favored (2.7%) General / -134.3,-171.2	6.9% (*p30*) chi angles: 60.8,44.4	0.086Å	-	-
A 124		THR	50	-	Favored (5.98%) General / -125.9,29.1	56.2% (*p*) chi angles: 56.2	0.055Å	-	-
A 125		GLU	50	-	Favored (39.97%) General / -93.7,129.7	67.1% (*mm-40*) chi angles: 303.2,306.2,317.5	0.043Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 126		GLU	50	-	Favored (42.78%) General / -62.1,148.9	15.7% (*pt-20*) chi angles: 66.9,177.3,295.9	0.016Å	-	-
A 127		ARG	50	-	Favored (49.66%) General / -125.7,146.7	33.7% (*mmt-85*) chi angles: 300.3,300.5,202.8,291.7	0.097Å	-	-
A 128		ASN	50	-	Favored (17.26%) General / -114.3,11.2	55.2% (*p30*) chi angles: 64.7,15.8	0.11Å	-	-
A 129		THR	50	-	Favored (50.99%) General / -136.3,154.1	76% (*p*) chi angles: 60.1	0.018Å	-	-

A 130	PHE	50	-	Favored (22.79%) General / -64.6,124.8	64.7% (*m-85*) chi angles: 286.1,280.6	0.051Å	-	-
A 131	HIS	50	-	Favored (42.07%) General / -115.2,145.8	28% (*m80*) chi angles: 288.8,61.3	0.065Å	OUTLIER(S) worst is CG-- ND1: 4.49 σ	OUTLIER(S) worst is CB- CG-CD2: 4.267 σ
A 132	VAL	50	-	Favored (19.86%) Isoleucine or valine / -77.0,138.8	13.8% (*p*) chi angles: 64.9	0.104Å	-	-
A 133	ILE	50	-	Favored (4.28%) Isoleucine or valine / -96.8,94.9	66.3% (*mt*) chi angles: 304.7,171.5	0.068Å	-	-
A 134	SER	50	-	Favored (35.45%) General / -70.8,-6.1	31.7% (*p*) chi angles: 52.4	0.151Å	-	-
A 135	PHE	50	-	Favored (76.53%) General / -55.4,-46.5	67.9% (*t80*) chi angles: 172.2,85.5	0.025Å	-	-
A 136	PHE	50	-	Favored (36.95%) General / -78.9,132.8	93.5% (*m-85*) chi angles: 297.2,283.4	0.023Å	-	-
A 137	THR	50	-	Favored (3.89%) General / -129.9,-176.3	29.7% (*p*) chi angles: 70.5	0.041Å	-	-
A 138	SER	50	-	Favored (57.31%) General / -63.2,-15.6	71.5% (*p*) chi angles: 57.8	0.098Å	-	-
A 139	GLU	50	-	Favored (61.08%) General / -73.3,-13.3	0% chi angles: 74.6,105.9,320	0.173Å	-	-
A 140	HIS	50	-	Favored (6.36%) General / -103.6,95.9	44.2% (*m80*) chi angles: 308.1,100	0.065Å	OUTLIER(S) worst is CG-- ND1: 4.509 σ	-
A 141	LYS	50	-	Favored (13.02%) General / -86.4,101.3	64.3% (*mmtt*) chi angles: 298.7,311.1,188.2,195.1	0.048Å	-	-

A 142	ILE	50	-	Favored (25.96%) Isoleucine or valine / -76.2,120.3	43.1% (*mm*) chi angles: 307.1,303	0.081Å	-	-	
A 143	LYS	50	-	Favored (17.7%) General / -85.2,-39.5	86.9% (*tttt*) chi angles: 183.4,186.1,175.9,180.5	0.029Å	-	-	
A 144	GLN	50	-	Favored (17.61%) General / -156.0,141.3	64.4% (*tt0*) chi angles: 184,180.4,30	0.091Å	-	-	
A 145	LEU	50	-	Favored (30.06%) General / -113.1,152.0	96.1% (*mt*) chi angles: 294.8,174.3	0.084Å	-	-	

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 146		SER	50	-	Favored (30.68%) General / -153.4,152.1	22.6% (*t*) chi angles: 186.5	0.02Å	-	-
A 147		ALA	50	-	Favored (10.28%) General / -155.5,131.9	-	0.071Å	-	-
A 148		GLY	50	-	Favored (9.68%) Glycine / -114.7,-148.8	-	-	-	-
A 149		SER	50	-	Favored (7.02%) General / -79.5,98.9	28.2% (*t*) chi angles: 185.3	0.034Å	-	-
A 150		ASN	50	-	Favored (6.48%) General / 69.5,22.2	17.9% (*m-20*) chi angles: 314.3,322.9	0.027Å	-	-
A 151		THR	50	-	Favored (48.81%) General / -126.5,150.4	81.3% (*p*) chi angles: 61.1	0.021Å	-	-
A 152		SER	50	-	Favored (36.74%) General / -142.9,148.3	70.7% (*m*) chi angles: 295.8	0.097Å	-	-
				0.426Å	Favored				

A 153	ALA	50	HB1 with A 195 ILE HD13	(25.23%) General / -149.1,142.5	-	0.074Å	-	-
A 154	ALA	50	-	Favored (32.19%) General / -133.2,126.7	-	0.046Å	-	-
A 155	LEU	50	-	Favored (56.63%) General / -113.4,129.0	69.1% (*tp*) chi angles: 177.3,62.2	0.063Å	-	-
A 156	THR	50	-	Favored (16.26%) General / -91.0,159.2	47.9% (*p*) chi angles: 66.1	0.016Å	-	-
A 157	GLU	50	-	Favored (67.62%) General / -58.2,-31.7	70.6% (*mm-40*) chi angles: 290.9,296.8,347	0.019Å	-	-
A 158	ASP	50	-	Favored (25.59%) General / -89.2,9.4	21% (*p-10*) chi angles: 75.8,352.1	0.141Å	-	-
A 159	GLY	50	-	Favored (38.6%) Glycine / 86.8,24.4	-	-	-	-
A 160	ARG	50	-	Favored (34%) General / -93.5,136.2	83.7% (*mtm180*) chi angles: 289.9,172.8,292.6,160	0.049Å	-	-
A 161	LEU	50	0.522Å HD21 with A 195 ILE HD12	Favored (56.72%) General / -115.4,129.9	58.9% (*tp*) chi angles: 179.1,59.4	0.056Å	-	-
A 162	PHE	50	-	Favored (51.53%) General / -124.6,130.0	89.8% (*m-85*) chi angles: 300.6,273.2	0.066Å	-	-
A 163	MET	50	-	Favored (49.54%) General / -131.3,153.4	72.4% (*mtp*) chi angles: 304.7,184,80.9	0.006Å	-	-
A 164	TRP	50	-	Favored (20.7%) General / -163.4,158.1	33% (*p90*) chi angles: 63.4,99.6	0.052Å	-	-
A 165	GLY	50	-	Favored (17.6%) Glycine / 112.2,-143.8	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 166		ASP	50	-	Favored (41.26%) General / -69.7,130.0	29.1% (t0) chi angles: 198.1,349.2	0.081Å	-	-
A 167		ASN	50	-	Favored (5.28%) General / -128.6,29.5	50.8% (t30) chi angles: 195,52.3	0.039Å	-	-
A 168		SER	50	-	Favored (68.93%) General / -63.4,-26.8	74.8% (p) chi angles: 58.2	0.062Å	-	-
A 169		GLU	50	-	Favored (11.23%) General / -120.0,23.0	67.3% (mm-40) chi angles: 287.8,304.4,332.5	0.053Å	-	-
A 170		GLY	50	0.419Å HA3 with A 233 ARG HA	Favored (70.61%) Glycine / 65.4,24.2	-	-	-	-
A 171		GLN	50	-	Favored (62.81%) General / -69.5,-14.3	12.3% (pm0) chi angles: 62.5,273.9,52.4	0.208Å	-	-
A 172		ILE	50	-	Favored (7.62%) Isoleucine or valine / -110.8,17.4	43.6% (pt) chi angles: 61.6,175	0.177Å	-	-
A 173		GLY	50	-	Favored (71.8%) Glycine / 56.4,37.0	-	-	-	-
A 174		LEU	50	-	Favored (6.24%) General / -109.2,30.8	70.5% (mt) chi angles: 292.7,181.7	0.09Å	-	-
A 175		LYS	50	-	Allowed (1.04%) General / 58.6,-133.7	45.2% (mttp) chi angles: 288.6,174.5,156.4,60	0.108Å	-	-
A 176		ASN	50	-	Favored (50.19%) General / -76.8,-5.9	90.7% (m-20) chi angles: 294.5,325.2	0.094Å	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 177	VAL 50	-	Favored (27.83%) Isoleucine or valine / -62.3,131.9	82.2% (*t*) chi angles: 174.7	0.057Å	-	-
A 178	SER 50	-	Favored (86.43%) General / -67.2,-39.1	47.6% (*p*) chi angles: 54.3	0.024Å	-	-
A 179	ASN 50	-	Allowed (0.87%) General / -179.6,159.2	10.8% (*p-10*) chi angles: 71.1,296.4	0.041Å	-	-
A 180	VAL 50	-	Favored (34.84%) Isoleucine or valine / -130.8,145.9	24.3% (*m*) chi angles: 293.4	0.083Å	-	-
A 181	CYS 50	-	Favored (32.75%) General / -105.5,7.1	84.3% (*m*) chi angles: 300.2	0.031Å	-	-
A 182	VAL 50	-	Favored (57.23%) Pre-proline / -142.3,151.1	27% (*m*) chi angles: 293.8	0.065Å	-	-
A 183	PRO 50	-	Favored (53.57%) Trans-proline / -55.5,132.7	88.4% (*Cg_exo*) chi angles: 330.1	0.072Å	-	-
A 184	GLN 50	-	Favored (54%) General / -122.2,139.2	50.7% (*tp60*) chi angles: 168,59.5,55	0.062Å	-	-
A 185	GLN 50	-	Favored (33.69%) General / -72.5,127.8	53% (*tt0*) chi angles: 193.2,173.7,347.7	0.03Å	-	-
# Alt Res	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
	Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 186	VAL 50	-	Favored (9.22%) Isoleucine or valine / -108.8,99.7	88.5% (*t*) chi angles: 177.8	0.045Å	-	-
A 187	THR 50	-	Favored (53.5%) General / -125.0,139.8	15.2% (*t*) chi angles: 188	0.052Å	-	-

A 188	ILE	50	0.442Å H with A 188 ILE HD13	Favored (8.81%) Isoleucine or valine / -109.5,11.9	0.1% chi angles: 71.8,305.6	0.101Å	-	-
A 189	GLY	50	-	Favored (26.96%) Glycine / 86.3,28.7	-	-	-	-
A 190	LYS	50	-	Favored (15.76%) Pre-proline / -144.0,139.2	57.9% (*mtpt*) chi angles: 294.6,179.4,62.1,169.6	0.068Å	-	-
A 191	PRO	50	-	Favored (71.95%) Trans-proline / -60.7,137.3	54.8% (*Cg_endo*) chi angles: 25.5	0.057Å	-	-
A 192	VAL	50	-	Favored (16.37%) Isoleucine or valine / -105.9,143.8	86% (*t*) chi angles: 177.4	0.085Å	-	-
A 193	SER	50	-	Favored (9.03%) General / -116.7,-21.6	75.8% (*p*) chi angles: 58.3	0.064Å	-	-
A 194	TRP	50	-	Favored (31.18%) General / -147.5,148.4	7.7% (*t-105*) chi angles: 209.2,270.7	0.106Å	-	-
A 195	ILE	99.99	0.522Å HD12 with A 161 LEU HD21	Favored (19.18%) Isoleucine or valine / -147.4,145.2	8.6% (*tt*) chi angles: 190.7,182.7	0.067Å	-	-
A 196	SER	50	0.406Å N with A 195 ILE HG12	Favored (23.38%) General / -141.4,130.5	34.7% (*t*) chi angles: 183	0.04Å	-	-
A 197	CYS	50	-	Favored (13.31%) General / -103.5,103.4	72.9% (*m*) chi angles: 297	0.055Å	-	-
A 198	GLY	50	-	Favored (6.47%) Glycine / -70.2,-167.4	-	-	-	-
A 199	TYR	50	-	Favored (52.06%) General /	8.7% (*m-85*) chi angles: 278,59.2	0.065Å	-	-

-69.8,-49.5

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 200		TYR	50	-	Favored (5.85%) General / -129.3,11.2	12.3% (*m-85*) chi angles: 319.1,292.3	0.021Å	-	-
A 201		HIS	50	-	Favored (36.28%) General / -154.8,156.4	24.6% (*p-80*) chi angles: 74.9,291.6	0.013Å	OUTLIER(S) worst is CG--ND1: 4.263 σ	OUTLIER(S) worst is CB-CG-CD2: 4.859 σ
A 202		SER	50	-	Favored (34.23%) General / -134.2,161.7	70.1% (*m*) chi angles: 297.3	0.03Å	-	-
A 203		ALA	50	-	Favored (33.67%) General / -151.1,152.6	-	0.051Å	-	-
A 204		PHE	50	-	Favored (43.42%) General / -141.1,158.8	17.5% (*p90*) chi angles: 64.3,75.1	0.084Å	-	-
A 205		VAL	50	-	Favored (74.37%) Isoleucine or valine / -116.8,127.6	48.5% (*t*) chi angles: 182.7	0.059Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 206		THR	50	-	Favored (34.43%) General / -76.2,155.5	72.2% (*p*) chi angles: 59	0.047Å	-	-
A 207		THR	50	-	Favored (62.3%) General / -58.2,-26.0	72.4% (*p*) chi angles: 63.4	0.038Å	-	-
A 208		ASP	50	-	Favored (30.07%) General / -90.9,9.5	6.4% (*p-10*) chi angles: 77.9,333.7	0.136Å	-	-
A 209		GLY	50	0.518Å HA3 with A 244 LYS HG3	Favored (14.22%) Glycine / 87.6,32.1	-	-	-	-
A 210		GLU	50	-	Favored (32.17%) General / -106.0,144.8	85.6% (*mt-10*) chi angles: 294.6,184.7,330.4	0.049Å	-	-

A 211	LEU	50	-	Favored (52.39%) General / -105.8,126.6	61.9% (*tp*) chi angles: 176.4,64.6	0.048Å	-	-
A 212	TYR	50	-	Favored (54.45%) General / -119.0,135.8	66% (*m-85*) chi angles: 290.5,79.3	0.035Å	-	-
A 213	VAL	50	0.71Å HG21 with A 222 LEU O	Favored (36.51%) Isoleucine or valine / -128.6,152.3	28.5% (*m*) chi angles: 295.3	0.017Å	-	-
A 214	PHE	50	-	Favored (2.68%) General / -171.0,147.7	11.3% (*p90*) chi angles: 47.1,278.5	0.011Å	-	-
A 215	GLY	50	-	Favored (20.02%) Glycine / 134.1,-150.5	-	-	-	-
A 216	GLU	50	-	Favored (40.21%) Pre-proline / -61.4,118.8	49.8% (*tt0*) chi angles: 189.2,182.8,35.8	0.055Å	-	-
A 217	PRO	50	-	Allowed (0.94%) Trans-proline / -80.8,40.0	35.5% (*Cg_endo*) chi angles: 36.9	0.024Å	-	-
A 218	GLU	50	-	Favored (37.83%) General / -117.0,150.9	76.4% (*mm-40*) chi angles: 301.5,301.7,326.2	0.04Å	-	-
A 219	ASN	50	-	Favored (9.78%) General / 66.0,14.8	81.2% (*m-20*) chi angles: 300.5,319.6	0.062Å	-	-
A 220	GLY	50	-	Favored (58.06%) Glycine / 61.4,19.9	-	-	-	-
A 221	LYS	50	-	Favored (62.96%) General / -69.9,-14.9	55.8% (*pttt*) chi angles: 60.5,190.2,178,185.5	0.107Å	-	-
A 222	LEU	50	0.71Å O with A 213 VAL HG21	Favored (50.39%) General / -77.5,-23.6	46.8% (*mt*) chi angles: 300.8,187.4	0.076Å	-	-
				Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 223		GLY	50	0.482Å HA2 with A 284 SER O	(72.91%) Glycine / 64.5,28.2	-	-	-	-
A 224		LEU	50	-	Favored (30.77%) Pre-proline / -105.5,145.4	93.9% (*mt*) chi angles: 295.1,171.8	0.052Å	-	-
A 225		PRO	50	-	Favored (84.05%) Trans-proline / -58.8,148.4	38.1% (*Cg_endo*) chi angles: 23.4	0.057Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 226		ASN	50	-	Favored (55.48%) General / -53.8,-33.4	8.1% (*t30*) chi angles: 203.7,72.7	0.045Å	-	-
A 227		GLN	50	0.461Å H with A 227 GLN NE2	Favored (64.77%) General / -65.0,-17.8	3.2% (*mp0*) chi angles: 323.9,80.5,57	0.084Å	-	-
A 228		LEU	50	-	Favored (18.88%) General / -101.4,-12.1	80.4% (*mt*) chi angles: 299.8,182.1	0.023Å	-	-
A 229		LEU	50	-	Favored (67.62%) General / -60.7,-27.1	94.3% (*mt*) chi angles: 294.3,176.9	0.064Å	-	-
A 230		GLY	50	-	Favored (64.33%) Glycine / -59.7,-27.6	-	-	-	-
A 231		ASN	50	-	Favored (4.28%) General / -105.3,32.4	57% (*t30*) chi angles: 199.8,35.8	0.095Å	-	-
A 232		HIS	50	-	Favored (60.92%) General / -62.5,-18.0	24.3% (*p80*) chi angles: 67,93.1	0.048Å	OUTLIER(S) worst is CG-- ND1: 4.23 σ	-
A 233		ARG	50	0.419Å HA with A 170 GLY HA3	Favored (59.77%) General / -81.3,-8.6	12.5% (*mtp85*) chi angles: 316,188.7,97.8,101.1	0.047Å	-	-
A 234		THR	50	-	Favored (28.4%) Pre-proline /	28.8% (*m*) chi angles: 307.5	0.064Å	-	-

-117.3,141.3

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 235	PRO 50	-		Favored (13.18%) Trans-proline / -58.2,123.2	85.1% (*Cg_exo*) chi angles: 331.1	0.071Å	-	-
A 236	GLN 50	-		Favored (49.44%) General / -121.8,143.4	41% (*mt-30*) chi angles: 294.8,183.3,100	0.042Å	-	-
A 237	LEU 50	-		Favored (49.71%) General / -66.3,133.1	64% (*tp*) chi angles: 178.3,64.2	0.063Å	-	-
A 238	VAL 50	-		Allowed (2%) Isoleucine or valine / -96.4,88.7	58.9% (*t*) chi angles: 180.8	0.031Å	-	-
A 239	SER 50	-		Favored (59.9%) General / -76.2,-16.2	55.6% (*p*) chi angles: 55.3	0.089Å	-	-
A 240	GLU 50	-		Favored (67.04%) General / -63.5,-22.7	48.7% (*mm-40*) chi angles: 282.1,300.8,290.9	0.148Å	-	-
A 241	ILE 50	-		Favored (10.82%) Pre-proline / -86.1,106.8	72.2% (*mt*) chi angles: 303.6,172.4	0.067Å	-	-
A 242	PRO 50	-		Allowed (1.01%) Trans-proline / -68.3,-49.0	94.3% (*Cg_endo*) chi angles: 30.3	0.091Å	-	-
A 243	GLU 50	-		Favored (19.97%) General / -79.4,168.1	14.7% (*pm0*) chi angles: 76.2,281.4,32.9	0.111Å	-	-
A 244	LYS 50	0.518Å HG3 with A 209 GLY HA3		Favored (11.07%) General / -60.7,121.0	62.8% (*tttp*) chi angles: 180.7,179,180.5,60	0.116Å	-	-
A 245	VAL 50	-		Favored (10.58%) Isoleucine or valine / -81.2,144.4	97.2% (*t*) chi angles: 178.3	0.062Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364

A 246	ILE	50	-	Favored (4.56%) Isoleucine or valine / -115.7,-48.1	71.7% (*mt*) chi angles: 303.5,173	0.059Å	-	-
A 247	GLN	50	0.502Å HB2 with A 258 LEU HB3	Favored (51.43%) General / -135.9,153.5	81.8% (*mt-30*) chi angles: 295.5,179.7,22.4	0.061Å	-	-
A 248	VAL	50	-	Favored (30.95%) Isoleucine or valine / -140.0,142.9	12.4% (*p*) chi angles: 65.8	0.074Å	-	-
A 249	ALA	50	-	Favored (37.39%) General / -136.2,133.7	-	0.049Å	-	-
A 250	CYS	50	-	Favored (55.78%) General / -116.9,133.6	81% (*m*) chi angles: 300.8	0.041Å	-	-
A 251	GLY	50	-	Favored (15.04%) Glycine / -107.6,-149.2	-	-	-	-
A 252	GLY	50	-	Favored (3.07%) Glycine / -65.0,-65.2	-	-	-	-
A 253	GLU	50	-	Favored (7.97%) General / -125.7,12.8	70% (*mm-40*) chi angles: 302.3,305.2,327.2	0.02Å	-	-
A 254	HIS	50	-	Favored (31.55%) General / -134.2,162.7	7.8% (*p-80*) chi angles: 71.8,309	0.055Å	OUTLIER(S) worst is CD2--NE2: 4.097 σ	OUTLIER(S) worst is CB-CG-CD2: 5.029 σ
A 255	THR	50	-	Favored (49.66%) General / -132.1,142.8	44.9% (*m*) chi angles: 305.3	0.075Å	-	-
A 256	VAL	50	-	Favored (63.43%) Isoleucine or valine / -126.0,135.6	46.9% (*t*) chi angles: 183.2	0.046Å	-	-
A 257	VAL	50	-	Favored (61.46%) Isoleucine or valine /	59% (*t*) chi angles: 180.9	0.063Å	-	-

-128.3,135.9

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 258		LEU	50	0.502Å HB3 with A 247 GLN HB2	Favored (28.49%) General / -113.5,115.7	61.4% (*tp*) chi angles: 178.9,64.7	0.05Å	-	-
A 259		THR	50	-	Favored (4.07%) General / -106.4,-179.9	20.6% (*p*) chi angles: 73.1	0.009Å	-	-
A 260		GLU	50	-	Favored (70.14%) General / -64.8,-29.2	18.1% (*pt-20*) chi angles: 56.7,186.3,340.5	0.083Å	-	-
A 261		ASN	50	-	Favored (10.55%) General / -94.7,-38.9	66% (*m-20*) chi angles: 298.8,348.3	0.038Å	-	-
A 262		ALA	50	0.812Å HB2 with A 293 ARG HE	Favored (6.33%) General / -159.7,-177.4	-	0.089Å	-	-
A 263		VAL	50	-	Favored (57.68%) Isoleucine or valine / -113.1,133.8	61.5% (*t*) chi angles: 180.1	0.058Å	-	-
A 264		TYR	50	-	Favored (47.11%) General / -119.8,144.8	86.4% (*m-85*) chi angles: 292.8,82.8	0.094Å	-	-
A 265		THR	50	-	Favored (47.96%) General / -133.1,156.2	72% (*p*) chi angles: 63.8	0.024Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 266		PHE	50	-	Favored (10.91%) General / -165.5,153.2	20.4% (*p90*) chi angles: 48.1,272.9	0.078Å	-	-
A 267		GLY	50	-	Favored (17.7%) Glycine / 119.7,-144.9	-	-	-	-
A 268		LEU	50	0.606Å HD22 with A 270 GLN	Favored (55.57%) General /	0.3% chi angles: 229.2,194.6	0.111Å	-	-

				HG3	-110.4,130.4				
A 269	GLY	50	0.454Å HA3 with A 274 LEU HG	Allowed (0.68%) Glycine / -132.5,60.1	-	-	-	-
A 270	GLN	50	0.606Å HG3 with A 268 LEU HD22	Favored (69.27%) General / -62.5,-27.6	0% chi angles: 334.6,86.4,279	0.1Å	-	-
A 271	PHE	50	-	Favored (34.79%) General / -104.7,10.1	19.4% (*m-85*) chi angles: 311.7,304.4	0.067Å	-	-
A 272	GLY	50	-	Favored (64.95%) Glycine / 78.9,22.9	-	-	-	-
A 273	GLN	50	-	Favored (61.06%) General / -72.6,-12.5	15.3% (*pm0*) chi angles: 63.6,270.1,47.6	0.183Å	-	-
A 274	LEU	50	0.454Å HG with A 269 GLY HA3	Favored (45.12%) General / -78.7,-28.0	79.1% (*mt*) chi angles: 296.2,182.1	0.046Å	-	-
A 275	GLY	50	-	Favored (92.59%) Glycine / 64.9,36.0	-	-	-	-
A 276	LEU	50	-	Favored (32.06%) General / -105.9,7.3	95.8% (*mt*) chi angles: 295.2,175.9	0.035Å	-	-
A 277	GLY	50	-	Favored (12.18%) Glycine / 111.3,-164.0	-	-	-	-
A 278	THR	50	-	Favored (31.62%) General / -105.4,12.4	62% (*p*) chi angles: 56.7	0.042Å	-	-
A 279	PHE	50	-	Favored (6.13%) General / -120.3,-23.7	47.4% (*m-85*) chi angles: 283,79.2	0.024Å	-	-
A 280	LEU	50	-	Favored (12.83%) General / -119.2,106.9	29.6% (*tp*) chi angles: 190.1,63.3	0.039Å	-	-
A 281	PHE	50	-	Favored (16.53%) General /	22.3% (*m-30*) chi angles: 303.7,314.3	0.022Å	-	-

-104.6,-12.3

A 282		GLU	50	-	Favored (43.88%) General / -144.5,155.8	2.6% (*pp20?*) chi angles: 68.5,72.4,33.8	0.07Å	-	-
A 283		THR	50	-	Favored (2.04%) General / -163.4,122.3	14.8% (*t*) chi angles: 187.2	0.073Å	-	-
A 284		SER	50	0.482Å O with A 223 GLY HA2	Favored (55.22%) General / -77.0,-21.1	74.7% (*p*) chi angles: 58.2	0.073Å	-	-
A 285		GLU	50	-	Favored (42.28%) Pre-proline / -111.5,150.5	0.6% chi angles: 64.1,279,288.2	0.088Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 286		PRO	50	-	Favored (48.18%) Trans-proline / -56.1,131.8	80% (*Cg_exo*) chi angles: 330.5	0.075Å	-	-
A 287		LYS	50	-	Favored (54%) General / -124.4,139.3	52.1% (*mttp*) chi angles: 281.3,181.3,170.4,56.3	0.018Å	-	-
A 288		VAL	50	-	Favored (31.09%) Isoleucine or valine / -72.5,133.8	96.1% (*t*) chi angles: 178.3	0.03Å	-	-
A 289		ILE	50	-	Allowed (0.69%) Isoleucine or valine / -74.5,91.8	59.8% (*mt*) chi angles: 305.9,174.1	0.031Å	-	-
A 290		GLU	50	-	Favored (67.25%) General / -60.8,-26.3	77% (*mm-40*) chi angles: 292.6,300.3,340.6	0.038Å	-	-
A 291		ASN	50	-	Favored (71.86%) General / -59.5,-33.9	21.3% (*m120*) chi angles: 309.7,107.2	0.037Å	-	-
A 292		ILE	50	-	Favored (2.58%) Isoleucine or	2.3% (*pp*) chi angles: 44.4,70.2	0.111Å	-	-

				valine / -117.2,29.5				
A 293	ARG	50	0.812Å HE with A 262 ALA HB2	Favored (66.53%) General / -65.3,-20.7	0.2% chi angles: 269.9,293,213.5,49.3	0.167Å	-	-
A 294	ASP	50	-	Favored (50.28%) General / -77.5,-24.1	82.2% (*m-20*) chi angles: 294.9,348.8	0.109Å	-	-
A 295	GLN	50	-	Favored (23.65%) General / -88.3,149.7	25.4% (*mp0*) chi angles: 283.3,67.5,47.6	0.038Å	-	-
A 296	THR	50	-	Favored (13.57%) General / -100.5,102.4	63.4% (*m*) chi angles: 303.5	0.016Å	-	-
A 297	ILE	50	-	Favored (25.54%) Isoleucine or valine / -79.3,135.5	43.5% (*mm*) chi angles: 306.2,303.4	0.072Å	-	-
A 298	SER	50	-	Favored (10.83%) General / -111.2,-23.5	94.6% (*p*) chi angles: 63.5	0.032Å	-	-
A 299	TYR	50	-	Favored (18.68%) General / -152.5,139.1	69.6% (*t80*) chi angles: 186.9,75.3	0.06Å	-	-
A 300	ILE	50	-	Favored (25.33%) Isoleucine or valine / -121.9,148.5	49.5% (*pt*) chi angles: 61.6,171.6	0.049Å	-	-
A 301	SER	50	-	Favored (24.95%) General / -150.0,143.1	36.7% (*t*) chi angles: 182.3	0.06Å	-	-
A 302	CYS	50	-	Favored (51.85%) General / -124.5,141.8	89.7% (*m*) chi angles: 295.2	0.085Å	-	-
A 303	GLY	50	-	Favored (30.88%) Glycine / -98.4,-165.1	-	-	-	-
A 304	GLU	50	-	Favored (94.73%) General / -63.4,-44.4	61.1% (*tt0*) chi angles: 183.5,182.6,29.8	0.01Å	-	-

# Alt	Res		High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 305	ASN	50	-		Favored (3.64%) General / -134.5,21.1	77.3% (*m-20*) chi angles: 291.7,305.1	0.079Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 306		HIS	50	-	Favored (16.39%) General / -146.6,170.7	42.3% (*p-80*) chi angles: 74,280.5	0.103Å	OUTLIER(S) worst is CG--ND1: 4.522 σ	OUTLIER(S) worst is CB-CG-CD2: 4.619 σ
A 307		THR	50	-	Favored (45.57%) General / -136.9,146.5	51.7% (*m*) chi angles: 304.8	0.084Å	-	-
A 308		ALA	50	-	Favored (49.14%) General / -131.7,139.8	-	0.039Å	-	-
A 309		LEU	50	-	Favored (54.01%) General / -125.4,137.2	32.2% (*mt*) chi angles: 311.6,176.6	0.119Å	-	-
A 310		ILE	50	-	Favored (72.56%) Isoleucine or valine / -115.6,125.0	65.4% (*mt*) chi angles: 303.9,175.6	0.022Å	-	-
A 311		THR	50	-	Favored (21.05%) General / -79.1,167.4	17.2% (*p*) chi angles: 74.7	0.048Å	-	-
A 312		ASP	50	-	Favored (62.51%) General / -65.6,-15.2	21.4% (*p-10*) chi angles: 67.5,330.9	0.093Å	-	-
A 313		ILE	50	-	Favored (9.73%) Isoleucine or valine / -105.0,-3.1	45.6% (*pt*) chi angles: 63,168.7	0.157Å	-	-
A 314		GLY	50	-	Favored (27.82%) Glycine / 97.5,18.6	-	-	-	-
A 315		LEU	50	-	Favored (32.4%) General / -78.9,149.4	88.5% (*mt*) chi angles: 300.6,178.6	0.047Å	-	-

A 316	MET	50	-	Favored (53.81%) General / -125.5,136.9	53.9% (*ttp*) chi angles: 187.1,171.1,63.8	0.06Å	-	-
A 317	TYR	50	-	Favored (54.75%) General / -123.0,136.2	81.9% (*m-85*) chi angles: 291,82.7	0.07Å	-	-
A 318	THR	50	-	Favored (46.13%) General / -132.4,156.8	58.7% (*p*) chi angles: 62.6	0.02Å	-	-
A 319	PHE	50	-	Favored (5.73%) General / -166.4,145.4	21.9% (*p90*) chi angles: 50.6,277.4	0.045Å	-	-
A 320	GLY	50	-	Favored (18.04%) Glycine / 127.0,-150.7	-	-	-	-
A 321	ASP	50	-	Favored (33.34%) General / -61.7,127.8	51.8% (*t0*) chi angles: 182.8,14.7	0.071Å	-	-
A 322	GLY	50	-	Favored (52.66%) Glycine / -101.8,-2.5	-	-	-	-
A 323	ARG	50	-	Favored (27.31%) General / -52.6,138.8	88.8% (*mtt180*) chi angles: 279.2,177.7,164.2,172	0.048Å	-	-
A 324	HIS	50	0.532Å O with A 18 GLY HA2	Favored (7.07%) General / 66.6,10.0	72.3% (*m-70*) chi angles: 305.6,303.9	0.026Å	OUTLIER(S) worst is CG-- ND1: 4.611 σ	-
A 325	GLY	50	-	Favored (91.08%) Glycine / 63.0,34.9	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 326		LYS	50	-	Favored (62.38%) General / -71.4,-17.5	63.6% (*pttt*) chi angles: 62.5,183,178.2,182.3	0.122Å	-	-
A 327		LEU	50	-	Favored (66.96%) General /	72.6% (*mt*) chi angles: 291.8,180.4	0.094Å	-	-

				-62.3,-23.9				
A 328	GLY	50	0.438Å HA2 with A 17 PHE CD1	Favored (66.15%) Glycine / 70.8,37.9	-	-	-	-
A 329	LEU	50	-	Favored (20.08%) General / -91.4,-23.2	96.1% (*mt*) chi angles: 297.5,174.6	0.032Å	-	-
A 330	GLY	50	-	Favored (78.27%) Glycine / 70.9,22.3	-	-	-	-
A 331	LEU	50	-	Favored (48.16%) General / -72.5,144.2	30.9% (*mt*) chi angles: 310.3,172.4	0.145Å	-	-
A 332	GLU	50	-	Favored (67.88%) General / -72.0,-33.3	30.8% (*tt0*) chi angles: 194,196.7,330.4	0.078Å	-	-
A 333	ASN	50	-	Favored (40.02%) General / -103.6,120.0	26% (*m120*) chi angles: 305.6,123.2	0.042Å	-	-
A 334	PHE	50	-	Favored (21.72%) General / -85.3,154.8	11.6% (*m-30*) chi angles: 309.3,321.7	0.067Å	-	-
A 335	THR	50	-	Favored (6.9%) General / -166.2,148.4	8.9% (*t*) chi angles: 183.2	0.027Å	-	-
A 336	ASN	50	-	Favored (58.56%) General / -64.9,142.1	94.9% (*m-20*) chi angles: 293.1,342.3	0.025Å	-	-
A 337	HIS	50	-	Favored (56.28%) General / -118.4,131.2	57.7% (*m-70*) chi angles: 284.2,262.5	0.024Å	OUTLIER(S) worst is CG-- ND1: 4.419 σ	-
A 338	PHE	50	-	Favored (16.37%) General / -104.6,-12.6	71% (*m-85*) chi angles: 287.9,82.1	0.087Å	-	-
A 339	ILE	50	-	Favored (71.91%) Pre-proline / -125.3,152.9	48.1% (*pt*) chi angles: 63.3,171.7	0.051Å	-	-
A 340	PRO	50	-	Favored (16.48%) Trans-proline /	94.5% (*Cg_exo*) chi angles: 329.8	0.068Å	-	-

-53.6,124.7

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 341		THR	50	-	Favored (56.14%) General / -118.8,132.6	91.5% (*m*) chi angles: 302.4	0.051Å	-	-
A 342		LEU	50	-	Favored (35.23%) General / -66.2,128.2	60.3% (*tp*) chi angles: 180.3,64	0.037Å	-	-
A 343		CYS	50	-	Favored (6.24%) General / -79.6,72.7	78.1% (*m*) chi angles: 301	0.042Å	-	-
A 344		SER	50	-	Favored (65.55%) General / -62.6,-21.3	72.2% (*p*) chi angles: 57.9	0.06Å	-	-
A 345		ASN	50	-	Favored (24.17%) General / -56.9,-20.6	17.2% (*p-10*) chi angles: 55.9,314.9	0.038Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 346		PHE	50	-	Favored (21.96%) General / -107.6,18.0	49.9% (*m-85*) chi angles: 283.3,285	0.015Å	-	-
A 347		LEU	50	-	Favored (69.21%) General / -59.4,-31.4	31.7% (*mt*) chi angles: 281.1,176.1	0.134Å	-	-
A 348		ARG	50	-	Favored (20.83%) General / -87.3,9.3	64.5% (*mtt-85*) chi angles: 296.6,184.9,180.9,245.2	0.04Å	-	-
A 349		PHE	50	-	Favored (30.08%) General / -125.5,160.2	73.9% (*m-85*) chi angles: 291.9,80.4	0.061Å	-	-
A 350		ILE	50	-	Favored (18.79%) Isoleucine or valine / -106.4,105.5	70.8% (*mt*) chi angles: 303.6,171.3	0.047Å	-	-
A 351		VAL	50	-	Favored (29.67%) Isoleucine or valine / -69.0,126.8	76.5% (*t*) chi angles: 179.2	0.045Å	-	-

A 352	LYS	50	-	Favored (5.62%) General / -115.5,-32.3	67.5% (*mttm*) chi angles: 289.6,179.5,175.6,292.2	0.076Å	-	-
A 353	LEU	50	0.457Å HB2 with A 364 PHE HB3	Favored (35.62%) General / -141.2,145.4	76.7% (*mt*) chi angles: 301.8,173.7	0.056Å	-	-
A 354	VAL	50	-	Favored (20.19%) Isoleucine or valine / -146.6,144.6	8.8% (*p*) chi angles: 68.4	0.075Å	-	-
A 355	ALA	50	-	Favored (38.36%) General / -138.8,140.0	-	0.069Å	-	-
A 356	CYS	50	-	Favored (54.31%) General / -118.6,135.7	69.3% (*m*) chi angles: 301.7	0.06Å	-	-
A 357	GLY	50	-	Favored (13.84%) Glycine / -114.7,-162.3	-	-	-	-
A 358	GLY	50	-	Favored (58.07%) Glycine / -69.5,-45.9	-	-	-	-
A 359	CYS	50	-	Favored (4.5%) General / -132.1,21.6	31.8% (*p*) chi angles: 64.3	0.071Å	-	-
A 360	HIS	50	-	Favored (17.89%) General / -166.2,163.3	35% (*p-80*) chi angles: 65.8,292.9	0.019Å	OUTLIER(S) worst is CD2--NE2: 4.323 σ	OUTLIER(S) worst is CB-CG-CD2: 5.174 σ
A 361	MET	50	-	Favored (30.03%) General / -146.9,146.0	58.6% (*ttp*) chi angles: 186.8,177.7,64.6	0.087Å	-	-
A 362	VAL	50	-	Favored (70.37%) Isoleucine or valine / -124.8,133.1	63.9% (*t*) chi angles: 179.9	0.075Å	-	-
A 363	VAL	50	-	Favored (49.47%) Isoleucine or valine / -129.2,140.3	40% (*t*) chi angles: 184.9	0.051Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 364		PHE	50	0.457Å HB3 with A 353 LEU HB2	Favored (15.76%) General / -115.4,107.9	19.2% (*t80*) chi angles: 176.9,46.7	0.024Å	-	-
A 365		ALA	50	-	Favored (47.82%) General / -124.2,147.8	-	0.038Å	-	-
			Avg: 50.27	Clashscore: 5.12	Outliers: 0 of 362	Poor rotamers: 8 of 301	Outliers: 0 of 319	Outliers: 13 of 364	Outliers: 8 of 364
A 366		ALA	50	-	Favored (23.46%) Pre-proline / -117.3,132.6	-	0.029Å	-	-
A 367		PRO	50	-	Favored (90.68%) Trans-proline / -64.2,146.6	85.6% (*Cg_endo*) chi angles: 30	0.025Å	-	-
A 368		HIS	50	-	Favored (90.61%) General / -60.1,-40.8	22.9% (*m-70*) chi angles: 272.8,271.7	0.064Å	OUTLIER(S) worst is CG--ND1: 4.287 σ	-
A 369		ARG	99.99	0.778Å HB2 with A 369 ARG NH1	-	0.6% chi angles: 210.7,142.7,293.5,80.8	0.084Å	-	-