

Viewing RDH12_mb_33-610-FFX1FH_reg-multi.table

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All-Atom	Clashscore, all atoms:	1.14		99 th percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the numbe	r of serious	steric ove	erlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	24	10.26%	Goal: <1%		
	Ramachandran outliers	17	6.16%	Goal: <0.05%		
	Ramachandran favored	213	77.17%	Goal: >98%		
Protein Geometry	MolProbity score [^]	2.36		55 th percentile [*] (N=27675, 0Å - 99Å)		
geomeay	Cβ deviations >0.25Å	12	4.63%	Goal: 0		
	Bad backbone bonds:	0 / 2208	0.00%	Goal: 0%		
	Bad backbone angles:	37 / 2985	1.24%	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 R	les	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 124.27		Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
33	TI	HR	101.21	0.673Å N with 36 GLN HE21	-	12.1% (<i>t</i>) chi angles: 185.4	0.246Å	-	OUTLIER(S) worst is C-N-CA: 4.504σ
34	A	SN	126.06	-	Favored (2.65%) General / -48.6,-27.1	20.8% (<i>p-10</i>) chi angles: 59.8,318	0.075Å	-	-
35	V	AL	63.88	-	Favored (17.57%) Isoleucine or valine / -51.8,-35.4	48.7% (<i>t</i>) chi angles: 168.4	0.102Å	-	-
36	G	LN	169.63	0.673Å HE21 with 33 THR N	Favored (10.98%) General / -86.1,98.7	43% (<i>mt-30</i>) chi angles: 306.2,169.9,80.6	0.043Å	-	-
					Favored (52.91%)	94% (mt)			

^{* 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.

2/19/2015			Viewing RDH12_mb_33-	-610-FFX1FH_reg-multi.table - Mo	olProbity		
37	LEU 112.63	-	Pre-proline / -144.4,159.2	chi angles: 294.9,177.7	0.103Å	-	-
38	PRO 117.63	-	Favored (9.37%) Trans-proline / -86.5,157.9	38.2% (<i>Cg_endo</i>) chi angles: 36.7	0.075Å	-	-
39	GLY 107.62	-	Favored (35.4%) Glycine / -60.1,153.1	-	-	-	-
40	LYS 241.57	-	Favored (12.09%) General / -159.5,176.4	0% chi angles: 20.2,61.5,197.4,71.3	0.134Å	-	-
41	VAL 174.29	-	Allowed (0.37%) Isoleucine or valine / -132.8,52.9	14.5% (<i>p</i>) chi angles: 64.3	0.165Å	-	-
42	VAL 86.48	-	Favored (13.99%) Isoleucine or valine / -54.0,138.1	71.6% (<i>t</i>) chi angles: 173.8	0.089Å	-	-
43	VAL 127.51	-	Favored (35.32%) Isoleucine or valine / -110.7,111.2	22.5% (<i>m</i>) chi angles: 302.8	0.142Å	-	-
44	ILE 72.86	-	Favored (45.99%) Isoleucine or valine / -104.9,115.0	62.3% (<i>mt</i>) chi angles: 302.2,179	0.05Å	-	-
45	THR 49.61	-	Favored (5.5%) General / -71.2,109.8	73.1% (<i>p</i>) chi angles: 58.9	0.132Å	-	-
46	GLY 57.86	-	Favored (42.53%) Glycine / -86.8,-166.5	-	-	-	-
47	ALA 112.55	-	OUTLIER (0.02%) General / -171.1,9.6	-	0.022Å	-	-
48	ASN 89.79	-	Allowed (0.66%) General / 37.2,47.4	5.3% (<i>m-20</i>) chi angles: 294.4,23.4	0.084Å	-	-
			Favored				

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49	THR	58.21	-	(33.87%) General / -107.8,145.3	61.5% (<i>m</i>) chi angles: 303.8	0.07Å	-	-
50	GLY	55.63	-	Favored (93.93%) Glycine / -57.4,-42.8	-	-	-	-
51	ILE	170.53	-	Favored (65.88%) Isoleucine or valine / -62.5,-34.6	0% chi angles: 189.5,268.6	0.253Å	-	-
52	GLY	48.34	-	Favored (91.59%) Glycine / -64.6,-35.1	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 124.27		Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
53	LYS	111.57	-	Favored (97.89%) General / -60.7,-43.4	49.1% (<i>tttp</i>) chi angles: 187.5,188.1,171.7,76.3	0.08Å	-	-
54	GLU	129.58	-	Favored (81.16%) General / -58.8,-48.5	43% (<i>mt-10</i>) chi angles: 298.9,178,266.5	0.108Å	-	-
55	THR	165.86	-	Favored (75.82%) General / -65.8,-33.4	16.8% (<i>p</i>) chi angles: 46.7	0.162Å	-	-
56	ALA	60.53	-	Favored (76.13%) General / -69.9,-37.8	-	0.065Å	-	-
57	ARG	159.86	-	Favored (68.85%) General / -70.5,-31.7	7.2% (ttt85) chi angles: 216.3,190.6,181.1,113.4	0.139Å	-	-
58	GLU	154.28	-	Favored (20.19%) General / -48.1,-52.5	5.8% (<i>tp10</i>) chi angles: 173.7,71.9,108.2	0.042Å	-	-
59	LEU	93.02	-	Favored (66.25%) General / -73.0,-39.1	22.9% (<i>mt</i>) chi angles: 300,160.2	0.087Å	-	-
				Favored				

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60	ALA 57.5	-	(23.5%) General / -80.1,-42.5	-	0.108Å	-	-
61	SER 52.86	-	Favored (69.71%) General / -60.7,-30.1	51.2% (<i>m</i>) chi angles: 300.2	0.129Å	-	-
62	ARG 141.07	-	Allowed (1.51%) General / -105.0,40.5	13.9% (<i>mmm180</i>) chi angles: 302.3,315.8,309.9,135	0.153Å	-	-
63	GLY 49.05	-	Allowed (1.08%) Glycine / 88.0,90.4	-	-	-	-
64	ALA 67.18	-	Favored (2.27%) General / -172.7,151.2	-	0.083Å	-	-
65	ARG 127.01	-	Allowed (0.76%) General / -105.5,67.3	66.9% (<i>mtp180</i>) chi angles: 295.8,168.4,81.6,184	0.06Å	-	-
66	VAL 63.89	-	Favored (3.76%) Isoleucine or valine / -55.4,147.7	74.3% (t) chi angles: 174	0.05Å	-	-
67	TYR 197.65	-	Favored (55.07%) General / -121.5,135.2	37.6% (<i>t80</i>) chi angles: 164,75.1	0.067Å	-	-
68	ILE 59.25	-	Favored (17.66%) Isoleucine or valine / -110.4,144.9	90.1% (<i>mt</i>) chi angles: 298.4,167.6	0.081Å	-	-
69	ALA 63.09	-	Favored (11.87%) General / -122.4,107.3	-	0.108Å	-	-
70	CYS 85.61	-	Favored (13.42%) General / -149.5,173.6	8.7% (t) chi angles: 197.3	0.075Å	-	-
71	ARG 92.77	-	Favored (13.98%) General / -89.8,-38.2	19.5% (<i>ttm180</i>) chi angles: 188.4,198.9,297.2,193.7	0.047Å	-	-

72

ASP 52.25

(5.63%)General /

-91.9,73.3

55.7% (t0) chi angles: 187.4,9.6 0.113Å

Clash > Cβ **Bond Bond** Alt Res High B Ramachandran **Rotamer** 0.4Å deviation lengths angles Outliers: Avg: Clashscore: Outliers: 17 of Poor rotamers: 24 of Outliers: Outliers: 34 12 of 1.14 234 0 of 278 of 278 124.27 276 259 Favored (5.1%) 69.3% (t) Isoleucine or 73 VAL 43.52 0.104Å valine / chi angles: 171.7 -66.6,-58.8 Favored 2.9% (tm?) (94.82%)0.074Å 74 LEU 120.77 chi angles: 188.9,275.6 General / -59.9,-43.2 Favored 2.7% (ttmp?) (57.86%)75 LYS 92.14 0.075Å chi angles: General / 201.7,189.6,304.8,79.5 -77.9,-17.0 Favored (32.94%)76 GLY 28.71 Glycine / -82.0,-31.1 Favored 2.3% (tp10) (43.37%)0.06Å 77 GLU 73.29 chi angles: General / 206.3,67.9,297.9 -78.7,-36.5 **Favored** 55.6% (p) (48.52%)0.116Å 78 SER 28.67 chi angles: 55.3 General / -55.9,-26.8 Favored (23.36%)0.045Å 79 ALA 36.58 General / -108.3,16.2 Favored (4.8%) 0.095Å 80 ALA 66.25 General / -121.6,-27.1 Allowed 59.7% (p) (0.6%)0.097Å SER 195.76 81 chi angles: 72.7 General / -82.1,-162.9 **Favored** 0.3% (19.49%)0.144Å 82 GLU 265.7 chi angles: General / 86.1,75.2,57.2 -108.8,156.5 Allowed (0.13%)52.2% (*mt*) 0.054Å 83 ILE 88.92 Isoleucine or chi angles: 305.7,178.7

valine / -144.1,62.5

84	ARG 198.75	-	Favored (21.79%) General / 59.9,37.2	97.8% (mtt180) chi angles: 290.9,186.2,174.4,186.1	0.141Å	-	OUTLIER(S) worst is C-N- CA: 4.16 σ
85	VAL 77.25	-	OUTLIER (0%) Isoleucine or valine / 163.4,130.2	0.9% chi angles: 136.8	0.063Å	-	-
86	ASP 128.54	0.452Å OD2 with 89 ASN HA	Allowed (0.46%) General / -59.5,106.4	0.9% chi angles: 295.8,49.1	0.043Å	-	-
87	THR 87.12	-	Favored (56.76%) General / -75.5,-23.0	0.5% chi angles: 95.7	0.283Å	-	OUTLIER(S) worst is N- CA-CB: 4.217
88	LYS 69.92	-	Favored (31.23%) General / -142.8,140.1	49.6% (<i>mttp</i>) chi angles: 289.6,189,190.5,76.5	0.069Å	-	-
89	ASN 57.49	0.452Å HA with 86 ASP OD2	Favored (24.29%) General / -69.8,124.5	18.8% (<i>m120</i>) chi angles: 283.6,112.9	0.078Å	-	-
90	SER 164.78	-	Allowed (0.15%) General / 73.2,154.4	42.4% (<i>t</i>) chi angles: 181.1	0.094Å	-	-
91	GLN 82.79	-	Favored (20.56%) General / -58.9,124.7	96.6% (<i>mt-30</i>) chi angles: 292.6,172.9,342.5	0.097Å	-	-
92	VAL 61.77	-	Favored (69.54%) Isoleucine or valine / -126.8,127.0	78.4% (<i>t</i>) chi angles: 179.2	0.067Å	-	-
#	Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
93	LEU 148.87	-	Favored (28.28%) General / -118.5,156.9	2.5% (mm?) chi angles: 294.6,317.6	0.031Å	-	-

			_	_	•		
94	VAL 116.56	-	Favored (54.52%) Isoleucine or valine / -134.0,135.8	7.6% (p) chi angles: 59.1	0.092Å	-	-
95	ARG 134.86	-	Favored (11.84%) General / -121.0,168.2	91.1% (<i>mtm180</i>) chi angles: 293.6,177.3,291.3,173.4	0.053Å	-	-
96	LYS 110.69	-	Favored (2.5%) General / -74.8,92.3	12.8% (<i>tmtt?</i>) chi angles: 199.2,280.7,186.6,180.3	0.061Å	-	-
97	LEU 74.49	-	Favored (23.34%) General / -109.7,111.7	29.8% (<i>tp</i>) chi angles: 167.8,66.4	0.091Å	-	-
98	ASP 63.07	-	Favored (53.69%) General / -108.6,127.1	51.5% (<i>t0</i>) chi angles: 188.4,13.6	0.029Å	-	-
99	LEU 81.38	-	Favored (29.81%) General / -82.2,2.8	5.1% (<i>mt</i>) chi angles: 294.9,143.6	0.105Å	-	-
100	SER 66.61	-	Favored (27.96%) General / -97.1,-9.5	16.7% (<i>m</i>) chi angles: 307.4	0.071Å	-	-
101	ASP 64.01	-	Favored (5.09%) General / -131.8,100.4	10.2% (<i>t0</i>) chi angles: 164.8,11.5	0.061Å	-	-
102	THR 107.33	-	Favored (68.15%) General / -58.5,-31.8	14% (<i>t</i>) chi angles: 190	0.213Å	-	-
103	LYS 66.57	-	Favored (99.07%) General / -61.8,-42.5	96.2% (<i>mttt</i>) chi angles: 289.8,187,175.7,183.1	0.144Å	-	-
104	SER 88.71	-	Favored (57.85%) General / -75.6,-26.6	54.6% (<i>p</i>) chi angles: 73.6	0.204Å	-	-
105	ILE 131.35	-	Favored (86.67%) Isoleucine or valine / -63.6,-39.8	0.4% chi angles: 236.3,295.5	0.226Å	-	-
			Favored	10.6% (<i>mmm180</i>)			

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106	ARG	134.57	-	(78.54%) General / -69.1,-40.4	chi angles: 279.8,289.7,293,113.8	0.109Å	-	-
107	ALA	23.77	-	Favored (85.66%) General / -58.2,-46.5	-	0.09Å	-	-
108	PHE	63.38	-	Favored (79.21%) General / -69.0,-38.5	16% (<i>t80</i>) chi angles: 172.8,47.7	0.2Å	-	-
109	ALA	42.58	-	Favored (67.05%) General / -58.0,-31.6	-	0.114Å	-	-
110	GLU	80.26	-	Favored (40.4%) General / -79.5,-35.2	55.1% (<i>mm-40</i>) chi angles: 282.6,310.7,311.3	0.106Å	-	-
111	GLY	36.4	-	Allowed (0.24%) Glycine / -67.9,28.4	-	-	-	OUTLIER(S) worst is C-N-CA: 4.256σ
112	РНЕ	80.44	-	Favored (8.18%) General / -163.9,143.9	7.8% (<i>m-30</i>) chi angles: 281.9,140.2	0.093Å	-	-
# Al	t Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: (124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
113	LEU	134.77	-	Favored (60.94%) General / -70.5,-47.3	45.3% (<i>tp</i>) chi angles: 180.5,56.1	0.065Å	-	-
114	ALA	51.84	_	Allowed (0.08%) General/	-	0.08Å	-	-
				-177.6,113.6				
115	GLU	119.5	-		4.5% (<i>pm0</i>) chi angles: 55.1,263.7,61.9	0.114Å	-	-

-90.0,147.9

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129	MET	125.09	-	Favored (40.47%) General / -137.9,140.6	38.2% (ttp) chi angles: 179.9,159.9,62.2	0.148Å	-	OUTLIER(S) worst is C-N-CA: 4.545σ
130	MET	139.48	-	OUTLIER (0.02%) General / 56.9,-8.9	0% chi angles: 241.5,206.2,201.4	0.177Å	-	-
131	CYS	40.41	-	Favored (12.92%) Pre-proline / -63.0,164.6	31.2% (p) chi angles: 65.3	0.069Å	-	-
132	PRO	63.86	-	Favored (13.28%) Trans-proline / -63.4,167.3	13.1% (<i>Cg_exo</i>) chi angles: 323.3	0.099Å	-	-
# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	_	Bond angles
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133	TYR	139.16	-	Favored (5.27%) General / -53.7,152.4	62.5% (<i>t80</i>) chi angles: 177.2,64.9	0.047Å	-	-
134	SER	54.02	-	Allowed (0.16%) General / 175.2,154.9	4.7% (p) chi angles: 42.3	0.035Å	-	-
135	LYS	72.92	-	Favored (16.25%) General / -100.9,158.1	43.5% (mtmt) chi angles: 297.8,200.6,303.7,179.3	0.091Å	-	-
136	THR	33.03	-	Favored (9.88%) General / -79.2,176.2	22.5% (p) chi angles: 49.3	0.05Å	-	-
137	ALA	34.67	-	Favored (78.2%) General / -66.8,-34.6	-	0.098Å	-	-
138	ASP	77.41	-	Allowed (0.17%) General / -67.1,9.9	4.5% (<i>m</i> -20) chi angles: 310.9,353.3	0.034Å	-	OUTLIER(S) worst is CA- CB-CG: 4.856 σ
139	GLY	39.01	-	Favored (2.54%) Glycine / 82.0,-36.0	-	-	-	-

2/19/2013			Viewing KDH12_inb_5	5-010-FFA1FH_leg-liluli1.table - Mic	orrobity		
140	PHE 102.17	-	Allowed (0.21%) General / -43.5,150.6	35.4% (<i>m-85</i>) chi angles: 307.4,300.4	0.141Å	-	-
141	GLU 147.02	-	Favored (26.9%) General / -69.3,125.5	0.2% chi angles: 94.4,74.8,359.6	0.112Å	-	-
142	THR 128.56	-	Favored (56.6%) General / -51.1,-39.6	15.9% (p) chi angles: 46.3	0.102Å	-	-
143	HIS 88.83	-	Favored (23.14%) General / -72.8,-3.1	14.4% (<i>m80</i>) chi angles: 313.5,76.4	0.114Å	-	-
144	LEU 96.48	-	Favored (3.8%) General / -117.3,-36.2	30.3% (<i>tp</i>) chi angles: 186.2,70.1	0.036Å	-	-
145	GLY 44.64	-	Favored (22.95%) Glycine / -67.3,-53.9	-	-	-	-
146	VAL 115.9	-	Favored (15.99%) Isoleucine or valine / -76.4,-24.5	3.6% (<i>m</i>) chi angles: 313.7	0.227Å	-	-
147	ASN 82.24	-	Favored (30.43%) General / -85.0,-20.5	38.5% (<i>m-20</i>) chi angles: 294.9,2.8	0.103Å	-	-
148	HIS 107.98	-	Allowed (0.48%) General / -139.1,-65.7	14.1% (<i>t60</i>) chi angles: 172.4,43.6	0.131Å	-	-
149	LEU 124.52	-	Favored (81.51%) General / -67.2,-43.6	2.9% (<i>mm</i> ?) chi angles: 289.6,314.4	0.16Å	-	-
150	GLY 29.97	-	Favored (99.08%) Glycine / -61.0,-40.9	-	-	-	-
151	HIS 65.7	-	Favored (77.62%) General / -63.2,-34.4	63.8% (<i>m80</i>) chi angles: 284.6,88.2	0.131Å	-	-
152	PHE 59.27	-	Favored (79.5%) General /	76.1% (<i>t80</i>) chi angles: 178.3,69	0.076Å	-	-

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153		LEU	98.03	-	Favored (96.94%) General / -60.4,-43.3	57.3% (<i>mt</i>) chi angles: 307.2,179.8	0.089Å	-	-
154	ļ	LEU	52.29	-	Favored (93.21%) General / -59.6,-44.8	41.3% (<i>tp</i>) chi angles: 185.3,58.5	0.026Å	-	-
155	;	THR	47.6	-	Favored (84.61%) General / -66.7,-37.4	77.8% (<i>m</i>) chi angles: 297.1	0.181Å	-	-
156	•	TYR	104.02	-	Favored (64.55%) General / -62.4,-52.2	60.7% (<i>t80</i>) chi angles: 172.4,67.8	0.056Å	-	-
157	,	LEU	59.98	-	Favored (81.77%) General / -66.2,-36.0	83.8% (<i>mt</i>) chi angles: 300.1,173.6	0.132Å	-	-
158	3	LEU	83.5	-	Favored (50.87%) General / -80.3,-17.8	81% (<i>mt</i>) chi angles: 302,180.7	0.164Å	-	-
159)	LEU	77.13	-	Favored (72.93%) General / -68.9,-33.0	37.3% (<i>mt</i>) chi angles: 284.8,162.2	0.136Å	-	-
160)	GLU	71.75	-	Favored (3.3%) General / -72.7,-58.5	0.4% chi angles: 149.9,29.6,45.9	0.133Å	-	-
161		ARG	90.56	-	Favored (99.57%) General / -62.6,-42.5	96.7% (<i>mtt180</i>) chi angles: 286.9,188.4,178.3,171.7	0.185Å	-	-
162		LEU	151.09	-	Favored (7.95%) General / -89.4,68.5	0% chi angles: 310,34.7	0.076Å	-	OUTLIER(S) worst is C-N- CA: 4.514 σ
163	;	LYS	231.57	-	Allowed (0.29%) General / -46.6,154.6	0% chi angles: 205.6,147.1,266.1,62.1	0.162Å	-	OUTLIER(S) worst is C-N- CA: 5.173 σ

164	VAL 160.06	-	Allowed (1.55%) Isoleucine or valine / -46.6,-31.6	5.9% (<i>p</i>) chi angles: 75	0.181Å	-	-
165	SER 51.06	-	Allowed (0.06%) General / -85.7,-101.5	77.9% (p) chi angles: 58.9	0.193Å	-	-
166	ALA 54.33	-	Favored (3.02%) Pre-proline / -69.2,-31.9	-	0.161Å	-	-
167	PRO 228.32	-	OUTLIER (0.09%) Trans-proline / -61.5,72.3	0.9% chi angles: 320.9	0.063Å	-	OUTLIER(S) worst is C-N-CA: 4.683σ
168	ALA 103.41	-	OUTLIER (0.01%) General / 25.3,-126.1	-	0.235Å	-	-
169	ARG 235.77	-	Favored (41.97%) General / -153.1,161.9	0% chi angles: 291.1,89.1,224.5,206	0.087Å	-	-
170	VAL 75.62	-	Allowed (1.77%) Isoleucine or valine / -94.9,166.6	72.1% (<i>t</i>) chi angles: 171.9	0.15Å	-	-
171	VAL 90.06	-	Favored (31.83%) Isoleucine or valine / -119.9,143.3	3.6% (<i>t</i>) chi angles: 156.7	0.082Å	-	-
172	ASN 74.14	-	Favored (50.24%) General / -125.8,145.4	0% chi angles: 339.9,124.5	0.027Å	-	OUTLIER(S) worst is CA- CB-CG: 5.358 σ
# Al	lt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: (124.27	Clashscore 1.14	: Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
173	VAL 77.62	-	Favored (57.54%) Isoleucine or valine / -125.1,120.1	6.3% (<i>t</i>) chi angles: 193.8	0.055Å	-	-
			Allowed				

2/19/2015			Viewing RDH12_mb_3	3-610-FFX1FH_reg-multi.table - Mo	lProbity		
174	SER 143.26	-	(0.34%) General / -109.0,-133.7	95.5% (p) chi angles: 66.7	0.171Å	-	-
175	SER 107.93	-	Favored (30.64%) General / -158.2,167.1	42.8% (<i>t</i>) chi angles: 177.9	0.036Å	-	-
176	VAL 169.83	-	Favored (12.89%) Isoleucine or valine / -80.6,-13.5	3.2% (<i>p</i>) chi angles: 80.1	0.162Å	-	-
1 <i>77</i>	ALA 104.75	-	Allowed (0.21%) General / -61.0,0.5	-	0.04Å	-	-
178	HIS 136.37	-	Allowed (1.03%) General / -65.6,2.2	29.7% (<i>p-80</i>) chi angles: 78.6,275.4	0.186Å	-	OUTLIER(S) worst is CA- CB-CG: 5.411 σ
179	HIS 105.73	-	Favored (58.51%) General / -77.2,-17.4	3.7% (<i>t-80</i>) chi angles: 203.4,316.4	0.059Å	-	OUTLIER(S) worst is CA- CB-CG: 5.288 σ
180	ILE 157.37	-	Allowed (0.29%) Isoleucine or valine / -142.4,-13.4	2.4% (<i>tp</i>) chi angles: 213.5,79.3	0.149Å	-	-
181	GLY 63.94	-	Favored (48.1%) Glycine / -64.5,144.2	-	-	-	-
182	LYS 87.5	-	Favored (36.97%) General / -123.7,155.9	54.9% (<i>mtmt</i>) chi angles: 297.4,195,293.3,183.9	0.044Å	-	-
183	ILE 138.76	-	Favored (37.42%) Pre-proline / -118.8,89.1	44.9% (<i>mm</i>) chi angles: 300.9,296.2	0.05Å	-	-
184	PRO 120.69	-	Allowed (0.3%) Trans-proline / -90.8,105.8	47.7% (<i>Cg_endo</i>) chi angles: 35.3	0.038Å	-	-
185	PHE 115.05	-	Favored (94.71%) General / -60.6,-41.5	95.8% (<i>m-85</i>) chi angles: 297.8,282.3	0.163Å	-	-

2/19/2015			Viewing RDH12_mb_3	3-610-FFX1FH_reg-multi.table - Mo	lProbity		
186	HIS 90.21	-	Favored (77.92%) General / -66.8,-34.5	47.8% (<i>t-80</i>) chi angles: 192,265.7	0.101Å	-	-
187	ASP 180.94	-	Allowed (1.07%) General / -111.0,46.4	83.2% (<i>m-20</i>) chi angles: 296.5,340.7	0.066Å	-	-
188	LEU 97.32	-	Favored (41.74%) General / -81.2,-20.1	3.6% (<i>tp</i>) chi angles: 220.5,69.7	0.135Å	-	-
189	GLN 140.17	-	Favored (2.85%) General / -136.9,5.8	0.9% chi angles: 303.7,88.8,254.6	0.082Å	-	-
190	SER 196.77	-	Favored (13.46%) General / -78.8,172.6	8.9% (<i>t</i>) chi angles: 193.3	0.05Å	-	OUTLIER(S) worst is C-N- CA: 5.703 σ
191	GLU 141.52	-	OUTLIER (0%) General / -56.2,12.7	0% chi angles: 55.3,36.4,259.3	0.068Å	-	-
192	LYS 115.39	_	Favored (6.19%)	45.6% (mmtm) chi angles:	0.118Å	_	OUTLIER(S) worst is C-N-
			General / -79.6,72.0	292.6,300.4,187.6,304.5			CA: 4.246 σ
# A	Alt Res High B	Clash > 0.4Å		292.6,300.4,187.6,304.5	Cβ deviation	Bond lengths	CA: 4.246 σ Bond angles
# A	Alt Res High B	0.4Å	-79.6,72.0 Ramachandran	292.6,300.4,187.6,304.5	Сβ	lengths	Bond
# A	Alt Res High B Avg: (0.4Å Clashscore:	-79.6,72.0 Ramachandran : Outliers: 17 of	292.6,300.4,187.6,304.5 Rotamer Poor rotamers: 24 of	C β deviation Outliers: 12 of	lengths Outliers:	Bond angles Outliers: 34
	Alt Res High B Avg: 0 124.27	0.4Å Clashscore:	-79.6,72.0 Ramachandran Outliers: 17 of 276 Favored (2.48%) General /	292.6,300.4,187.6,304.5 Rotamer Poor rotamers: 24 of 234 61.3% (mmt-85) chi angles:	Cβ deviation Outliers: 12 of 259	lengths Outliers:	Bond angles Outliers: 34
193	Alt Res High B Avg: 0 124.27 ARG 112.01	0.4Å Clashscore:	-79.6,72.0 Ramachandran Outliers: 17 of 276 Favored (2.48%) General / 45.5,61.7 Favored (2.07%) General /	292.6,300.4,187.6,304.5 Rotamer Poor rotamers: 24 of 234 61.3% (<i>mmt-85</i>) chi angles: 315.4,301.1,176.8,270.6 45% (<i>t80</i>)	Cβ deviation Outliers: 12 of 259 0.156Å	lengths Outliers:	Bond angles Outliers: 34
193 194	Avg: 0 124.27 ARG 112.01 TYR 91.21	0.4Å Clashscore:	-79.6,72.0 Ramachandran : Outliers: 17 of 276 Favored (2.48%) General / 45.5,61.7 Favored (2.07%) General / -40.4,132.1 Favored (50.08%) General /	292.6,300.4,187.6,304.5 Rotamer Poor rotamers: 24 of 234 61.3% (<i>mmt-85</i>) chi angles: 315.4,301.1,176.8,270.6 45% (<i>t80</i>) chi angles: 175,93.7	Cβ deviation Outliers: 12 of 259 0.156Å	lengths Outliers:	Bond angles Outliers: 34

2/19/2015			Viewing RDH12_mb_	33-610-FFX1FH_reg-multi.table - Mo	lProbity		
197	GLY 51.63	-	(12.32%) Glycine / -73.0,-50.6	-	-	-	-
198	PHE 72.95	-	Favored (57.48%) General / -75.3,-24.8	55.6% (<i>m-85</i>) chi angles: 282.4,89.9	0.196Å	-	-
199	ALA 42.08	-	Favored (98.28%) General / -63.6,-41.4	-	0.073Å	-	-
200	TYR 78.18	-	Favored (73.7%) General / -66.0,-47.7	37.5% (<i>t80</i>) chi angles: 174.3,58.3	0.061Å	-	-
201	CYS 60.18	-	Favored (95.11%) General / -60.0,-43.7	95.1% (<i>m</i>) chi angles: 293.9	0.154Å	-	-
202	HIS 75.92	-	Favored (80.91%) General / -64.1,-35.5	2.9% (<i>p-80</i>) chi angles: 90.6,301.2	0.199Å	-	OUTLIER(S) worst is CA- CB-CG: 8.376 σ
203	SER 101.46	-	Favored (25.03%) General / -83.6,-34.7	16% (<i>m</i>) chi angles: 308	0.042Å	-	-
204	LYS 143.54	-	Favored (56.41%) General / -83.8,-11.9	70.5% (<i>mmtt</i>) chi angles: 297.8,307.4,192.2,184.1	0.27Å	-	-
205	LEU 132.3	-	Favored (78.03%) General / -64.7,-47.5	0.8% chi angles: 194.6,305.9	0.04Å	-	-
206	ALA 49.87	-	Favored (70.16%) General / -55.6,-39.0	-	0.094Å	-	-
207	ASN 81.16	-	Favored (69.9%) General / -67.2,-30.1	1.6% (<i>m120</i>) chi angles: 290.1,193.5	0.194Å	-	OUTLIER(S) worst is CA- CB-CG: 8.081 σ
208	VAL 152.71	-	Favored (55.04%) Isoleucine or valine / -70.4,-33.8	15.6% (<i>m</i>) chi angles: 305.8	0.277Å	-	OUTLIER(S) worst is N- CA-CB: 4.266 σ
			Favored				

2/19/2015			Viewing RDH12_mb_33	3-610-FFX1FH_reg-multi.table - Mo	olProbity		
209	LEU 71.19	-	(28.19%) General / -82.8,-31.8	56% (<i>mt</i>) chi angles: 307.9,177.8	0.086Å	-	-
210	PHE 78.7	-	Favored (70.04%) General / -56.5,-37.2	84.7% (<i>t80</i>) chi angles: 181.7,73.1	0.088Å	-	-
211	THR 69.96	-	Favored (50.07%) General / -49.8,-48.8	7.3% (<i>m</i>) chi angles: 314.7	0.071Å	-	-
212	ARG 182.06	-	Favored (44.17%) General / -79.8,-21.5	7.3% (tpm_?) chi angles: 185,60.7,275.5,187	0.086Å	-	-
# /	Alt Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
213	GLU 102.08	-	Favored (14.56%) General / -90.8,-35.8	36.3% (<i>tp10</i>) chi angles: 177.9,51.8,13.9	0.118Å	-	-
214	LEU 144.29	-	Favored (94.29%) General / -60.2,-45.1	61% (<i>tp</i>) chi angles: 176.9,59.7	0.079Å	-	-
215	ALA 61.08	-	Favored (20.67%) General / -73.2,-2.2	-	0.081Å	-	-
216	LYS 146.29	-	Favored (29.11%) General / -79.7,-40.4	3.7% (tmmm?) chi angles: 182.9,278.4,305.9,300.1	0.143Å	-	-
217	ARG 70.09	-	Favored (26.34%) General / -82.6,-36.2	43.5% (<i>tpt85</i>) chi angles: 179.5,59.6,189.4,98.5	0.201Å	-	-
218	LEU 139	-	Favored (6.04%) General / -87.8,60.7	10.2% (<i>mp</i>) chi angles: 280.1,59.5	0.122Å	-	-
219	GLN 89.88	-	Favored (5.21%) General / -119.6,-28.9	8.1% (<i>tp60</i>) chi angles: 193.8,52,96.2	0.065Å	-	-
			Allowed (0.3%)				

2/19/2015			Viewing RDH12_mb_33	3-610-FFX1FH_reg-multi.table - Mo	lProbity		
220	GLY 45.97	-	Glycine / -130.1,87.5	-	-	-	-
221	THR 130.17	-	Allowed (0.13%) General / -154.8,-63.8	2.6% (p) chi angles: 39.2	0.085Å	-	-
222	GLY 54.18	-	Allowed (0.84%) Glycine / 130.6,-52.0	-	-	-	-
223	VAL 132.42	-	Favored (20.94%) Isoleucine or valine / -68.7,139.2	17.9% (<i>m</i>) chi angles: 291.7	0.108Å	-	-
224	THR 155.12	-	Allowed (0.66%) General / -158.5,-157.9	13.4% (<i>t</i>) chi angles: 190.6	0.319Å	-	OUTLIER(S) worst is C- CA-CB: 4.354 σ
225	THR 133.18	-	Favored (39.77%) General / -144.1,151.6	13.5% (<i>t</i>) chi angles: 190.4	0.106Å	-	-
226	TYR 124.84	-	Favored (3.11%) General / -112.9,-177.3	14.7% (<i>m-30</i>) chi angles: 294.1,354.5	0.041Å	-	OUTLIER(S) worst is CA- CB-CG: 4.207 σ
227	ALA 85.56	-	Favored (26.56%) General / -162.1,165.9	-	0.059Å	-	-
228	VAL 158.02	-	Allowed (0.52%) Isoleucine or valine / -148.7,-178.1	8.5% (<i>p</i>) chi angles: 70.4	0.136Å	-	-
229	HIS 152.9	-	Allowed (1.57%) Pre-proline / -166.4,130.0	24.9% (<i>p80</i>) chi angles: 73.7,83	0.05Å	-	-
230	PRO 164.25	-	Favored (2%) Trans-proline / -81.7,109.3	94% (<i>Cg_endo</i>) chi angles: 30.8	0.017Å	-	-
231	GLY 98.78	-	Favored (91.6%) Glycine / -65.8,-44.8	-	-	-	-

18% (m)

(77.16%)

232	VAI	. 157.39	-	Isoleucine or valine / -61.8,-37.0	18% (<i>m</i>) chi angles: 291.8	0.221Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
233	VAI	₋ 181.19	-	Favored (7.63%) Isoleucine or valine / -105.1,13.7	60.9% (<i>t</i>) chi angles: 181.2	0.21Å	-	-
234	ARC	G 269.11	-	Favored (21.35%) General / -109.3,17.6	10.5% (<i>mmt85</i>) chi angles: 290.3,288.5,169.1,117.6	0.198Å	-	-
235	SER	136.67	-	Favored (3.42%) General / -119.2,-177.8	0.3% chi angles: 241.4	0.145Å	-	-
236	GLU	J 224.8	-	Allowed (0.99%) General / -87.9,41.3	30% (<i>mp0</i>) chi angles: 307.3,71.8,12.9	0.061Å	-	-
237	LEU	328.28	-	Favored (36%) General / -80.7,135.5	10.3% (<i>mp</i>) chi angles: 279.4,58.3	0.044Å	-	-
238	VAI	₋ 361.18	-	OUTLIER (0.04%) Isoleucine or valine / -79.9,-157.8	28.2% (<i>m</i>) chi angles: 301.4	0.253Å	-	OUTLIER(S) worst is C-N- CA: 4.94 σ
239	ARC	374.78	-	OUTLIER (0.01%) General / -4.0,98.6	99.7% (<i>mtt180</i>) chi angles: 295.9,181.2,177.8,179	0.052Å	-	-
240	HIS	277.74	-	Allowed (0.37%) General / -147.9,-14.4	4.9% (<i>p-80</i>) chi angles: 56.2,245.3	0.064Å	-	-
241	SER	148.65	-	Allowed (0.28%) General / 44.0,-139.7	20.3% (t) chi angles: 169.8	0.271Å	-	OUTLIER(S) worst is C- CA-CB: 4.575 σ
242	SER	133.54	-	Favored (15.32%) General / -116.6,13.5	55.8% (p) chi angles: 55.3	0.077Å	-	-

2/19/2015			Viewing RDH12_mb_33	3-610-FFX1FH_reg-multi.table - Mo	olProbity		
243	LEU 201.95	-	Allowed (1.88%) General / -86.6,49.8	51.8% (<i>mt</i>) chi angles: 306.8,183.1	0.058Å	-	-
244	LEU 277.91	-	Favored (18.84%) General / -86.1,109.4	0.5% chi angles: 275.1,28.9	0.025Å	-	-
245	CYS 110.49	-	Favored (18.98%) General / -60.9,155.8	73.5% (<i>m</i>) chi angles: 296.9	0.052Å	-	-
246	LEU 264.8	-	Favored (11.94%) General / -134.4,173.2	0.2% chi angles: 316.9,306.3	0.127Å	-	-
247	LEU 344.54	0.423Å HB2 with 283 SER HA	Favored (3.88%) General / -148.0,107.2	46% (<i>tp</i>) chi angles: 177,55.8	0.07Å	-	OUTLIER(S) worst is C-N-CA: 4.195σ
248	TRP 450.74	0.421Å HB2 with 247 LEU O	OUTLIER (0.01%) General / 160.1,172.8	1.7% (<i>t-105</i>) chi angles: 220,270.2	0.131Å	-	OUTLIER(S) worst is C-N- CA: 5.66 σ
249	ARG 426.24	-	OUTLIER (0.02%) General / 92.7,121.9	24% (<i>tpt85</i>) chi angles: 177.5,49.8,160.9,92.8	0.11Å	-	-
250	LEU 311.48	-	Allowed (1.47%) General / -48.0,149.1	49.3% (<i>tp</i>) chi angles: 184.8,62.5	0.066Å	-	-
251	PHE 250.74	-	Allowed (1.35%) General / -41.8,138.8	30.9% (<i>m</i> -85) chi angles: 304.2,305.3	0.097Å	-	-
252	SER 163.36	-	Favored (28.47%) Pre-proline / -118.6,140.6	15.2% (<i>m</i>) chi angles: 308.6	0.09Å	-	-
# Al	t Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
253	PRO 153.91	-	Allowed (1.26%) Trans-proline / -82.1,-30.4	63.1% (<i>Cg_endo</i>) chi angles: 34.2	0.056Å	-	-

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2/19/2013			viewing KDH12_inb_3	55-010-FFX1FH_leg-lilulii.table - Mio	orrobity		
254	PHE 183.36	-	Favored (13.23%) General / -48.2,135.4	20.2% (<i>m-85</i>) chi angles: 315.5,116.7	0.052Å	-	-
255	VAL 139.98	-	Allowed (0.66%) Isoleucine or valine / -105.5,-178.9	27.7% (<i>m</i>) chi angles: 295.6	0.159Å	-	-
256	LYS 305.67	-	Favored (16.93%) General / 61.7,35.7	98.5% (<i>mttt</i>) chi angles: 297,180.3,179,180.6	0.15Å	-	-
257	THR 276.04	-	Favored (7.65%) General / -81.8,96.5	58.1% (<i>p</i>) chi angles: 56.4	0.025Å	-	-
258	ALA 210.82	-	OUTLIER (0.01%) General / -67.5,-145.8	-	0.222Å	-	-
259	ARG 213.72	-	Favored (5.38%) General / -130.7,13.6	40.3% (ptt180) chi angles: 61.4,182.2,180.6,181.2	0.049Å	-	-
260	GLU 247.55	-	Favored (24.42%) General / -92.9,112.5	7.8% (<i>mp0</i>) chi angles: 309.5,64.2,52.8	0.053Å	-	-
261	GLY 105.41	-	Favored (61.71%) Glycine / -73.3,-31.1	-	-	-	-
262	ALA 78.65	-	Favored (78.28%) General / -55.9,-46.7	-	0.026Å	-	-
263	GLN 161.92	-	Favored (98.51%) General / -63.5,-42.1	9% (<i>tt0</i>) chi angles: 197.7,205.5,315	0.062Å	-	-
264	THR 202.67	-	Favored (71.9%) General / -63.1,-30.8	6.8% (<i>p</i>) chi angles: 42.7	0.192Å	-	-
265	SER 84.86	-	Favored (78.2%) General / -69.1,-37.1	57.4% (<i>m</i>) chi angles: 299.4	0.102Å	-	-
			Favored				

2/19/2015			Viewing RDH12_mb_33	3-610-FFX1FH_reg-multi.table - Mo	olProbity		
266	LEU 87.95	-	(80.53%) General / -65.5,-35.3	89.5% (<i>mt</i>) chi angles: 299.8,178.9	0.122Å	-	-
267	HIS 94.4	-	Favored (97.79%) General / -62.1,-41.0	13% (<i>m-70</i>) chi angles: 287.6,228.8	0.102Å	-	-
268	CYS 116.65	-	Favored (71.45%) General / -63.4,-30.3	6.4% (<i>t</i>) chi angles: 199.9	0.112Å	-	-
269	ALA 131.85	-	Favored (56.49%) General / -77.1,-7.8	-	0.097Å	-	OUTLIER(S) worst is C-N- CA: 5.728 σ
270	LEU 308.31	-	OUTLIER (0%) General / 128.4,7.2	9.3% (<i>tp</i>) chi angles: 193.6,43.8	0.215Å	-	-
271	ALA 133.76	-	Favored (12.15%) General / -73.1,0.2	-	0.18Å	-	-
272	GLU 143.4	-	Favored (9.46%) General /	4.1% (<i>pt-20</i>) chi angles: 85.5,163.8,257.2	0.164Å	-	-
			-151.8,178.4	001071.0010720712			
# Al	t Res High B	Clash > 0.4Å	-151.8,178.4 Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
# Al		0.4Å	Ramachandran			lengths	angles Outliers: 34
# Al 273	Avg:	0.4Å Clashscore:	Ramachandran Outliers: 17 of	Rotamer Poor rotamers: 24 of	deviation Outliers: 12 of	lengths Outliers:	angles Outliers: 34
	Avg: 0 124.27	0.4Å Clashscore:	Ramachandran Outliers: 17 of 276 Favored (4.57%) Glycine /	Rotamer Poor rotamers: 24 of	deviation Outliers: 12 of	lengths Outliers:	angles Outliers: 34
273	Avg: 0 124.27 GLY 71.24	0.4Å Clashscore:	Ramachandran Outliers: 17 of 276 Favored (4.57%) Glycine / -79.5,117.7 Favored (5.24%) General /	Rotamer Poor rotamers: 24 of 234 - 29.5% (mt)	deviation Outliers: 12 of 259	lengths Outliers:	angles Outliers: 34 of 278 - OUTLIER(S) worst is C-N-
273 274	Avg: 0 124.27 GLY 71.24 LEU 210.77	0.4Å Clashscore:	Ramachandran Outliers: 17 of 276 Favored (4.57%) Glycine / -79.5,117.7 Favored (5.24%) General / -146.5,-176.6 OUTLIER (0%) Pre-proline /	Rotamer Poor rotamers: 24 of 234 - 29.5% (mt) chi angles: 289.7,158.8 2.6% (tm-20) chi angles:	deviation Outliers: 12 of 259	lengths Outliers:	angles Outliers: 34 of 278 - OUTLIER(S) worst is C-N-

2/19/2015			Viewing RDH12_mb_3 General /	3-610-FFX1FH_reg-multi.table - Mo	lProbity		
			-53.8,151.7				
278	SER 125.06	-	Favored (42.53%) General / -74.7,138.0	40.6% (<i>t</i>) chi angles: 181.4	0.062Å	-	-
279	GLY 95.24	-	Favored (35.41%) Glycine / 179.0,-166.1	-	-	-	-
280	LYS 167.75	-	Favored (5.46%) General / -117.0,175.7	33.4% (<i>mttm</i>) chi angles: 263.3,188.6,180.2,293.1	0.044Å	-	-
281	TYR 159.78	-	Favored (33.51%) General / -73.1,-48.7	1.2% (<i>t80</i>) chi angles: 176.4,118.5	0.071Å	-	OUTLIER(S) worst is CA- CB-CG: 4.483 σ
282	PHE 226.87	-	Favored (14.41%) General / -99.0,-25.9	33.2% (<i>t80</i>) chi angles: 194.7,91	0.054Å	-	OUTLIER(S) worst is C-N-CA: 4.177σ
283	SER 265	0.423Å HA with 247 LEU HB2	OUTLIER (0%) General / 112.9,-42.3	47.4% (<i>t</i>) chi angles: 180.1	0.205Å	-	OUTLIER(S) worst is N- CA-CB: 4.215 σ
284	ASP 112.42	-	Favored (4.08%) General / -130.8,-4.1	0.8% chi angles: 328,295.7	0.057Å	-	-
285	CYS 124.36	-	Favored (2.45%) General / -166.9,-173.7	7.1% (p) chi angles: 49.3	0.07Å	-	-
286	LYS 198.14	-	Allowed (0.19%) General / 68.7,-163.3	55.6% (<i>mttp</i>) chi angles: 304.9,174.1,184.6,71.5	0.268Å	-	OUTLIER(S) worst is C- CA-CB: 4.223
287	ARG 169.79	-	OUTLIER (0.03%) General / -82.0,-132.9	10.5% (<i>ptp180</i>) chi angles: 58.7,170.5,75.3,220	0.294Å	-	OUTLIER(S) worst is C- CA-CB: 4.176 σ
288	THR 258.81	-	Favored (20.12%) General / -111.1,157.3	22% (p) chi angles: 49.1	0.048Å	-	-
289	TRP 288.47	-	Allowed (1%) General / -175.5,149.5	58.3% (<i>t-105</i>) chi angles: 172.1,243	0.107Å	-	OUTLIER(S) worst is C-N- CA: 4.106 σ
			OUTLIER				

2/19/2015			Viewing RDH12_mb_33	3-610-FFX1FH_reg-multi.table - Mo	olProbity		
290	VAL 243.63	-	(0.03%) Isoleucine or valine / -93.2,-145.5	2.7% (<i>p</i>) chi angles: 81.1	0.319Å	-	OUTLIER(S) worst is C- CA-CB: 4.866 σ
291	SER 177.14	-	Allowed (1.96%) Pre-proline / -156.8,109.8	16% (<i>m</i>) chi angles: 283.2	0.047Å	-	-
292	PRO 130.67	-	Favored (6.27%) Trans-proline / -84.5,-15.3	12.9% (<i>Cg_endo</i>) chi angles: 39.7	0.04Å	-	-
# A	It Res High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	•	Bond angles
	Avg: (124.27	Clashscore: 1.14	Outliers: 17 of 276	Poor rotamers: 24 of 234	Outliers: 12 of 259	Outliers: 0 of 278	Outliers: 34 of 278
293	ARG 189.56	-	Favored (2.45%) General / -73.0,98.0	7.6% (<i>mmt180</i>) chi angles: 259.6,281.2,179.3,159.2	0.053Å	-	-
294	ALA 74.64	-	Allowed (1.2%) General / -139.4,-11.8	-	0.061Å	-	-
295	ARG 114.88	-	Allowed (1.97%) General / -85.7,50.5	73.6% (ttt180) chi angles: 192.8,177.8,178.1,179.4	0.079Å	-	-
296	ASN 64.72	-	Favored (2.62%) General / -149.4,97.2	12% (<i>m120</i>) chi angles: 293.6,153	0.099Å	-	OUTLIER(S) worst is CA- CB-CG: 7.402 σ
297	ASN 84.45	-	Favored (20.62%) General / -83.9,-38.9	16.7% (<i>p-10</i>) chi angles: 58.4,303.1	0.102Å	-	-
298	LYS 89.34	-	Favored (61.25%) General / -72.2,-23.3	36.1% (<i>mttm</i>) chi angles: 300.1,201.6,166.1,284.1	0.222Å	-	-
299	THR 103.53	-	Favored (70.49%) General / -60.2,-31.8	1.7% (<i>p</i>) chi angles: 37.2	0.124Å	-	-
300	ALA 40.25	-	Favored (13.86%)	-	0.078Å	-	-

2/19/2015			Viewing RDH12_mb_33 General / -97.8,-28.5	8-610-FFX1FH_reg-multi.table - Mc	lProbity		
301	GLU 86.77	-	Favored (65.15%) General / -73.6,-34.7	4.2% (<i>pt-20</i>) chi angles: 84.9,203.6,34.5	0.2Å	-	-
302	ARG 72.72	-	Favored (67.21%) General / -68.7,-28.9	15.9% (<i>tpp180</i>) chi angles: 166.6,55.8,72.6,173.2	0.163Å	-	-
303	LEU 56.07	-	Favored (73.41%) General / -66.4,-32.2	17.6% (<i>tp</i>) chi angles: 192.7,72	0.101Å	-	-
304	TRP 70.38	-	Favored (53.68%) General / -63.2,-53.4	47.6% (<i>t-105</i>) chi angles: 177,271.5	0.088Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.28 σ
305	ASN 69.55	-	Favored (58.32%) General / -76.3,-19.3	0.4% chi angles: 96.8,289.1	0.27Å	-	-
306	VAL 85.59	-	Allowed (0.73%) Isoleucine or valine / -73.9,5.5	0.3% chi angles: 94.9	0.209Å	-	-
307	SER 48.37	-	Favored (23.99%) General / -100.6,-7.4	17.2% (<i>m</i>) chi angles: 307.3	0.089Å	-	-
308	CYS 77.9	-	Favored (9.81%) General / -118.1,-16.2	6% (p) chi angles: 48	0.159Å	-	-
309	GLU 23.43	-	Favored (57.44%) General / -78.3,-16.8	55.4% (<i>mt-10</i>) chi angles: 298.8,168.4,313.4	0.082Å	-	-
310	LEU 34.93	-	-	53.5% (<i>mt</i>) chi angles: 306.2,173.7	0.079Å	-	-