



# Viewing NR2E3\_sm\_206-408H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	34.6	11 <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	3	1.69%	Goal: <1%
	Ramachandran outliers	11	5.47%	Goal: <0.05%
	Ramachandran favored	185	92.04%	Goal: >98%
	MolProbity score^	2.68		37 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	2.05%	Goal: 0
	Bad backbone bonds:	12 / 1627	0.74%	Goal: 0%
	Bad backbone angles:	18 / 2207	0.82%	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: Clashscore: 34.6 Outliers: 11 of 57.88 Poor rotamers: 3 of 177 Outliers: 4 of 195 Outliers: 7 of 203 Outliers: 16 of 203								
A 206	SER	50	-	-	36.6% (t) chi angles: 182.3	0.018Å	-	-
A 207	SER	50	-	Favored (88.73%) Pre-proline / -65.0,125.2	50.5% (m) chi angles: 301.6	0.01Å	-	-
A 208	PRO	50	-	Favored (71.19%) Trans-proline / -62.7,-35.1	50.9% (Cg_endo) chi angles: 25.1	0.112Å	-	-
A 209	TYR	99.99	0.543Å CD2 with A 209 TYR O	Favored (27.04%) General / 56.6,36.1	31.6% (t80) chi angles: 164.6,86	0.111Å	-	-
A 210	SER	99.99	-	Favored (42.63%) General / -59.1,129.5	34.2% (t) chi angles: 183.2	0.042Å	-	-
Favored								

A 211	SER	99.99	-	(30.76%) General / -88.3,139.2	33.2% ( <i>t</i> ) chi angles: 183.7	0.038Å	-	-
A 212	SER	99.99	0.417Å CA with A 226 ARG HH12	Favored (50.89%) General / -62.0,146.1	22.8% ( <i>t</i> ) chi angles: 186.7	0.03Å	-	-
A 213	SER	99.99	-	Favored (85.09%) Pre-proline / -59.1,128.4	22.6% ( <i>t</i> ) chi angles: 186.6	0.016Å	-	-
A 214	PRO	99.99	-	Favored (22.15%) Trans-proline / -63.3,-42.5	86% ( <i>Cg_endo</i> ) chi angles: 30	0.022Å	-	-
A 215	CYS	99.99	-	Favored (27.53%) General / -89.5,142.6	39.9% ( <i>t</i> ) chi angles: 175.4	0.097Å	-	-
A 216	GLY	50	-	Favored (45.24%) Glycine / 70.3,3.1	-	-	-	-
A 217	LEU	50	-	OUTLIER (0%) General / 38.1,116.7	52.6% ( <i>tp</i> ) chi angles: 179.2,67.6	0.103Å	-	-
A 218	ASP	50	-	Favored (55.05%) General / -57.5,133.2	74.4% ( <i>m-20</i> ) chi angles: 298.5,342.4	0.018Å	-	-
A 219	SER	50	-	Favored (16.08%) General / -79.3,170.8	91.5% ( <i>p</i> ) chi angles: 62.8	0.037Å	-	-
A 220	ILE	50	0.544Å HD12 with A 274 SER OG	Favored (47.58%) Isoleucine or valine / -63.5,-29.6	13.5% ( <i>tt</i> ) chi angles: 190.8,177.9	0.132Å	-	-
A 221	HIS	50	-	Favored (61.63%) General / -74.7,-40.1	62.8% ( <i>m170</i> ) chi angles: 296.5,162.8	0.084Å	OUTLIER(S) worst is CG-- ND1: 4.453 σ	-
A 222	GLU	50	-	Favored (76.79%) General / -63.0,-34.1	11.2% ( <i>mt-10</i> ) chi angles: 265.9,197.1,22.7	0.055Å	-	-
A 223	THR	50	-	Favored (78.63%) General / -69.2,-39.6	44.8% ( <i>p</i> ) chi angles: 66.5	0.054Å	-	-

A 224	SER	50	-	Favored (95.07%) General / -64.8,-40.3	48.5% (t) chi angles: 179.5	0.037Å	-	-
A 225	ALA	50	-	Favored (89.44%) General / -64.3,-38.0	-	0.023Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 226	ARG	50	0.442Å HG2 with A 230 MET CE	Favored (91.86%) General / -65.7,-40.0	60.5% (ttp180) chi angles: 186.9,175.2,62.1,192.4	0.019Å	-	-
A 227	LEU	50	0.431Å O with A 230 MET HG2	Favored (86.02%) General / -64.9,-37.0	60% (mt) chi angles: 294,184.2	0.033Å	-	-
A 228	LEU	50	-	Favored (52.85%) General / -71.5,-47.9	59.9% (tp) chi angles: 178.3,59.2	0.05Å	-	-
A 229	PHE	50	-	Favored (74.96%) General / -66.4,-33.1	31.9% (m-85) chi angles: 278.6,290.7	0.084Å	-	OUTLIER(S) worst is CA-CB-CG: 4.323 σ
A 230	MET	50	0.442Å CE with A 226 ARG HG2	Favored (76.56%) General / -68.4,-34.8	21.5% (ptp) chi angles: 67.6,180.3,58.3	0.062Å	-	-
A 231	ALA	50	-	Favored (98.83%) General / -63.4,-41.3	-	0.036Å	-	-
A 232	VAL	50	-	Favored (62.64%) Isoleucine or valine / -71.7,-46.3	92.2% (t) chi angles: 178	0.076Å	-	-
A 233	LYS	99.99	-	Favored (91.49%) General / -60.9,-40.0	98.9% (mttt) chi angles: 292.9,182.5,179.2,181.3	0.027Å	-	-
A 234	TRP	50	-	Favored (97.82%) General / -61.5,-44.0	73.3% (t90) chi angles: 172,80.6	0.037Å	-	-
A	ALA	50	-	Favored (89.23%)	-	0.018Å	-	-

235				General / -63.1,-38.0				
A 236	LYS	50	0.436Å HG2 with A 408 PHE CE1	Favored (63.9%) General / -67.9,-16.1	56.2% ( <i>mtmt</i> ) chi angles: 293.5,181.4,295.2,178	0.031Å	-	-
A 237	ASN	50	-	Favored (12.38%) General / -114.3,-12.9	21.2% ( <i>m120</i> ) chi angles: 288.8,95.8	0.099Å	-	-
A 238	LEU	50	0.668Å HD12 with A 239 PRO HD2	Favored (93.61%) Pre-proline / -71.6,151.5	24.5% ( <i>tp</i> ) chi angles: 186.2,72.6	0.031Å	-	-
A 239	PRO	50	0.668Å HD2 with A 238 LEU HD12	Favored (13.39%) Trans-proline / -49.7,147.6	49.8% ( <i>Cg_exo</i> ) chi angles: 326.6	0.103Å	-	-
A 240	VAL	50	0.699Å HG11 with A 345 LEU HD22	Allowed (0.12%) Isoleucine or valine / 69.8,-43.5	7.2% ( <i>p</i> ) chi angles: 74.1	0.22Å	-	-
A 241	PHE	50	-	Favored (80.11%) General / -57.1,-42.2	81.6% ( <i>t80</i> ) chi angles: 181.2,83.3	0.047Å	-	-
A 242	SER	50	-	Favored (65.85%) General / -67.0,-23.1	67.3% ( <i>m</i> ) chi angles: 296.7	0.054Å	-	-
A 243	SER	50	-	Favored (44.41%) General / -85.4,-15.0	22.2% ( <i>t</i> ) chi angles: 187.9	0.025Å	-	-
A 244	LEU	50	-	Favored (70.86%) Pre-proline / -60.0,150.2	87.8% ( <i>mt</i> ) chi angles: 298.6,180.3	0.044Å	-	-
A 245	PRO	50	-	Favored (95.05%) Trans-proline / -57.5,141.4	46.4% ( <i>Cg_endo</i> ) chi angles: 24.7	0.025Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
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A 246	PHE	50	-	Favored (65.49%) General /	52.8% ( <i>p90</i> ) chi angles: 61.8,86.9	0.026Å	-	-
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A 247	ARG	50	0.572Å HH21 with A 337 LYS HG2	-56.2,-33.6 Favored (81.03%) General / -67.1,-36.0	30.2% ( <i>ptt-85</i> ) chi angles: 62.3,174.2,178.9,281.2	0.093Å	-	-
A 248	ASP	50	-	Favored (86.5%) General / -66.8,-38.4	97.8% ( <i>m-20</i> ) chi angles: 288.1,348.2	0.064Å	-	-
A 249	GLN	50	0.54Å OE1 with A 408 PHE CZ	Favored (97.8%) General / -63.9,-41.4	57.4% ( <i>mt-30</i> ) chi angles: 302.2,194.5,50.6	0.074Å	OUTLIER(S) worst is CD-- OE1: 5.756 σ	OUTLIER(S) worst is CB- CG-CD: 4.179 σ
A 250	VAL	50	0.501Å O with A 254 GLU HG3	Favored (92.66%) Isoleucine or valine / -66.0,-43.5	99.3% ( <i>t</i> ) chi angles: 176.5	0.044Å	-	-
A 251	ILE	50	0.689Å HG22 with A 333 THR HB	Favored (79.52%) Isoleucine or valine / -59.7,-50.6	61.1% ( <i>mt</i> ) chi angles: 287.1,164.9	0.141Å	-	-
A 252	LEU	50	0.815Å HA with A 333 THR HG21	Favored (91.44%) General / -59.0,-43.3	95.2% ( <i>mt</i> ) chi angles: 293.9,175.3	0.032Å	-	-
A 253	LEU	50	-	Favored (70.09%) General / -71.9,-36.5	43.7% ( <i>mt</i> ) chi angles: 282.8,170.7	0.087Å	-	-
A 254	GLU	50	0.664Å HA with A 404 LEU HD22	Favored (82.38%) General / -60.4,-37.9	57% ( <i>mt-10</i> ) chi angles: 290.2,178.7,303.1	0.054Å	-	-
A 255	GLU	50	0.502Å HB3 with A 333 THR HG22	Favored (33.63%) General / -79.8,-38.1	9.9% ( <i>tm-20</i> ) chi angles: 178.6,289.7,325.1	0.084Å	-	-
A 256	ALA	50	-	Favored (19.72%) General / -105.7,-5.8	-	0.01Å	-	-
A 257	TRP	50	0.478Å HB3 with A 404 LEU HD21	Favored (64.43%) General / -54.4,-36.8	32.6% ( <i>p-90</i> ) chi angles: 75.2,262.9	0.089Å	-	-
A 258	SER	50	0.443Å HB2 with A 386 ILE HD12	Favored (65.59%) General / -72.7,-32.2	91.4% ( <i>p</i> ) chi angles: 62.8	0.083Å	-	-

A 259	GLU	50	-	Favored (73.92%) General / -70.5,-40.1	54.2% ( <i>mt-10</i> ) chi angles: 300.7,178.8,36.7	0.049Å	-	-
A 260	LEU	50	-	Favored (79.05%) General / -68.2,-36.1	97% ( <i>mt</i> ) chi angles: 297.3,178.2	0.032Å	-	-
A 261	PHE	50	-	Favored (89.17%) General / -61.5,-46.6	79.3% ( <i>t80</i> ) chi angles: 177.7,85.9	0.058Å	-	-
A 262	LEU	50	0.624Å HD11 with A 306 THR OG1	Favored (95.86%) General / -64.4,-42.9	6.8% ( <i>tt</i> ) chi angles: 193.2,163.1	0.069Å	-	-
A 263	LEU	50	-	Favored (83.83%) General / -62.5,-36.9	56.3% ( <i>mt</i> ) chi angles: 284.7,168.7	0.006Å	-	-
A 264	GLY	50	-	Favored (70.62%) Glycine / -68.5,-44.9	-	-	-	-
A 265	ALA	50	-	Favored (89.19%) General / -59.0,-42.0	-	0.023Å	-	-
<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: 57.88</div> <div>Clashscore: 34.6</div> <div>Outliers: 11 of 201</div> <div>Poor rotamers: 3 of 177</div> <div>Outliers: 4 of 195</div> <div>Outliers: 7 of 203</div> <div>Outliers: 16 of 203</div> </div>								
A 266	ILE	50	0.918Å HG22 with A 307 ILE HA	Favored (82.65%) Isoleucine or valine / -68.5,-44.8	27.2% ( <i>pt</i> ) chi angles: 55.8,164.5	0.026Å	-	-
A 267	GLN	50	0.738Å N with A 266 ILE HG13	Favored (84.74%) General / -65.5,-36.7	64% ( <i>tt0</i> ) chi angles: 181.4,174.4,29.5	0.035Å	-	-
A 268	TRP	50	-	Favored (57.56%) General / -91.5,0.0	99.5% ( <i>m95</i> ) chi angles: 292.6,98.6	0.019Å	OUTLIER(S) worst is NE1-- CE2: 4.41 σ	
A 269	SER	50	0.851Å HA with A 311 ARG NH2	Favored (22.95%) General / 59.0,39.8 Favored	66.3% ( <i>m</i> ) chi angles: 298.4	0.132Å	-	-

A 270	LEU	50	0.414Å HD23 with A 271 PRO O	(47.68%) Pre-proline / -56.4,122.1	9.9% ( <i>tt</i> ) chi angles: 185.8,154.8	0.068Å	-	-
A 271	PRO	50	0.414Å O with A 270 LEU HD23	Favored (44.48%) Trans-proline / -53.3,131.7	96.8% ( <i>Cg_exo</i> ) chi angles: 329.3	0.057Å	-	-
A 272	LEU	50	0.762Å HD13 with A 304 GLN HG2	Favored (7.33%) General / -114.2,-28.3	3.6% ( <i>pp</i> ) chi angles: 71.7,83.2	0.124Å	-	-
A 273	ASP	99.99	-	Favored (4.35%) General / -103.2,31.3	42.9% ( <i>t0</i> ) chi angles: 192.9,336.6	0.07Å	-	-
A 274	SER	50	0.743Å C with A 276 PRO HD3	Favored (18.74%) General / -98.7,153.4	40.9% ( <i>p</i> ) chi angles: 53.8	0.096Å	-	-
A 275	CYS	50	0.435Å N with A 276 PRO HD3	OUTLIER (0%) Pre-proline / 83.0,-3.8	51.2% ( <i>m</i> ) chi angles: 306.8	0.153Å	-	-
A 276	PRO	50	0.743Å HD3 with A 274 SER C	Favored (60.02%) Trans-proline / -64.7,-27.6	87.9% ( <i>Cg_exo</i> ) chi angles: 331.6	0.116Å	-	OUTLIER(S) worst is CA- N-CD: 4.382 σ
A 277	LEU	50	-	Allowed (0.56%) General / -50.8,-65.4	78.7% ( <i>mt</i> ) chi angles: 297.8,169.8	0.042Å	-	-
A 278	LEU	99.99	-	Allowed (0.08%) General / -54.2,-71.5	95.6% ( <i>mt</i> ) chi angles: 296.4,173.7	0.02Å	-	-
A 279	ALA	99.99	-	OUTLIER (0.03%) Pre-proline / -5.8,84.8	-	0.033Å	-	-
A 280	PRO	99.99	-	OUTLIER (0.05%) Trans-proline / -50.9,101.7	55% ( <i>Cg_exo</i> ) chi angles: 326.9	0.039Å	-	-
A 281	PRO	99.99	0.446Å HA with A 294 THR HG22	OUTLIER (0.02%) Trans-proline / -46.5,92.4	61.1% ( <i>Cg_exo</i> ) chi angles: 327.3	0.018Å	-	-
A 282	GLU	99.99	-	Favored (45.37%) General / -72.3,148.4	92% ( <i>mt-10</i> ) chi angles: 297.3,181.2,335.8	0.028Å	-	-

A 283	ALA	99.99	0.433Å HA with A 292 ARG HG2	Favored (56.85%) General / -92.2,2.0	-	0.034Å	-	-
A 284	SER	99.99	-	OUTLIER (0%) General / 17.4,-73.7	71.7% ( <i>p</i> ) chi angles: 57.8	0.111Å	-	-
A 285	ALA	99.99	-	Favored (52.28%) General / -133.0,147.1	-	0.076Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 286	ALA	99.99	-	Favored (3.62%) General / -145.9,102.2	-	0.019Å	-	-
A 287	GLY	99.99	-	Favored (3.48%) Glycine / -105.0,-110.2	-	-	-	-
A 288	GLY	99.99	-	Favored (10.49%) Glycine / -88.5,-33.3	-	-	-	-
A 289	ALA	99.99	-	Favored (13.7%) General / -119.5,166.0	-	0.093Å	-	-
A 290	GLN	99.99	0.623Å HE22 with A 292 ARG HH21	Favored (19.05%) General / -111.2,158.4	51.3% ( <i>tt0</i> ) chi angles: 180.3,185.4,61.9	0.07Å	-	-
A 291	GLY	99.99	0.489Å N with A 290 GLN HG2	Favored (9.62%) Glycine / -160.2,144.0	-	-	-	-
A 292	ARG	99.99	0.623Å HH21 with A 290 GLN HE22	Favored (26.36%) General / -138.2,165.6	99.6% ( <i>mtt180</i> ) chi angles: 292.1,184.1,183.6,177	0.092Å	-	-
A 293	LEU	99.99	-	Favored (47.32%) General / -119.9,144.6	78.8% ( <i>mt</i> ) chi angles: 299.1,171.2	0.141Å	-	-
A	THR	99.99	0.446Å HG22 with A	Favored (16.35%)	67.2% ( <i>p</i> )	0.112Å	-	OUTLIER(S) worst is O-C-



294			281 PRO HA	General / -159.1,144.8	chi angles: 59.5			N: 5.273 $\sigma$
A 295	LEU	99.99	0.674Å HD13 with A 297 SER O	OUTLIER (0%) General / 136.3,-141.1	15.2% ( <i>mt</i> ) chi angles: 295.7,154.5	0.28Å	-	OUTLIER(S) worst is C-N- CA: 8.4 $\sigma$
A 296	ALA	50	0.638Å O with A 295 LEU HB2	OUTLIER (0%) General / 48.1,161.8	-	0.257Å	-	OUTLIER(S) worst is O-C- N: 4.722 $\sigma$
A 297	SER	99.99	0.674Å O with A 295 LEU HD13	OUTLIER (0.01%) General / -75.0,-135.0	88.1% ( <i>p</i> ) chi angles: 61.7	0.176Å	-	-
A 298	MET	50	0.478Å SD with A 300 THR HB	Allowed (0.46%) General / -153.7,31.2	3.4% ( <i>tpt</i> ) chi angles: 213.7,76.2,175.1	0.119Å	-	-
A 299	GLU	50	0.452Å HB2 with A 297 SER OG	OUTLIER (0%) General / -22.4,-30.7	44.4% ( <i>mt-10</i> ) chi angles: 291.2,170.2,292.7	0.16Å	-	-
A 300	THR	50	0.636Å O with A 304 GLN HG3	Favored (60.87%) General / -54.8,-33.0	24.6% ( <i>m</i> ) chi angles: 309	0.103Å	-	-
A 301	ARG	50	0.835Å HA with A 304 GLN OE1	Favored (86.27%) General / -65.2,-37.1	0.3% chi angles: 160,272.5,158.5,166.3	0.307Å	-	-
A 302	VAL	50	-	Favored (19.81%) Isoleucine or valine / -80.2,-40.1	59.6% ( <i>t</i> ) chi angles: 180.3	0.112Å	-	-
A 303	LEU	50	0.421Å HB2 with A 385 ARG NH1	Favored (76.59%) General / -59.5,-36.8	29.9% ( <i>tp</i> ) chi angles: 186.6,69.9	0.056Å	-	-
A 304	GLN	50	0.835Å OE1 with A 301 ARG HA	Favored (71.75%) General / -59.8,-51.0	84.4% ( <i>mt-30</i> ) chi angles: 288.4,171.7,301	0.074Å	-	OUTLIER(S) worst is OE1- CD-NE2: 5.457 $\sigma$
A 305	GLU	50	-	Favored (59.29%) General / -50.8,-48.8	18.8% ( <i>tt0</i> ) chi angles: 167.2,198.6,316.4	0.088Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
Avg:			57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 306	THR	50	0.624Å OG1 with A 262 LEU	Favored (83.02%) General /		38% ( <i>p</i> )	0.067Å	-	-

HD11

-66.6,-36.6

chi angles: 53.1

A 307	ILE	50	0.918Å HA with A 266 ILE HG22	Favored (89.42%) Isoleucine or valine / -65.5,-40.9	3.8% ( <i>pt</i> ) chi angles: 74.1,194	0.18Å	-	-
A 308	SER	50	-	Favored (72.41%) General / -71.1,-37.3	74.8% ( <i>m</i> ) chi angles: 294.9	0.015Å	-	-
A 309	ARG	50	-	Favored (77.67%) General / -67.0,-34.4	99.4% ( <i>mtt180</i> ) chi angles: 290.5,183.2,177.2,180.7	0.02Å	-	-
A 310	PHE	50	0.72Å CD2 with A 266 ILE HD13	Favored (56.2%) General / -77.0,-36.4	1.6% ( <i>m-85</i> ) chi angles: 292.2,35.3	0.021Å	-	-
A 311	ARG	50	0.851Å NH2 with A 269 SER HA	Favored (74.72%) General / -70.0,-35.8	99.6% ( <i>mtt180</i> ) chi angles: 293.9,183.5,180.6,180.8	0.007Å	-	-
A 312	ALA	50	-	Favored (77.59%) General / -66.0,-34.2	-	0.055Å	-	-
A 313	LEU	50	0.585Å HD23 with A 374 LEU HD11	Favored (60.26%) General / -75.9,-13.1	7.6% ( <i>tp</i> ) chi angles: 205.4,44.4	0.121Å	-	-
A 314	ALA	50	-	Favored (29.35%) General / 56.7,40.2	-	0.062Å	-	-
A 315	VAL	50	0.486Å HB with A 320 PHE CZ	Favored (14.21%) Isoleucine or valine / -52.3,133.9	59.3% ( <i>t</i> ) chi angles: 180.9	0.079Å	-	-
A 316	ASP	50	0.565Å HB2 with A 317 PRO HD2	Favored (8.58%) Pre-proline / -101.2,168.8	17.8% ( <i>p30</i> ) chi angles: 75.1,20	0.131Å	-	-
A 317	PRO	50	0.565Å HD2 with A 316 ASP HB2	Favored (87.53%) Trans-proline / -54.3,-39.3	78.6% ( <i>Cg_endo</i> ) chi angles: 29.8	0.079Å	-	-
A 318	THR	50	-	Favored (79.21%) General /	77.1% ( <i>p</i> ) chi angles: 58.6	0.048Å	-	-

A 319	GLU	50	-	-68.7,-41.5 Favored (89.95%) General / -65.1,-38.2	79% ( <i>mt-10</i> ) chi angles: 295.2,175.4,322	0.012Å	-	-
A 320	PHE	50	0.486Å CZ with A 315 VAL HB	Favored (96.93%) General / -61.5,-44.5	96.5% ( <i>m-85</i> ) chi angles: 292.7,275.9	0.081Å	-	-
A 321	ALA	50	-	Favored (95.27%) General / -64.3,-43.3	-	0.021Å	-	-
A 322	CYS	50	-	Favored (92.99%) General / -65.3,-42.4	89.7% ( <i>m</i> ) chi angles: 293.2	0.027Å	-	-
A 323	MET	50	0.466Å CE with A 371 LEU HD22	Favored (87.61%) General / -63.6,-37.5	66.6% ( <i>mtt</i> ) chi angles: 290.5,181.7,184.1	0.064Å	-	OUTLIER(S) worst is CG- SD-CE: 5.738 σ
A 324	LYS	50	0.428Å HG3 with A 320 PHE O	Favored (88.05%) General / -65.8,-38.1	83.1% ( <i>mttt</i> ) chi angles: 297.5,179.1,199.1,179.3	0.041Å	-	-
A 325	ALA	50	-	Favored (79.32%) General / -68.8,-40.7	-	0.021Å	-	-
<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: 57.88</div> <div>Clashscore: 34.6</div> <div>Outliers: 11 of 201</div> <div>Poor rotamers: 3 of 177</div> <div>Outliers: 4 of 195</div> <div>Outliers: 7 of 203</div> <div>Outliers: 16 of 203</div> </div>								
A 326	LEU	50	0.596Å HD21 with A 350 GLN N	Favored (98.56%) General / -63.5,-42.0	90.5% ( <i>mt</i> ) chi angles: 292.2,176.7	0.027Å	-	-
A 327	VAL	50	-	Favored (95.15%) Isoleucine or valine / -63.2,-46.7	37.8% ( <i>t</i> ) chi angles: 165.7	0.084Å	-	-
A 328	LEU	50	-	Favored (81.82%) General / -67.9,-42.1	50.7% ( <i>tp</i> ) chi angles: 183.3,59.9	0.039Å	-	-
A 329	PHE	50	-	Favored (5.74%) General / -89.1,61.2	27.2% ( <i>m-30</i> ) chi angles: 294.1,311.1	0.034Å	-	-

A 330	LYS	50	1.017Å HE3 with A 332 GLU HG2	Favored (40.92%) Pre-proline / -105.6,123.0	55.4% ( <i>tptt</i> ) chi angles: 187.4,65.3,175.4,170.5	0.063Å	-	-
A 331	PRO	50	0.719Å HD2 with A 330 LYS HD2	Favored (16.7%) Trans-proline / -68.0,-6.3	82.5% ( <i>Cg_endo</i> ) chi angles: 29.9	0.058Å	-	-
A 332	GLU	99.99	1.017Å HG2 with A 330 LYS HE3	Favored (66.17%) General / -66.5,-22.6	75.4% ( <i>mm-40</i> ) chi angles: 289.3,303.8,315.5	0.083Å	-	-
A 333	THR	50	0.815Å HG21 with A 252 LEU HA	Favored (53.29%) General / -65.7,134.5	62.1% ( <i>p</i> ) chi angles: 62.8	0.05Å	-	-
A 334	ARG	50	-	Favored (51.46%) General / -69.7,136.7	60.4% ( <i>ttm-85</i> ) chi angles: 180.6,182.9,292.7,277.5	0.078Å	-	-
A 335	GLY	50	-	Favored (60.78%) Glycine / 80.7,23.0	-	-	-	-
A 336	LEU	50	-	Favored (58.59%) General / -65.4,140.0	64.7% ( <i>mt</i> ) chi angles: 288.2,178.4	0.031Å	-	-
A 337	LYS	50	0.572Å HG2 with A 247 ARG HH21	Favored (17.5%) General / -89.7,-31.4	28.8% ( <i>tptp</i> ) chi angles: 184.7,63.9,180.3,64	0.015Å	-	-
A 338	ASP	50	-	Favored (52.7%) Pre-proline / -133.6,82.0	42.9% ( <i>t0</i> ) chi angles: 193.4,340.3	0.087Å	-	-
A 339	PRO	50	-	Favored (21%) Trans-proline / -65.9,-39.0	77.1% ( <i>Cg_endo</i> ) chi angles: 29.7	0.057Å	-	-
A 340	GLU	50	-	Favored (86.47%) General / -61.2,-38.4	11.6% ( <i>pt-20</i> ) chi angles: 66.3,175.7,59.7	0.062Å	-	-
A 341	HIS	50	-	Favored (73.56%) General / -69.5,-43.2	54.3% ( <i>t60</i> ) chi angles: 184,51.1	0.005Å	OUTLIER(S) worst is CG-- ND1: 4.454 σ	OUTLIER(S) worst is CB- CG-CD2: 4.749 σ
A 342	VAL	50	-	Favored (87.58%) Isoleucine or	81.6% ( <i>t</i> ) chi angles: 174.6	0.072Å	-	-

A 343	GLU	50	-	valine /	83.2% ( <i>mt-10</i> )	0.034Å	-	-
				-65.1,-40.0 Favored (83.67%) General / -66.6,-36.9				
A 344	ALA	50	-		-	0.025Å	-	-
				Favored (82.08%) General / -62.2,-36.5				
A 345	LEU	50	0.699Å HD22 with A 240 VAL HG11	Favored (71.16%) General / -71.5,-36.5	97% ( <i>mt</i> ) chi angles: 292.7,174	0.024Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 346	GLN	50	-	Favored (74.28%) General / -70.3,-36.6	45% ( <i>tt0</i> ) chi angles: 195.2,182.3,48	0.028Å	-	-
A 347	ASP	50	-	Favored (98.77%) General / -63.3,-43.2	37.6% ( <i>t70</i> ) chi angles: 183.6,57	0.015Å	-	-
A 348	GLN	50	0.5Å HA with A 351 VAL HG12	Favored (90.05%) General / -63.0,-38.2	52.7% ( <i>tt0</i> ) chi angles: 182.7,183.5,57.8	0.02Å	-	-
A 349	SER	50	0.579Å O with A 352 MET HG2	Favored (69.21%) General / -72.0,-34.7	49.5% ( <i>m</i> ) chi angles: 300.9	0.06Å	-	-
A 350	GLN	50	0.596Å N with A 326 LEU HD21	Favored (30.84%) General / -82.0,-31.9	0% chi angles: 69.3,104.5,149.5	0.141Å	-	-
A 351	VAL	50	0.5Å HG12 with A 348 GLN HA	Favored (84.92%) Isoleucine or valine / -65.9,-39.5	8.2% ( <i>p</i> ) chi angles: 70.3	0.129Å	-	-
A 352	MET	50	0.579Å HG2 with A 349 SER O	Favored (89.07%) General / -66.3,-39.1	18.9% ( <i>ptp</i> ) chi angles: 71,181.2,57.1	0.084Å	-	-
A 353	LEU	50	-	Favored (81.92%) General /	63.5% ( <i>tp</i> ) chi angles: 178.7,60.8	0.029Å	-	-

A 354	SER	50	-	-66.9,-44.0 Favored (89.78%) General / -59.6,-41.1	35.9% ( <i>t</i> ) chi angles: 182.5	0.03Å	-	-	
A 355	GLN	50	-	Favored (73.98%) General / -70.3,-40.8	94.6% ( <i>mt-30</i> ) chi angles: 293.9,183.4,331	0.034Å	-	-	
A 356	HIS	50	-	Favored (73.86%) General / -62.0,-50.0	82.1% ( <i>t60</i> ) chi angles: 183.3,76.2	0.049Å	OUTLIER(S) worst is CG-- ND1: 8.342 $\sigma$	OUTLIER(S) worst is CB- CG-CD2: 4.155 $\sigma$	
A 357	SER	50	-	Favored (87.64%) General / -65.9,-38.0	32.1% ( <i>t</i> ) chi angles: 184.5	0.01Å	-	-	
A 358	LYS	50	-	Favored (69.97%) General / -68.8,-31.1	38.3% ( <i>ttpt</i> ) chi angles: 187.9,180.3,64,181.2	0.028Å	-	-	
A 359	ALA	50	-	Favored (20.19%) General / -85.1,-37.5	-	0.029Å	-	-	
A 360	HIS	50	-	Favored (18.9%) General / -89.4,-29.7	75% ( <i>m80</i> ) chi angles: 292.8,76.9	0.028Å	OUTLIER(S) worst is CG-- CD2: 5.28 $\sigma$	OUTLIER(S) worst is ND1- CG-CD2: 4.005 $\sigma$	
A 361	HIS	50	-	Favored (28.08%) Pre-proline / -125.7,59.6	98.8% ( <i>m-70</i> ) chi angles: 298.6,285.6	0.054Å	OUTLIER(S) worst is CG-- ND1: 4.687 $\sigma$	OUTLIER(S) worst is CB- CG-CD2: 4.111 $\sigma$	
A 362	PRO	50	-	Favored (76.12%) Trans-proline / -62.1,-24.0	86.5% ( <i>Cg_endo</i> ) chi angles: 30	0.081Å	-	-	
A 363	SER	50	-	Favored (42.59%) General / -99.2,9.9	70.1% ( <i>m</i> ) chi angles: 295.9	0.052Å	-	-	
A 364	GLN	50	-	Favored (46.95%) Pre-proline / -122.8,75.5	77.4% ( <i>mt-30</i> ) chi angles: 294.6,182.7,47.1	0.024Å	-	-	
A 365	PRO	50	-	Favored (76.68%) Trans-proline / -62.0,-24.3	72.5% ( <i>Cg_endo</i> ) chi angles: 29.2	0.096Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles

Avg: Clashscore: 57.88				Outliers: 11 of 201		Poor rotamers: 3 of 177		Outliers: 4 of 195		Outliers: 7 of 203		Outliers: 16 of 203	
A 366	VAL	50	-	Favored (9%) Isoleucine or valine / -94.4,3.2		60.3% (t) chi angles: 181.6		0.08Å		-		-	
A 367	ARG	50	-	Favored (93.2%) General / -65.2,-39.6		52.7% (ttt85) chi angles: 188.4,180,179.9,72.3		0.049Å		-		-	
A 368	PHE	50	-	Favored (98.02%) General / -60.9,-43.8		51.5% (t80) chi angles: 175.1,62.8		0.024Å		-		-	
A 369	GLY	50	-	Favored (97.02%) Glycine / -64.5,-39.7		-		-		-		-	
A 370	LYS	50	-	Favored (93.38%) General / -64.4,-39.2		98.1% (mttt) chi angles: 290.7,184.7,178.4,182.2		0.042Å		-		-	
A 371	LEU	50	0.466Å HD22 with A 323 MET CE	Favored (79.61%) General / -67.0,-44.7		56.9% (mt) chi angles: 293.3,184.4		0.056Å		-		-	
A 372	LEU	50	-	Favored (76.5%) General / -67.0,-33.9		45.1% (mt) chi angles: 293.1,186.2		0.076Å		-		-	
A 373	LEU	50	-	Favored (61.24%) General / -69.1,-11.9		75.5% (mt) chi angles: 289.1,176.8		0.145Å		-		-	
A 374	LEU	50	0.585Å HD11 with A 313 LEU HD23	Favored (63.58%) General / -69.7,-24.6		87.1% (mt) chi angles: 292.7,178.3		0.035Å		-		-	
A 375	LEU	50	-	Favored (34.13%) Pre-proline / -67.6,-42.0		84.7% (mt) chi angles: 300.9,179.8		0.117Å		-		-	
A 376	PRO	50	-	Favored (98.17%) Trans-proline / -58.1,-36.2		82.3% (Cg_exo) chi angles: 330.4		0.07Å		-		-	
A 377	SER	50	-	Favored (80.26%) General / -68.8,-39.0		50.1% (m) chi angles: 301.1		0.021Å		-		-	

A 378	LEU	50	0.73Å O with A 381 ILE HG12	Favored (94.84%) General / -63.4,-39.6	86.2% ( <i>mt</i> ) chi angles: 292.4,178.2	0.077Å	-	-
A 379	ARG	50	0.875Å HH22 with A 330 LYS HG2	Favored (66.35%) General / -66.2,-22.4	18.7% ( <i>tpp85</i> ) chi angles: 186.3,58.5,70.1,78.2	0.097Å	-	-
A 380	PHE	50	-	Favored (20.71%) General / -91.1,-22.4	2.5% ( <i>m-85</i> ) chi angles: 285.9,36.6	0.062Å	-	-
A 381	ILE	50	0.808Å HB with A 385 ARG NH2	Favored (12.95%) Isoleucine or valine / -55.0,126.8	12.9% ( <i>pt</i> ) chi angles: 75.6,169.1	0.091Å	-	-
A 382	THR	50	0.612Å O with A 385 ARG HG2	Favored (33.24%) General / -80.0,128.2	29.9% ( <i>p</i> ) chi angles: 70.4	0.151Å	-	-
A 383	ALA	50	-	Favored (86.24%) General / -60.1,-39.5	-	0.039Å	-	-
A 384	GLU	50	0.495Å O with A 388 LEU HD13	Favored (89.62%) General / -60.1,-40.5	12% ( <i>pt-20</i> ) chi angles: 63.1,177.7,59.7	0.076Å	-	-
A 385	ARG	50	0.808Å NH2 with A 381 ILE HB	Favored (82.96%) General / -67.5,-37.5	33% ( <i>ptt85</i> ) chi angles: 73.6,189.6,171.3,68.9	0.094Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 386	ILE	50	0.443Å HD12 with A 258 SER HB2	Favored (91.52%) Isoleucine or valine / -64.6,-41.2	79.1% ( <i>mt</i> ) chi angles: 296.7,177	0.073Å	-	-
A 387	GLU	50	-	Favored (91.96%) General / -65.6,-42.2	89.6% ( <i>mt-10</i> ) chi angles: 297.6,172.7,332.2	0.02Å	-	-
A 388	LEU	50	0.495Å HD13 with A 384 GLU O	Favored (82.31%) General / -66.0,-36.1	11.2% ( <i>mp</i> ) chi angles: 274.4,61.9	0.032Å	-	-
				Favored				



A 389	LEU	50	0.453Å HB2 with A 385 ARG O	Favored (65.49%) General / -72.8,-40.9	6.2% ( <i>tp</i> ) chi angles: 219.1,54.2	0.087Å	-	-
A 390	PHE	50	-	Favored (3.69%) General / -125.2,-26.1	86% ( <i>m-85</i> ) chi angles: 301.9,282.9	0.038Å	-	-
A 391	PHE	50	0.462Å CG with A 400 MET HE3	Favored (14.66%) General / -113.8,0.9	67.1% ( <i>m-85</i> ) chi angles: 288.9,286.9	0.102Å	-	-
A 392	ARG	50	0.727Å HA with A 396 GLY O	Favored (81.29%) General / -56.7,-44.0	27.3% ( <i>ptt-85</i> ) chi angles: 61.7,171.2,179.3,281.9	0.114Å	-	-
A 393	LYS	50	-	Favored (73.95%) General / -69.0,-33.6	62.8% ( <i>mttp</i> ) chi angles: 290.4,184.6,180.6,62.1	0.034Å	-	-
A 394	THR	50	0.429Å OG1 with A 395 ILE HG12	Favored (39.6%) General / -79.8,-34.8	82.4% ( <i>p</i> ) chi angles: 60.7	0.042Å	-	-
A 395	ILE	99.99	0.553Å CG2 with A 398 THR HG23	Allowed (0.82%) Isoleucine or valine / -131.4,-26.1	38.5% ( <i>mm</i> ) chi angles: 299.4,305.8	0.206Å	-	OUTLIER(S) worst is N- CA-CB: 4.208 σ
A 396	GLY	50	0.746Å HA3 with A 397 ASN HB3	Favored (8.89%) Glycine / 100.7,-126.4	-	-	-	OUTLIER(S) worst is C-N- CA: 7.199 σ
A 397	ASN	50	0.746Å HB3 with A 396 GLY HA3	OUTLIER (0%) General / 106.6,-84.3	25.2% ( <i>t-20</i> ) chi angles: 181,302.1	0.149Å	-	OUTLIER(S) worst is CA- CB-CG: 5.758 σ
A 398	THR	50	0.553Å HG23 with A 395 ILE CG2	Favored (88.15%) Pre-proline / -76.2,123.9	0.5% chi angles: 162.4	0.288Å	-	-
A 399	PRO	50	-	Favored (88.82%) Trans-proline / -57.5,139.0	94.9% ( <i>Cg_exo</i> ) chi angles: 329.3	0.082Å	-	-
A 400	MET	99.99	0.462Å HE3 with A 391 PHE CG	Favored (74.61%) General / -56.3,-40.7 Favored	21.1% ( <i>mmt</i> ) chi angles: 285,300.7,173.4	0.046Å	-	-

A 401	GLU	50	0.778Å HA with A 404 LEU HD13	(66.97%) General / -59.4,-28.5	2.4% ( <i>pp20?</i> ) chi angles: 64.4,69.3,25.8	0.175Å	-	-	
A 402	LYS	50	-	Favored (60.96%) General / -72.5,-23.1	26.3% ( <i>tptp</i> ) chi angles: 188.9,60.5,185.1,66.4	0.039Å	-	-	
A 403	LEU	50	-	Favored (20.84%) General / -99.8,-11.3	84.3% ( <i>mt</i> ) chi angles: 289.3,173.6	0.048Å	-	-	
A 404	LEU	50	0.778Å HD13 with A 401 GLU HA	Favored (81.29%) General / -57.8,-41.1	8.7% ( <i>mp</i> ) chi angles: 268,66.4	0.041Å	-	OUTLIER(S) worst is CD1- CG-CD2: 4.487 $\sigma$	
A 405	CYS	50	-	Favored (99.47%) General / -61.3,-42.9	46.9% ( <i>t</i> ) chi angles: 185.2	0.022Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 57.88	Clashscore: 34.6	Outliers: 11 of 201	Poor rotamers: 3 of 177	Outliers: 4 of 195	Outliers: 7 of 203	Outliers: 16 of 203
A 406	ASP	50	-	-	Favored (91.67%) General / -65.4,-39.0	79.1% ( <i>m-20</i> ) chi angles: 288.5,357.1	0.045Å	-	-
A 407	MET	50	-	-	Favored (97.54%) General / -64.0,-41.3	63.5% ( <i>mtt</i> ) chi angles: 294.5,182.2,176.5	0.035Å	-	-
A 408	PHE	99.99	0.54Å CZ with A 249 GLN OE1	-	-	74.5% ( <i>t80</i> ) chi angles: 185.9,77.7	0.06Å	-	-

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