

Viewing cdh23_mb_24-233_FFX1Hmulti.table

When finished, you should close this window.

Hint: Use File | Save As... to save a copy of this page.

All-Atom	Clashscore, all atoms:	0.62		99 th percentile* (N=1784, all resolutions)
Contacts	Clashscore is the number	of serious	steric ov	erlaps (> 0.4 Å) per 1000 atoms.
	Poor rotamers	3	1.60%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	192 92.31%		Goal: >98%
Protein Geometry	MolProbity score [^]	1.34		98 th percentile* (N=27675, 0Å - 99Å)
geometry	Cβ deviations >0.25Å	2	1.01%	Goal: 0
	Bad backbone bonds:	0 / 1681	0.00%	Goal: 0%
	Bad backbone angles:	9 / 2302	0.39%	Goal: <0.1%

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

[^] 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	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers: 2 of 199		
24	GLN	81.62	-	-	4.6% (pp0?) chi angles: 64.2,89.9,26.9	0.088Å	-	OUTLIER(S) worst is NE2-CD-OE1: 6.156σ
25	VAL	85.44	-	Favored (35.15%) Isoleucine or valine /-82.0,130.8	10.7% (<i>p</i>) chi angles: 67.3	0.057Å	-	-
26	ASN	52.34	-	Favored (34.39%) General / -57.0,144.4	56.3% (<i>t</i> 30) chi angles: 185.5,42.7	0.059Å	-	-
27	ARG	99.93	-	Favored (27.37%) General /	60.1% (mtm180) chi angles: 288.3,155.9,298,190.2	0.086Å	-	-

^{* 100&}lt;sup>th</sup> 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.

			-133.1,124.3				
28	LEU 86.21	-	Favored (98.1%) Pre-proline / -66.2,149.2	3.9% (<i>mm</i> ?) chi angles: 284.9,297.4	0.053Å	-	-
29	PRO 83.6	-	Favored (19.06%) Trans-proline / -79.4,145.8	64.5% (<i>Cg_endo</i>) chi angles: 27.7	0.052Å	-	-
30	PHE 57.73	-	Favored (53.2%) General / -124.7,135.6	44.5% (<i>p90</i>) chi angles: 55.4,90.7	0.049Å	-	-
31	PHE 97.12	-	Favored (51.48%) General / -64.4,132.9	27.8% (<i>m</i> -85) chi angles: 306.5,305.1	0.083Å	-	-
32	THR 82.88	-	Favored (18.95%) General / -92.2,-24.8	46% (<i>p</i>) chi angles: 55.2	0.086Å	-	-
33	ASN 73.23	-	Favored (53.68%) General / -56.7,137.7	63.5% (<i>m</i> -20) chi angles: 276.5,334.6	0.06Å	-	-
34	HIS 57.37	-	Favored (57.99%) General / -78.4,-8.0	81% (<i>t60</i>) chi angles: 181.1,61.5	0.104Å	-	-
35	PHE 96.1	-	Favored (60.61%) General / -74.8,-13.7	11.3% (<i>p90</i>) chi angles: 57.4,71.2	0.196Å	-	-
36	PHE 79.92	-	Favored (59.97%) General / -76.2,-15.9	97.3% (<i>m-85</i>) chi angles: 294.1,273.8	0.081Å	-	-
37	ASP 76.11	-	Favored (17.23%) General / -99.9,-18.2	2.4% (<i>m-20</i>) chi angles: 320,332.7	0.065Å	-	OUTLIER(S) worst is CA- CB-CG: 4.739 σ
38	THR 158.65	-	Allowed (0.58%) General / -126.6,-78.0	13.7% (<i>p</i>) chi angles: 45.7	0.166Å	-	-
39	TYR 80.9	-	Allowed (0.34%) General / 175.4,169.5	49.3% (<i>p90</i>) chi angles: 61.6,85.6	0.043Å	-	-

40	LEU	63.86	-	Favored (10.24%) General / -130.6,108.9	66.3% (<i>tp</i>) chi angles: 179.3,62.4	0.077Å	-	-
41	LEU	43.91	-	Favored (34.06%) General / -83.2,137.4	37.7% (<i>tp</i>) chi angles: 180.4,70.6	0.081Å	-	-
42	ILE	42.97	-	Favored (21.34%) Isoleucine or valine / -139.7,125.2	17.6% (<i>mt</i>) chi angles: 315.2,172.2	0.095Å	-	-
43	SER	92.25	-	Favored (43.43%) General / -73.2,148.9	58.8% (<i>p</i>) chi angles: 55.8	0.028Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187		Outliers: 0 of 210	Outliers: 9 of 210
44	GLU	80.4	-	Favored (59.47%) General / -74.5,-21.6	7.8% (pt-20) chi angles: 50.1,200.1,321.5	0.252Å	-	-
45	ASP	152.55	-	Allowed (0.31%) General / -44.2,-26.4	21.1% (<i>m-20</i>) chi angles: 269.1,345.4	0.081Å	-	-
46	THR	61.33	-	Favored (14.96%) Pre-proline / -57.6,116.7	54.5% (<i>m</i>) chi angles: 294.8	0.032Å	-	-
47	PRO	140.82	-	Favored (8.21%) Trans-proline / -81.9,134.1	95.3% (<i>Cg_endo</i>) chi angles: 30.7	0.026Å	-	-
48	VAL	96.22	-	Favored (5.98%) Isoleucine or valine /-48.6,130.8	15% (<i>m</i>) chi angles: 289.4	0.078Å	-	-
49	GLY	22.83	-	Favored (38.99%) Glycine / 102.5,-22.0	-	-	-	-
50	SER	32.5	-	Favored (39.99%) General /	22.9% (<i>t</i>) chi angles: 186.9	0.042Å	-	-

			-73.6,153.9				
51	SER 48.87	-	Favored (18.44%) General / -83.0,111.0	58.1% (<i>p</i>) chi angles: 55.7	0.05Å	-	-
52	VAL 66.44	-	Favored (91.99%) Isoleucine or valine /-64.1,-47.0	54.6% (<i>t</i>) chi angles: 170	0.033Å	-	-
53	THR 116.4	-	Allowed (0.87%) General / -167.1,-167.1	12.2% (<i>t</i>) chi angles: 191.4	0.186Å	-	-
54	GLN 51.47	-	Favored (33.69%) General / -139.8,136.2	62.8% (tt0) chi angles: 183.7,183.1,7.7	0.096Å	-	-
55	LEU 110.31	-	Favored (19.38%) General / -84.7,111.2	7.4% (<i>mp</i>) chi angles: 266.9,69.9	0.039Å	-	-
56	LEU 103.98	-	Favored (43.47%) General / -97.9,126.7	2.7% (mm?) chi angles: 294,315.6	0.038Å	-	-
57	ALA 38.19	-	Favored (51.16%) General / -131.8,152.2	-	0.089Å	-	-
58	GLN 46.46	-	Favored (53.97%) General / -125.5,138.4	27.8% (<i>tp60</i>) chi angles: 182.3,63.8,87.8	0.09Å	-	-
59	ASP 91.47	-	Favored (13.15%) General / -101.8,162.1	2.1% (<i>t70</i>) chi angles: 213.1,295.9	0.023Å	-	-
60	MET 90.65	-	Favored (27.39%) General / -99.8,-6.2	22.5% (<i>mmp</i>) chi angles: 305.2,281.1,90.8	0.082Å	-	-
61	ASP 88.61	-	Favored (12.18%) General / -109.8,-21.8	0.6% chi angles: 316.8,4	0.101Å	-	OUTLIER(S) worst is CA- CB-CG: 4.695 σ
62	ASN 60.37	-	Allowed (1.17%) General / 74.6,29.3	15.6% (<i>m-80</i>) chi angles: 307.2,267.9	0.154Å	-	-

63	ASP	52.47	-	Favored (83.87%) Pre-proline / -72.9,143.1	80.9% (<i>m-20</i>) chi angles: 294.6,327.9	0.048Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers: 2 of 199		Outliers: 9 of 210
64	PRO	67.81	-	Favored (26.76%) Trans-proline / -56.0,127.6	1.2% (<i>Cg_exo</i>) chi angles: 321.2	0.046Å	-	-
65	LEU	73.97	-	Favored (13.7%) General / -97.5,161.6	38.8% (<i>mt</i>) chi angles: 305.5,186.9	0.035Å	-	-
66	VAL	49.27	-	Favored (61.93%) Isoleucine or valine /-130.3,134.8	85.1% (<i>t</i>) chi angles: 174.9	0.038Å	-	-
67	PHE	139.58	-	Favored (23.63%) General / -108.7,153.3	98.3% (<i>m-85</i>) chi angles: 296.8,91.9	0.056Å	-	-
68	GLY	27.81	-	Favored (32.29%) Glycine / -162.8,-174.1	-	-	-	-
69	VAL	90.38	-	Favored (34.73%) Isoleucine or valine /-129.0,146.1	13.5% (<i>p</i>) chi angles: 65	0.116Å	-	-
70	SER	38.32	-	Favored (50.67%) General / -127.3,145.8	47.8% (<i>t</i>) chi angles: 179.8	0.065Å	-	-
71	GLY	23.09	-	Favored (9.39%) Glycine / 94.2,138.8	-	-	-	-
72	GLU	44.49	-	Favored (77.3%) General / -69.5,-37.8	5% (<i>mp0</i>) chi angles: 304.3,90.9,309	0.132Å	-	-
73	GLU	37.49	-	Favored (66.49%) General /	83.7% (tt0) chi angles: 187,178.4,11.4	0.104Å	-	-

74	ALA 26	5.68	-	-73.1,-37.9 Favored (95.12%) General / -60.7,-41.4	-	0.064Å	-	-
75	SER 33	3.46	-	Favored (43.54%) General / -79.9,-21.8	79.3% (p) chi angles: 59.7	0.15Å	-	-
76	ARG 14	9.79	-	Favored (4.22%) General / -56.0,-59.9	72.6% (ttt-85) chi angles: 178.5,188.7,176.7,274.9	0.128Å	-	-
77	PHE 69	9.43	-	Favored (56.24%) General / -77.2,-33.2	74.1% (<i>m-85</i>) chi angles: 286.6,268.6	0.141Å	-	-
78	PHE 64	1.16	-	Favored (49.89%) General / -128.6,151.1	70.4% (<i>m</i> -85) chi angles: 302.9,289.1	0.101Å	-	-
79	ALA 3	7.6	-	Favored (37%) General / -123.4,155.7	-	0.037Å	-	-
80	VAL 39	9.09	-	Favored (65.64%) Isoleucine or valine /-126.5,134.7	43.5% (<i>t</i>) chi angles: 184.1	0.088Å	-	-
81	GLU 48	3.49	-	Favored (71.16%) Pre-proline / -72.0,118.9	58.5% (<i>mt-10</i>) chi angles: 293.9,193.4,319.3	0.076Å	-	-
82	PRO 163	2.43	-	Favored (59.16%) Trans-proline / -51.1,-40.8	4.9% (<i>Cg</i> _exo) chi angles: 322	0.052Å	-	-
83	ASP 66	5.86	-	Favored (20.23%) General / -87.6,-30.8	0.5% chi angles: 319,56.6	0.077Å	-	-
#	Alt Res Hig	gh B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		wg: 5.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers:	•	Outliers: 9 of 210
84	THR 83	3.11	-	Favored (8.12%) General /	70.8% (p) chi angles: 64	0.042Å	-	-

85	GLY 32.71	-	-100.6,-39.0 Favored (65.68%) Glycine / 92.4,5.0	-	-	-	-
86	VAL 37.48	-	Favored (31.9%) Isoleucine or valine / -66.3,130.7	54% (<i>t</i>) chi angles: 169.2	0.068Å	-	-
87	VAL 42.35	-	Favored (54.97%) Isoleucine or valine /-104.6,120.4	46.1% (<i>t</i>) chi angles: 183.5	0.082Å	-	-
88	TRP 70.58	-	Favored (43.29%) General / -121.4,149.2	69.1% (<i>p</i> -90) chi angles: 58.1,270.1	0.095Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.117 σ
89	LEU 69.41	-	Favored (29.12%) General / -81.2,124.2	29.1% (<i>tp</i>) chi angles: 188.8,67.8	0.049Å	-	-
90	ARG 152.38	-	Favored (13.36%) General / -92.9,-35.4	18.6% (<i>mtm180</i>) chi angles: 301.9,208.1,308.9,129.1	0.116Å	-	-
91	GLN 86.67	-	Favored (75.69%) Pre-proline / -133.3,150.6	2% (<i>mm-40</i>) chi angles: 303,281.4,242	0.076Å	-	-
92	PRO 79.58	-	Favored (56.48%) Trans-proline / -59.2,152.9	83.2% (<i>Cg_exo</i>) chi angles: 331.8	0.076Å	-	-
93	LEU 58.13	-	Favored (18.72%) General / -89.1,156.6	87.6% (<i>mt</i>) chi angles: 300.7,178.9	0.031Å	-	-
94	ASP 68.71	-	Allowed (1.54%) General / -160.4,107.1	31% (<i>t0</i>) chi angles: 171,357.7	0.111Å	-	-
95	ARG 140.18	-	Favored (50.79%) General / -77.3,-24.3	4% (<i>ttp85</i>) chi angles: 186.7,212.4,45.4,50	0.049Å	-	OUTLIER(S) worst is CD- NE-CZ: 6.522 σ
96	GLU 108.85	-	Favored (78.64%) General / -68.3,-43.0	11.3% (<i>tm-20</i>) chi angles: 195.7,292.8,331	0.069Å	-	-

97	THR	131.16	-	Favored (76.8%) General / -67.6,-45.0	26.3% (<i>m</i>) chi angles: 291.7	0.099Å	-	-
98	LYS	87.73	-	Allowed (0.77%) General / -166.9,112.4	37.2% (ttmt) chi angles: 195,175.3,300.3,187.4	0.058Å	-	-
99	SER	69.66	-	Favored (62.65%) General / -74.3,-31.7	89.8% (<i>p</i>) chi angles: 62.5	0.095Å	-	-
100	GLU	67.79	-	Favored (43.74%) General / -151.4,160.5	1.1% (<i>pt-20</i>) chi angles: 69,142.4,318.1	0.039Å	-	-
101	РНЕ	69.04	-	Favored (4.45%) General / -169.8,177.4	13.1% (<i>p90</i>) chi angles: 54.1,105.2	0.066Å	-	-
102	THR	38.29	-	Favored (54.49%) General / -121.2,137.8	13.1% (<i>t</i>) chi angles: 186.1	0.095Å	-	-
103	VAL	42.3	-	Favored (18.36%) Isoleucine or valine /-118.3,159.9	35.3% (<i>m</i>) chi angles: 298.1	0.051Å	-	-
	VAL		- Clash > 0.4Å	(18.36%) Isoleucine or valine	• ,	0.051Å Cβ deviation	- Bond lengths	- Bond angles
			0.4Å	(18.36%) Isoleucine or valine /-118.3,159.9 Ramachandran	chi angles: 298.1	Cβ deviation	lengths Outliers:	
	Alt Res	High B Avg:	0.4Å Clashscore:	(18.36%) Isoleucine or valine /-118.3,159.9 Ramachandran Outliers: 0 of	chi angles: 298.1 Rotamer Poor rotamers: 3 of	Cβ deviation Outliers:	lengths Outliers:	Outliers: 9
# #	Alt Res GLU	High B Avg: 75.22	0.4Å Clashscore:	(18.36%) Isoleucine or valine /-118.3,159.9 Ramachandran Outliers: 0 of 208 Favored (50.77%) General /	Rotamer Poor rotamers: 3 of 187 44.1% (mt-10) chi angles:	C β deviation Outliers: 2 of 199	lengths Outliers:	Outliers: 9
# <i>A</i>	Alt Res GLU PHE	High B Avg: 75.22 36.81	0.4Å Clashscore:	(18.36%) Isoleucine or valine /-118.3,159.9 Ramachandran Outliers: 0 of 208 Favored (50.77%) General / -113.3,137.9 Favored (41.26%) General /	chi angles: 298.1 Rotamer Poor rotamers: 3 of 187 44.1% (<i>mt-10</i>) chi angles: 283.6,198.3,18.4 73.4% (<i>m-85</i>)	Cβ deviation Outliers: 2 of 199 0.04Å	lengths Outliers:	Outliers: 9

			/ -145.8,131.4	chi angles: 61.1			
108	SER 60.68	-	Favored (27.43%) General / -117.0,156.5	33.5% (<i>t</i>) chi angles: 175.3	0.088Å	-	-
109	ASP 128.21	-	Favored (17.58%) General / -111.4,2.6	20.5% (<i>p30</i>) chi angles: 50.6,14.5	0.046Å	-	-
110	HIS 110.97	-	Allowed (0.87%) General / 85.2,-8.3	68.6% (<i>m80</i>) chi angles: 302.7,88.2	0.233Å	-	-
111	GLN 91.36	-	Favored (5.55%) General / -105.5,-41.2	9.9% (<i>mt-30</i>) chi angles: 295.2,146.9,104.4	0.031Å	-	-
112	GLY 28.45	-	Favored (7.34%) Glycine / -141.8,-157.9	-	-	-	-
113	VAL 94.2	-	Favored (2.92%) Isoleucine or valine / -163.8,147.3	12.1% (<i>p</i>) chi angles: 66	0.065Å	-	-
114	ILE 101.58	-	Favored (24.38%) Isoleucine or valine / -121.0,153.2	2.2% (<i>pp</i>) chi angles: 65,100	0.06Å	-	-
115	THR 40.22	-	Favored (35.75%) General / -121.1,154.8	77.9% (p) chi angles: 58.5	0.049Å	-	-
116	ARG 84.23	-	Favored (24.34%) General / -146.9,138.7	75.2% (<i>mtp180</i>) chi angles: 282,172.3,63.7,193.3	0.046Å	-	-
117	LYS 82.7	-	Favored (32.48%) General / -78.6,151.3	61.4% (<i>mttm</i>) chi angles: 288.5,192.6,178.4,306.1	0.051Å	-	-
118	VAL 44.96	-	Favored (28.45%) Isoleucine or valine / -124.1,150.0	57.7% (<i>t</i>) chi angles: 180.6	0.059Å	-	-
119	ASN 46.36	-	Favored (24.53%)	59.3% (m-20)	0.078Å	-	-

				General / -104.5,111.7	chi angles: 308.7,313.2			
120	ILE	63.75	-	Favored (47.01%) Isoleucine or valine /-100.0,131.7	18.7% (<i>mt</i>) chi angles: 287.6,186.1	0.071Å	-	-
121	GLN	35.64	-	Favored (53.67%) General / -118.8,137.0	57.1% (tt0) chi angles: 180.2,187.1,353.3	0.089Å	-	-
122	VAL	37.68	-	Favored (40.8%) Isoleucine or valine /-94.7,131.7	32.7% (<i>t</i>) chi angles: 186	0.06Å	-	-
123	GLY	29.62	-	Favored (4.44%) Glycine / -93.5,113.2	-	-	-	-
# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers: 2 of 199		Outliers: 9 of 210
124	ASP	65.62	-	Favored (11.94%) General / -47.0,129.7	38.7% (<i>t70</i>) chi angles: 187.7,57.1	0.113Å	-	-
125	VAL	73.03	-	Allowed (0.23%) Isoleucine or valine / -128.9,-159.3	26.3% (<i>m</i>) chi angles: 301.9	0.271Å	-	-
126	ASN	78.77	-	Favored (2.05%) General / -119.2,83.6	6% (<i>t30</i>) chi angles: 198.9,85.7	0.091Å	-	-
127	ASP	214.23	-	Favored (15%) General / -98.8,-24.5	1.3% (<i>m-20</i>) chi angles: 318.8,255.8	0.074Å	-	-
128	ASN	82.64	-	Favored (16.68%) General / -103.5,158.0	49.9% (<i>m-80</i>) chi angles: 285.6,274.5	0.033Å	-	-
129	ALA	46.45	-	Favored (43.34%) Pre-proline/	-	0.034Å	-	-
				-111.5,151.5				

		THR HG21	Trans-proline / -60.4,124.3	chi angles: 326.8			
131	THR 37.29	-	Favored (12.05%) General / -84.0,101.8	72.3% (p) chi angles: 59	0.026Å	-	-
132	PHE 61.66	0.465Å CE2 with 218 THR HG23	Favored (9.13%) General / -56.5,154.0	67.6% (<i>m</i> -85) chi angles: 290.9,290.2	0.052Å	-	-
133	HIS 53.81	-	Favored (38.32%) General / -138.0,137.8	44.6% (<i>m-70</i>) chi angles: 306.2,312.1	0.079Å	-	-
134	ASN 69.5	-	Allowed (0.31%) General / 78.0,34.2	10.2% (<i>m120</i>) chi angles: 306.2,84.3	0.16Å	-	-
135	GLN 65.35	-	Favored (78.19%) Pre-proline / -77.0,159.6	33.9% (<i>mt-30</i>) chi angles: 284.4,192.2,100.8	0.061Å	-	-
136	PRO 153.58	-	Favored (19.61%) Cis-proline / -75.2,129.8	33.2% (<i>Cg_exo</i>) chi angles: 341.1	0.074Å	-	-
137	TYR 83.63	-	Favored (40.97%) General / -75.6,133.2	22.7% (<i>m-30</i>) chi angles: 301.3,318.3	0.067Å	-	-
138	SER 34.64	-	Favored (11.58%) General / -164.9,152.7	35.1% (<i>t</i>) chi angles: 182.8	0.057Å	-	-
139	VAL 92.47	-	Favored (12.94%) Isoleucine or valine /-155.1,144.1	12.7% (<i>p</i>) chi angles: 65.5	0.097Å	-	-
140	ARG 104.86	-	Favored (37.91%) General / -110.6,119.0	8.6% (<i>tpt180</i>) chi angles: 184.1,71.2,185.1,228.4	0.075Å	-	-
141	ILE 52.97	-	Favored (70.31%) Pre-proline / -128.3,149.0	23.9% (<i>pt</i>) chi angles: 67.3,180	0.051Å	-	-
142	PRO 66.58	-	Favored (80.94%) Trans-proline /	72.7% (<i>Cg_exo</i>) chi angles: 328	0.084Å	-	-

				00.0,132.2				
143	GLU	72.48	-	Favored (78.22%) General / -60.3,-36.6	11.4% (<i>pt-20</i>) chi angles: 51,191,320.9	0.137Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 3 of	Outliers:	Outliers:	Outliers: 9
		75.22	0.62	208	187	2 of 199	0 of 210	of 210
144	ASN	105.61	-	Allowed (0.61%) General / -80.4,21.6	47.5% (<i>p30</i>) chi angles: 61.1,21.9	0.133Å	-	-
145	THR	54.8	-	Favored (79%) Pre-proline / -63.9,122.8	45.3% (<i>m</i>) chi angles: 293.5	0.026Å	-	-
146	PRO	137.42	-	Favored (32.35%) Trans-proline / -72.3,139.7	23.2% (<i>Cg_endo</i>) chi angles: 19.8	0.063Å	-	-

-66.8,152.2

Favored

154	VAL	52.51	-	/-147.1,112.3 Allowed (1.44%)	30% (m)	0.089Å	_	_
4	4.63.1	T 6 00		Isoleucine or valine /-74.3,170.5 Favored (16.84%)	chi angles: 301.1 21.8% (<i>t-20</i>)	0.050		
155	ASN	56.83	-	General / -151.6,135.9 Favored	chi angles: 183.5,249.5	0.068Å	-	-
156	ALA	40.66	-	(44.69%) General / -142.6,154.8	-	0.064Å	-	-
157	THR	40.26	-	Favored (11.51%) General / -127.5,171.5	40.7% (p) chi angles: 53.9	0.025Å	-	-
158	ASP	72	-	Favored (4.1%) Pre-proline / -153.8,126.8	10.4% (<i>t0</i>) chi angles: 202.6,320	0.15Å	-	-
159	PRO	91.11	-	Favored (9.32%) Trans-proline / -85.3,-5.8	3.7% (<i>Cg_endo</i>) chi angles: 41.5	0.018Å	-	-
160	ASP	58.09	-	Favored (47.26%) General / -69.8,150.1	11% (<i>m-20</i>) chi angles: 305.3,359.4	0.045Å	-	-
161				Favored	20.20/ (mat)			
101	LEU	53.93	-	(11.86%) General / -86.7,170.4	20.3% (<i>mt</i>) chi angles: 314.8,175.1	0.115Å	-	-
162		53.9328.45	-	General /	, ,	0.115Å -	-	-
	GLY		-	General / -86.7,170.4 Allowed (0.79%) Glycine /	, ,	0.115Å - 0.122Å	-	-
162 163	GLY	28.45 38.26	- - Clash > 0.4Å	General / -86.7,170.4 Allowed (0.79%) Glycine / 60.5,-105.3 Favored (28.13%) General /	chi angles: 314.8,175.1	-	- Bond lengths	- Bond angles
162 163	GLY	28.45 38.26	0	General / -86.7,170.4 Allowed (0.79%) Glycine / 60.5,-105.3 Favored (28.13%) General / -86.5,-20.4	chi angles: 314.8,175.1	- 0.122Å Cβ deviation	lengths Outliers:	Outliers: 9

165	GLY 64.96	-	-77.7,-33.3 Favored (84.61%) Glycine / -75.6,-8.8	-	-	-	-
166	SER 109.85	-	Favored (13.45%) General / -94.7,101.6	74% (m) chi angles: 294	0.042Å	-	-
167	VAL 51.87	-	Favored (3.41%) Isoleucine or valine / -94.3,153.7	57.9% (<i>t</i>) chi angles: 180.6	0.096Å	-	-
168	LEU 55.4	-	Favored (45.51%) General / -133.5,137.2	78.9% (<i>mt</i>) chi angles: 294.6,181	0.048Å	-	-
169	TYR 59.58	-	Favored (32.2%) General / -102.5,143.4	63.1% (<i>m</i> -85) chi angles: 306.8,279.2	0.08Å	-	-
170	SER 41.36	-	Favored (12.31%) General / -143.6,172.8	21.7% (t) chi angles: 188.1	0.035Å	-	-
171	PHE 58.66	-	Favored (17.83%) General / -94.5,153.7	33.3% (<i>m</i> -85) chi angles: 287.2,304	0.028Å	-	-
172	GLN 58.33	-	Favored (9.66%) Pre-proline / -137.2,100.1	10.8% (<i>tp-100</i>) chi angles: 185,59.7,250.8	0.05Å	-	-
173	PRO 74.31	-	Favored (78.26%) Cis-proline / -76.1,168.1	27.1% (<i>Cg_endo</i>) chi angles: 37.7	0.078Å	-	-
174	PRO 62.21	-	Favored (41.66%) Trans-proline / -51.0,133.9	0.7% chi angles: 320.7	0.073Å	-	-
175	SER 38.11	-	Favored (19.77%) General / -83.1,165.2	22.3% (t) chi angles: 187.9	0.027Å	-	-
176	GLN 137.76	-	Favored (13.44%) General / -103.9,-22.8	4.4% (<i>tp60</i>) chi angles: 178.3,63.6,107.7	0.082Å	-	-

177	РНЕ	93.29	-	Favored (21.88%) General / -90.7,-21.0	96.9% (<i>m-85</i>) chi angles: 294.4,91	0.123Å	-	-
178	РНЕ	78.45	-	Favored (37.38%) General / -143.7,149.6	13% (<i>m-85</i>) chi angles: 315.5,269.7	0.079Å	-	-
179	ALA	43.33	-	Favored (11.3%) General / -120.1,168.3	-	0.033Å	-	-
180	ILE	51.1	-	Favored (46.58%) Isoleucine or valine / -137.2,137.3	19.7% (tt) chi angles: 189.7,165.1	0.112Å	-	-
181	ASP	49.52	-	Favored (15.22%) General / -72.0,118.7	17.3% (<i>t0</i>) chi angles: 189.1,313.1	0.052Å	-	-
182	SER	48.92	-	Favored (70.62%) General / -59.8,-32.4	90.5% (p) chi angles: 62.6	0.128Å	-	-
183	ALA	54.9	-	Favored (14.64%) General / -101.6,-21.8	-	0.073Å	-	-
		54.9 High B	- Clash > 0.4Å	(14.64%) General /	- Rotamer	0.073Å Cβ deviation	- Bond lengths	- Bond angles
		High B Avg:	0.4Å	(14.64%) General / -101.6,-21.8 Ramachandran	Rotamer Poor rotamers: 3 of	Cβ deviation	lengths	Outliers: 9
		High B	0.4Å	(14.64%) General / -101.6,-21.8 Ramachandran Outliers: 0 of 208		Cβ deviation	lengths Outliers:	
	t Res	High B Avg:	0.4Å Clashscore:	(14.64%) General / -101.6,-21.8 Ramachandran Outliers: 0 of	Poor rotamers: 3 of	Cβ deviation Outliers:	lengths Outliers:	Outliers: 9
# Al	t Res	High B Avg: 75.22	0.4Å Clashscore:	(14.64%) General / -101.6,-21.8 Ramachandran Outliers: 0 of 208 Favored (12.67%) General /	Poor rotamers: 3 of 187 74.9% (mtt85) chi angles:	C β deviation Outliers: 2 of 199	lengths Outliers:	Outliers: 9
# Al	ARG	High B Avg: 75.22	0.4Å Clashscore:	(14.64%) General / -101.6,-21.8 Ramachandran Outliers: 0 of 208 Favored (12.67%) General / -102.3,-27.7 Favored (84.47%)	Poor rotamers: 3 of 187 74.9% (mtt85) chi angles:	C β deviation Outliers: 2 of 199	lengths Outliers:	Outliers: 9

			/ -105.5,125.0 Favored				
188	THR 121.47	-	(45.57%) General / -118.0,144.4	31.8% (<i>p</i>) chi angles: 51.5	0.069Å	-	-
189	VAL 77.26	-	Favored (34.08%) Isoleucine or valine /-69.0,131.2	54.4% (<i>t</i>) chi angles: 170	0.039Å	-	-
190	ILE 235.96	-	Favored (2.36%) Isoleucine or valine /-109.9,-30.6	37.7% (<i>mm</i>) chi angles: 294.7,298.8	0.075Å	-	-
191	ARG 142.54	-	Favored (46.6%) General / -130.9,155.5	60.9% (<i>ttt180</i>) chi angles: 186,179.5,166.6,200.7	0.108Å	-	-
192	GLU 72.8	-	Favored (46.91%) General / -58.5,143.1	5.3% (<i>pm0</i>) chi angles: 77,300.8,341.6	0.053Å	-	OUTLIER(S) worst is CB- CG-CD: 4.553 σ
193	LEU 116.33	-	Favored (16.28%) General / -109.5,160.4	3% (<i>mp</i>) chi angles: 304.7,102	0.034Å	-	-
194	ASP 66.27	-	Favored (3.04%) General / -156.0,112.0	12.9% (<i>t0</i>) chi angles: 167.4,355.6	0.133Å	-	OUTLIER(S) worst is CA- CB-CG: 4.154 σ
195	TYR 55.37	-	Favored (74.94%) General / -66.0,-33.1	90% (<i>t80</i>) chi angles: 175.9,78.7	0.117Å	-	-
196	GLU 104.79	-	Favored (66.68%) General / -68.5,-47.6	10.3% (<i>tm-20</i>) chi angles: 197.3,292.4,337.2	0.063Å	-	-
197	THR 120.01	-	Favored (77.42%) General / -67.3,-34.4	32.4% (<i>m</i>) chi angles: 292.5	0.13Å	-	-
198	THR 51.94	-	Favored (2.8%) General / -159.1,116.9	23% (<i>m</i>) chi angles: 291	0.036Å	-	-
199	GLN 105.07	-	Favored (45.34%) General / -79.1,-22.3	6% (<i>mp0</i>) chi angles: 300.6,86.3,69.4	0.082Å	-	-

200	ALA	41.48	-	Favored (2.48%) General / -169.3,141.3	-	0.094Å	-	-
201	TYR	131.03	-	Favored (48.33%) General / -110.4,137.3	70.4% (<i>m-85</i>) chi angles: 302.4,82.9	0.06Å	-	-
202	GLN	51.67	-	Favored (2.46%) General / -116.3,86.3	92.3% (<i>mm-40</i>) chi angles: 307.7,300.1,305.3	0.04Å	-	-
203	LEU	50.11	-	Favored (36.48%) General / -90.2,129.5	51.2% (<i>mt</i>) chi angles: 308,180.6	0.051Å	-	-
# A	lt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers: 2 of 199		Outliers: 9 of 210
204	THR	33.55	-	Favored (22.67%) General / -73.9,122.5	22.1% (<i>m</i>) chi angles: 309.8	0.048Å	-	-
205	VAL	35.6	-	Favored (55.14%) Isoleucine or valine / -102.2,123.1	93.3% (<i>t</i>) chi angles: 175.6	0.054Å	-	-
206	ASN	46.65	-	Favored (43.27%) General / -100.8,134.8	46.9% (<i>t30</i>) chi angles: 180.5,56.6	0.066Å	-	-
207	ALA	43.48	-	Favored (16.31%) General / -128.5,114.1	-	0.024Å	-	-
208	THR	42.76	-	Favored (21.19%) General / -108.6,155.0	4.4% (t) chi angles: 174.6	0.068Å	-	-
209	ASP	70.36	-	Favored (4.17%) General / -85.7,-172.6	4.1% (<i>p30</i>) chi angles: 63.8,86.3	0.174Å	-	-
210	GLN	122.57	-	Favored (21.15%) General /	81% (<i>mt-30</i>) chi angles:	0.052Å	-	-

			-111.5,8.5	291.8,181.4,25.9			
211	ASP 87.47	-	Favored (13.65%) General / -56.9,151.9	35.6% (<i>t70</i>) chi angles: 186.5,233.6	0.109Å	-	-
212	LYS 81.41	-	Favored (29.47%) General / -102.7,-1.8	35.9% (<i>mmtm</i>) chi angles: 320.4,298.2,181.9,285.4	0.115Å	-	-
213	THR 131.14	-	Favored (4.45%) General / -115.8,-35.5	28.7% (p) chi angles: 70.8	0.175Å	-	-
214	ARG 164.59	-	Favored (2.16%) Pre-proline / -160.3,82.8	13.4% (<i>ptt180</i>) chi angles: 59.9,178.6,191.2,222.2	0.075Å	-	-
215	PRO 82.52	-	Favored (8.14%) Trans-proline / -75.6,124.3	71.6% (<i>Cg_endo</i>) chi angles: 29.5	0.023Å	-	-
216	LEU 56.57	-	Favored (15.01%) General / -93.3,160.0	47.8% (<i>mt</i>) chi angles: 300.7,166.7	0.106Å	-	-
217	SER 90.84	-	Favored (4.91%) General / -151.0,114.7	88.1% (<i>p</i>) chi angles: 61.7	0.049Å	-	-
218	THR 112.63	0.533Å HG21 with 130 PRO O	Favored (13.86%) General / -95.2,162.1	13.5% (<i>t</i>) chi angles: 186.5	0.088Å	-	-
219	LEU 46.72	-	Favored (46.55%) General / -132.8,136.8	68% (mt) chi angles: 304.5,181.7	0.054Å	-	-
220	ALA 32.88	-	Favored (10.29%) General / -124.5,171.0	-	0.026Å	-	-
221	ASN 55.36	-	Favored (47.67%) General / -117.9,142.1	36.9% (<i>t30</i>) chi angles: 178.5,37.7	0.062Å	-	-
			Favored (13.96%)	61.2% (<i>tp</i>)			

222	LEU	62.85	-	General / -121.0,108.5	chi angles: 176.6,60.1	0.065Å	-	-
223	ALA	37.28	-	Favored (10.77%) General / -90.5,96.7	-	0.034Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 75.22	Clashscore: 0.62	Outliers: 0 of 208	Poor rotamers: 3 of 187	Outliers: 2 of 199		Outliers: 9 of 210
224	ILE	100.15	-	Favored (17.38%) Isoleucine or valine /-86.8,107.9	3.7% (<i>mp</i>) chi angles: 299.5,102	0.029Å	-	-
225	ILE	98.57	-	Favored (43.67%) Isoleucine or valine /-93.6,129.7	23% (<i>mm</i>) chi angles: 308.2,311	0.056Å	-	-
226	ILE	105.11	-	Favored (10.66%) Isoleucine or valine /-90.2,143.7	42.5% (<i>mm</i>) chi angles: 302.4,305.8	0.1Å	-	-
227	THR	41.17	-	Favored (24.45%) General / -94.9,112.8	18.5% (<i>m</i>) chi angles: 310.9	0.058Å	-	-
228	ASP	44.94	-	Favored (2.11%) General / -45.5,119.4	34.3% (<i>t0</i>) chi angles: 198.9,6.3	0.201Å	-	-
229	VAL	106.42	-	Allowed (0.39%) Isoleucine or valine / -121.6,-165.5	7.6% (<i>m</i>) chi angles: 309.2	0.243Å	-	-
230	GLN	133.03	-	Favored (3.55%) General / -103.6,90.1	42.1% (<i>tp60</i>) chi angles: 178.2,53.8,72.3	0.057Å	-	-
231	ASP	152.15	-	Favored (35.4%) General / -101.4,-0.5	21.4% (<i>m</i> -20) chi angles: 279.8,14.8	0.129Å	-	-
232	MET	125.71	-	Favored (32.68%) General / -84.2,139.0	56.9% (<i>mtt</i>) chi angles: 304,176.7,182.1	0.091Å	-	OUTLIER(S) worst is C-N- CA: 4.741 σ

233 ASP 26.11

-

61.4% (*m-20*) chi angles: 278.8,0.1

0.108Å

 $\begin{array}{c} OUTLIER(S)\\ worst is CA-\\ CB-CG: 5.159\\ \sigma\end{array}$

About MolProbity | Website for the Richardson Lab | Using ecloud x-H | Internal reference 4.1-537