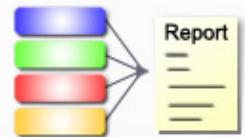


# Protein Structure Validation Suite (PSVS)



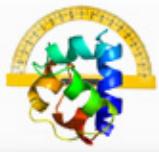
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## PSVS report for Final\_model\_1

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# PSVS report for Final\_model\_1



Protein Structure Validation Suite  
(PSVS)



# **Software Environment**

## **Software for structure quality evaluation:**

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.12 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-2.3
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4

## **MolProbity programs:**

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14
probe	Version 2.6

## **Other Software:**

PERL	Version 5.16.3
convert	ImageMagick 6.7.8
ps2pdf	Ghostscript 9.25
htmldoc	v1.8.28
gnuplot	Version 4.6.2
jpegtopnm	netpbm-progs 10.79.00
pnmcrop	netpbm-progs 10.79.00
pnmtojpeg	netpbm-progs 10.79.00

Updated on March, 2020

# Structure Quality Analysis for NAME

Analyses performed for all residues.

Procheck analysis, RMSD calculation and structure superimposition are based on all residues

NESG ID: NAME

PDB ID:

Deposition date:

Common Name:

Class:

Length (a.a.): 379

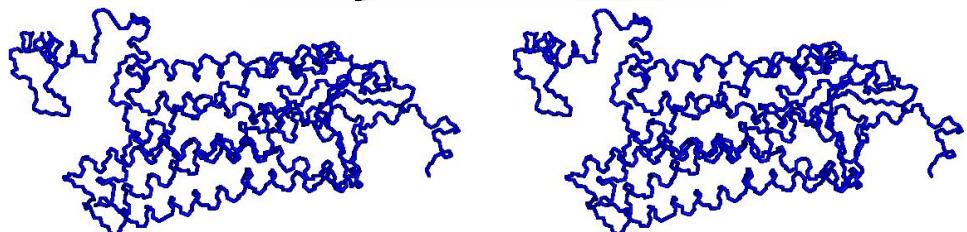
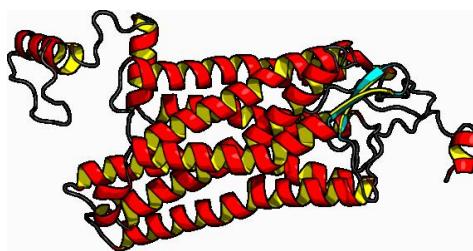
Organism:

SwissProt /  
TrEMBL ID:

# models: 1

Oligomerization: dimer

Molecular weight: 41198



## Secondary Structure Elements:

*Inter-chain break(s) between 379 & 390*

alpha helices:

beta strands:

## Ramachandran Plot Summary for selected residues<sup>3</sup> from Procheck

*Most favoured regions    Additionally allowed regions    Generously allowed regions    Disallowed regions*

88.7%                  9.8%                  0.3%                  1.2%

## Ramachandran Plot Summary for selected residues<sup>3</sup> from Richardson Lab's Molprobity

*Most favoured regions    Allowed regions    Disallowed regions    [View plot](#) [View model summary](#)*

91.7%                  4.8%                  3.5%

## Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) <sup>3</sup>	Procheck (all) <sup>3</sup>	MolProbity	Clashscore
---------	----------	---------------	---------------------------------	-----------------------------	------------	------------

Raw score	0.05	0.05	0.04	0.08	55.29
-----------	------	------	------	------	-------

Z-score <sup>1</sup>	-6.58	-2.48	0.47	0.47	-7.96
----------------------	-------	-------	------	------	-------

## Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

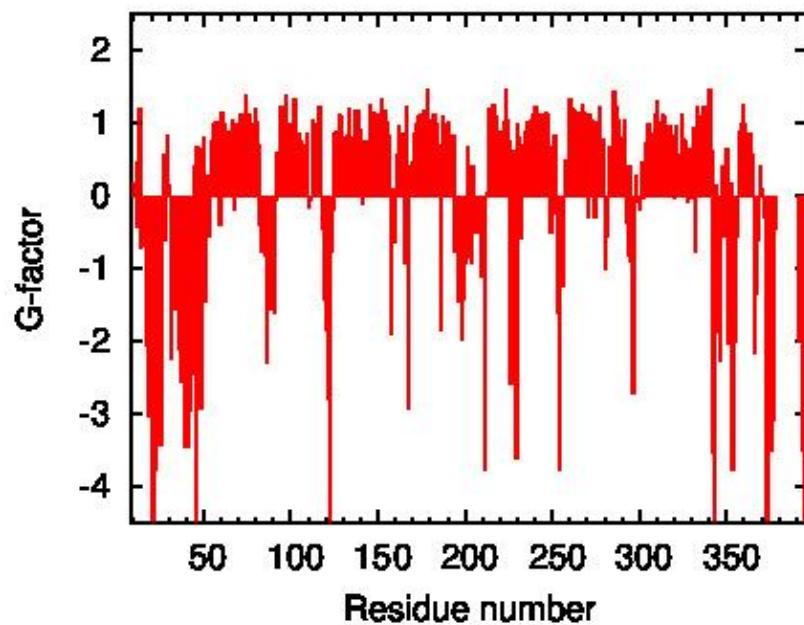
RMS deviation for bond angles: 1.8 °

RMS deviation for bond lengths: 0.013 Å

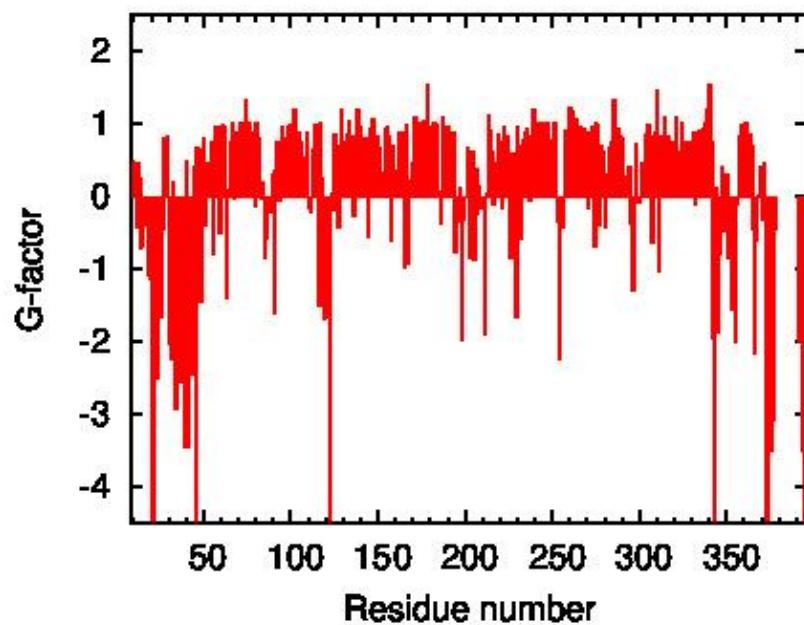
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>3</sup>Selected residues: all

Procheck G-factor for phi-psi

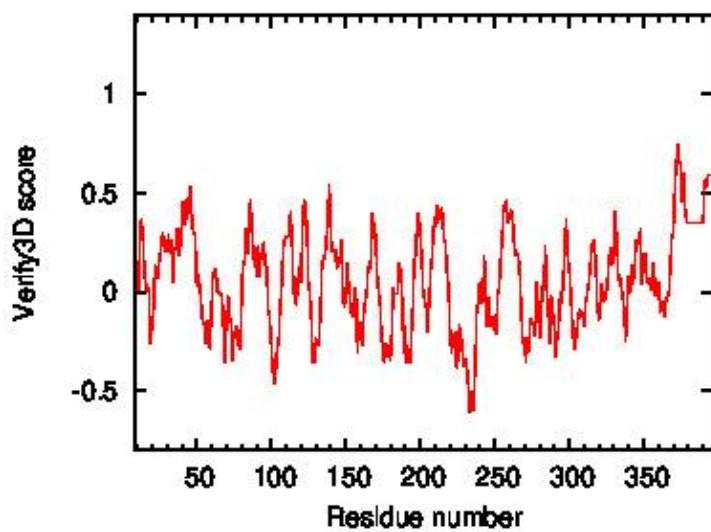


Procheck G-factor for all dihedral angles

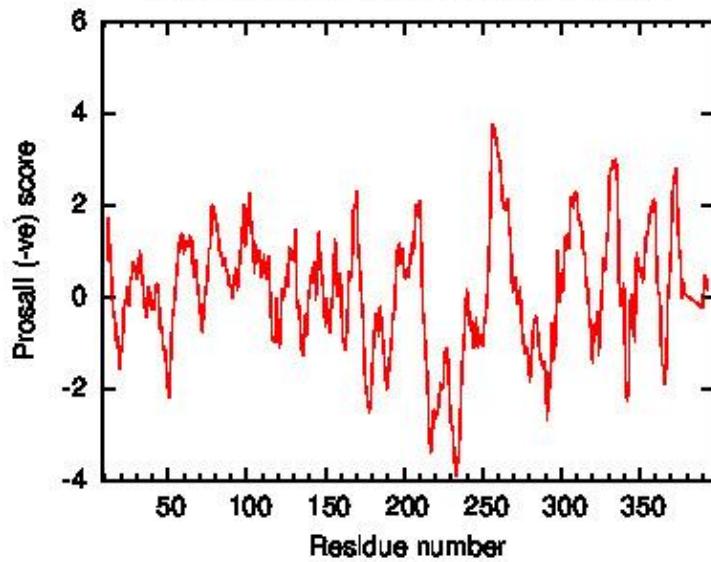


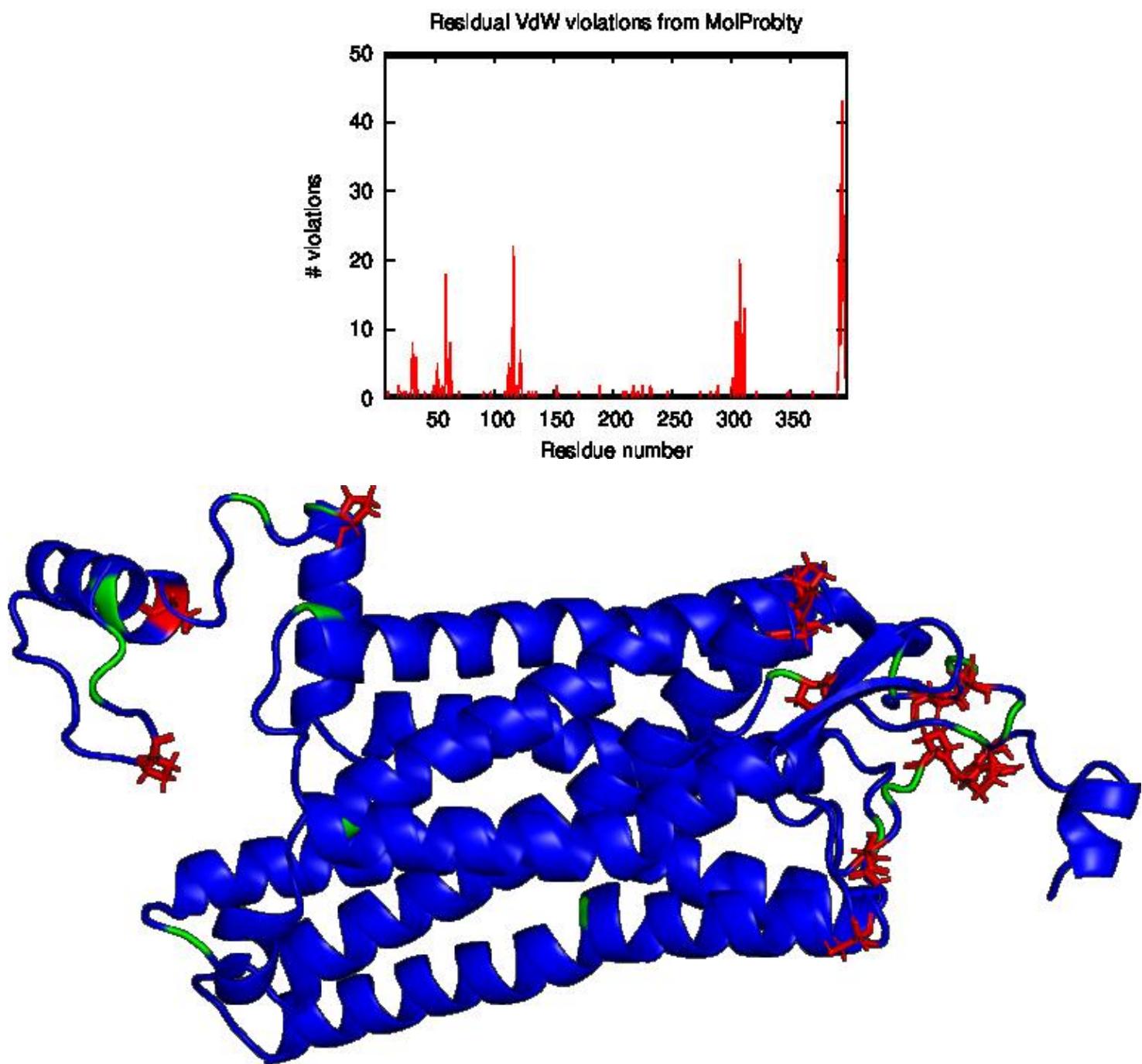
PSVS Software Environment

Verify3D score over window of 7 residues



ProsaII (-ve) score over window of 7 residues





**Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)**

**References:**

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## PSVS Software Environment

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6. Sippl MJ, "Calculation of conformation ensembles from potentials of mean force". *J Mol Biol* 1990, 213:859-883
7. Laskowski RA et al, "AQUA and PROCHECK\_NMR: programs for checking the quality of proteins structures solved by NMR". *J Biomolec NMR* 1996, 8:477-486
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14. Guntert P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA". *J. Mol. Biol* 1997, 273:283-298
15. Lovell SC et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation". *Proteins* 2003, 50:437-450
16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features". *Biopolymers* 1983, 22:2577-2637
17. Bagaria A, Jaravine, V, Huang YJ, Montelione, GT, and Guntert, P "Protein structure validation by generalized linear model root-mean-square deviation prediction". *Protein Sci* 2012) 21:229-238.

# Summary of structure quality factors

---

Analyses performed for all residues.

Total structures computed	currently unknown		
Number of structures used	1		
Structure Quality Factors - overall statistics			
	Mean score	SD	Z-score <sup>g</sup>
Procheck G-factor <sup>e</sup> (phi / psi only)	0.04	N/A	0.47
Procheck G-factor <sup>e</sup> (all dihedral angles)	0.08	N/A	0.47
Verify3D	0.05	0.0000	-6.58
ProsaII (-ve)	0.05	0.0000	-2.48
MolProbity clashscore	55.29	0.0000	-7.96
Ramachandran Plot Summary from Procheck			
Most favoured regions	88.7%		
Additionally allowed regions	9.8%		
Generously allowed regions	0.3%		
Disallowed regions	1.2%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	91.7%		
Allowed regions	4.8%		
Disallowed regions	3.5%		

---

<sup>f</sup> Residues selected based on: all residues

*Selected residue ranges: all*

<sup>g</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

Generated using PSVS 1.5

# Detailed results of Final\_model\_1 by PSSM

## Output from PDBStat

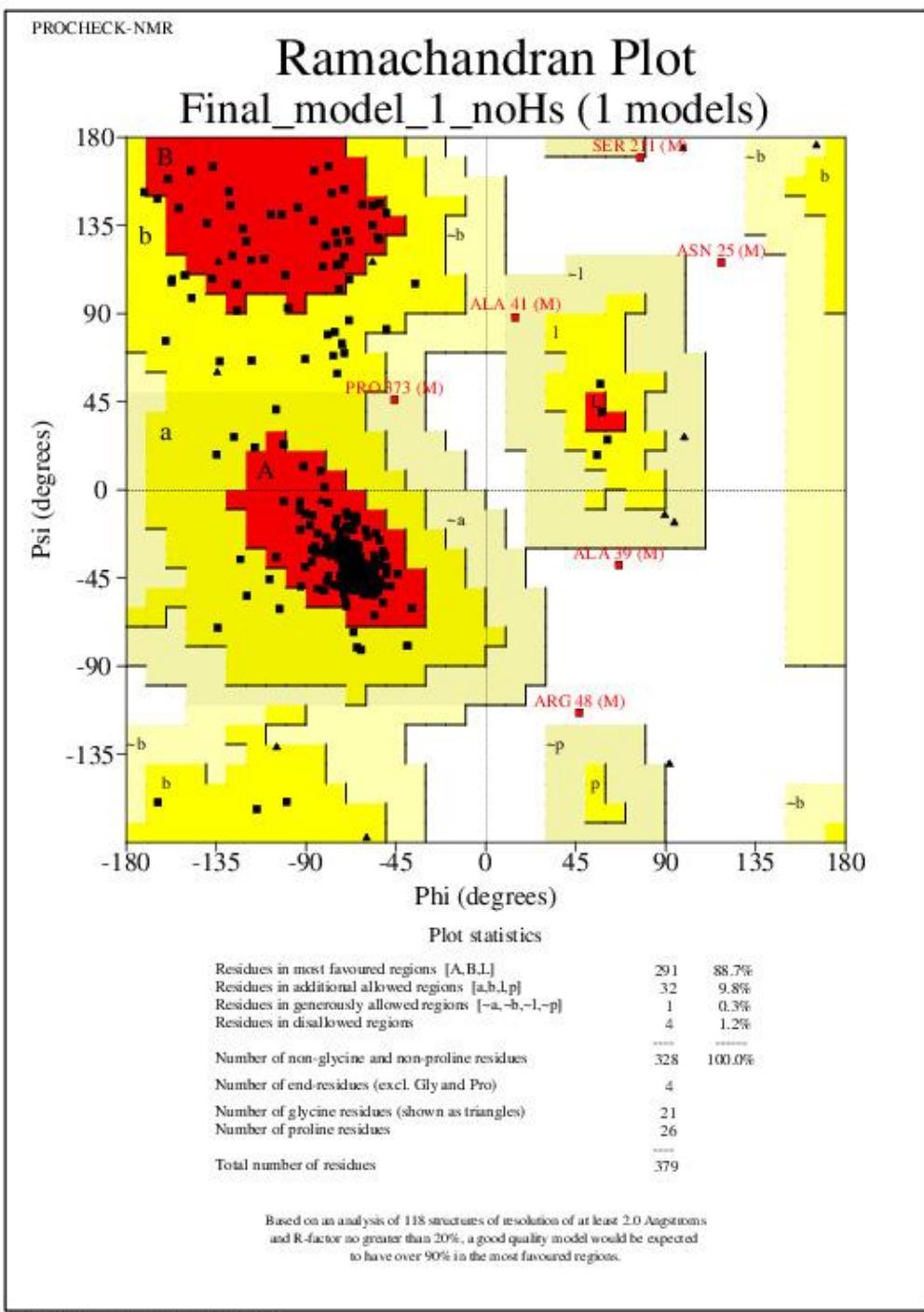
## Output from PROCHECK

### Ramachandran Plot for all models

#### Text summary of Ramachandran Plot

```
+-----<<< P   R   O   C   H   E   C   K       S   U   M   M   A   R   Y   >>>-----+
|                                         |
| Final_model_1_noHs_000.rin      0.0                         379 residues |
|                                         |
*| Ramachandran plot:    88.7% core     9.8% allow     0.3% gener     1.2% disall |
|                                         |
*| All Ramachandrans:    21 labelled residues (out of 375) |
+| Chir-chi2 plots:        5 labelled residues (out of 190) |
```

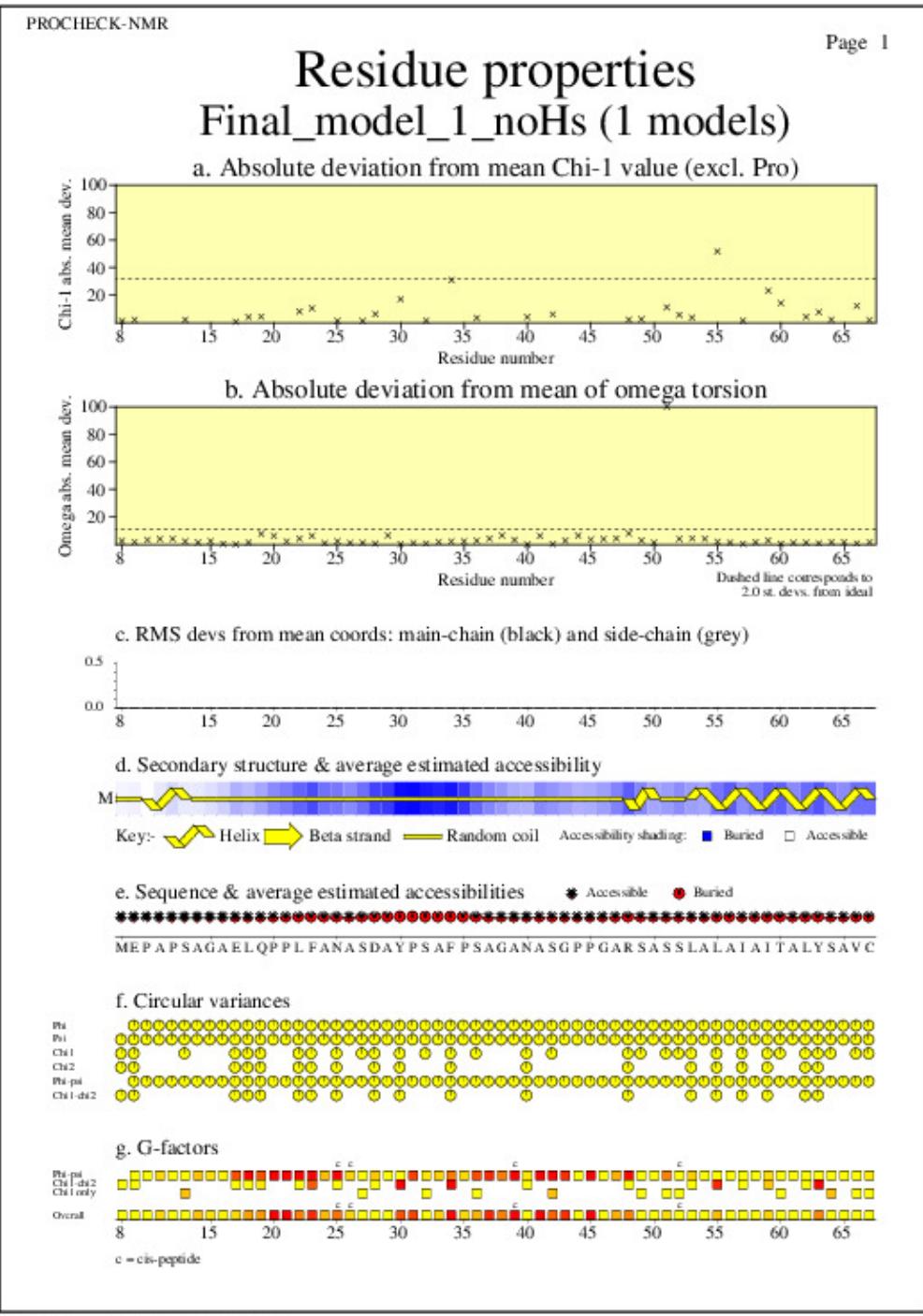
#### JPEG image for all model Ramachandran Plot



Final\_model\_1\_noHs\_01\_ramachand.ps

## Residue Properties for all models

JPEG for all model Residue Properties - page \$num\_n



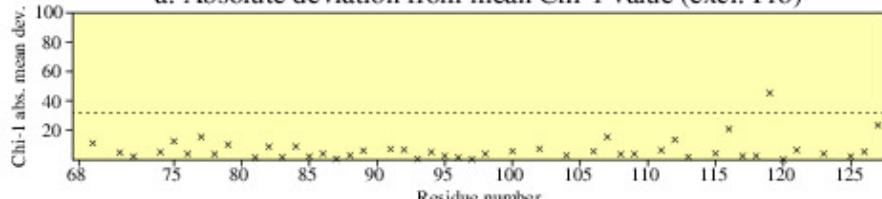
JPEG for all model Residue Properties - page \$num\_n

PROCHECK-NMR

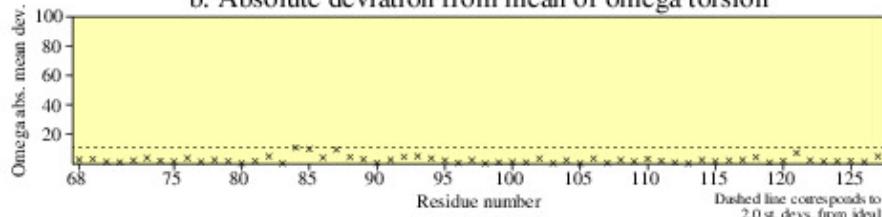
Page 2

## Residue properties Final\_model\_1\_noHs (1 models)

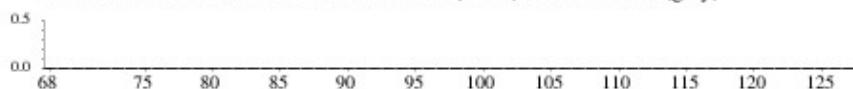
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



d. Secondary structure &amp; average estimated accessibility



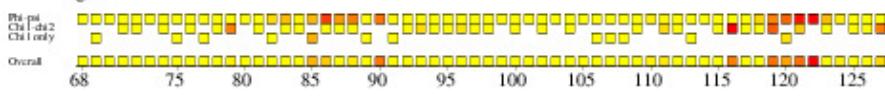
e. Sequence &amp; average estimated accessibilities



f. Circular variances



g. G-factors



Final\_model\_1\_noHs\_10\_residprop.ps

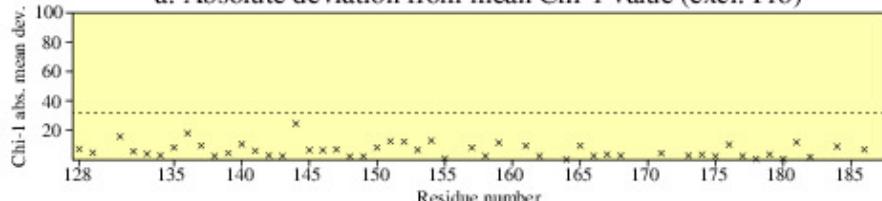
**JPEG for all model Residue Properties - page \$num\_n**

PROCHECK-NMR

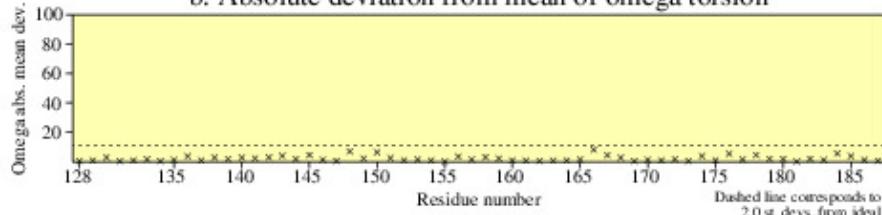
Page 3

## Residue properties Final\_model\_1\_noHs (1 models)

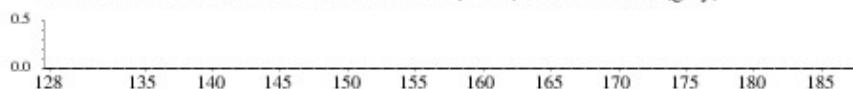
a. Absolute deviation from mean Chi-1 value (excl. Pro)



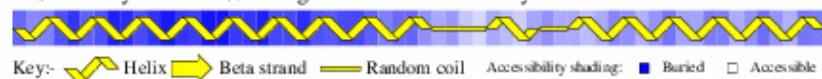
b. Absolute deviation from mean of omega torsion



c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



d. Secondary structure &amp; average estimated accessibility

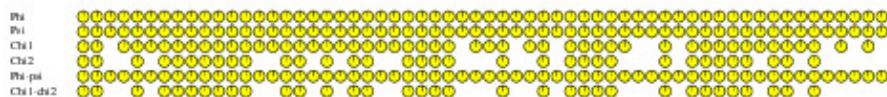


Accessibility shading: Buried Accessible

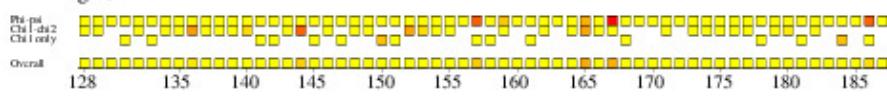
e. Sequence &amp; average estimated accessibilities



f. Circular variances



g. G-factors



Final\_model\_1\_noHs\_10\_residprop.ps

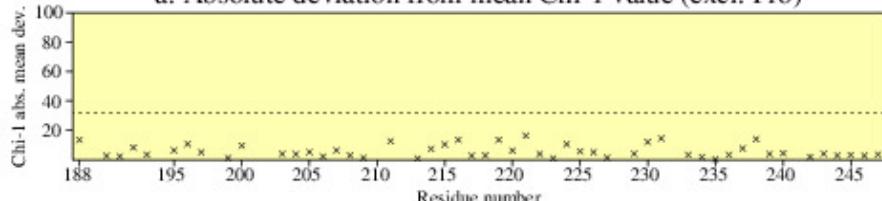
**JPEG for all model Residue Properties - page \$num\_n**

PROCHECK-NMR

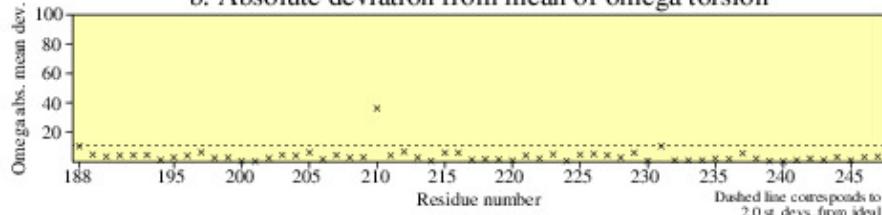
Page 4

## Residue properties Final\_model\_1\_noHs (1 models)

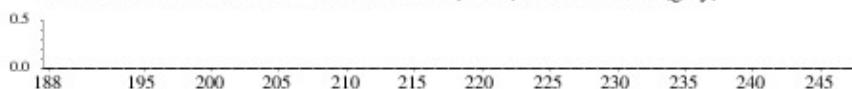
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



d. Secondary structure &amp; average estimated accessibility



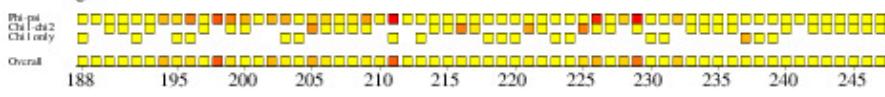
e. Sequence &amp; average estimated accessibilities



f. Circular variances



g. G-factors



Final\_model\_1\_noHs\_10\_residprop.ps

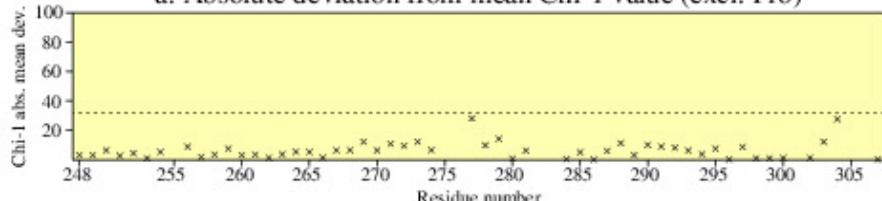
**JPEG for all model Residue Properties - page \$num\_n**

PROCHECK-NMR

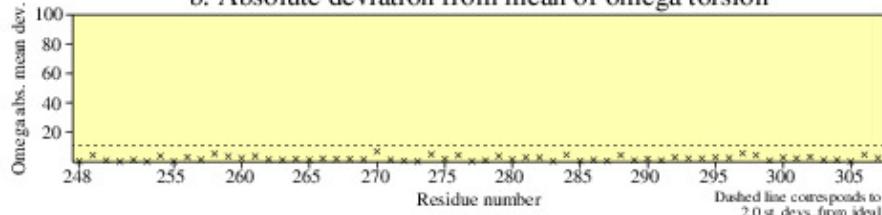
Page 5

## Residue properties Final\_model\_1\_noHs (1 models)

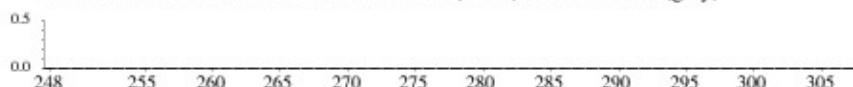
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



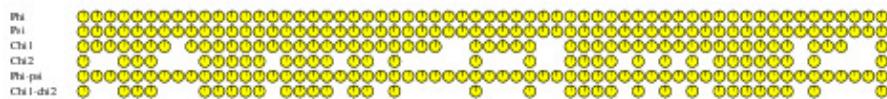
d. Secondary structure &amp; average estimated accessibility



e. Sequence &amp; average estimated accessibilities



f. Circular variances



g. G-factors

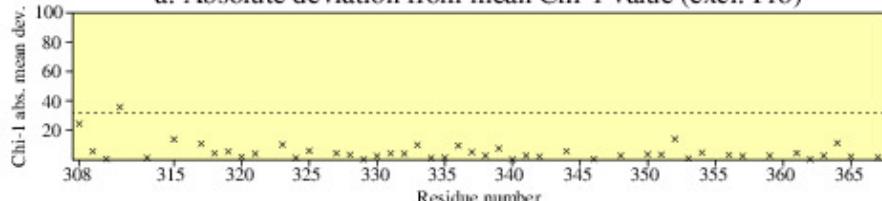


Final\_model\_1\_noHs\_10\_residprop.ps

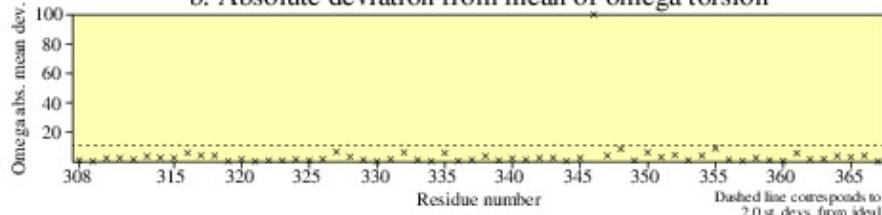
**JPEG for all model Residue Properties - page \$num\_n**

## Residue properties Final\_model\_1\_noHs (1 models)

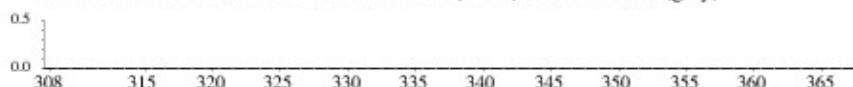
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. RMS devs from mean coords: main-chain (black) and side-chain (grey)



d. Secondary structure &amp; average estimated accessibility



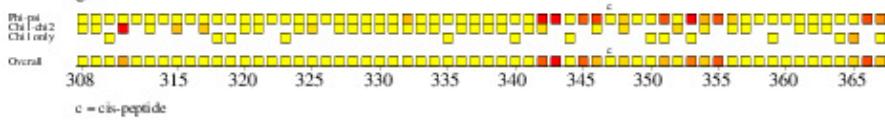
e. Sequence &amp; average estimated accessibilities



f. Circular variances

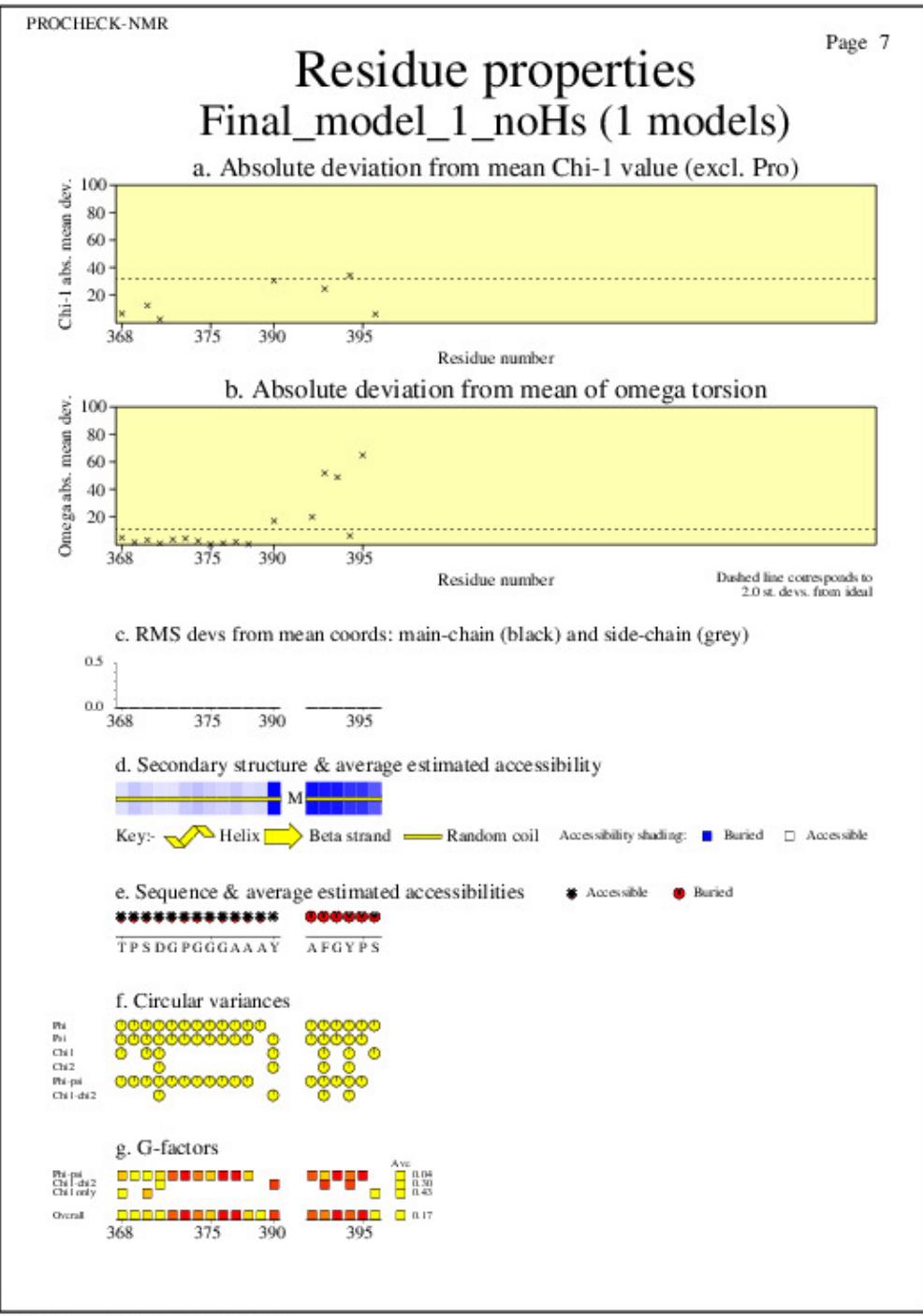


g. G-factors



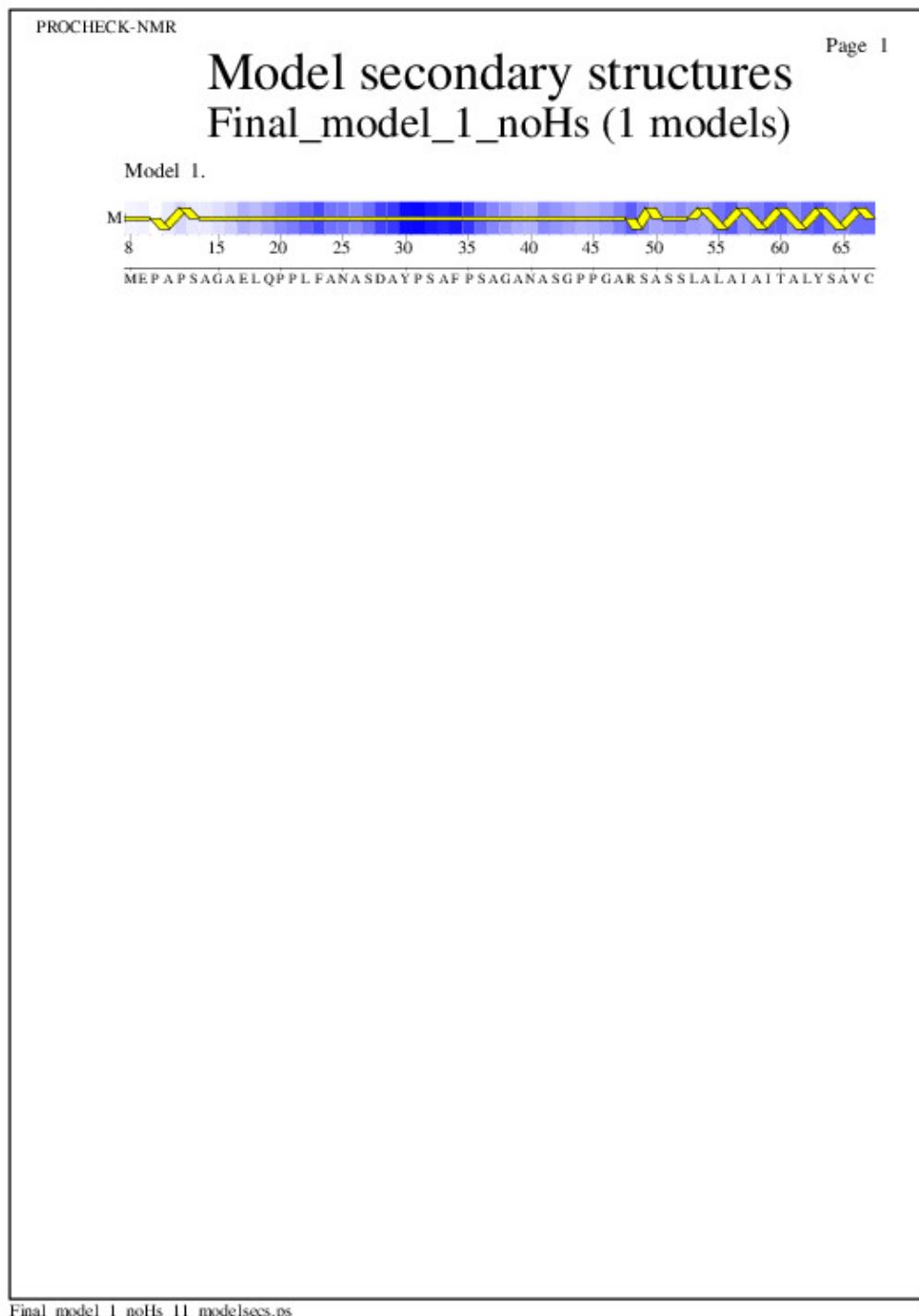
Final\_model\_1\_noHs\_10\_residprop.ps

**JPEG for all model Residue Properties - page \$num\_n**



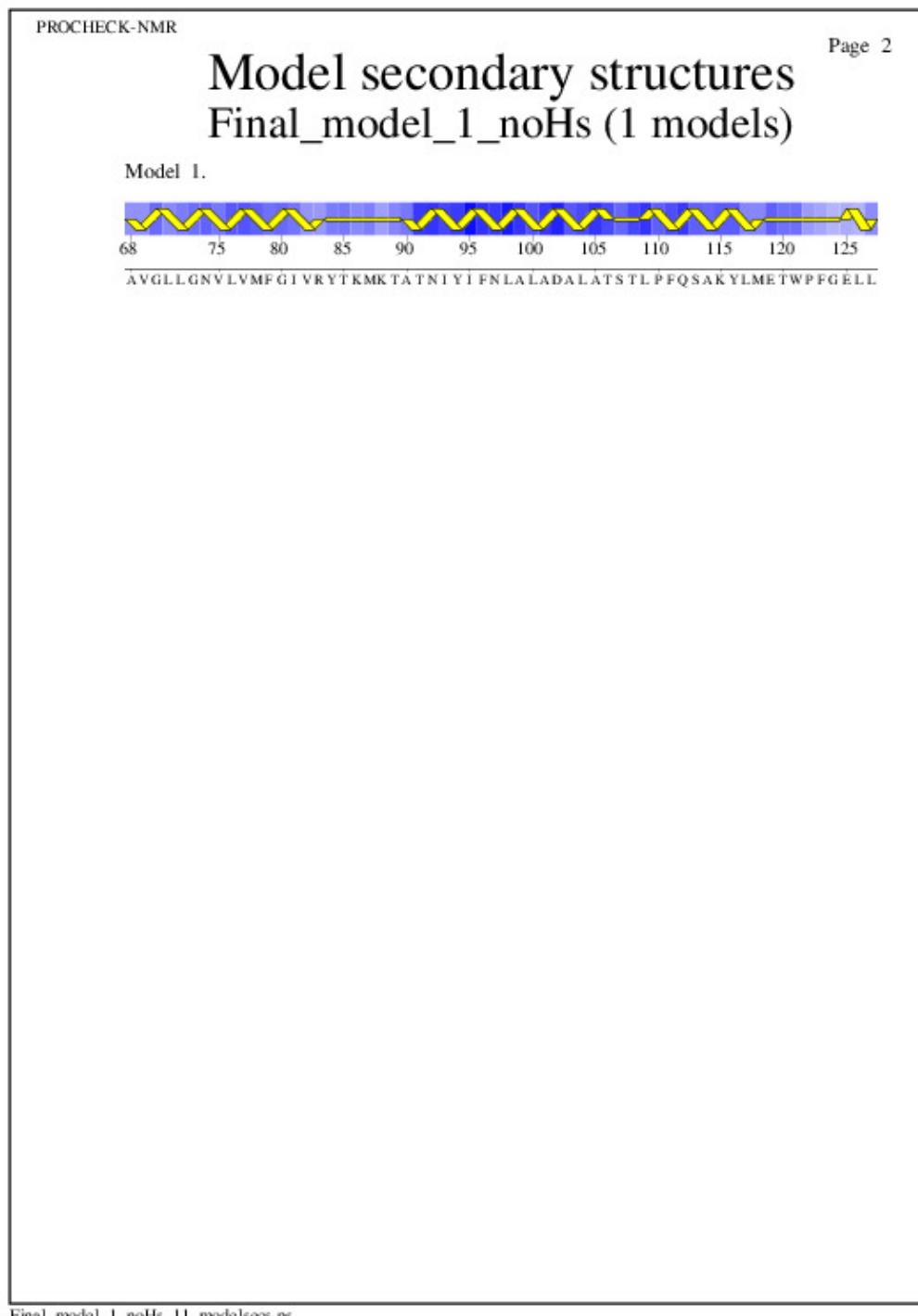
## Model Secondary Structures from Procheck

JPEG for Model Secondary Structures - page \$num\_n



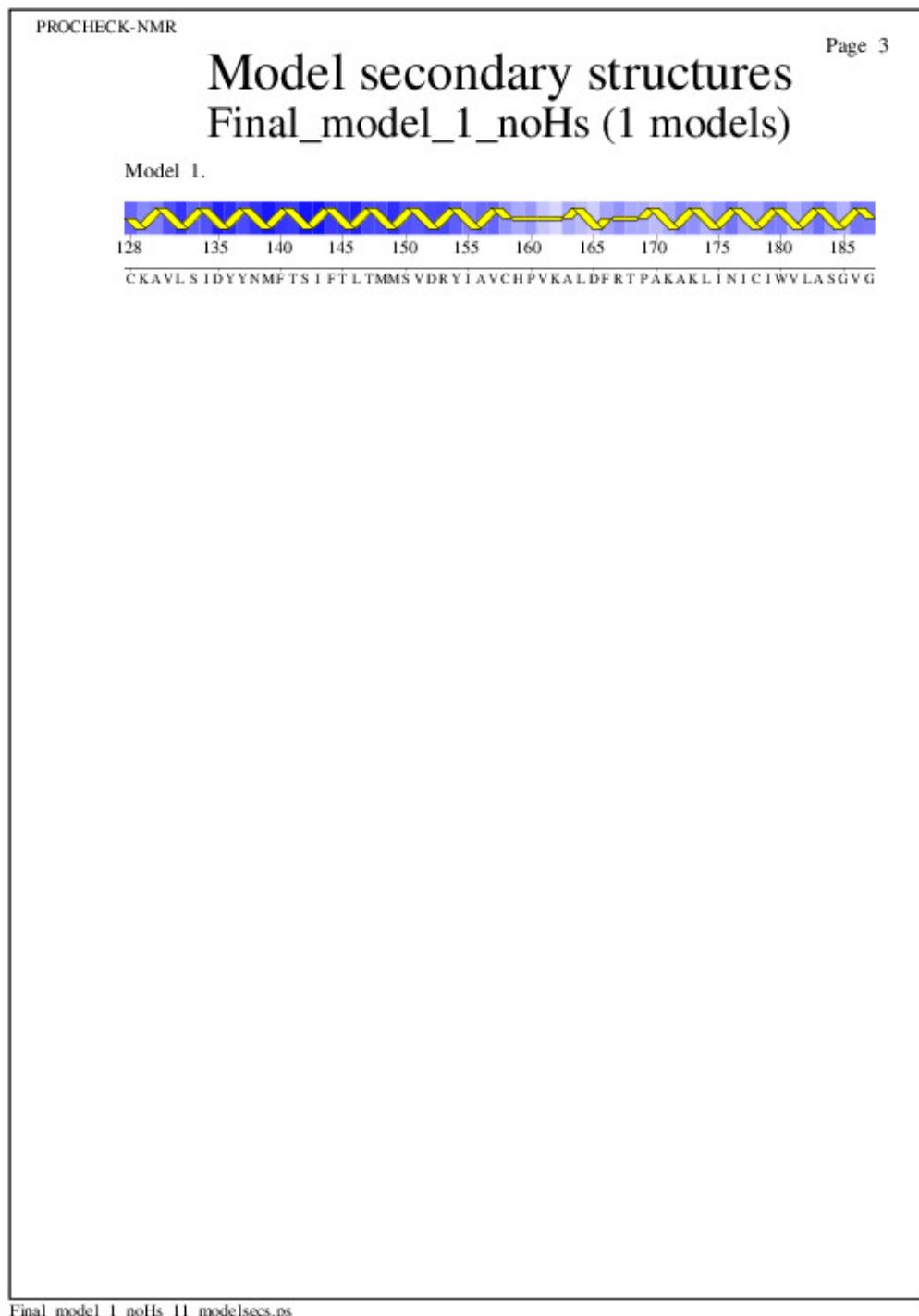
Final\_model\_1\_noHs\_11\_modsecs.ps

JPEG for Model Secondary Structures - page \$num\_n



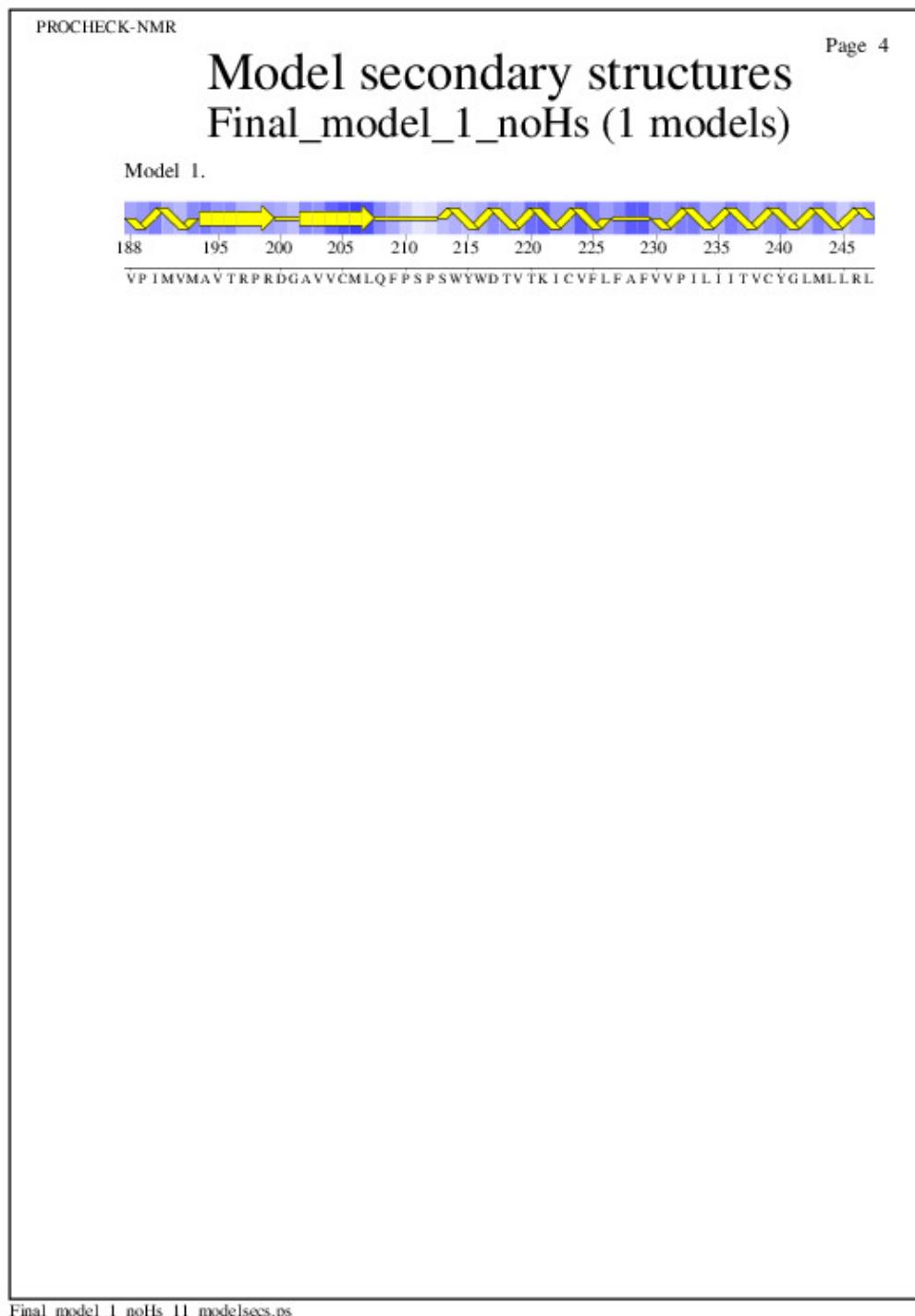
Final\_model\_1\_noHs\_11\_modsecs.ps

JPEG for Model Secondary Structures - page \$num\_n



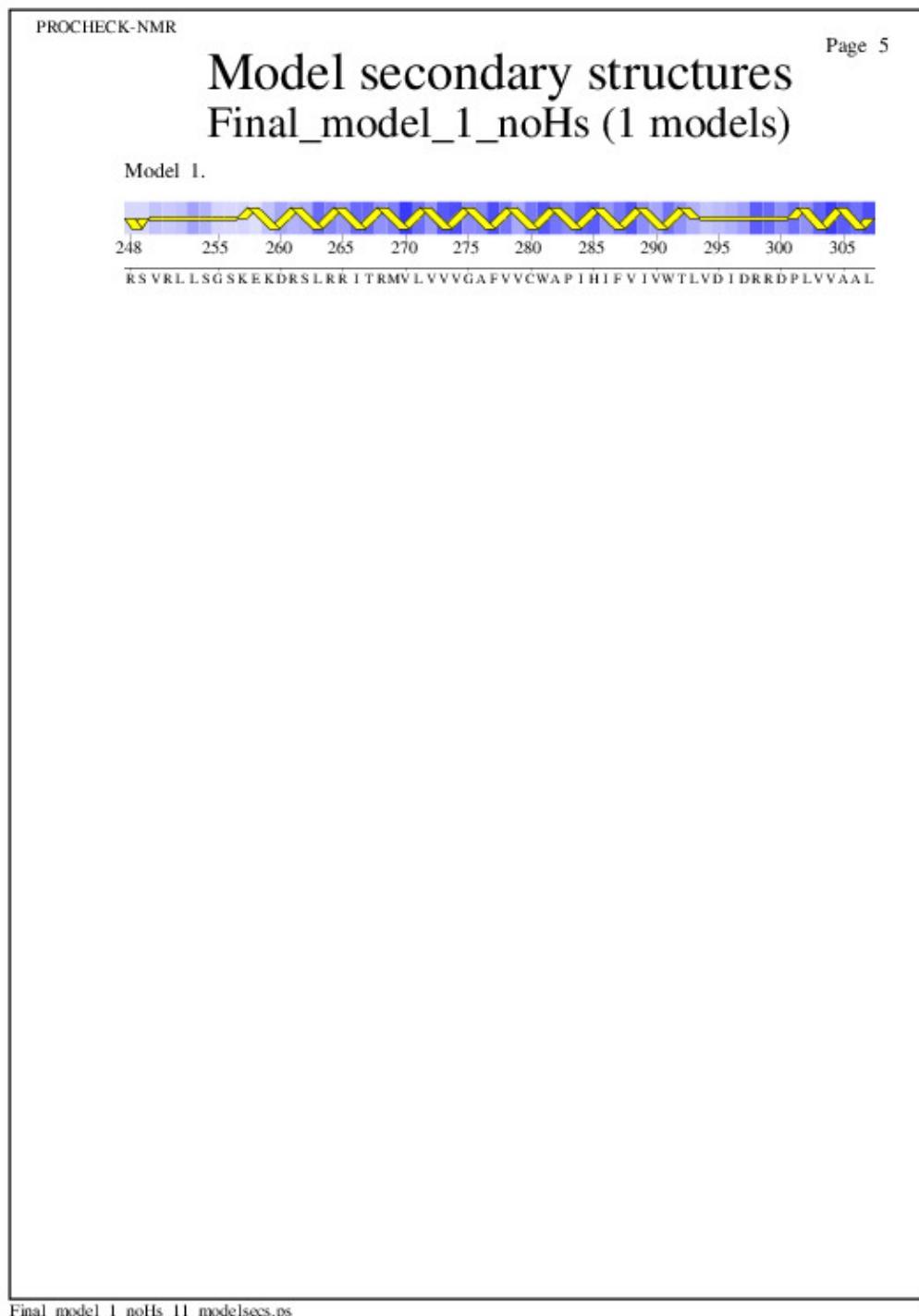
Final\_model\_1\_noHs\_11\_modsecs.ps

JPEG for Model Secondary Structures - page \$num\_n

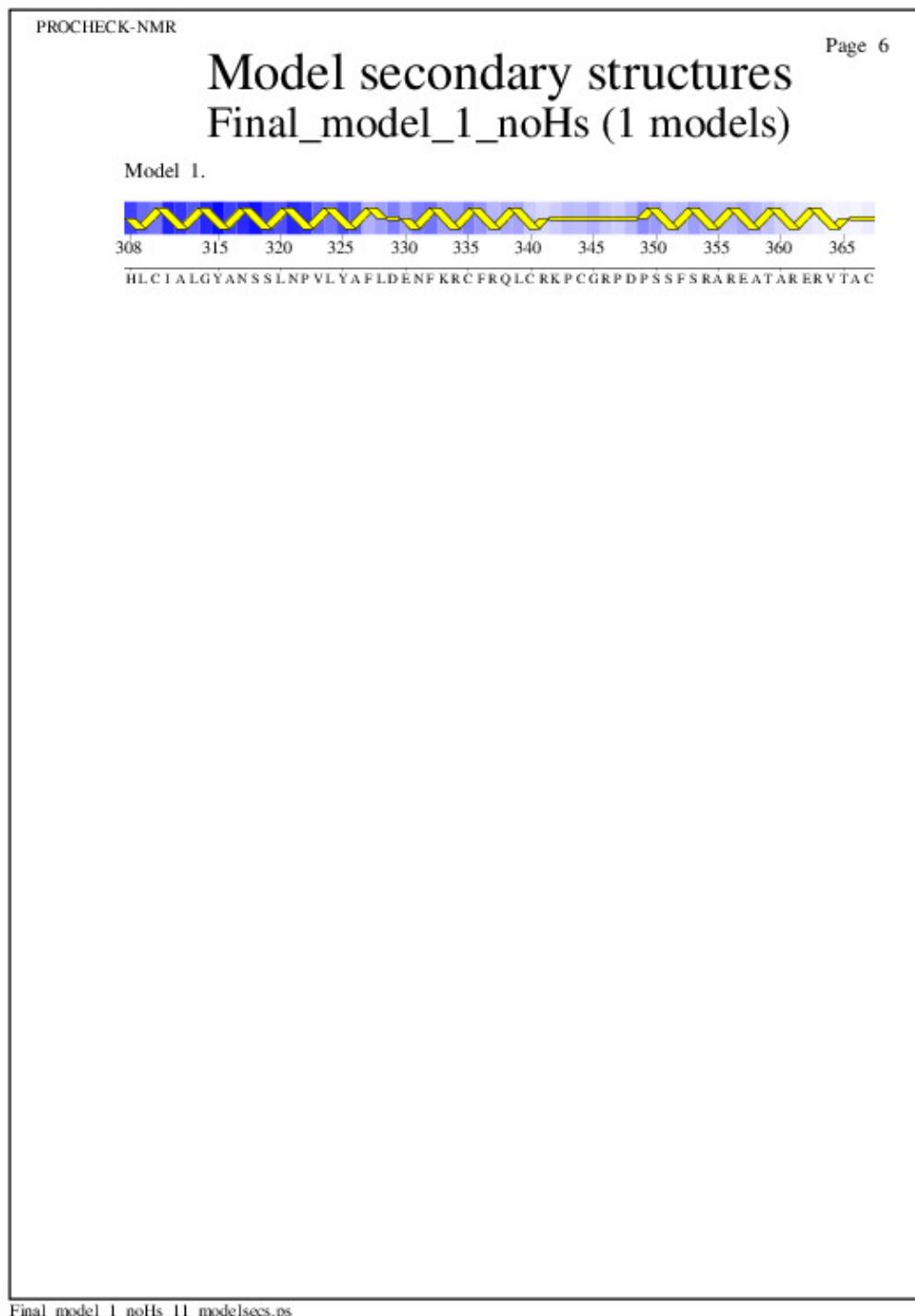


Final\_model\_1\_noHs\_11\_modsecs.ps

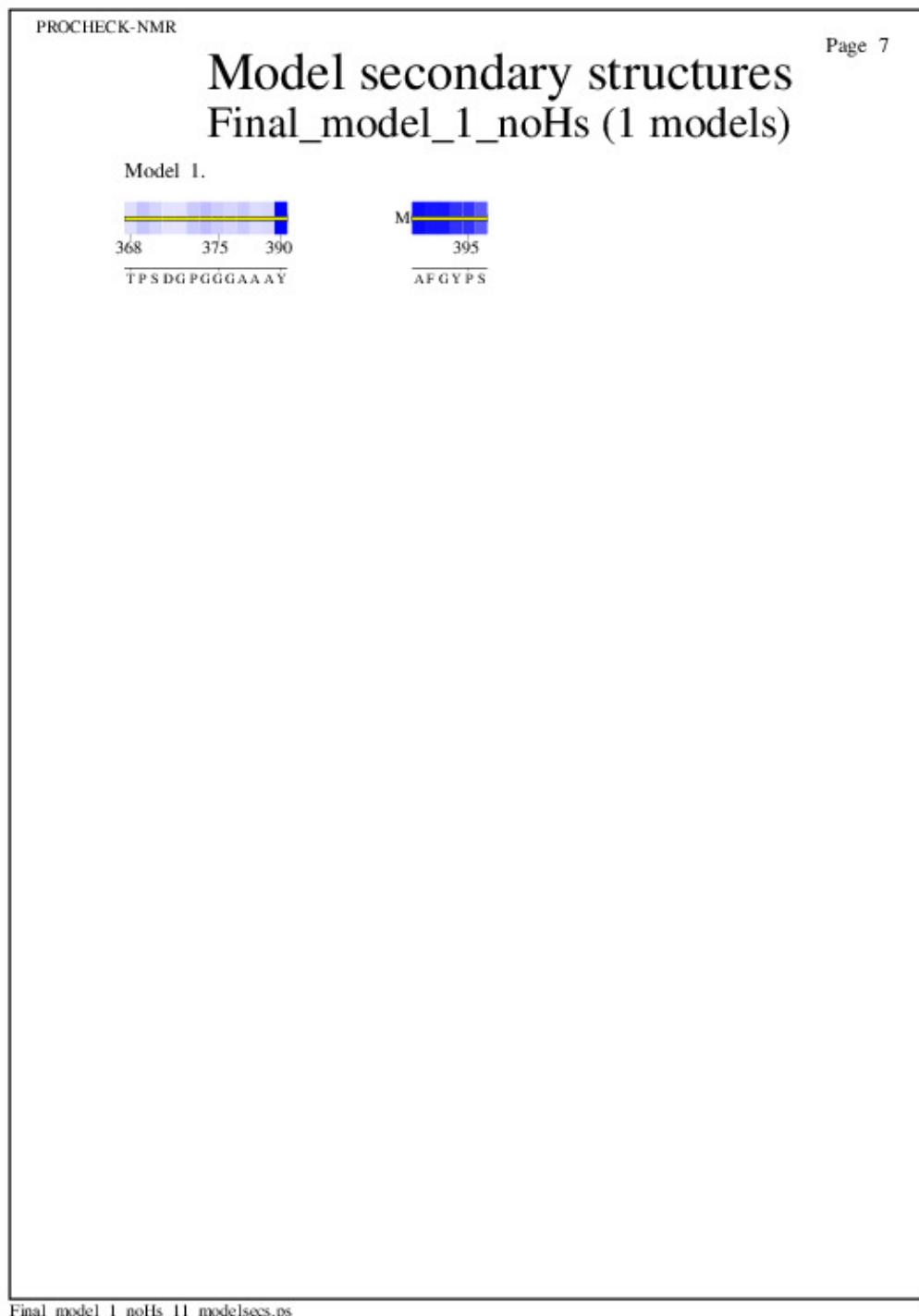
JPEG for Model Secondary Structures - page \$num\_n



JPEG for Model Secondary Structures - page \$num\_n

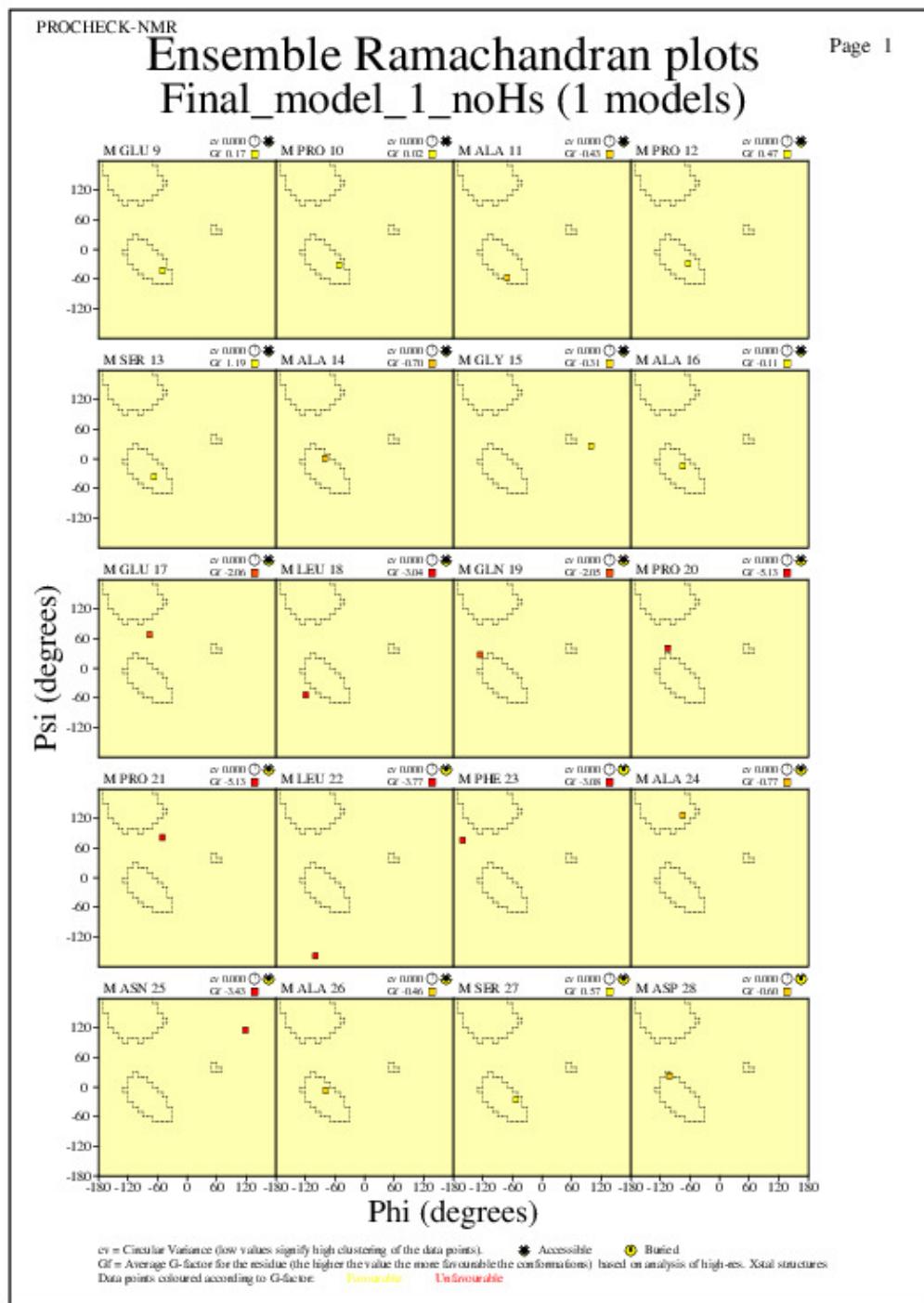


JPEG for Model Secondary Structures - page \$num\_n

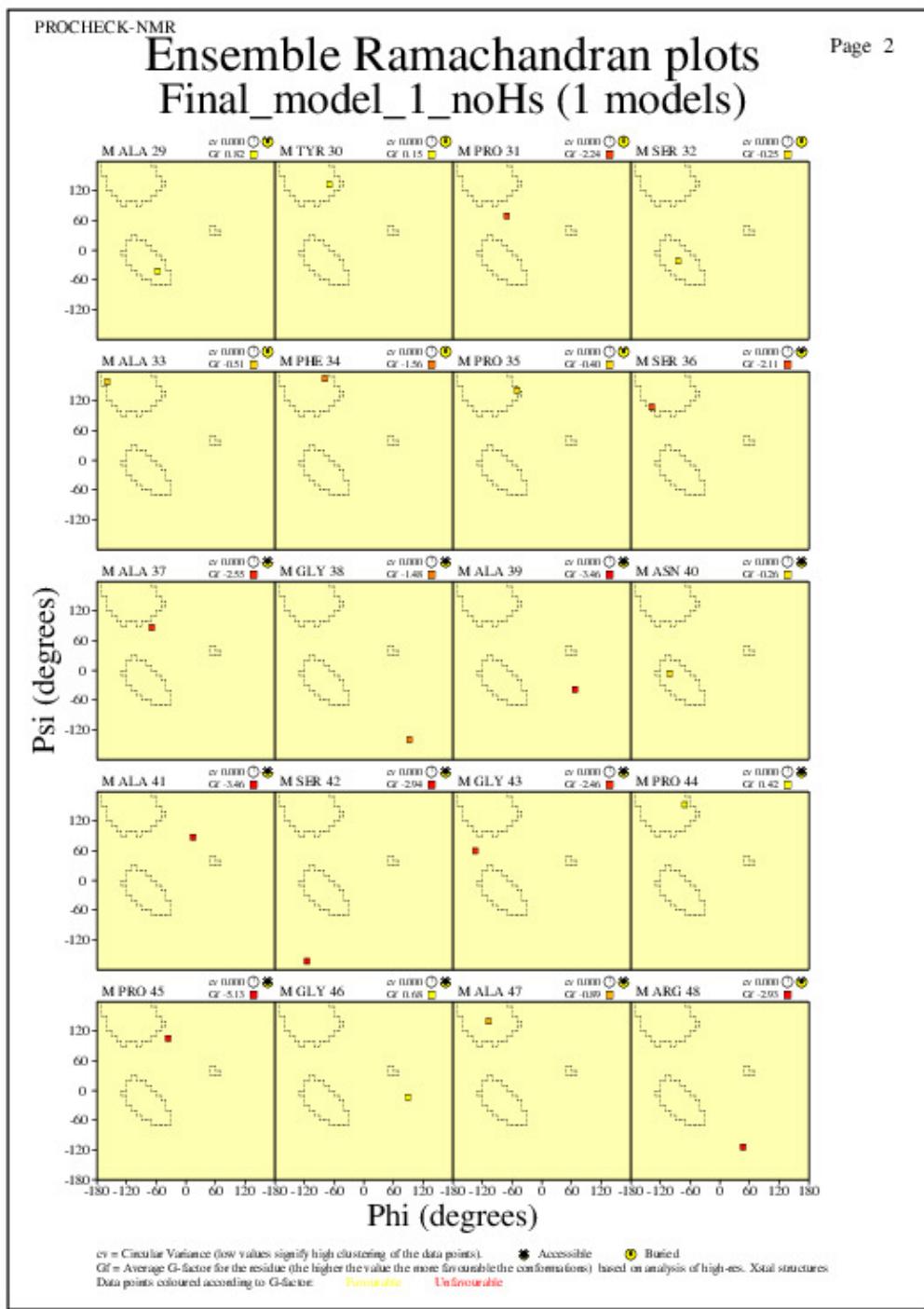


## Ramachandran Plots for each residue

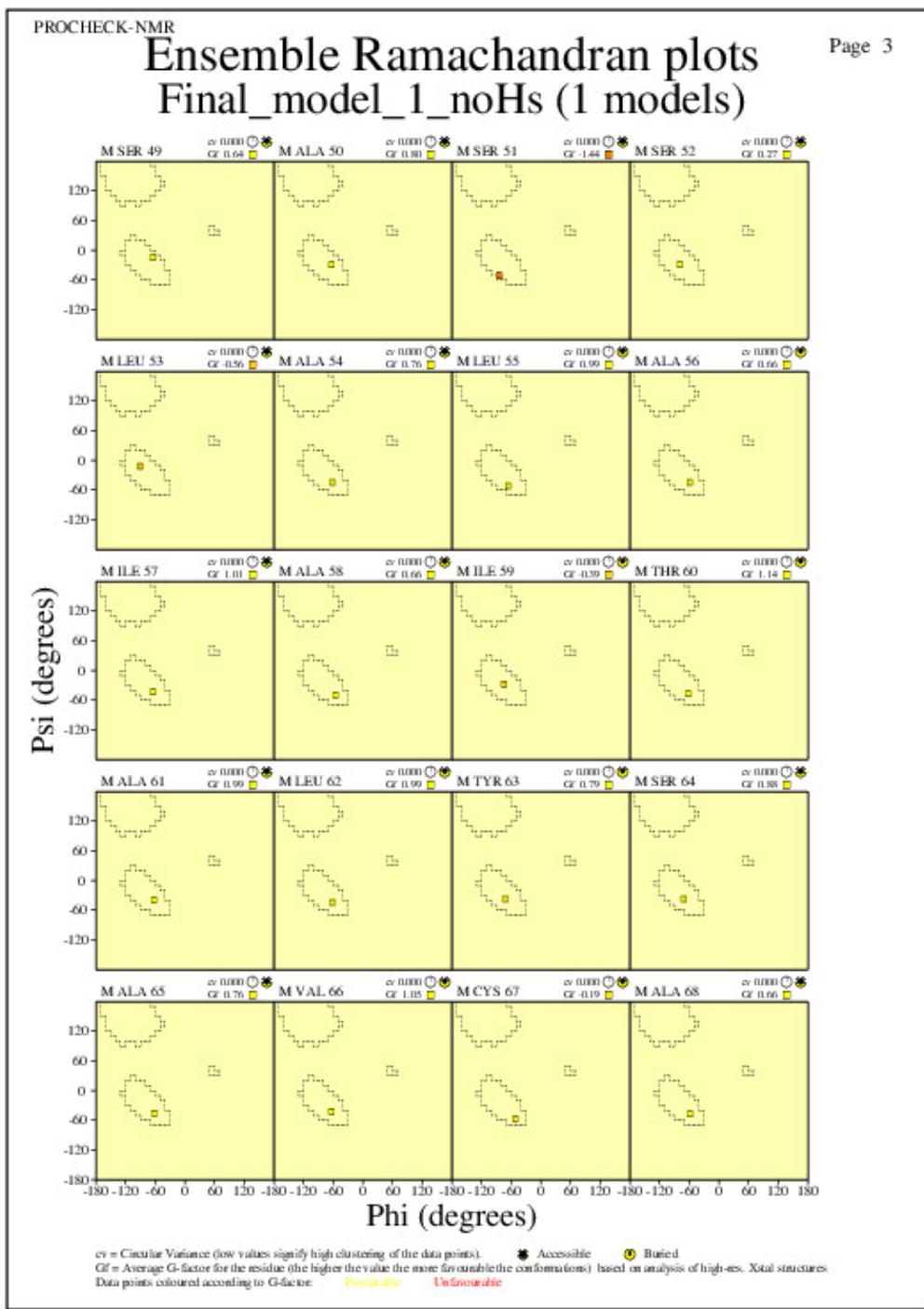
JPEG for residue Ramachandran Plots - page \$num\_n



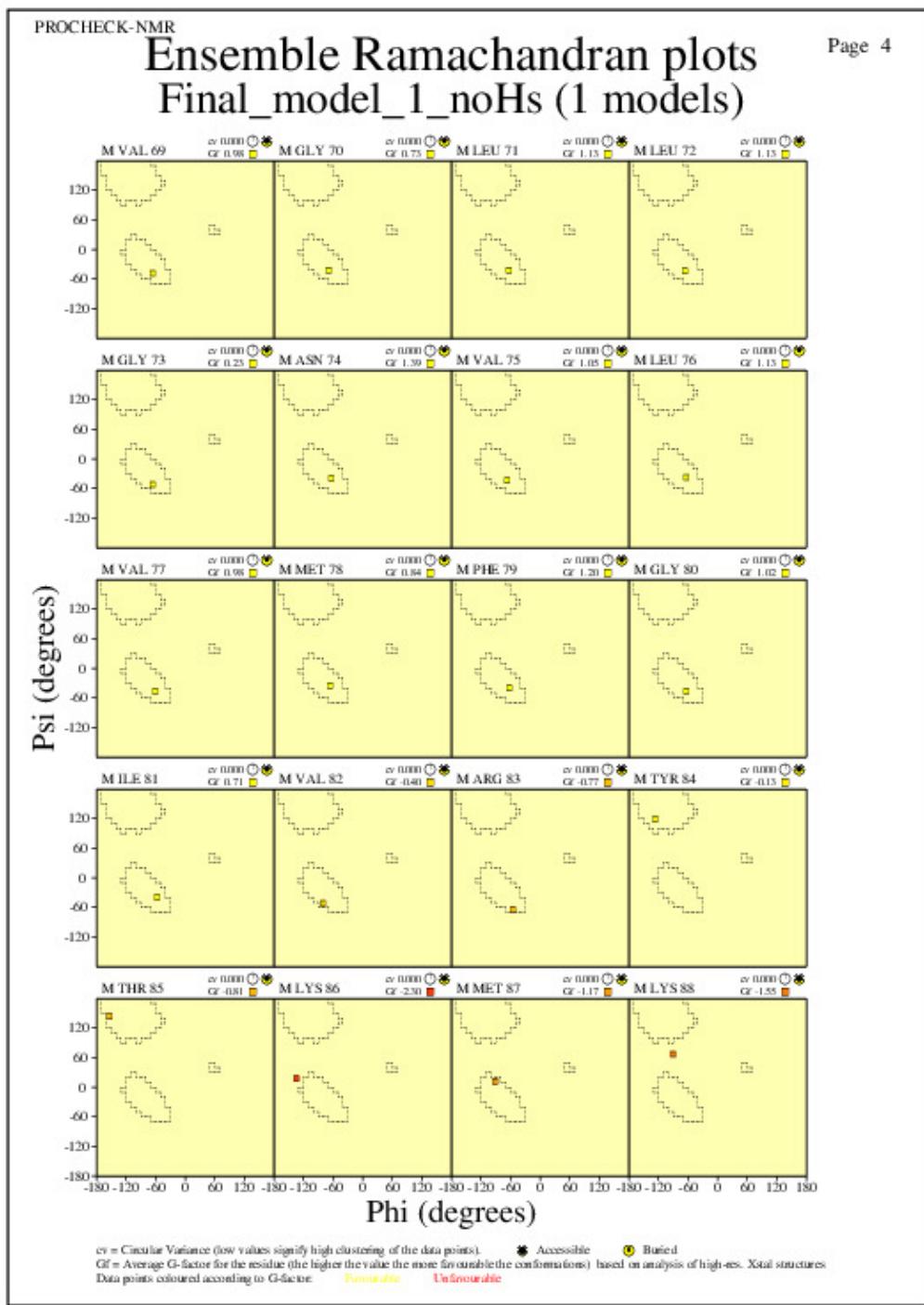
## JPEG for residue Ramachandran Plots - page \$num\_n



## JPEG for residue Ramachandran Plots - page \$num\_n

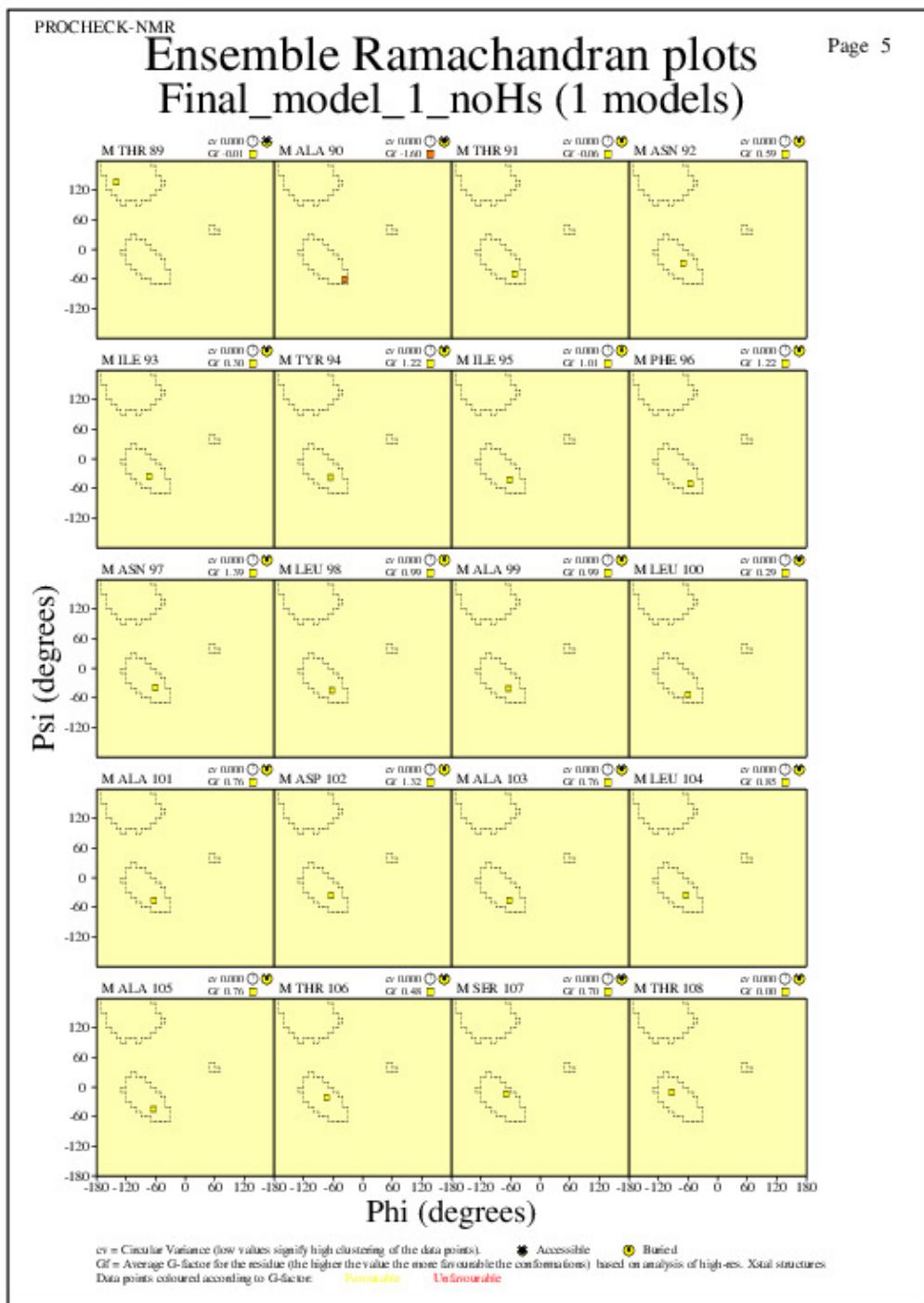


## JPEG for residue Ramachandran Plots - page \$num\_n



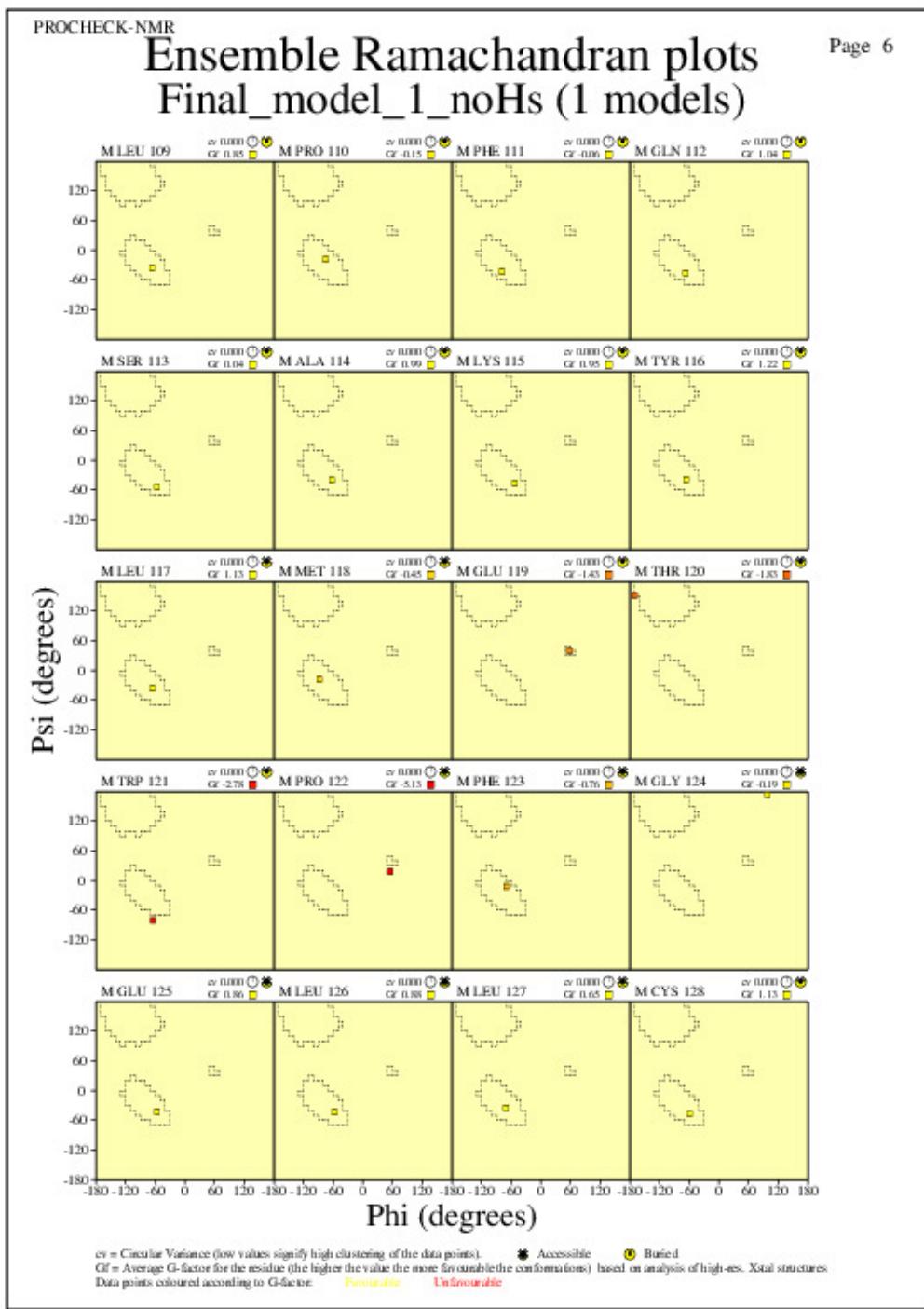
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



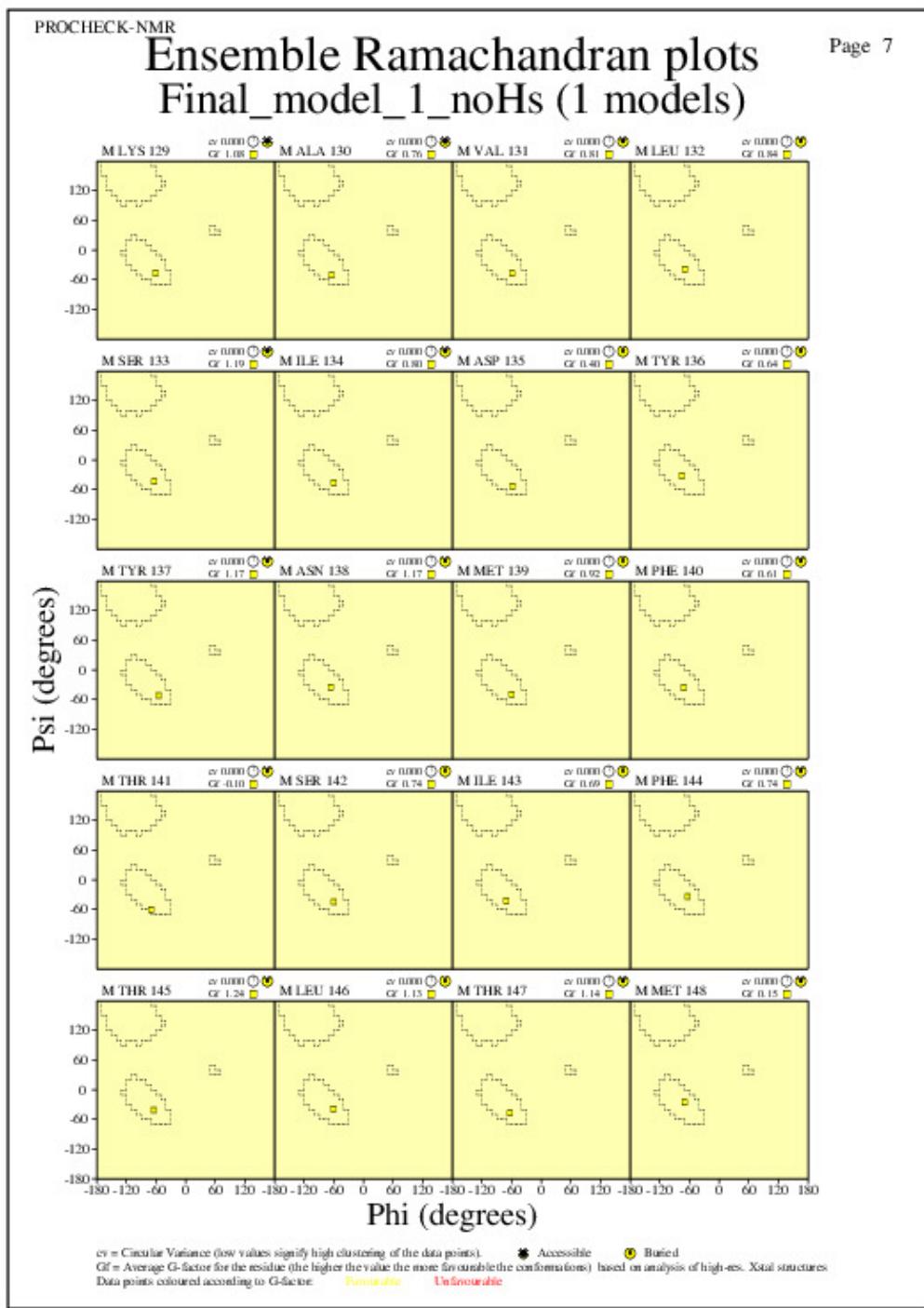
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



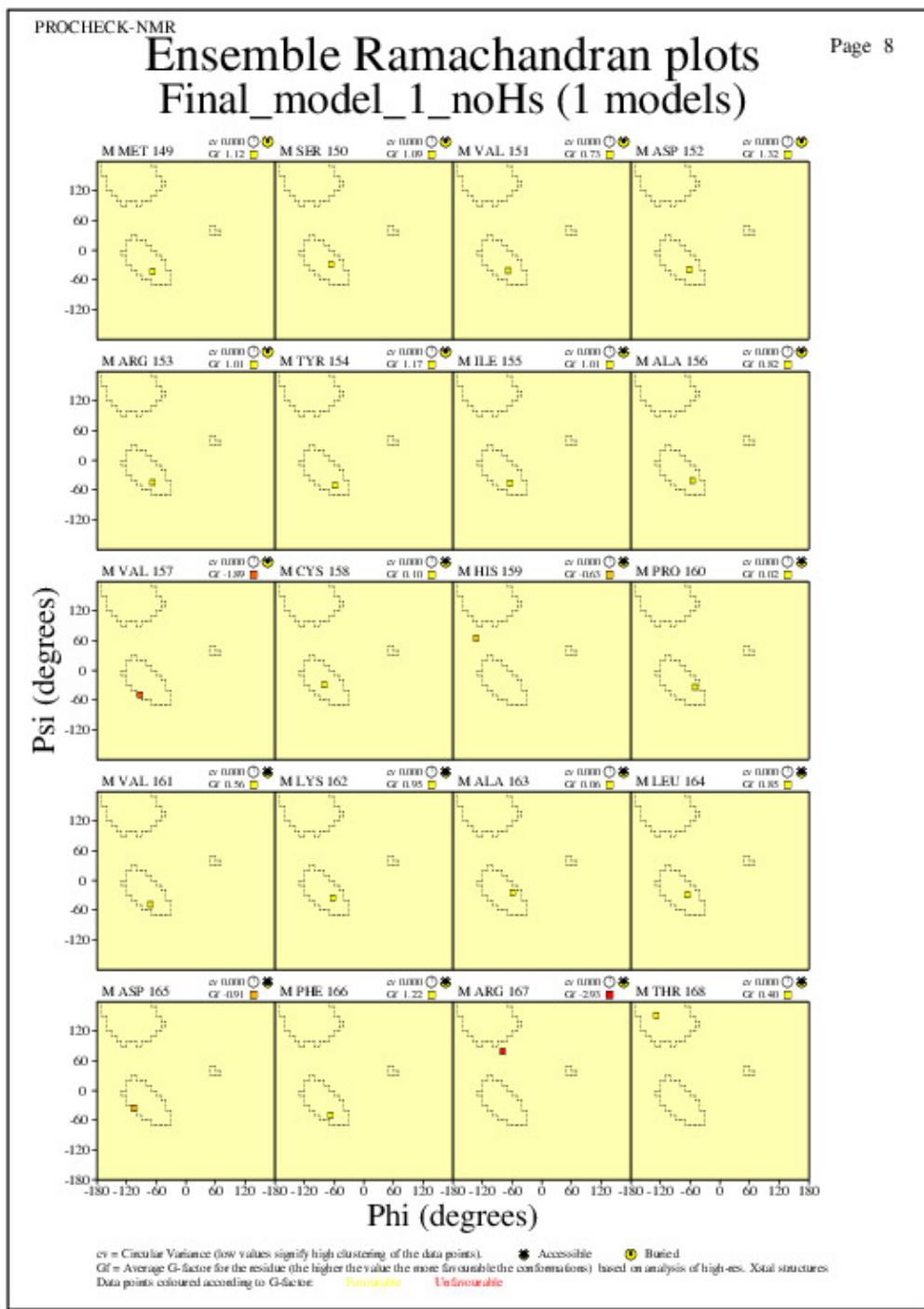
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



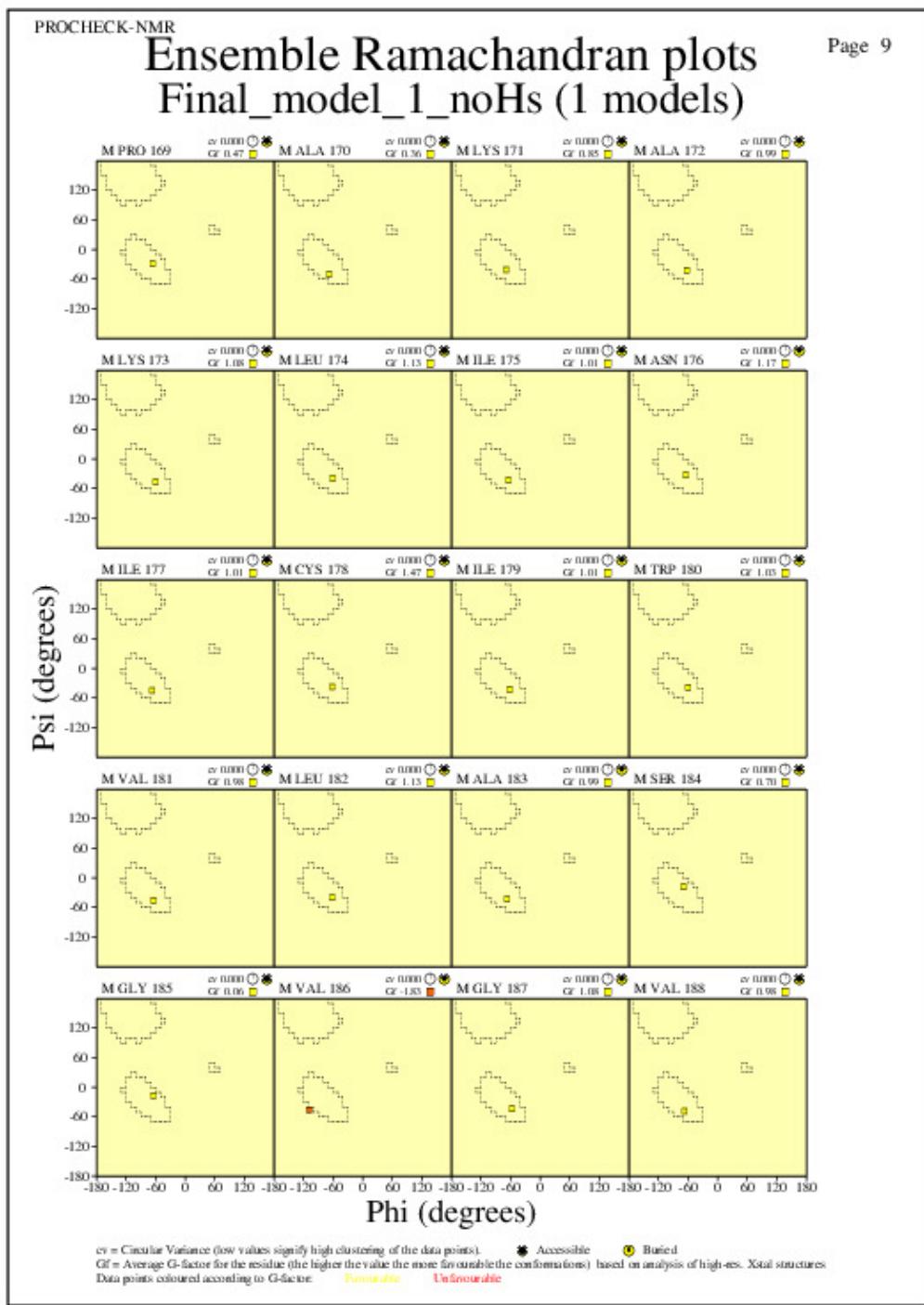
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n

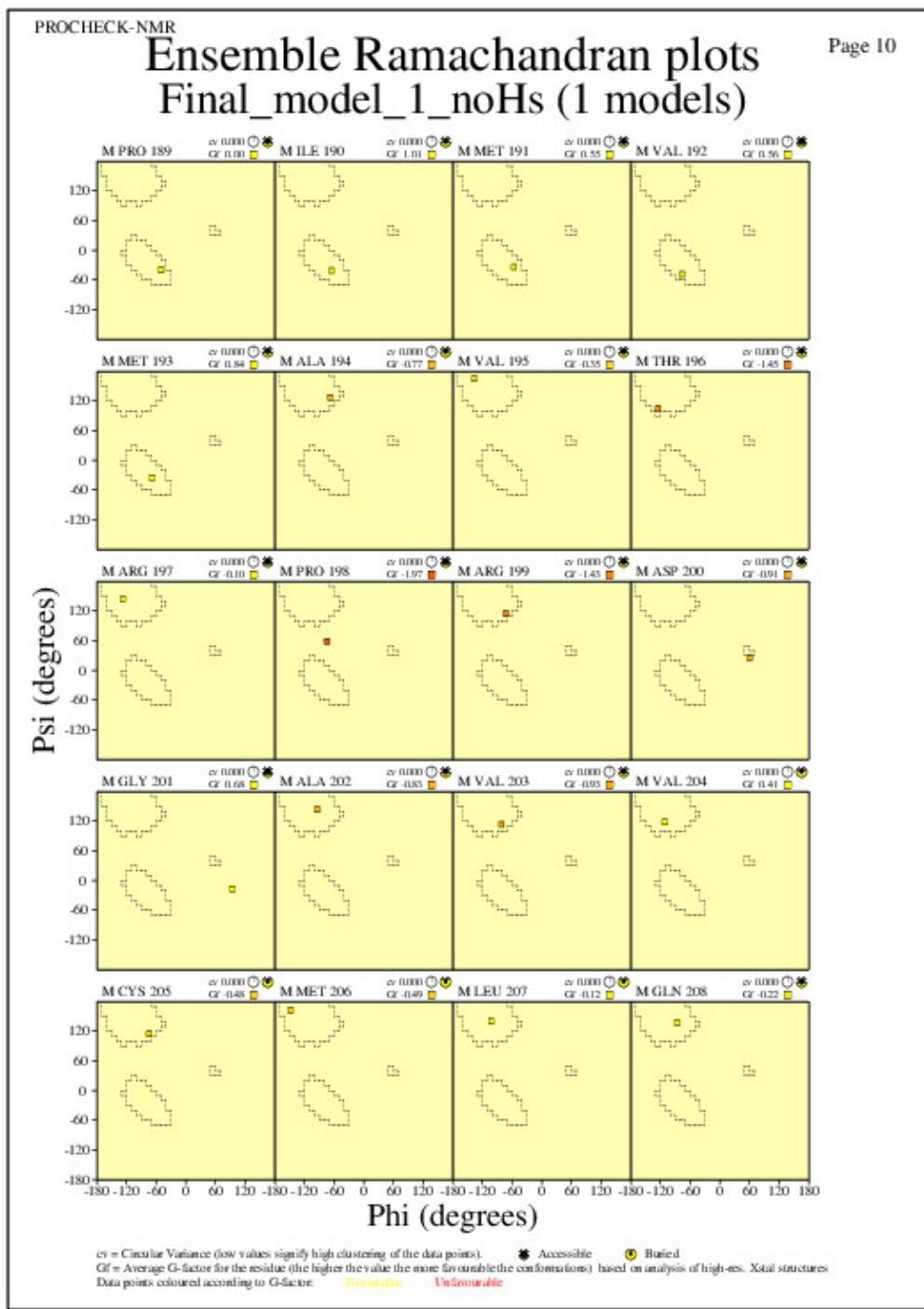


Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n

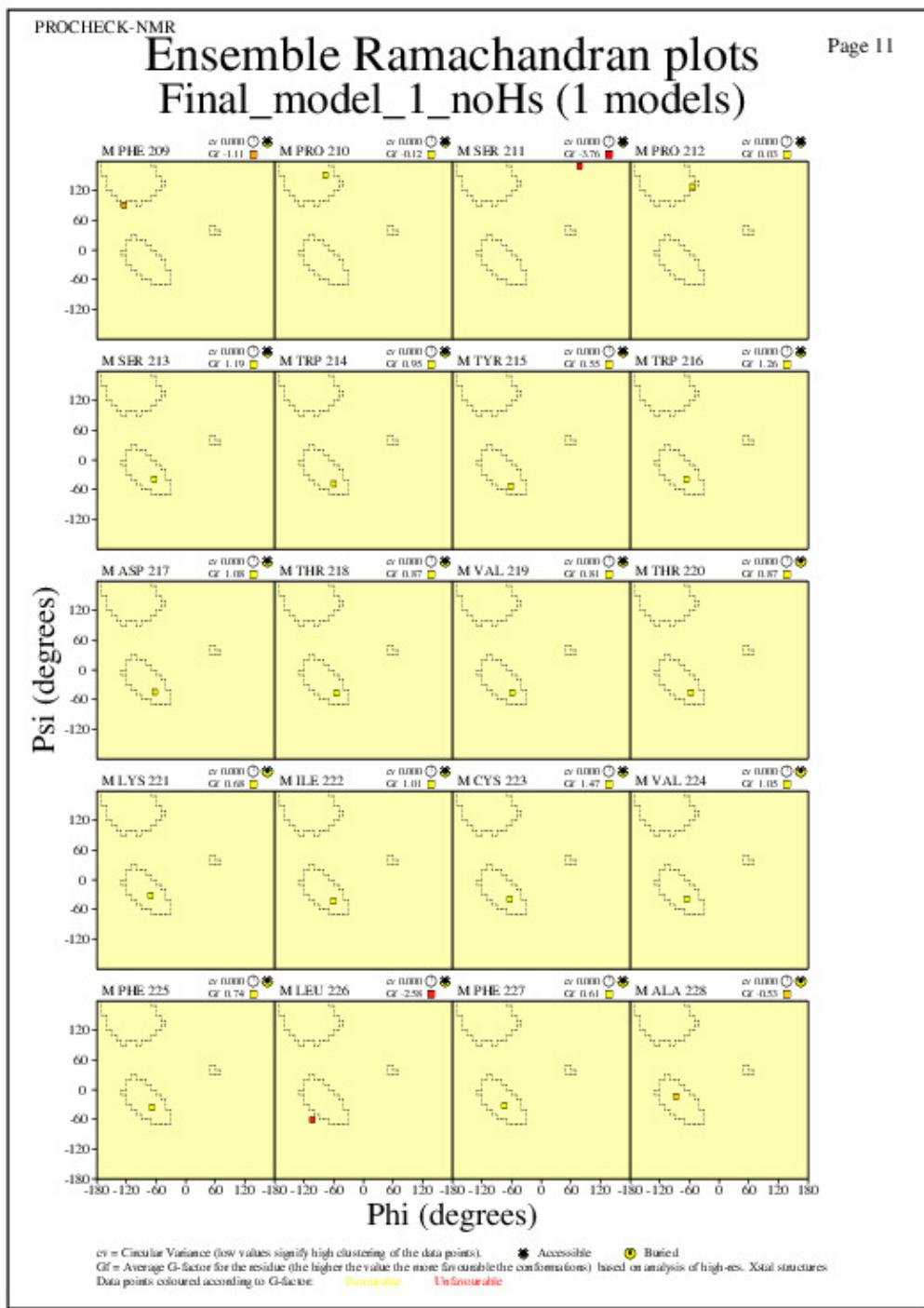


## JPEG for residue Ramachandran Plots - page \$num\_n



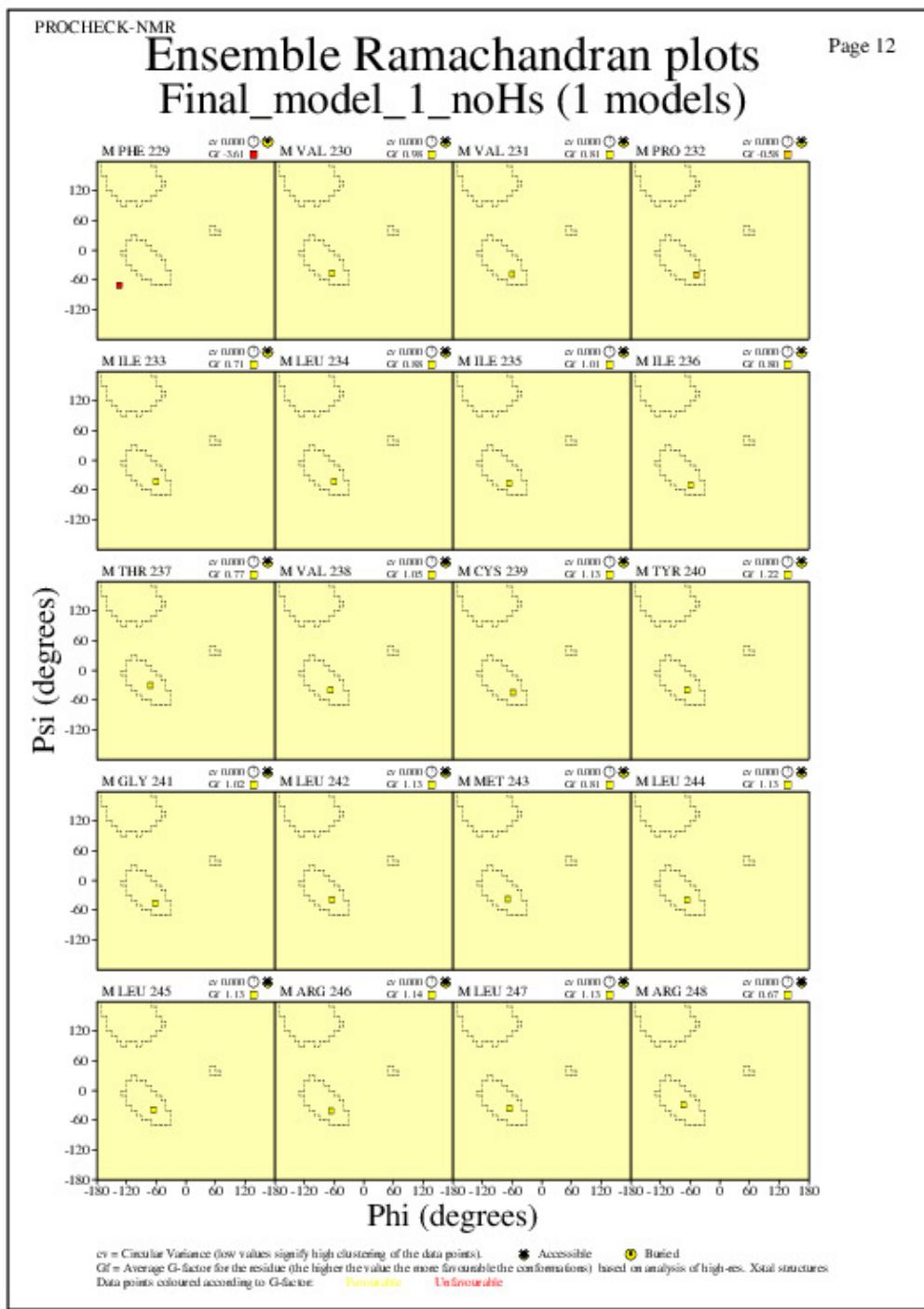
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



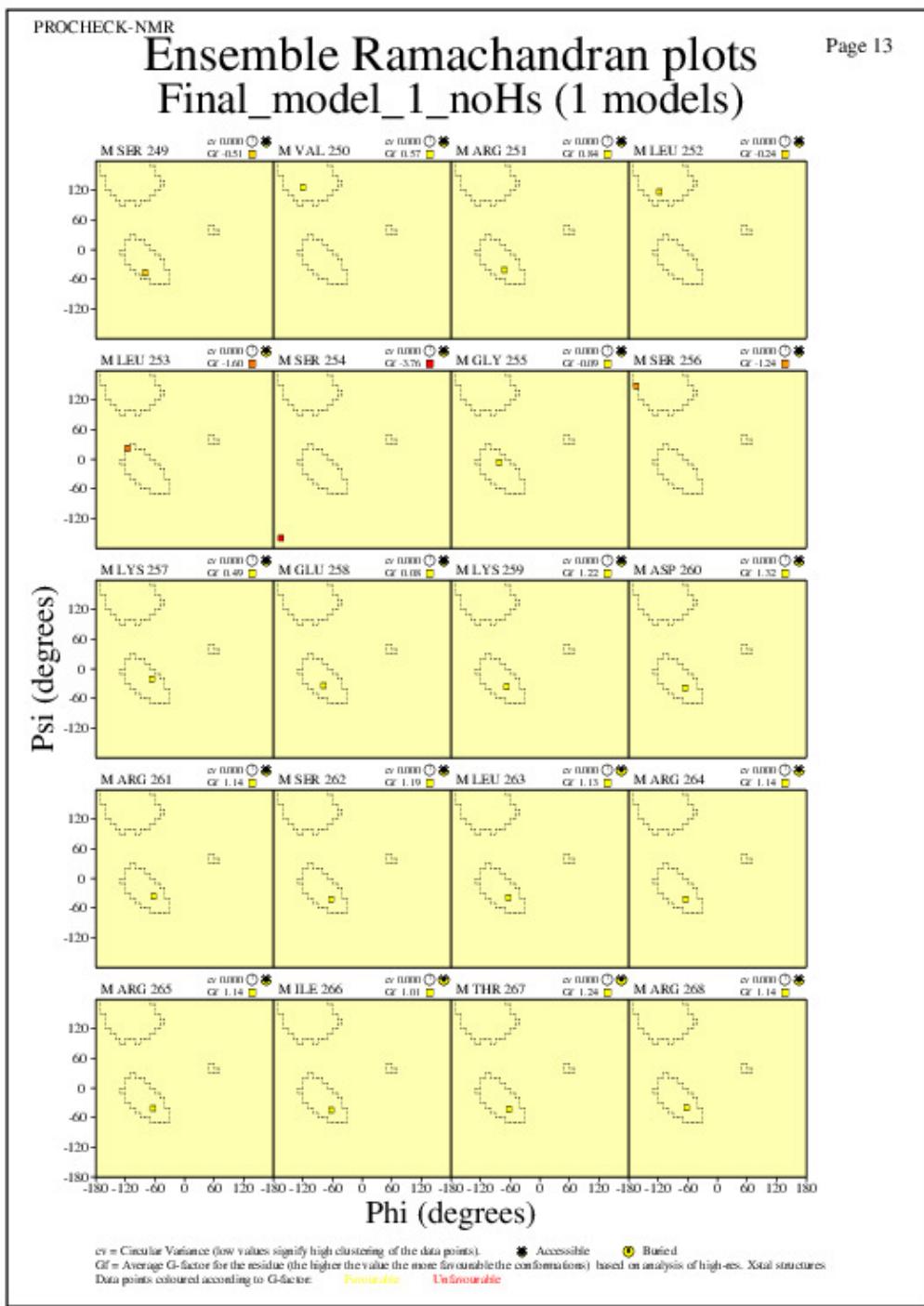
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



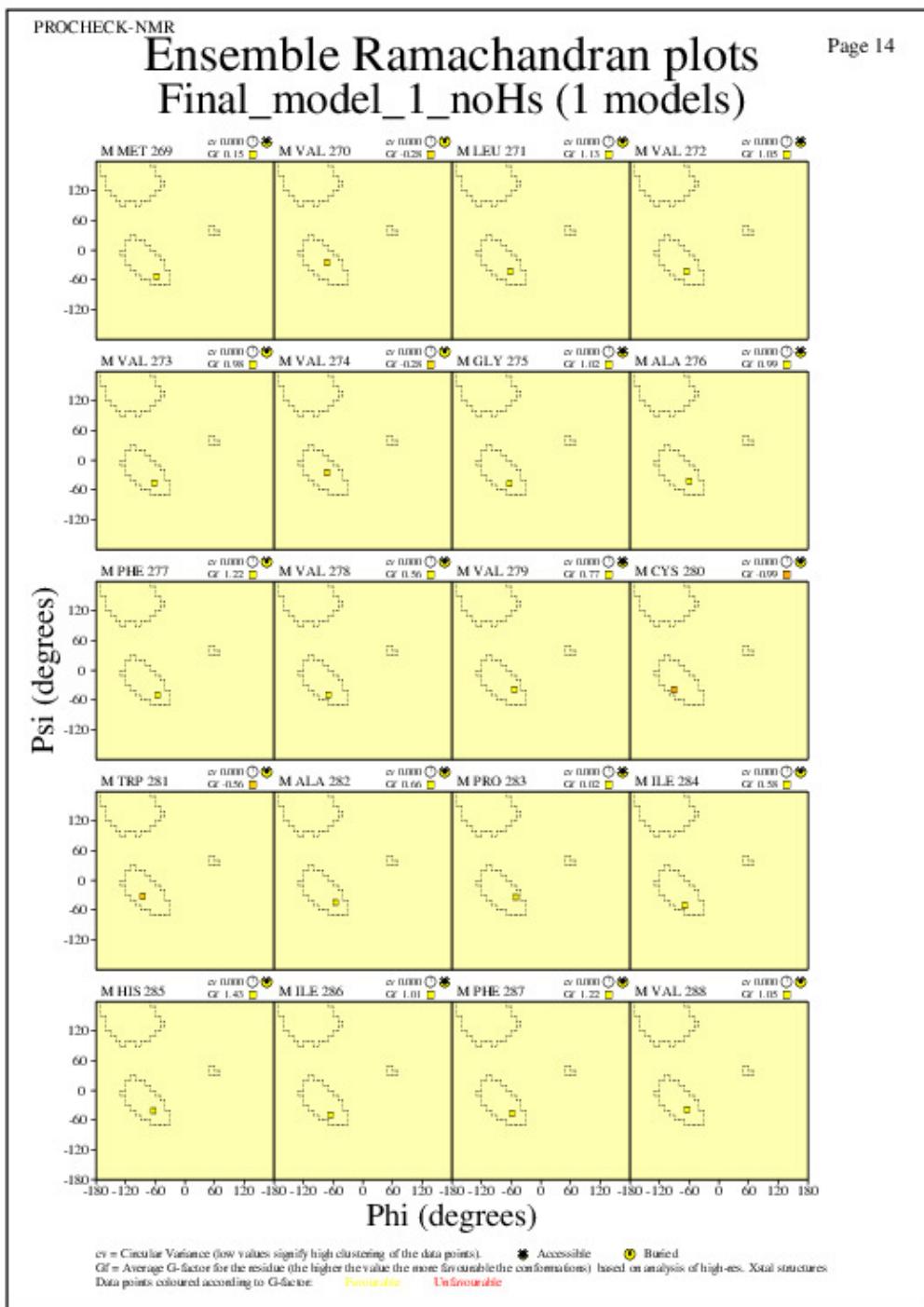
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n

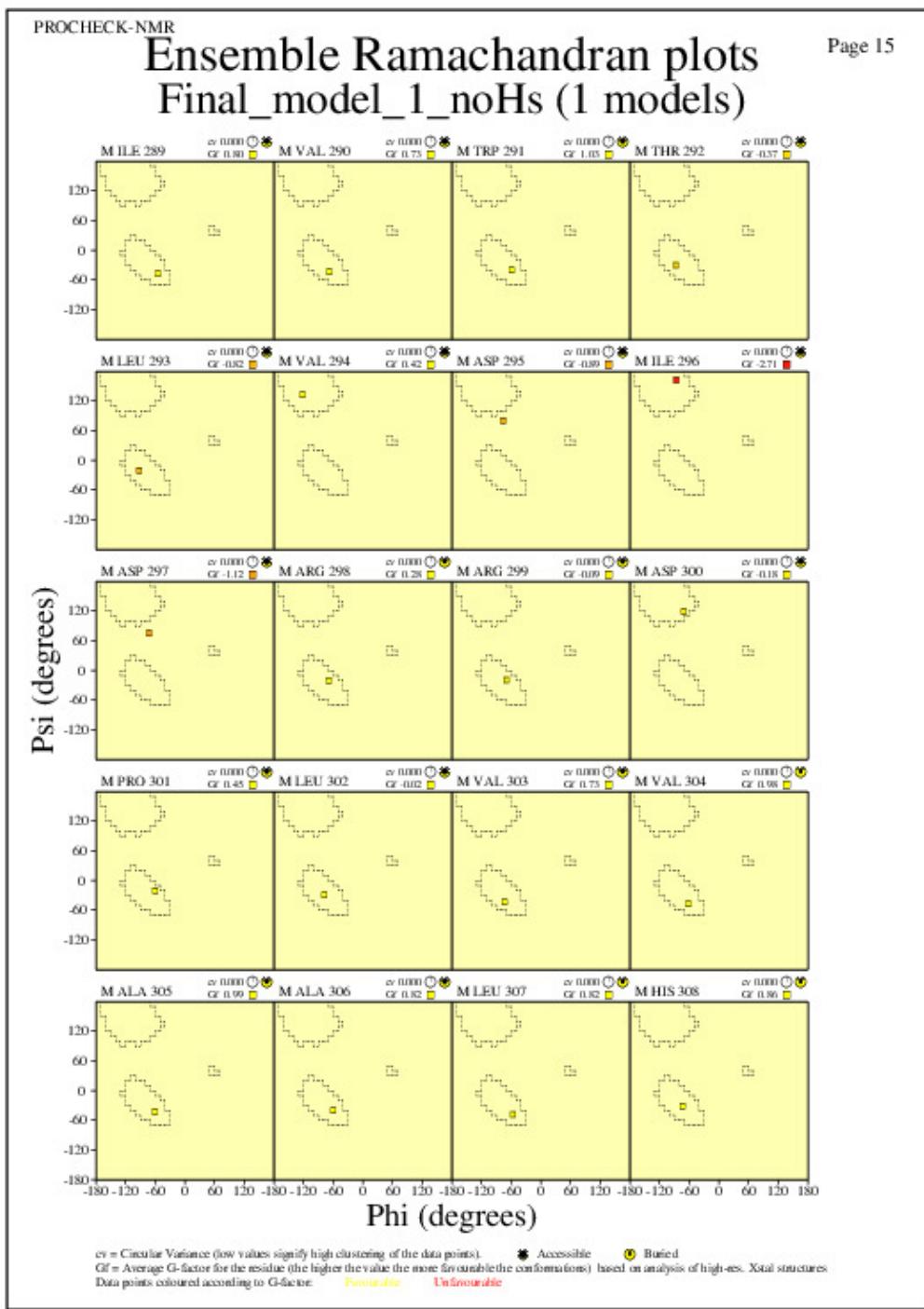


Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n

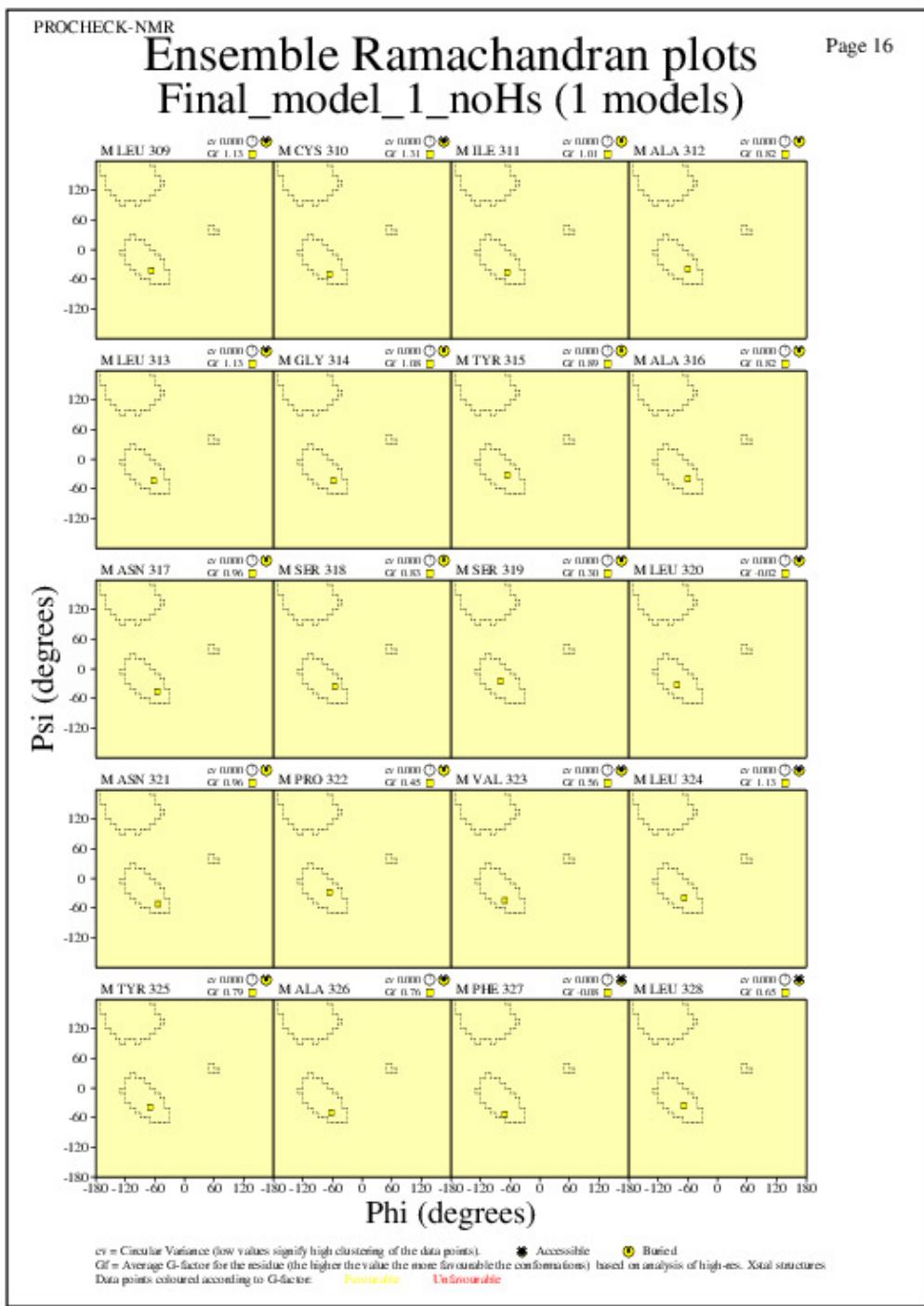


## JPEG for residue Ramachandran Plots - page \$num\_n



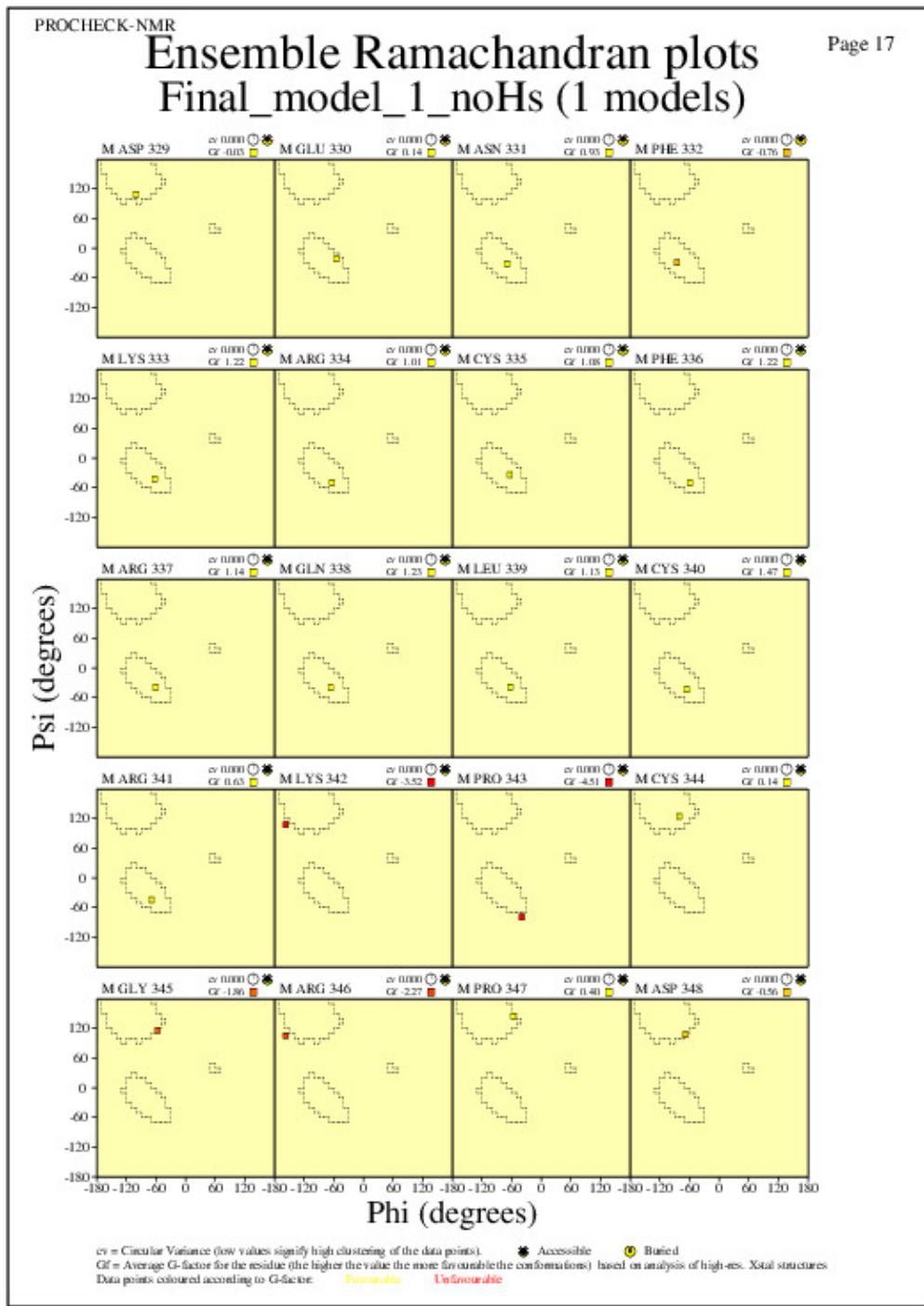
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



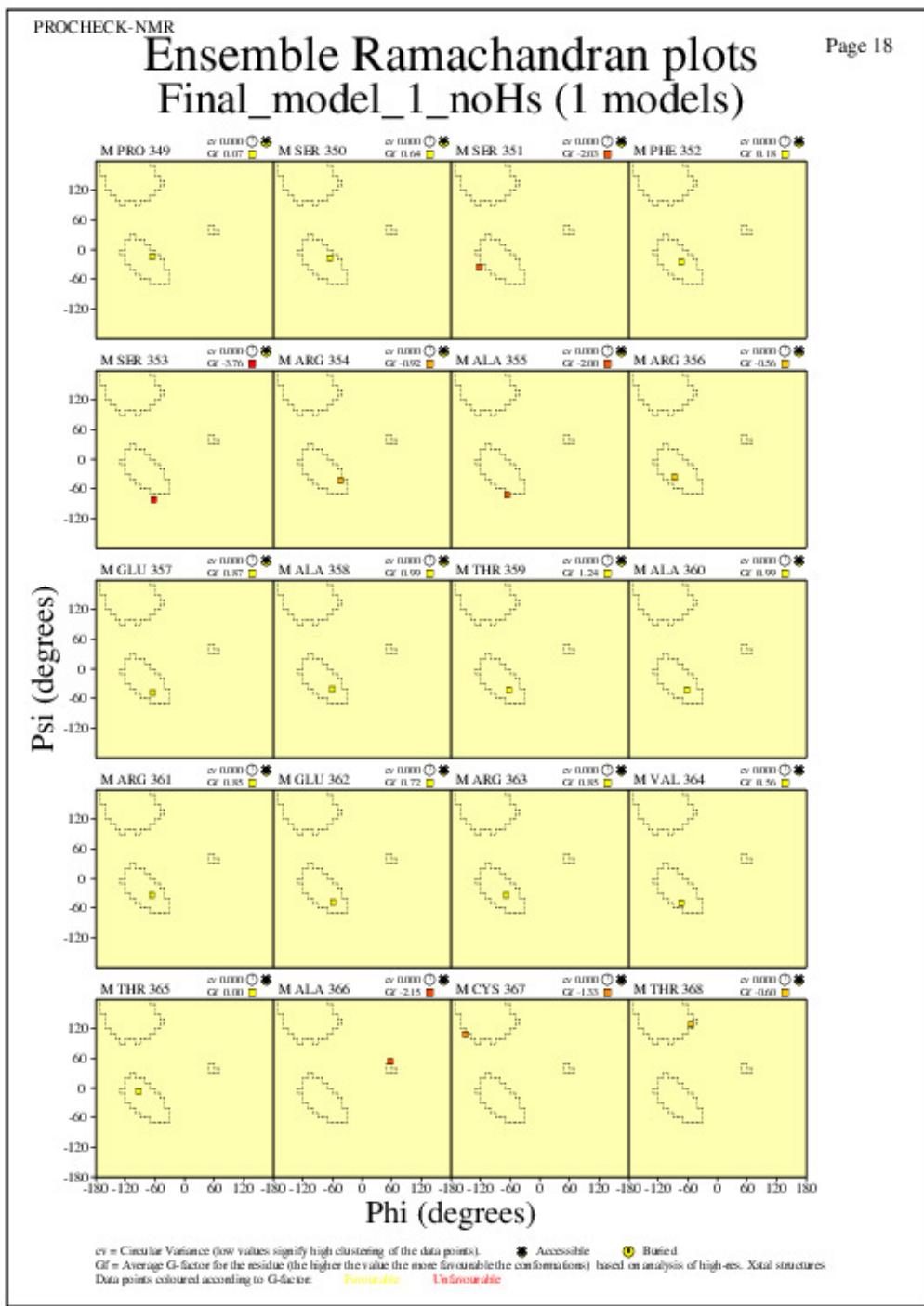
Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n

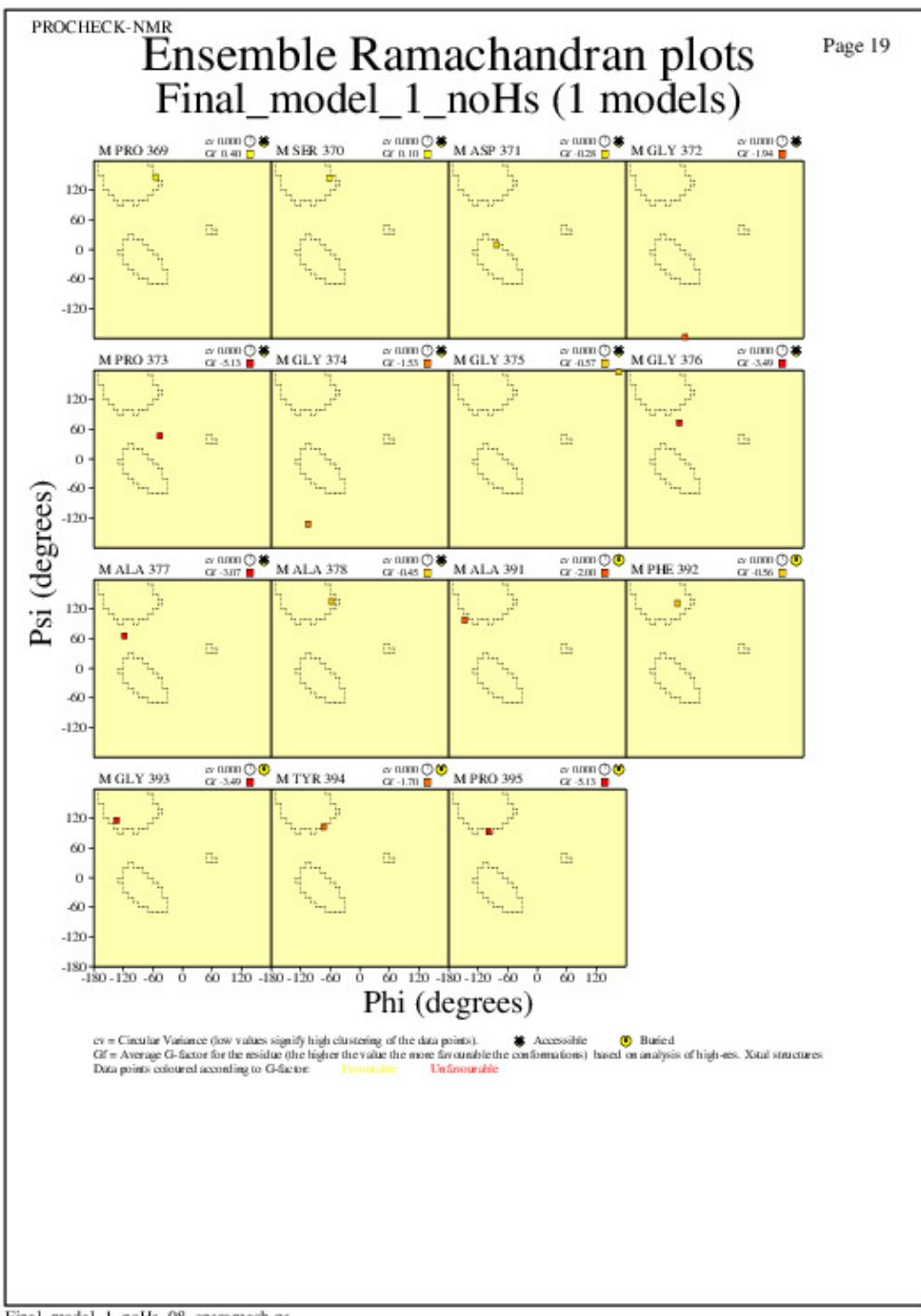


Final\_model\_1\_noHs\_08\_ensramach.ps

## JPEG for residue Ramachandran Plots - page \$num\_n



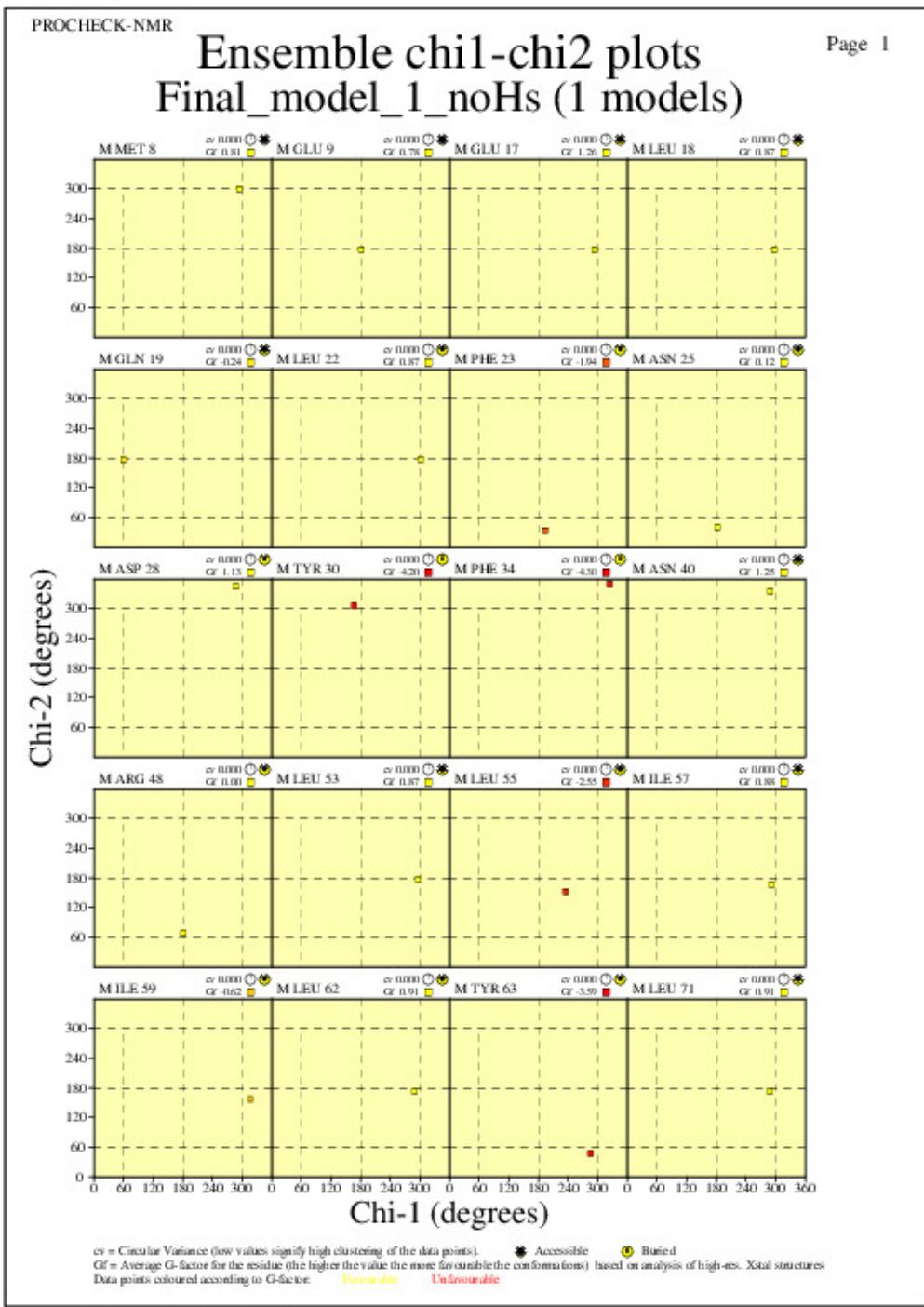
## JPEG for residue Ramachandran Plots - page \$num\_n



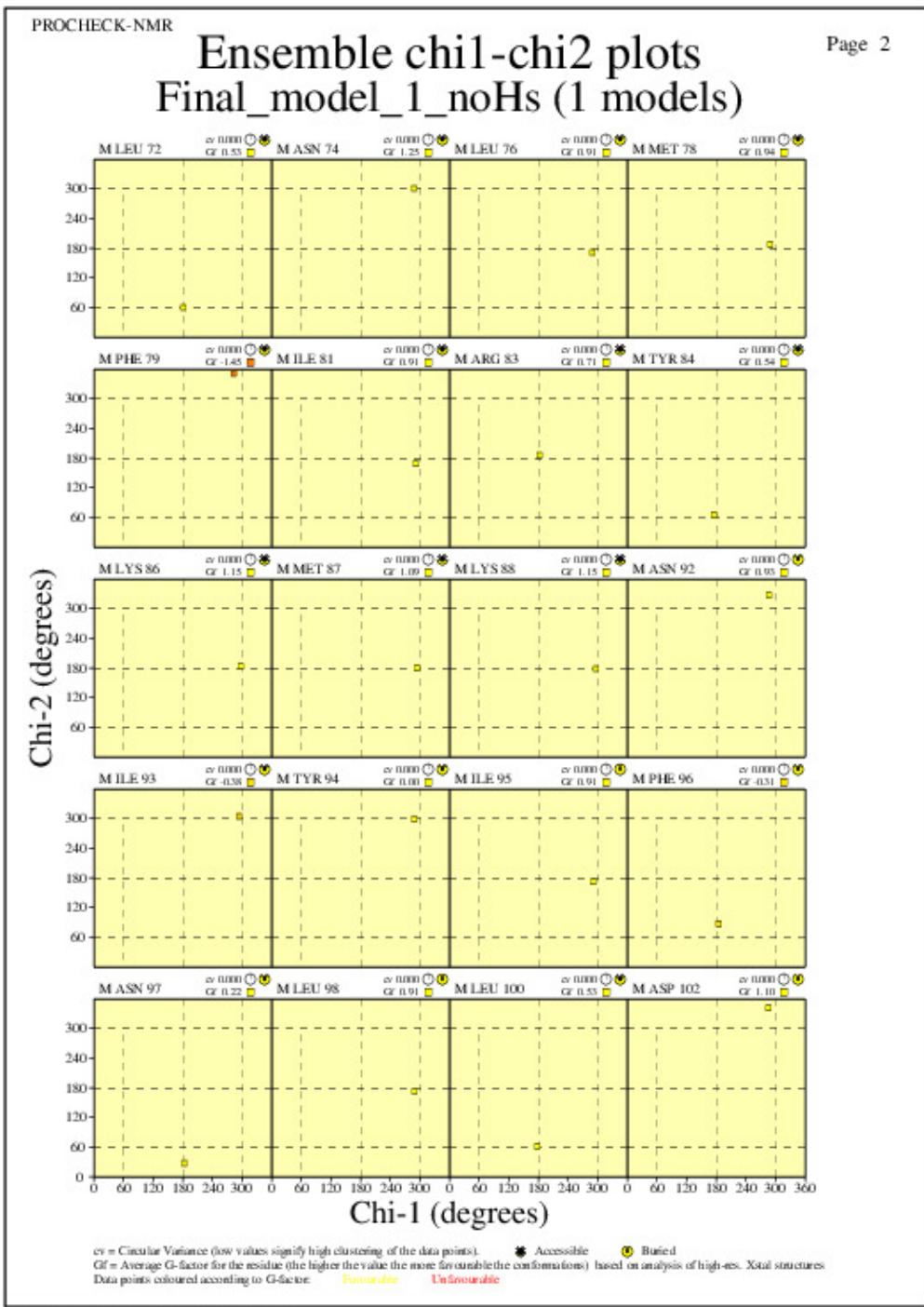
**Ramachandran analysis for each residue from Molprobit**

**Chi1-Chi2 Plots for each residue**

JPEG for residue Chi1-Chi2 Plots - page \$num\_n

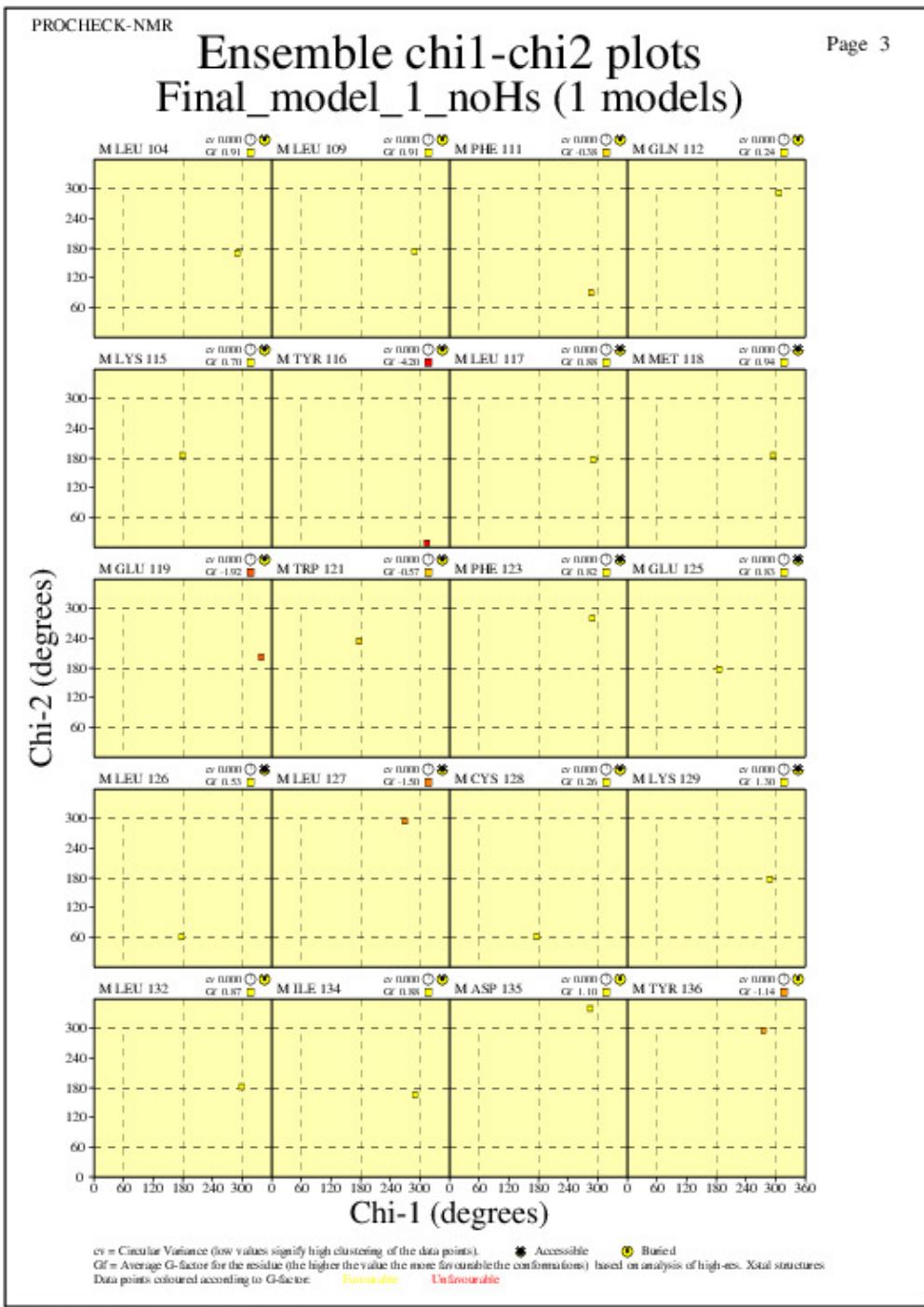


JPEG for residue Chi1-Chi2 Plots - page \$num\_n



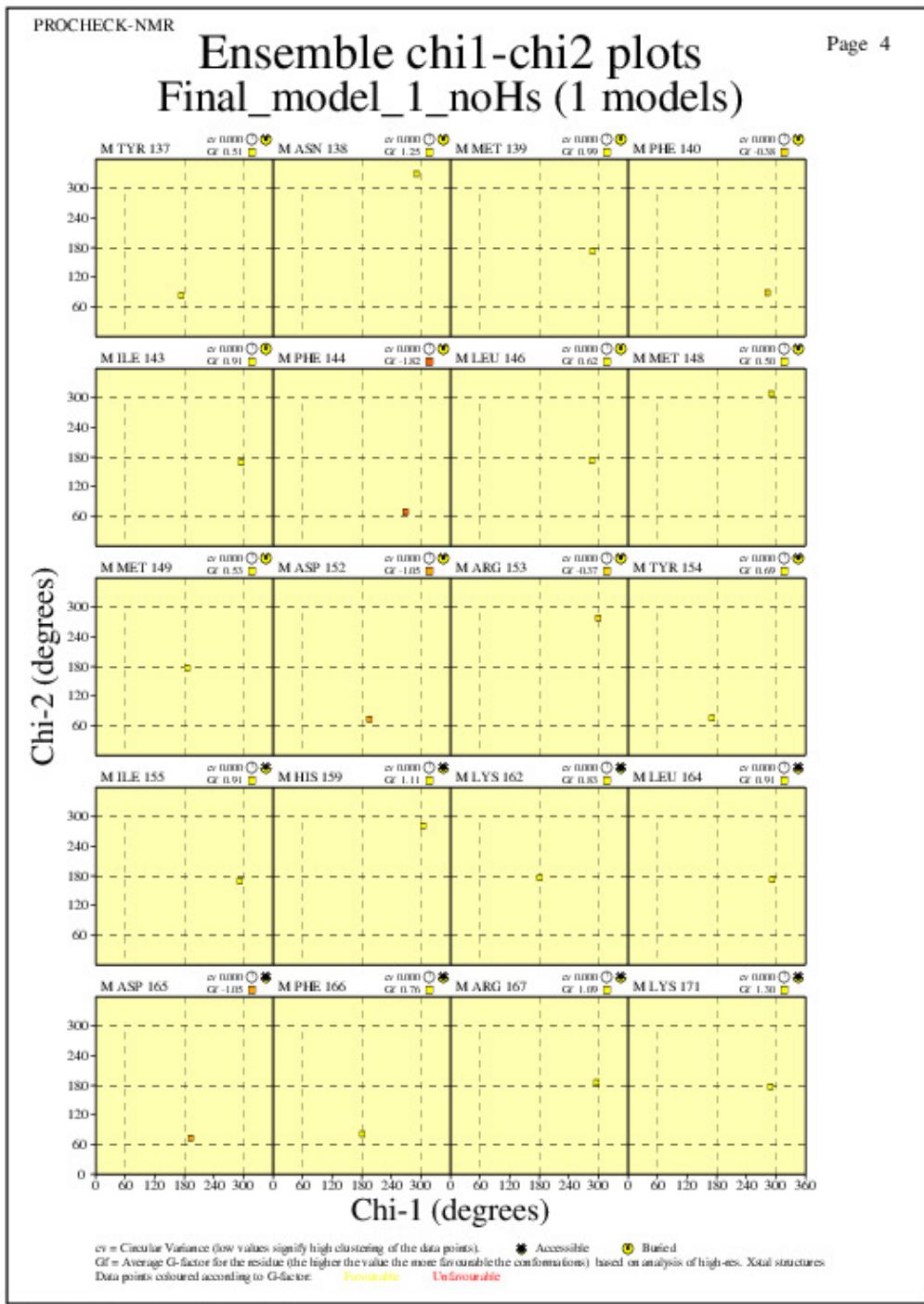
Final\_model\_1\_noHs\_09\_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num\_n



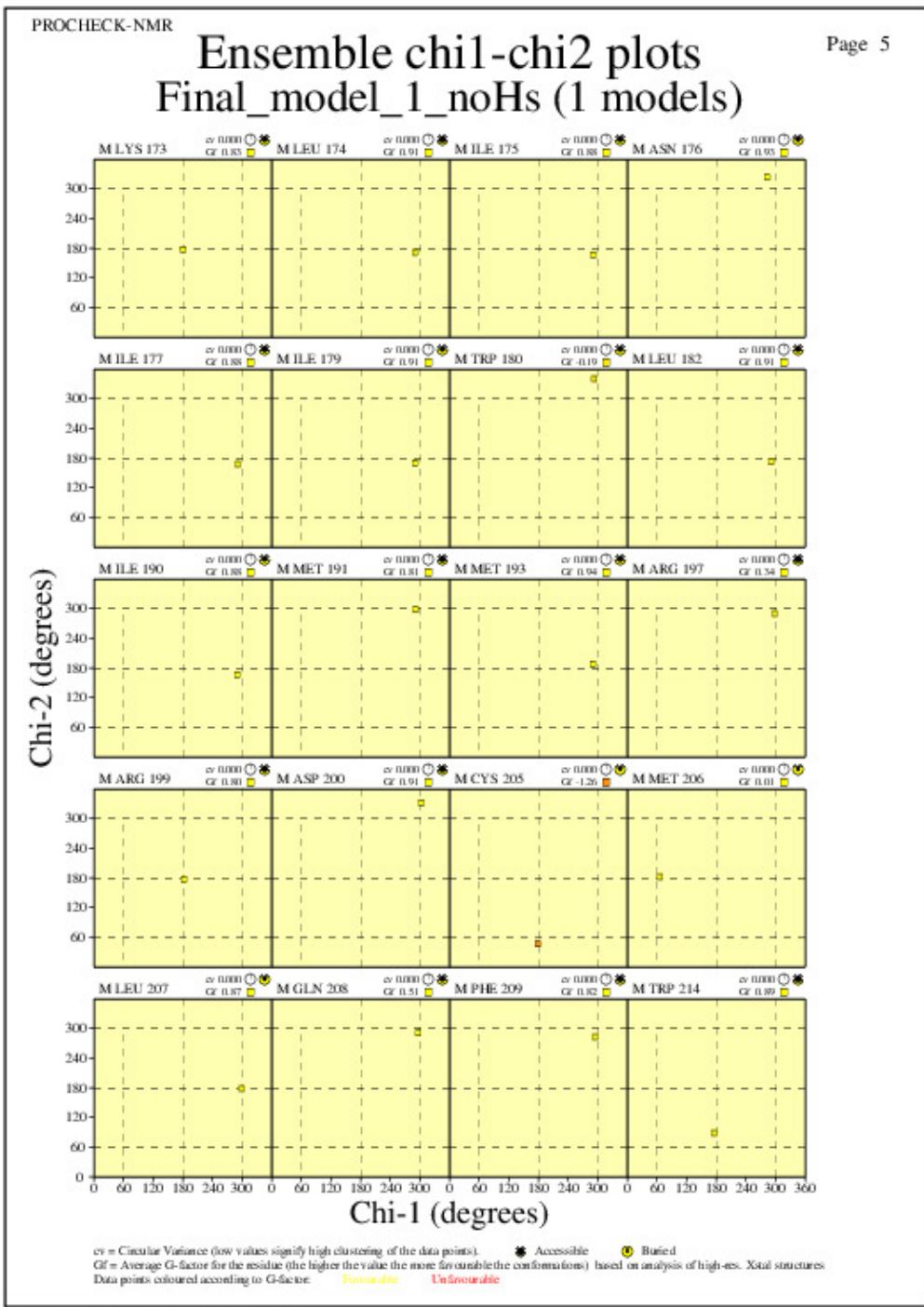
Final\_model\_1\_noHs\_09\_ensch1ch2.ps

**JPEG for residue Chi1-Chi2 Plots - page \$num\_n**



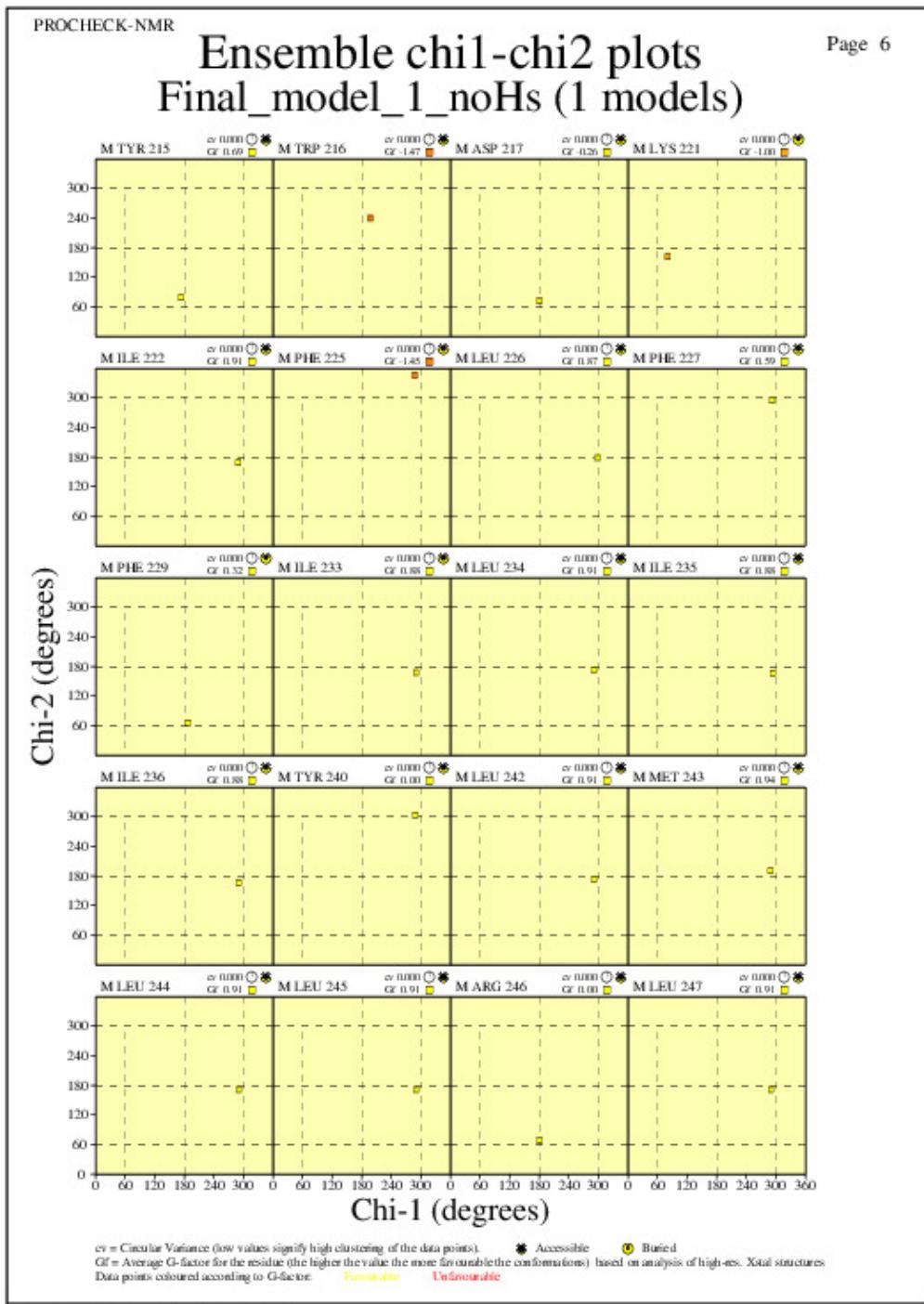
Final\_model\_1\_noHs\_09\_ensch1ch2.ps

**JPEG for residue Chi1-Chi2 Plots - page \$num\_n**



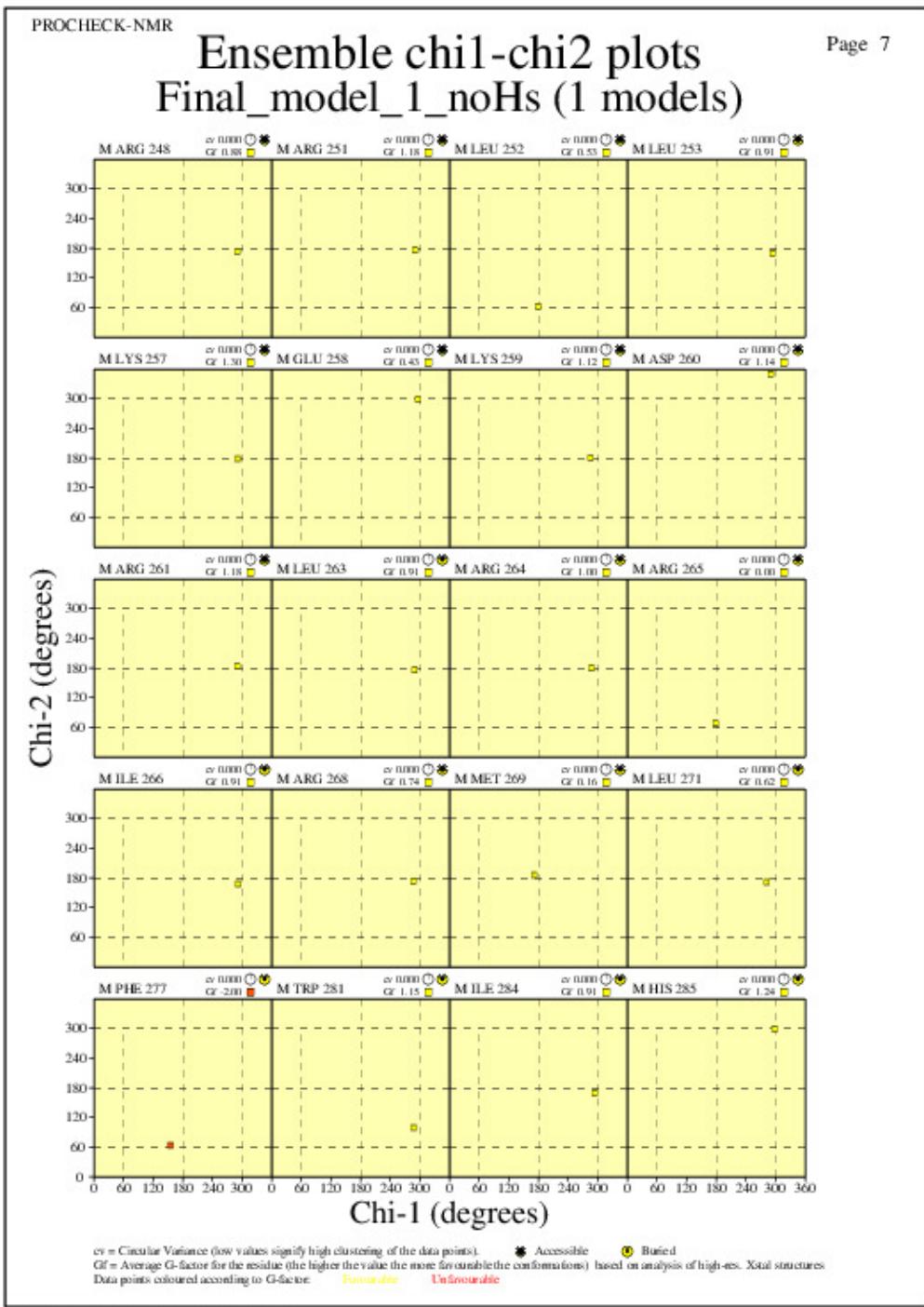
Final\_model\_1\_noHs\_09\_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num\_n



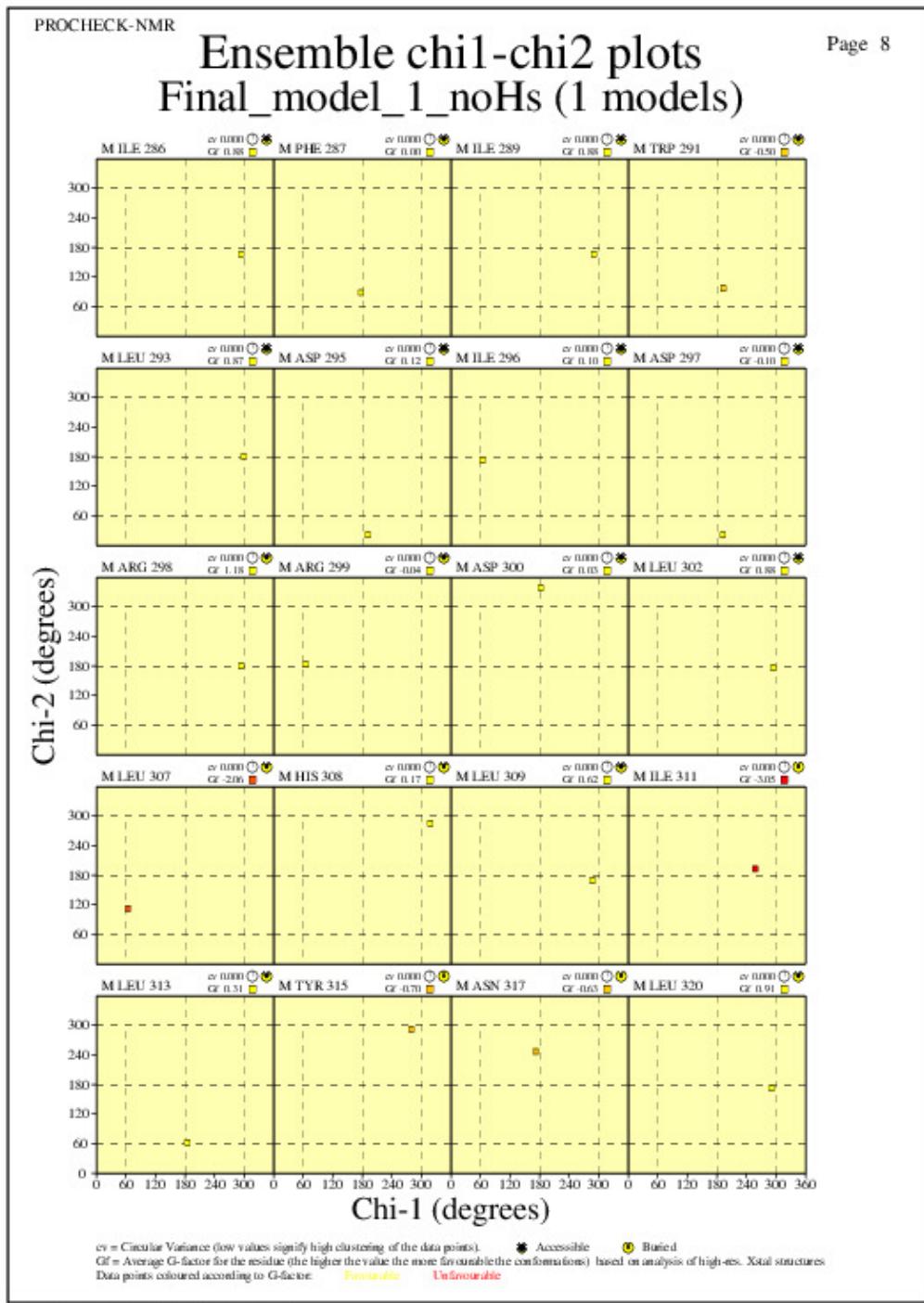
Final\_model\_1\_noHs\_09\_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num\_n

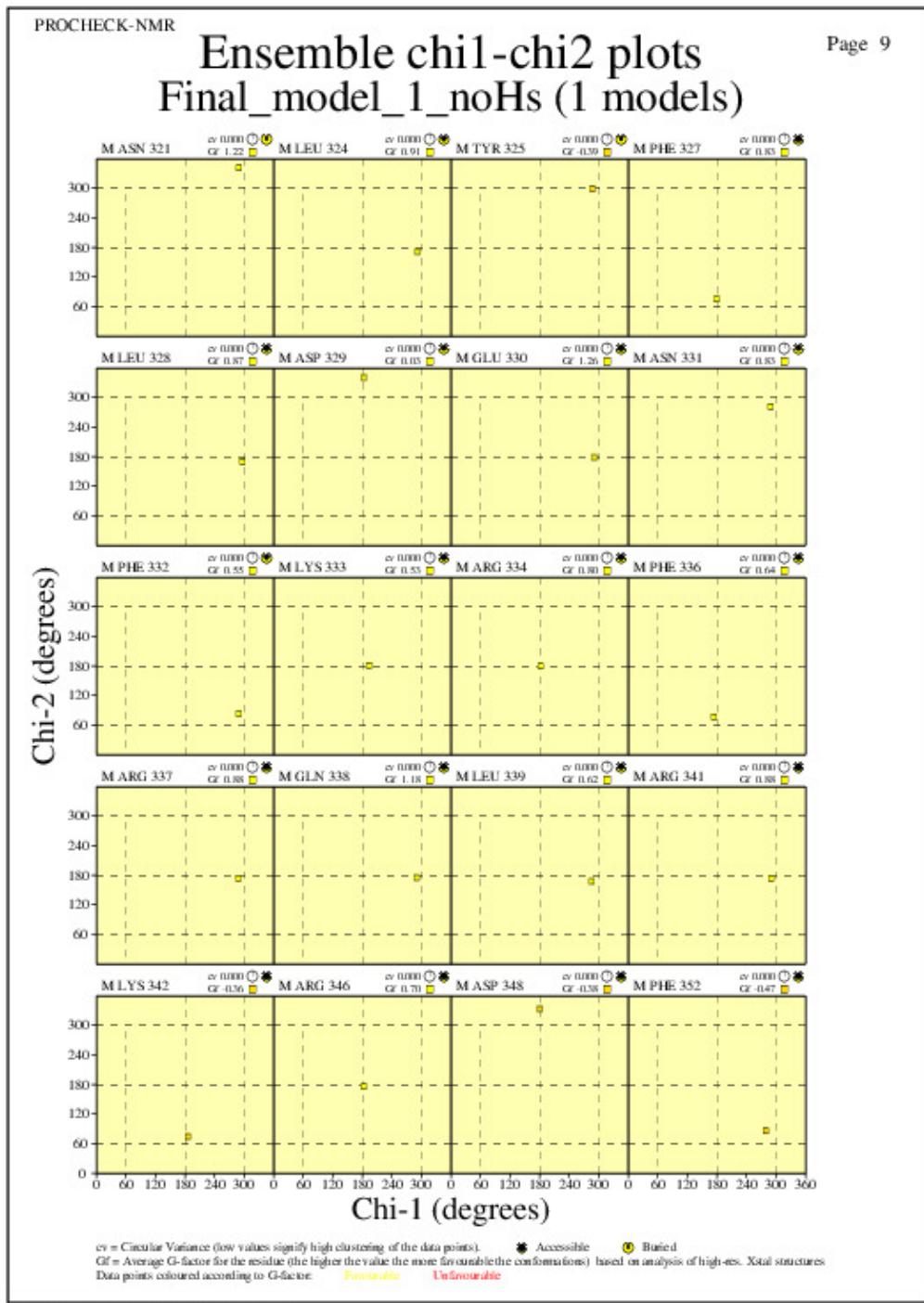


Final\_model\_1\_noHs\_09\_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num\_n

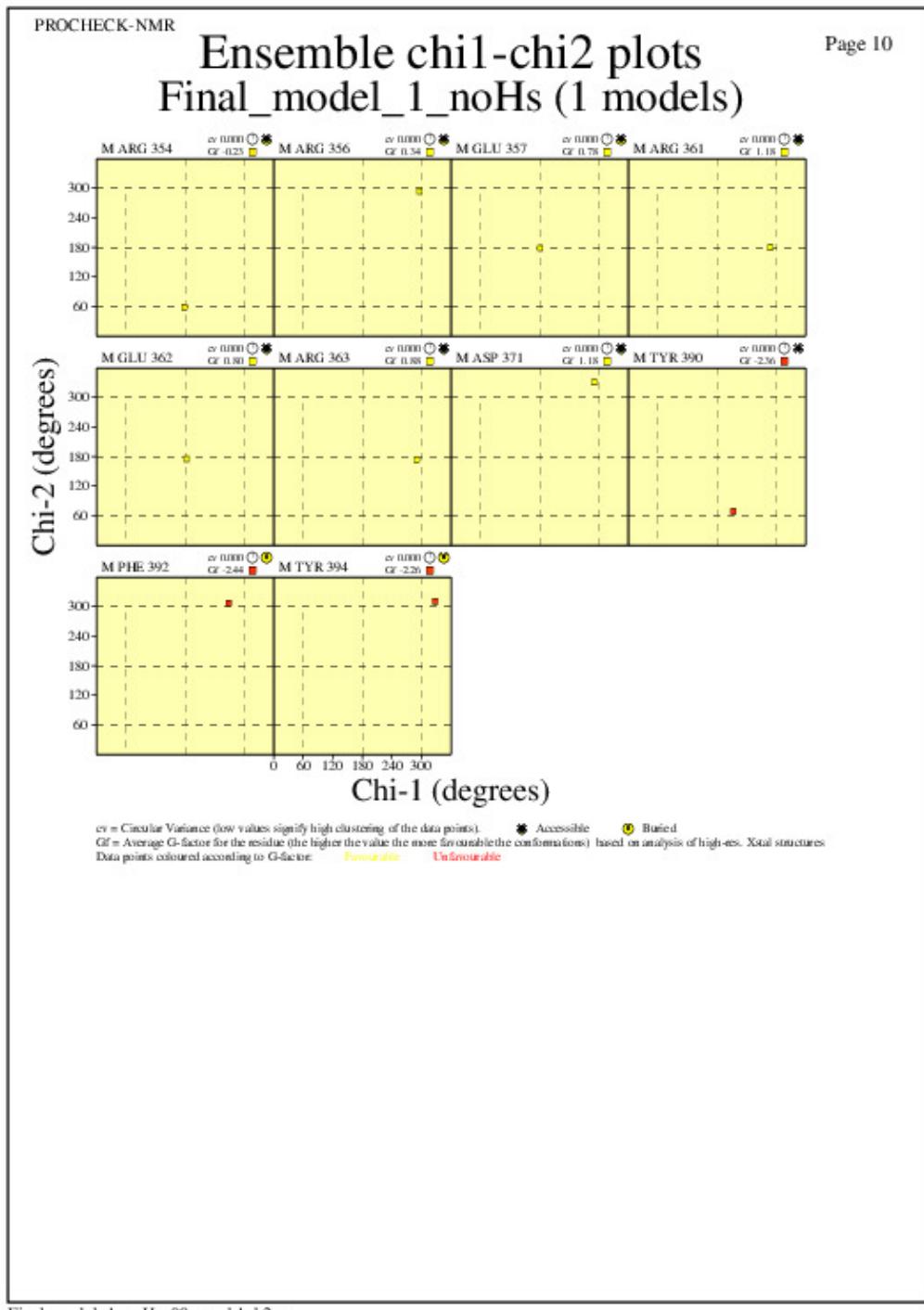


JPEG for residue Chi1-Chi2 Plots - page \$num\_n

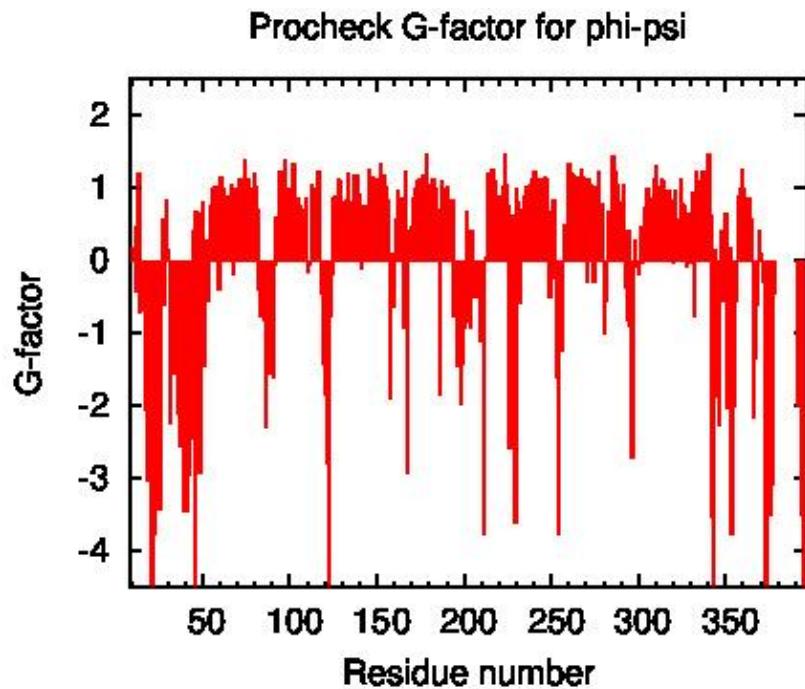


Final\_model\_1\_noHs\_09\_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num\_n



## Procheck G-factors for phi-psi for each residue

**JPEG image for residue phi-psi G-factors****Table of Procheck G-factors for phi-psi for ordered residues**

```
#phipsi_gfactor
#Residue\Model  average
9      0.17
10     0.02
11     -0.43
12     0.47
13     1.19
14     -0.70
15     -0.31
16     -0.11
17     -2.06
18     -3.04
19     -2.05
20     -5.13
21     -5.13
22     -3.77
23     -3.08
24     -0.77
25     -3.43
26     -0.46
27     0.57
28     -0.60
29     0.82
30     0.15
31     -2.24
32     -0.25
33     -0.51
34     -1.56
35     -0.40
36     -2.11
37     -2.55
38     -1.48
```

## PSVS Software Environment

39	-3.46
40	-0.26
41	-3.46
42	-2.94
43	-2.46
44	0.42
45	-5.13
46	0.68
47	-0.89
48	-2.93
49	0.64
50	0.80
51	-1.44
52	0.27
53	-0.56
54	0.76
55	0.99
56	0.66
57	1.01
58	0.66
59	-0.39
60	1.14
61	0.99
62	0.99
63	0.79
64	0.88
65	0.76
66	1.05
67	-0.19
68	0.66
69	0.98
70	0.73
71	1.13
72	1.13
73	0.23
74	1.39
75	1.05
76	1.13
77	0.98
78	0.84
79	1.20
80	1.02
81	0.71
82	-0.40
83	-0.77
84	-0.13
85	-0.81
86	-2.30
87	-1.17
88	-1.55
89	-0.01
90	-1.60
91	-0.06
92	0.59
93	0.30
94	1.22
95	1.01
96	1.22
97	1.39
98	0.99
99	0.99
100	0.29

## PSVS Software Environment

101	0.76
102	1.32
103	0.76
104	0.85
105	0.76
106	0.48
107	0.70
108	0.00
109	0.85
110	-0.15
111	-0.06
112	1.04
113	0.04
114	0.99
115	0.95
116	1.22
117	1.13
118	-0.45
119	-1.43
120	-1.83
121	-2.78
122	-5.13
123	-0.76
124	-0.19
125	0.86
126	0.88
127	0.65
128	1.13
129	1.08
130	0.76
131	0.81
132	0.84
133	1.19
134	0.80
135	0.40
136	0.64
137	1.17
138	1.17
139	0.92
140	0.61
141	-0.10
142	0.74
143	0.69
144	0.74
145	1.24
146	1.13
147	1.14
148	0.15
149	1.12
150	1.09
151	0.73
152	1.32
153	1.01
154	1.17
155	1.01
156	0.82
157	-1.89
158	0.10
159	-0.63
160	0.02
161	0.56
162	0.95

## PSVS Software Environment

163	0.06
164	0.85
165	-0.91
166	1.22
167	-2.93
168	0.40
169	0.47
170	0.36
171	0.85
172	0.99
173	1.08
174	1.13
175	1.01
176	1.17
177	1.01
178	1.47
179	1.01
180	1.03
181	0.98
182	1.13
183	0.99
184	0.70
185	0.06
186	-1.83
187	1.08
188	0.98
189	0.00
190	1.01
191	0.55
192	0.56
193	0.84
194	-0.77
195	-0.35
196	-1.45
197	-0.10
198	-1.97
199	-1.43
200	-0.91
201	0.68
202	-0.83
203	-0.93
204	0.41
205	-0.48
206	-0.49
207	-0.12
208	-0.22
209	-1.11
210	-0.12
211	-3.76
212	0.03
213	1.19
214	0.95
215	0.55
216	1.26
217	1.08
218	0.87
219	0.81
220	0.87
221	0.68
222	1.01
223	1.47
224	1.05

## PSVS Software Environment

225	0.74
226	-2.58
227	0.61
228	-0.53
229	-3.61
230	0.98
231	0.81
232	-0.58
233	0.71
234	0.88
235	1.01
236	0.80
237	0.77
238	1.05
239	1.13
240	1.22
241	1.02
242	1.13
243	0.81
244	1.13
245	1.13
246	1.14
247	1.13
248	0.67
249	-0.51
250	0.57
251	0.84
252	-0.24
253	-1.60
254	-3.76
255	-0.09
256	-1.24
257	0.49
258	0.08
259	1.22
260	1.32
261	1.14
262	1.19
263	1.13
264	1.14
265	1.14
266	1.01
267	1.24
268	1.14
269	0.15
270	-0.28
271	1.13
272	1.05
273	0.98
274	-0.28
275	1.02
276	0.99
277	1.22
278	0.56
279	0.77
280	-0.99
281	-0.56
282	0.66
283	0.02
284	0.58
285	1.43
286	1.01

## PSVS Software Environment

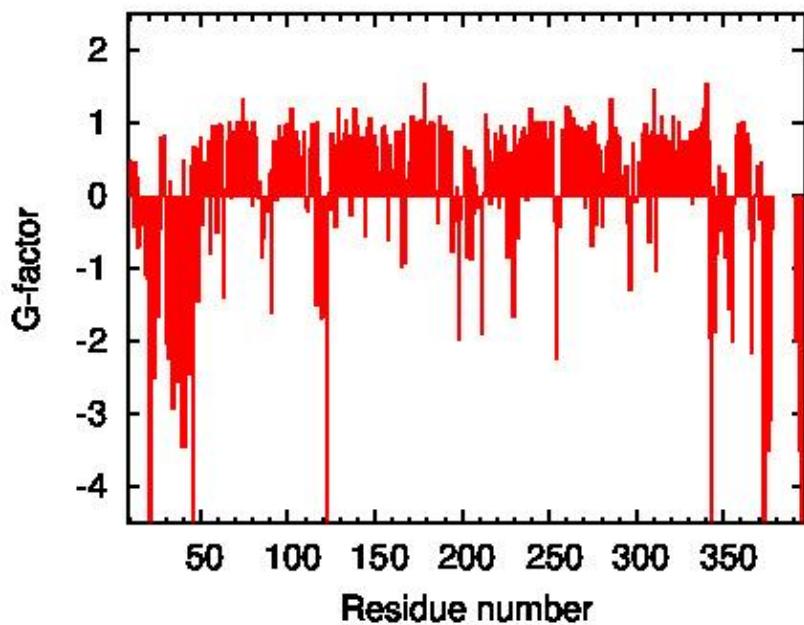
287	1.22
288	1.05
289	0.80
290	0.73
291	1.03
292	-0.37
293	-0.82
294	0.42
295	-0.89
296	-2.71
297	-1.12
298	0.28
299	-0.09
300	-0.18
301	0.45
302	-0.02
303	0.73
304	0.98
305	0.99
306	0.82
307	0.82
308	0.86
309	1.13
310	1.31
311	1.01
312	0.82
313	1.13
314	1.08
315	0.89
316	0.82
317	0.96
318	0.83
319	0.30
320	-0.02
321	0.96
322	0.45
323	0.56
324	1.13
325	0.79
326	0.76
327	-0.08
328	0.65
329	-0.03
330	0.14
331	0.93
332	-0.76
333	1.22
334	1.01
335	1.08
336	1.22
337	1.14
338	1.23
339	1.13
340	1.47
341	0.63
342	-3.52
343	-4.51
344	0.14
345	-1.86
346	-2.27
347	0.40
348	-0.56

## PSVS Software Environment

```
349      0.07
350      0.64
351     -2.03
352      0.18
353     -3.76
354     -0.92
355     -2.00
356     -0.56
357      0.87
358      0.99
359      1.24
360      0.99
361      0.85
362      0.72
363      0.85
364      0.56
365      0.00
366     -2.15
367     -1.33
368     -0.60
369      0.40
370      0.10
371     -0.28
372     -1.94
373     -5.13
374     -1.53
375     -0.57
376     -3.49
377     -3.07
378     -0.45
391     -2.00
392     -0.56
393     -3.49
394     -1.70
395     -5.13
#Reported_Model_Average 0.043
#Overall_Average_Reported      0.043
```

## Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

**Procheck G-factor for all dihedral angles****Table of Procheck G-factors for all dihedrals for ordered residues**

```
#alldih_gfactor
#Residue\Model    average
8      0.81
9      0.48
10     0.02
11     -0.43
12     0.47
13     0.24
14     -0.70
15     -0.31
16     -0.11
17     -0.40
18     -1.08
19     -1.14
20     -5.13
21     -5.13
22     -1.45
23     -2.51
24     -0.77
25     -1.65
26     -0.46
27     0.81
28     0.26
29     0.82
30     -2.02
31     -2.24
32     0.20
33     -0.51
34     -2.93
35     -0.40
36     -0.87
37     -2.55
38     -1.48
39     -3.46
40     0.49
```

## PSVS Software Environment

41	-3.46
42	-1.83
43	-2.46
44	0.42
45	-5.13
46	0.68
47	-0.89
48	-1.46
49	0.65
50	0.80
51	-0.39
52	0.47
53	0.15
54	0.76
55	-0.78
56	0.66
57	0.95
58	0.66
59	-0.50
60	0.95
61	0.99
62	0.95
63	-1.40
64	0.08
65	0.76
66	1.01
67	-0.03
68	0.66
69	0.89
70	0.73
71	1.02
72	0.83
73	0.23
74	1.32
75	0.86
76	1.02
77	0.74
78	0.89
79	-0.13
80	1.02
81	0.81
82	0.05
83	-0.03
84	0.21
85	-0.84
86	-0.57
87	-0.04
88	-0.20
89	0.31
90	-1.60
91	0.35
92	0.76
93	-0.04
94	0.61
95	0.96
96	0.45
97	0.80
98	0.95
99	0.99
100	0.41
101	0.76
102	1.21

## PSVS Software Environment

103	0.76
104	0.88
105	0.76
106	0.26
107	0.54
108	0.38
109	0.88
110	-0.15
111	-0.22
112	0.64
113	0.21
114	0.99
115	0.82
116	-1.49
117	1.01
118	0.25
119	-1.68
120	-1.06
121	-1.67
122	-5.13
123	0.03
124	-0.19
125	0.85
126	0.71
127	-0.42
128	0.70
129	1.19
130	0.76
131	0.39
132	0.86
133	1.03
134	0.84
135	0.75
136	-0.25
137	0.84
138	1.21
139	0.95
140	0.11
141	0.76
142	0.81
143	0.80
144	-0.54
145	0.94
146	0.88
147	1.06
148	0.33
149	0.82
150	0.19
151	0.66
152	0.14
153	0.32
154	0.93
155	0.96
156	0.82
157	-0.61
158	0.70
159	0.24
160	0.02
161	0.35
162	0.89
163	0.06
164	0.88

## PSVS Software Environment

165	-0.98
166	0.99
167	-0.92
168	0.22
169	0.47
170	0.36
171	1.08
172	0.99
173	0.96
174	1.02
175	0.95
176	1.05
177	0.94
178	1.53
179	0.96
180	0.42
181	0.86
182	1.02
183	0.99
184	-0.01
185	0.06
186	-0.38
187	1.08
188	0.95
189	0.00
190	0.95
191	0.68
192	0.74
193	0.89
194	-0.77
195	-0.19
196	-0.34
197	0.12
198	-1.97
199	-0.31
200	0.00
201	0.68
202	-0.83
203	-0.17
204	0.61
205	-0.87
206	-0.24
207	0.38
208	0.15
209	-0.15
210	-0.12
211	-1.89
212	0.03
213	1.12
214	0.92
215	0.62
216	-0.11
217	0.41
218	0.46
219	0.86
220	0.75
221	-0.16
222	0.96
223	0.80
224	0.82
225	-0.36
226	-0.85

## PSVS Software Environment

227	0.60
228	-0.53
229	-1.65
230	0.95
231	0.70
232	-0.58
233	0.79
234	0.89
235	0.94
236	0.84
237	-0.05
238	0.66
239	1.21
240	0.61
241	1.02
242	1.02
243	0.88
244	1.02
245	1.02
246	0.57
247	1.02
248	0.77
249	0.08
250	0.75
251	1.01
252	0.14
253	-0.34
254	-2.24
255	-0.09
256	-0.43
257	0.90
258	0.25
259	1.17
260	1.23
261	1.16
262	0.24
263	1.02
264	1.07
265	0.57
266	0.96
267	0.94
268	0.94
269	0.16
270	-0.15
271	0.88
272	0.59
273	0.95
274	-0.68
275	1.02
276	0.99
277	-0.39
278	0.69
279	0.63
280	-0.43
281	0.29
282	0.66
283	0.02
284	0.74
285	1.34
286	0.94
287	0.61
288	0.93

## PSVS Software Environment

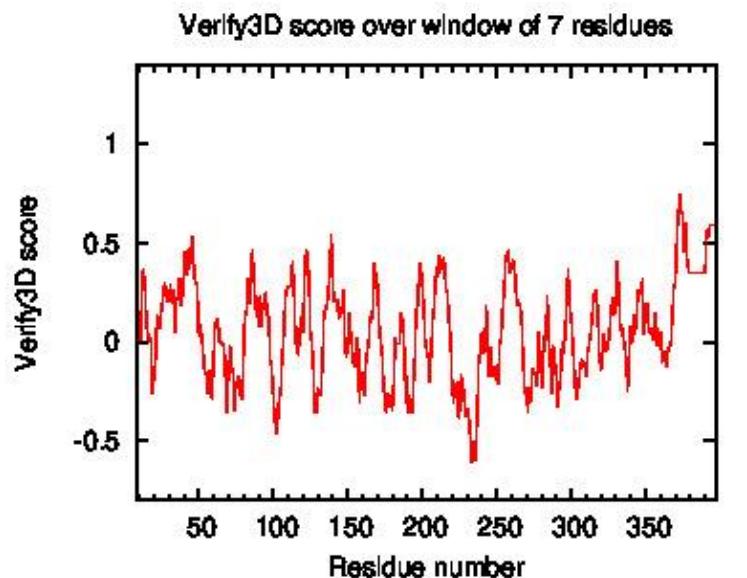
289	0.84
290	0.80
291	0.27
292	0.05
293	0.03
294	0.41
295	-0.38
296	-1.30
297	-0.61
298	0.73
299	-0.07
300	-0.07
301	0.45
302	0.43
303	0.85
304	0.48
305	0.99
306	0.82
307	-0.62
308	0.51
309	0.88
310	1.45
311	-1.02
312	0.82
313	0.72
314	1.08
315	0.09
316	0.82
317	0.17
318	0.75
319	0.48
320	0.45
321	1.09
322	0.45
323	0.62
324	1.02
325	0.20
326	0.76
327	0.38
328	0.76
329	0.00
330	0.70
331	0.88
332	-0.11
333	0.88
334	0.90
335	0.60
336	0.93
337	1.01
338	1.20
339	0.88
340	1.53
341	0.75
342	-1.94
343	-4.51
344	0.13
345	-1.86
346	-0.78
347	0.40
348	-0.47
349	0.07
350	0.30

```
351      -0.83
352      -0.14
353      -1.55
354      -0.58
355      -2.00
356      -0.11
357      0.83
358      0.99
359      0.86
360      0.99
361      1.01
362      0.76
363      0.86
364      0.69
365      -0.44
366      -2.15
367      -0.60
368      0.02
369      0.40
370      -0.31
371      0.45
372      -1.94
373      -5.13
374      -1.53
375      -0.57
376      -3.49
377      -3.07
378      -0.45
379      0.00
390      -2.36
391      -2.00
392      -1.50
393      -3.49
394      -1.98
395      -5.13
396      -0.03
#Reported_Model_Average 0.080
#Overall_Average_Reported      0.080
```

## Output from Verify3D

**Verify3D Score over a window of \$winsize\_s residues**

**JPEG image for Verify3D Score**

**Table of Verify3D scores for ordered residues across all models**

```
#verify3d
#Residue\Model  only_model
8      -1.30
9       0.04
10      0.25
11      0.14
12      0.44
13      0.34
14      0.14
15      1.10
16      0.14
17     -0.46
18     -1.14
19     -0.03
20      0.44
21     -0.11
22     -0.68
23      0.71
24      0.14
25      0.51
26     -0.25
27      0.17
28      0.51
29     -0.25
30      1.25
31     -0.11
32      0.17
33     -0.25
34      0.71
35     -0.11
36      0.17
37     -0.25
38      1.10
39      0.14
40      0.51
41     -0.25
42      0.17
43      1.10
```

## PSVS Software Environment

44	0.44
45	0.25
46	1.10
47	-0.25
48	0.71
49	0.34
50	-0.25
51	0.17
52	0.17
53	-0.68
54	0.14
55	0.29
56	-0.25
57	-0.94
58	0.14
59	-0.54
60	0.08
61	0.14
62	-0.68
63	1.25
64	0.34
65	0.14
66	-0.40
67	-0.81
68	0.14
69	-0.74
70	1.10
71	-0.68
72	-1.14
73	1.10
74	0.09
75	-0.74
76	-0.68
77	-0.40
78	0.23
79	-0.84
80	1.10
81	-0.54
82	-0.80
83	0.71
84	1.25
85	0.08
86	0.47
87	0.23
88	0.47
89	0.08
90	-0.25
91	0.08
92	0.51
93	-0.54
94	1.25
95	-0.54
96	0.71
97	0.09
98	0.29
99	-0.25
100	-0.68
101	-0.25
102	-0.83
103	-0.25
104	-0.68
105	-0.25

## PSVS Software Environment

106	0.08
107	0.17
108	0.08
109	0.29
110	0.44
111	0.71
112	0.10
113	0.17
114	0.14
115	0.08
116	1.25
117	-0.68
118	-0.83
119	-0.46
120	0.08
121	1.12
122	0.44
123	0.71
124	1.10
125	0.28
126	-0.68
127	-0.68
128	-0.81
129	0.08
130	-0.25
131	-0.40
132	0.29
133	0.17
134	-0.94
135	-0.83
136	1.25
137	1.25
138	0.09
139	0.23
140	0.71
141	0.08
142	0.17
143	-0.54
144	0.71
145	0.08
146	0.29
147	0.08
148	0.23
149	0.23
150	0.17
151	-0.74
152	-0.83
153	0.71
154	1.25
155	-0.54
156	-0.25
157	-0.40
158	-0.81
159	0.20
160	0.44
161	-0.80
162	0.47
163	-0.25
164	-1.14
165	0.23
166	0.71
167	0.71

## PSVS Software Environment

168	0.08
169	0.44
170	0.14
171	0.47
172	-0.25
173	0.47
174	-0.68
175	-0.54
176	0.09
177	-0.94
178	-0.35
179	-0.54
180	1.12
181	-0.80
182	-0.68
183	-0.25
184	0.17
185	1.10
186	-0.74
187	1.10
188	-0.80
189	0.44
190	-0.54
191	-0.83
192	-0.80
193	0.23
194	-0.25
195	-0.40
196	0.08
197	0.24
198	0.44
199	0.71
200	0.51
201	1.10
202	-0.25
203	-0.74
204	-0.40
205	-0.81
206	0.23
207	0.29
208	0.25
209	0.71
210	0.44
211	0.17
212	0.25
213	0.17
214	1.12
215	-0.43
216	1.12
217	0.51
218	0.08
219	-0.74
220	0.08
221	0.08
222	-0.94
223	-0.35
224	-0.40
225	0.71
226	-0.68
227	-0.84
228	-0.25
229	0.71

## PSVS Software Environment

230	-0.74
231	-0.74
232	-0.11
233	-0.54
234	-0.68
235	-0.94
236	-0.54
237	0.08
238	-0.80
239	-0.81
240	1.25
241	1.10
242	-0.68
243	0.23
244	-0.68
245	-0.68
246	0.71
247	0.29
248	-0.41
249	0.34
250	-0.74
251	-0.41
252	-0.68
253	0.29
254	0.17
255	1.10
256	0.17
257	0.47
258	0.28
259	0.47
260	0.51
261	0.24
262	0.34
263	0.29
264	0.71
265	0.24
266	-0.54
267	0.08
268	0.24
269	0.23
270	-0.40
271	-0.68
272	-0.74
273	-0.40
274	-0.74
275	1.10
276	-0.25
277	0.71
278	-0.74
279	-0.80
280	-0.81
281	1.12
282	-0.25
283	0.44
284	-0.54
285	1.04
286	-0.94
287	0.71
288	-0.40
289	-0.94
290	-0.74
291	1.12

## PSVS Software Environment

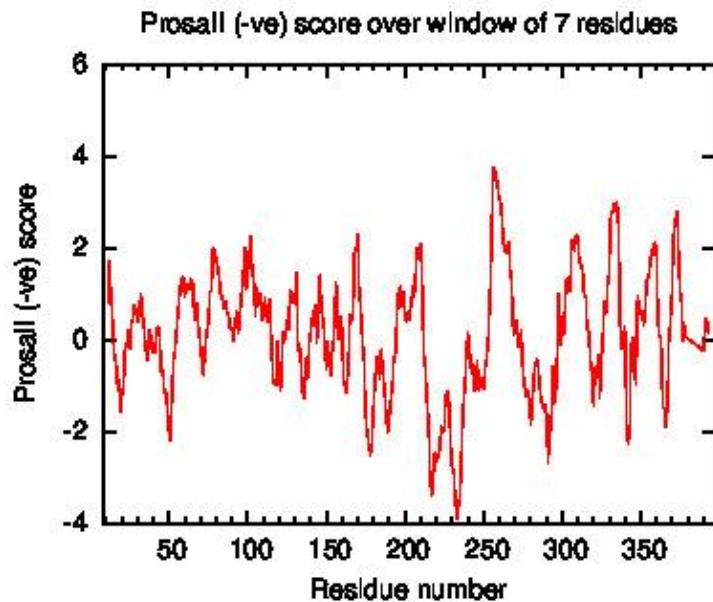
292	0.08
293	-0.68
294	-0.74
295	0.23
296	-0.54
297	0.51
298	0.71
299	0.71
300	0.51
301	0.44
302	-1.14
303	-0.74
304	-0.40
305	-0.25
306	-0.25
307	0.29
308	1.04
309	-0.68
310	-0.35
311	-0.54
312	-0.25
313	-0.68
314	1.10
315	1.25
316	-0.25
317	0.09
318	0.17
319	0.17
320	-0.68
321	0.09
322	-0.11
323	-0.74
324	0.29
325	1.25
326	-0.25
327	-0.84
328	0.29
329	0.51
330	0.04
331	0.51
332	0.71
333	0.08
334	0.71
335	-0.81
336	-0.84
337	0.24
338	0.10
339	0.29
340	-0.35
341	-0.41
342	0.47
343	0.25
344	-0.35
345	1.10
346	-0.41
347	0.25
348	0.51
349	0.44
350	0.17
351	0.17
352	-0.84
353	0.17

```
354      0.71
355     -0.25
356      0.24
357      0.28
358     -0.25
359      0.08
360      0.14
361     -0.41
362      0.28
363      0.24
364     -0.80
365      0.08
366      0.14
367     -0.35
368      0.08
369      0.44
370      0.34
371      0.23
372      1.10
373      0.25
374      1.10
375      1.10
376      1.10
377     -0.25
378      0.14
379     -0.25
390      1.25
391     -0.25
392      0.71
393      1.10
394      1.25
395     -0.11
396      0.17
#Reported_Model_Average 0.046
#Overall_Average_Reported      0.046
```

## Output from Prosall

### Prosall Score over a window of \$winsize\_s residues

JPEG image for Prosall Score



#### Table of Verify3D scores for ordered residues across all models

```
#verify3d
#Residue\Model  only_model
8      -1.30
9       0.04
10      0.25
11      0.14
12      0.44
13      0.34
14      0.14
15      1.10
16      0.14
17     -0.46
18     -1.14
19     -0.03
20      0.44
21     -0.11
22     -0.68
23      0.71
24      0.14
25      0.51
26     -0.25
27      0.17
28      0.51
29     -0.25
30      1.25
31     -0.11
32      0.17
33     -0.25
34      0.71
35     -0.11
36      0.17
37     -0.25
38      1.10
39      0.14
40      0.51
41     -0.25
42      0.17
```

## PSVS Software Environment

43	1.10
44	0.44
45	0.25
46	1.10
47	-0.25
48	0.71
49	0.34
50	-0.25
51	0.17
52	0.17
53	-0.68
54	0.14
55	0.29
56	-0.25
57	-0.94
58	0.14
59	-0.54
60	0.08
61	0.14
62	-0.68
63	1.25
64	0.34
65	0.14
66	-0.40
67	-0.81
68	0.14
69	-0.74
70	1.10
71	-0.68
72	-1.14
73	1.10
74	0.09
75	-0.74
76	-0.68
77	-0.40
78	0.23
79	-0.84
80	1.10
81	-0.54
82	-0.80
83	0.71
84	1.25
85	0.08
86	0.47
87	0.23
88	0.47
89	0.08
90	-0.25
91	0.08
92	0.51
93	-0.54
94	1.25
95	-0.54
96	0.71
97	0.09
98	0.29
99	-0.25
100	-0.68
101	-0.25
102	-0.83
103	-0.25
104	-0.68

## PSVS Software Environment

105	-0.25
106	0.08
107	0.17
108	0.08
109	0.29
110	0.44
111	0.71
112	0.10
113	0.17
114	0.14
115	0.08
116	1.25
117	-0.68
118	-0.83
119	-0.46
120	0.08
121	1.12
122	0.44
123	0.71
124	1.10
125	0.28
126	-0.68
127	-0.68
128	-0.81
129	0.08
130	-0.25
131	-0.40
132	0.29
133	0.17
134	-0.94
135	-0.83
136	1.25
137	1.25
138	0.09
139	0.23
140	0.71
141	0.08
142	0.17
143	-0.54
144	0.71
145	0.08
146	0.29
147	0.08
148	0.23
149	0.23
150	0.17
151	-0.74
152	-0.83
153	0.71
154	1.25
155	-0.54
156	-0.25
157	-0.40
158	-0.81
159	0.20
160	0.44
161	-0.80
162	0.47
163	-0.25
164	-1.14
165	0.23
166	0.71

## PSVS Software Environment

167	0.71
168	0.08
169	0.44
170	0.14
171	0.47
172	-0.25
173	0.47
174	-0.68
175	-0.54
176	0.09
177	-0.94
178	-0.35
179	-0.54
180	1.12
181	-0.80
182	-0.68
183	-0.25
184	0.17
185	1.10
186	-0.74
187	1.10
188	-0.80
189	0.44
190	-0.54
191	-0.83
192	-0.80
193	0.23
194	-0.25
195	-0.40
196	0.08
197	0.24
198	0.44
199	0.71
200	0.51
201	1.10
202	-0.25
203	-0.74
204	-0.40
205	-0.81
206	0.23
207	0.29
208	0.25
209	0.71
210	0.44
211	0.17
212	0.25
213	0.17
214	1.12
215	-0.43
216	1.12
217	0.51
218	0.08
219	-0.74
220	0.08
221	0.08
222	-0.94
223	-0.35
224	-0.40
225	0.71
226	-0.68
227	-0.84
228	-0.25

## PSVS Software Environment

229	0.71
230	-0.74
231	-0.74
232	-0.11
233	-0.54
234	-0.68
235	-0.94
236	-0.54
237	0.08
238	-0.80
239	-0.81
240	1.25
241	1.10
242	-0.68
243	0.23
244	-0.68
245	-0.68
246	0.71
247	0.29
248	-0.41
249	0.34
250	-0.74
251	-0.41
252	-0.68
253	0.29
254	0.17
255	1.10
256	0.17
257	0.47
258	0.28
259	0.47
260	0.51
261	0.24
262	0.34
263	0.29
264	0.71
265	0.24
266	-0.54
267	0.08
268	0.24
269	0.23
270	-0.40
271	-0.68
272	-0.74
273	-0.40
274	-0.74
275	1.10
276	-0.25
277	0.71
278	-0.74
279	-0.80
280	-0.81
281	1.12
282	-0.25
283	0.44
284	-0.54
285	1.04
286	-0.94
287	0.71
288	-0.40
289	-0.94
290	-0.74

## PSVS Software Environment

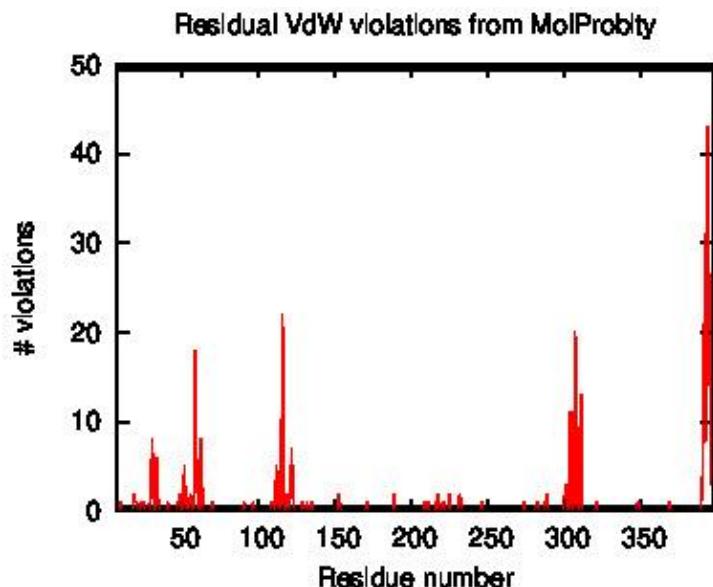
291	1.12
292	0.08
293	-0.68
294	-0.74
295	0.23
296	-0.54
297	0.51
298	0.71
299	0.71
300	0.51
301	0.44
302	-1.14
303	-0.74
304	-0.40
305	-0.25
306	-0.25
307	0.29
308	1.04
309	-0.68
310	-0.35
311	-0.54
312	-0.25
313	-0.68
314	1.10
315	1.25
316	-0.25
317	0.09
318	0.17
319	0.17
320	-0.68
321	0.09
322	-0.11
323	-0.74
324	0.29
325	1.25
326	-0.25
327	-0.84
328	0.29
329	0.51
330	0.04
331	0.51
332	0.71
333	0.08
334	0.71
335	-0.81
336	-0.84
337	0.24
338	0.10
339	0.29
340	-0.35
341	-0.41
342	0.47
343	0.25
344	-0.35
345	1.10
346	-0.41
347	0.25
348	0.51
349	0.44
350	0.17
351	0.17
352	-0.84

```
353      0.17
354      0.71
355     -0.25
356      0.24
357      0.28
358     -0.25
359      0.08
360      0.14
361     -0.41
362      0.28
363      0.24
364     -0.80
365      0.08
366      0.14
367     -0.35
368      0.08
369      0.44
370      0.34
371      0.23
372      1.10
373      0.25
374      1.10
375      1.10
376      1.10
377     -0.25
378      0.14
379     -0.25
390      1.25
391     -0.25
392      0.71
393      1.10
394      1.25
395     -0.11
396      0.17
#Reported_Model_Average 0.046
#Overall_Reported          0.046
```

## Output from MolProbit

### VdW violations from MAGE

#### JPEG image for MAGE VdW violation

**Table of MAGE VdW violations for ordered residues across all models**

```
#mage_clash
#Residue\Model  only_model
8.000 0
9.000 0
10.000 1
11.000 0
12.000 0
13.000 0
14.000 0
15.000 0
16.000 0
17.000 0
18.000 0
19.000 2
20.000 1
21.000 1
22.000 0
23.000 0
24.000 1
25.000 1
26.000 0
27.000 0
28.000 0
29.000 0
30.000 3
31.000 8
32.000 0
33.000 0
34.000 6
35.000 1
36.000 0
37.000 0
38.000 0
39.000 0
40.000 0
41.000 1
42.000 0
43.000 0
```

## PSVS Software Environment

44.000 0  
45.000 0  
46.000 0  
47.000 0  
48.000 1  
49.000 2  
50.000 0  
51.000 0  
52.000 5  
53.000 0  
54.000 0  
55.000 1  
56.000 2  
57.000 0  
58.000 0  
59.000 18  
60.000 5  
61.000 0  
62.000 0  
63.000 8  
64.000 0  
65.000 0  
66.000 0  
67.000 0  
68.000 0  
69.000 0  
70.000 1  
71.000 0  
72.000 0  
73.000 0  
74.000 0  
75.000 0  
76.000 0  
77.000 0  
78.000 0  
79.000 0  
80.000 0  
81.000 0  
82.000 0  
83.000 0  
84.000 0  
85.000 0  
86.000 0  
87.000 0  
88.000 0  
89.000 0  
90.000 0  
91.000 1  
92.000 0  
93.000 0  
94.000 0  
95.000 0  
96.000 0  
97.000 1  
98.000 0  
99.000 0  
100.000 0  
101.000 0  
102.000 0  
103.000 0  
104.000 0  
105.000 0

## PSVS Software Environment

106.000 0  
107.000 0  
108.000 0  
109.000 1  
110.000 1  
111.000 0  
112.000 5  
113.000 3  
114.000 0  
115.000 1  
116.000 22  
117.000 0  
118.000 0  
119.000 2  
120.000 0  
121.000 1  
122.000 7  
123.000 1  
124.000 0  
125.000 0  
126.000 0  
127.000 0  
128.000 0  
129.000 1  
130.000 0  
131.000 0  
132.000 1  
133.000 0  
134.000 0  
135.000 1  
136.000 0  
137.000 0  
138.000 0  
139.000 0  
140.000 0  
141.000 0  
142.000 0  
143.000 0  
144.000 0  
145.000 0  
146.000 0  
147.000 0  
148.000 0  
149.000 0  
150.000 0  
151.000 0  
152.000 0  
153.000 2  
154.000 0  
155.000 0  
156.000 0  
157.000 0  
158.000 0  
159.000 0  
160.000 0  
161.000 0  
162.000 0  
163.000 0  
164.000 0  
165.000 0  
166.000 0  
167.000 0

## PSVS Software Environment

168.000 0  
169.000 0  
170.000 0  
171.000 1  
172.000 0  
173.000 0  
174.000 0  
175.000 0  
176.000 0  
177.000 0  
178.000 0  
179.000 0  
180.000 0  
181.000 0  
182.000 0  
183.000 0  
184.000 0  
185.000 0  
186.000 0  
187.000 0  
188.000 0  
189.000 2  
190.000 0  
191.000 0  
192.000 0  
193.000 0  
194.000 0  
195.000 0  
196.000 0  
197.000 0  
198.000 0  
199.000 0  
200.000 0  
201.000 0  
202.000 0  
203.000 0  
204.000 0  
205.000 0  
206.000 0  
207.000 0  
208.000 0  
209.000 1  
210.000 0  
211.000 1  
212.000 0  
213.000 0  
214.000 0  
215.000 0  
216.000 1  
217.000 0  
218.000 2  
219.000 0  
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## PSVS Software Environment

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## PSVS Software Environment

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## PSVS Software Environment

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392.000 31
393.000 8
394.000 43
395.000 19
396.000 3
#Reported_Model_Average 0.833
#Overall_Average_Reported      0.833

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### **List of bad contacts calculated by MAGE**

5860	M	116	TYR	CD2	M	394	TYR	CD2	-1.632	0
5860	M	392	PHE	HA	M	31	PRO	CG	-1.592	0
5860	M	116	TYR	HD2	M	394	TYR	CG	-1.591	0
5860	M	116	TYR	HD2	M	394	TYR	CD2	-1.544	0
5860	M	116	TYR	CD2	M	394	TYR	CE2	-1.444	0
5860	M	394	TYR	CD1	M	116	TYR	1HB	-1.417	0
5860	M	116	TYR	CB	M	394	TYR	CD1	-1.363	0
5860	M	393	GLY	1HA	M	116	TYR	CE2	-1.359	0
5860	M	304	VAL	HA	M	307	LEU	CD2	-1.335	0
5860	M	307	LEU	1HD1	M	308	HIS	CE1	-1.330	0
5860	M	392	PHE	CA	M	31	PRO	2HG	-1.274	0
5860	M	394	TYR	CE2	M	116	TYR	CE2	-1.262	0
5860	M	116	TYR	CD2	M	394	TYR	CG	-1.243	0
5860	M	392	PHE	HA	M	31	PRO	CB	-1.229	0

### **VdW violations from MAGE**

## PSVS Software Environment

5860	M	60	THR	HA	M	394	TYR	CE1	-1.224	0
5860	M	116	TYR	CZ	M	393	GLY	1HA	-1.212	0
5860	M	60	THR	HA	M	394	TYR	CZ	-1.203	0
5860	M	394	TYR	CD2	M	59	ILE	HB	-1.185	0
5860	M	31	PRO	CG	M	392	PHE	CA	-1.145	0
5860	M	304	VAL	O	M	307	LEU	HG	-1.141	0
5860	M	392	PHE	HD2	M	31	PRO	2HB	-1.111	0
5860	M	394	TYR	CE1	M	60	THR	CA	-1.080	0
5860	M	394	TYR	CD2	M	59	ILE	CB	-1.053	0
5860	M	304	VAL	HA	M	307	LEU	3HD2	-1.049	0
5860	M	307	LEU	CD2	M	304	VAL	CA	-1.046	0
5860	M	56	ALA	HA	M	394	TYR	CB	-1.037	0
5860	M	59	ILE	CG2	M	394	TYR	CD2	-1.026	0
5860	M	311	ILE	1HG2	M	392	PHE	H	-1.021	0
5860	M	394	TYR	CG	M	59	ILE	HB	-1.020	0
5860	M	116	TYR	CD2	M	394	TYR	CZ	-1.010	0
5860	M	56	ALA	HA	M	394	TYR	1HB	-1.007	0
5860	M	395	PRO	2HB	M	34	PHE	HA	-1.007	0
5860	M	392	PHE	2HB	M	307	LEU	2HD1	-0.988	0
5860	M	59	ILE	CG2	M	394	TYR	HD2	-0.979	0
5860	M	307	LEU	3HD2	M	304	VAL	CA	-0.979	0
5860	M	307	LEU	CG	M	304	VAL	O	-0.978	0
5860	M	392	PHE	CB	M	307	LEU	2HD1	-0.974	0
5860	M	116	TYR	CE2	M	394	TYR	CD2	-0.971	0
5860	M	112	GLN	O	M	116	TYR	CD1	-0.967	0
5860	M	311	ILE	1HG2	M	392	PHE	N	-0.967	0
5860	M	60	THR	OG1	M	394	TYR	CD1	-0.961	0
5860	M	116	TYR	CB	M	394	TYR	CG	-0.952	0
5860	M	394	TYR	CD1	M	116	TYR	CD2	-0.952	0
5860	M	392	PHE	HA	M	31	PRO	2HG	-0.940	0
5860	M	308	HIS	HA	M	392	PHE	CB	-0.937	0
5860	M	308	HIS	CE1	M	307	LEU	CD1	-0.931	0
5860	M	392	PHE	HD2	M	31	PRO	CB	-0.927	0
5860	M	392	PHE	H	M	311	ILE	CG2	-0.917	0
5860	M	116	TYR	1HB	M	394	TYR	HD1	-0.899	0
5860	M	392	PHE	CD1	M	307	LEU	O	-0.898	0
5860	M	304	VAL	O	M	308	HIS	CD2	-0.897	0
5860	M	307	LEU	CD1	M	392	PHE	CD2	-0.883	0
5860	M	308	HIS	HA	M	392	PHE	1HB	-0.882	0
5860	M	394	TYR	CD1	M	116	TYR	CG	-0.877	0
5860	M	304	VAL	3HG1	M	395	PRO	1HG	-0.873	0
5860	M	308	HIS	ND1	M	392	PHE	C	-0.871	0
5860	M	394	TYR	CB	M	116	TYR	2HB	-0.863	0
5860	M	31	PRO	2HB	M	392	PHE	CD2	-0.862	0
5860	M	308	HIS	NE2	M	395	PRO	CD	-0.860	0
5860	M	116	TYR	CE2	M	393	GLY	CA	-0.855	0
5860	M	394	TYR	CE2	M	59	ILE	2HG2	-0.850	0
5860	M	116	TYR	CD2	M	394	TYR	N	-0.848	0
5860	M	307	LEU	CD2	M	304	VAL	O	-0.843	0
5860	M	31	PRO	CG	M	392	PHE	CD2	-0.840	0
5860	M	308	HIS	ND1	M	393	GLY	N	-0.837	0
5860	M	59	ILE	CD1	M	394	TYR	HA	-0.834	0
5860	M	308	HIS	2HB	M	59	ILE	CG2	-0.832	0
5860	M	392	PHE	CG	M	307	LEU	2HD1	-0.831	0
5860	M	393	GLY	CA	M	116	TYR	CZ	-0.831	0
5860	M	394	TYR	CG	M	116	TYR	CG	-0.826	0
5860	M	34	PHE	CA	M	395	PRO	2HB	-0.825	0
5860	M	392	PHE	CD1	M	311	ILE	CG1	-0.825	0
5860	M	304	VAL	HA	M	307	LEU	1HD2	-0.824	0
5860	M	395	PRO	2HD	M	308	HIS	CE1	-0.813	0
5860	M	392	PHE	CD1	M	311	ILE	2HG1	-0.807	0
5860	M	116	TYR	1HB	M	394	TYR	CE1	-0.805	0

## PSVS Software Environment

5860	M	392	PHE	CG	M	311	ILE	2HD1	-0.794	0
5860	M	60	THR	CA	M	394	TYR	CZ	-0.793	0
5860	M	116	TYR	CD2	M	394	TYR	CE1	-0.791	0
5860	M	31	PRO	2HG	M	392	PHE	CG	-0.788	0
5860	M	63	TYR	1HB	M	394	TYR	OH	-0.787	0
5860	M	394	TYR	CD2	M	59	ILE	2HG2	-0.783	0
5860	M	394	TYR	CE1	M	60	THR	OG1	-0.778	0
5860	M	304	VAL	CG1	M	395	PRO	1HD	-0.777	0
5860	M	63	TYR	CZ	M	392	PHE	O	-0.769	0
5860	M	112	GLN	O	M	116	TYR	CE1	-0.769	0
5860	M	394	TYR	CB	M	59	ILE	HB	-0.769	0
5860	M	308	HIS	NE2	M	304	VAL	3HG1	-0.767	0
5860	M	394	TYR	H	M	116	TYR	CB	-0.767	0
5860	M	55	LEU	1HD1	M	301	PRO	CB	-0.766	0
5860	M	308	HIS	CD2	M	59	ILE	3HD1	-0.766	0
5860	M	391	ALA	O	M	116	TYR	OH	-0.766	0
5860	M	116	TYR	HD1	M	116	TYR	N	-0.761	0
5860	M	394	TYR	CE1	M	60	THR	CB	-0.758	0
5860	M	392	PHE	CD2	M	307	LEU	2HD1	-0.756	0
5860	M	31	PRO	CB	M	392	PHE	CD2	-0.754	0
5860	M	56	ALA	CA	M	394	TYR	1HB	-0.753	0
5860	M	393	GLY	N	M	308	HIS	CE1	-0.752	0
5860	M	393	GLY	1HA	M	116	TYR	CD2	-0.751	0
5860	M	113	SER	HA	M	394	TYR	OH	-0.747	0
5860	M	394	TYR	CA	M	59	ILE	2HD1	-0.742	0
5860	M	392	PHE	CE2	M	31	PRO	2HD	-0.740	0
5860	M	392	PHE	N	M	63	TYR	OH	-0.736	0
5860	M	304	VAL	CA	M	307	LEU	1HD2	-0.735	0
5860	M	395	PRO	1HD	M	308	HIS	NE2	-0.733	0
5860	M	308	HIS	CE1	M	395	PRO	CD	-0.732	0
5860	M	34	PHE	CG	M	395	PRO	HA	-0.730	0
5860	M	31	PRO	1HB	M	393	GLY	N	-0.728	0
5860	M	116	TYR	CG	M	394	TYR	N	-0.725	0
5860	M	394	TYR	CE1	M	113	SER	HA	-0.725	0
5860	M	31	PRO	2HG	M	392	PHE	CB	-0.719	0
5860	M	59	ILE	2HD1	M	394	TYR	2HB	-0.713	0
5860	M	116	TYR	N	M	116	TYR	CD1	-0.712	0
5860	M	392	PHE	CD2	M	307	LEU	3HD1	-0.711	0
5860	M	30	TYR	C	M	30	TYR	CD2	-0.705	0
5860	M	113	SER	HA	M	394	TYR	CZ	-0.705	0
5860	M	116	TYR	2HB	M	394	TYR	CG	-0.704	0
5860	M	391	ALA	CB	M	112	GLN	2HG	-0.703	0
5860	M	392	PHE	CD2	M	31	PRO	2HG	-0.701	0
5860	M	34	PHE	N	M	34	PHE	CD1	-0.695	0
5860	M	395	PRO	2HB	M	34	PHE	CB	-0.690	0
5860	M	304	VAL	CG1	M	308	HIS	NE2	-0.689	0
5860	M	392	PHE	CD1	M	311	ILE	2HD1	-0.685	0
5860	M	394	TYR	CE2	M	116	TYR	HE2	-0.683	0
5860	M	307	LEU	CD2	M	304	VAL	C	-0.680	0
5860	M	31	PRO	1HG	M	391	ALA	C	-0.677	0
5860	M	31	PRO	1HG	M	391	ALA	O	-0.668	0
5860	M	392	PHE	O	M	63	TYR	OH	-0.668	0
5860	M	55	LEU	3HD1	M	395	PRO	O	-0.663	0
5860	M	394	TYR	CB	M	59	ILE	2HD1	-0.662	0
5860	M	311	ILE	HB	M	392	PHE	HD1	-0.661	0
5860	M	30	TYR	CD1	M	390	TYR	HA	-0.659	0
5860	M	311	ILE	CD1	M	392	PHE	CD1	-0.654	0
5860	M	116	TYR	2HB	M	394	TYR	1HB	-0.649	0
5860	M	304	VAL	3HG1	M	395	PRO	CG	-0.647	0
5860	M	34	PHE	CZ	M	119	GLU	HA	-0.646	0
5860	M	59	ILE	2HD1	M	394	TYR	HA	-0.644	0
5860	M	304	VAL	CG1	M	395	PRO	CG	-0.633	0

## PSVS Software Environment

5860 M 112 GLN 2HB	M 116 TYR OH	-0.631	0
5860 M 31 PRO CD	M 392 PHE CD2	-0.629	0
5860 M 395 PRO 1HG	M 304 VAL CG1	-0.628	0
5860 M 395 PRO 2HD	M 393 GLY O	-0.627	0
5860 M 31 PRO CB	M 392 PHE CA	-0.623	0
5860 M 391 ALA 3HB	M 112 GLN CD	-0.622	0
5860 M 312 ALA 2HB	M 63 TYR CE1	-0.619	0
5860 M 59 ILE 1HG2	M 308 HIS 2HB	-0.618	0
5860 M 30 TYR HD2	M 30 TYR C	-0.616	0
5860 M 34 PHE HD1	M 34 PHE N	-0.616	0
5860 M 305 ALA HA	M 308 HIS HD2	-0.616	0
5860 M 392 PHE 1HB	M 311 ILE HB	-0.615	0
5860 M 56 ALA O	M 394 TYR CD1	-0.614	0
5860 M 394 TYR HD2	M 59 ILE 1HG2	-0.608	0
5860 M 108 THR O	M 112 GLN 1HG	-0.606	0
5860 M 116 TYR CG	M 394 TYR CE1	-0.605	0
5860 M 56 ALA O	M 60 THR OG1	-0.603	0
5860 M 396 SER HA	M 52 SER O	-0.603	0
5860 M 31 PRO 2HD	M 392 PHE CD2	-0.601	0
5860 M 311 ILE CB	M 392 PHE HD1	-0.601	0
5860 M 394 TYR CD1	M 116 TYR 2HB	-0.594	0
5860 M 55 LEU 3HD2	M 59 ILE 1HD1	-0.591	0
5860 M 395 PRO CD	M 304 VAL CG1	-0.591	0
5860 M 392 PHE CE1	M 311 ILE 2HG1	-0.588	0
5860 M 392 PHE CA	M 63 TYR OH	-0.587	0
5860 M 394 TYR CB	M 56 ALA CA	-0.586	0
5860 M 31 PRO 2HG	M 392 PHE N	-0.582	0
5860 M 392 PHE 2HB	M 308 HIS CA	-0.582	0
5860 M 48 ARG O	M 396 SER 1HB	-0.581	0
5860 M 56 ALA HA	M 394 TYR 2HB	-0.581	0
5860 M 60 THR OG1	M 394 TYR HD1	-0.581	0
5860 M 395 PRO CB	M 35 PRO 2HD	-0.579	0
5860 M 307 LEU O	M 392 PHE HD1	-0.577	0
5860 M 308 HIS HA	M 392 PHE 2HB	-0.576	0
5860 M 391 ALA CA	M 311 ILE 3HD1	-0.574	0
5860 M 392 PHE CB	M 308 HIS CA	-0.572	0
5860 M 311 ILE CG2	M 63 TYR OH	-0.570	0
5860 M 307 LEU HG	M 308 HIS H	-0.563	0
5860 M 55 LEU CD2	M 59 ILE 1HD1	-0.557	0
5860 M 311 ILE 3HD1	M 391 ALA N	-0.557	0
5860 M 30 TYR CE1	M 132 LEU CD2	-0.555	0
5860 M 307 LEU CD1	M 392 PHE HD2	-0.555	0
5860 M 308 HIS CB	M 59 ILE CG2	-0.555	0
5860 M 395 PRO 2HD	M 393 GLY C	-0.554	0
5860 M 48 ARG 2HG	M 49 SER N	-0.550	0
5860 M 59 ILE C	M 394 TYR CE2	-0.550	0
5860 M 311 ILE 3HD1	M 390 TYR C	-0.549	0
5860 M 311 ILE HB	M 392 PHE CD1	-0.547	0
5860 M 59 ILE 3HG2	M 308 HIS 2HB	-0.546	0
5860 M 307 LEU CD1	M 308 HIS ND1	-0.546	0
5860 M 59 ILE 3HD1	M 394 TYR HA	-0.545	0
5860 M 308 HIS CB	M 59 ILE 1HG2	-0.542	0
5860 M 393 GLY O	M 395 PRO CD	-0.542	0
5860 M 31 PRO CG	M 392 PHE N	-0.540	0
5860 M 393 GLY H	M 308 HIS HE1	-0.540	0
5860 M 51 SER 1HB	M 52 SER HA	-0.537	0
5860 M 34 PHE 2HB	M 395 PRO 2HB	-0.536	0
5860 M 116 TYR HE2	M 392 PHE O	-0.536	0
5860 M 392 PHE CD2	M 307 LEU 1HB	-0.536	0
5860 M 35 PRO CD	M 395 PRO 2HB	-0.527	0
5860 M 31 PRO 2HB	M 307 LEU CD1	-0.526	0
5860 M 63 TYR HH	M 392 PHE C	-0.526	0

## PSVS Software Environment

5860	M	112	GLN	2HB	M	116	TYR	CZ	-0.523	0
5860	M	308	HIS	ND1	M	392	PHE	2HB	-0.520	0
5860	M	392	PHE	HD1	M	311	ILE	CG1	-0.516	0
5860	M	311	ILE	1HG2	M	391	ALA	HA	-0.511	0
5860	M	308	HIS	CG	M	59	ILE	3HD1	-0.508	0
5860	M	116	TYR	HA	M	34	PHE	HZ	-0.507	0
5860	M	307	LEU	1HD1	M	308	HIS	NE2	-0.505	0
5860	M	395	PRO	2HG	M	393	GLY	O	-0.504	0
5860	M	35	PRO	CD	M	395	PRO	CB	-0.503	0
5860	M	60	THR	HA	M	394	TYR	OH	-0.503	0
5860	M	304	VAL	C	M	307	LEU	3HD2	-0.501	0
5860	M	31	PRO	2HG	M	311	ILE	2HD1	-0.500	0
5860	M	307	LEU	3HD1	M	392	PHE	HD2	-0.499	0
5860	M	35	PRO	2HD	M	395	PRO	2HB	-0.498	0
5860	M	396	SER	CB	M	52	SER	2HB	-0.498	0
5860	M	59	ILE	HB	M	394	TYR	2HB	-0.494	0
5860	M	34	PHE	1HB	M	48	ARG	CD	-0.491	0
5860	M	31	PRO	CG	M	391	ALA	C	-0.490	0
5860	M	392	PHE	O	M	116	TYR	CE2	-0.490	0
5860	M	393	GLY	1HA	M	116	TYR	CE1	-0.489	0
5860	M	55	LEU	CD1	M	301	PRO	2HB	-0.488	0
5860	M	59	ILE	CD1	M	308	HIS	CD2	-0.484	0
5860	M	304	VAL	1HG1	M	395	PRO	1HB	-0.484	0
5860	M	392	PHE	CD1	M	311	ILE	CB	-0.484	0
5860	M	311	ILE	CG2	M	391	ALA	HA	-0.483	0
5860	M	308	HIS	N	M	307	LEU	HG	-0.482	0
5860	M	60	THR	3HG2	M	394	TYR	HE1	-0.478	0
5860	M	59	ILE	1HG2	M	308	HIS	CG	-0.476	0
5860	M	395	PRO	CB	M	304	VAL	1HG1	-0.470	0
5860	M	55	LEU	1HD1	M	301	PRO	2HB	-0.468	0
5860	M	391	ALA	CB	M	112	GLN	CG	-0.467	0
5860	M	392	PHE	CE2	M	307	LEU	1HB	-0.467	0
5860	M	49	SER	HA	M	52	SER	1HB	-0.461	0
5860	M	116	TYR	HA	M	34	PHE	CZ	-0.452	0
5860	M	312	ALA	N	M	311	ILE	2HG2	-0.449	0
5860	M	34	PHE	2HB	M	395	PRO	CB	-0.448	0
5860	M	63	TYR	OH	M	311	ILE	2HG2	-0.446	0
5860	M	394	TYR	H	M	116	TYR	2HB	-0.446	0
5860	M	392	PHE	2HB	M	307	LEU	CD1	-0.441	0
5860	M	392	PHE	1HB	M	63	TYR	OH	-0.440	0
5860	M	52	SER	2HB	M	396	SER	1HB	-0.439	0
5860	M	34	PHE	HA	M	395	PRO	CB	-0.436	0
5860	M	60	THR	3HG2	M	113	SER	1HB	-0.436	0
5860	M	307	LEU	1HD2	M	304	VAL	3HG1	-0.435	0
5860	M	112	GLN	2HG	M	391	ALA	1HB	-0.434	0
5860	M	301	PRO	1HD	M	300	ASP	HA	-0.434	0
5860	M	394	TYR	CE1	M	60	THR	N	-0.429	0
5860	M	59	ILE	O	M	394	TYR	CE2	-0.428	0
5860	M	392	PHE	CD1	M	307	LEU	C	-0.426	0
5860	M	393	GLY	O	M	395	PRO	CG	-0.425	0
5860	M	301	PRO	CB	M	55	LEU	CD1	-0.424	0
5860	M	396	SER	O	M	395	PRO	C	-0.422	0
5860	M	31	PRO	2HB	M	307	LEU	3HD1	-0.421	0
5860	M	31	PRO	N	M	30	TYR	CD2	-0.417	0
5860	M	63	TYR	OH	M	392	PHE	C	-0.417	0
5860	M	63	TYR	OH	M	392	PHE	CB	-0.416	0
5860	M	394	TYR	HE2	M	63	TYR	CD1	-0.416	0
5860	M	48	ARG	CG	M	49	SER	N	-0.414	0
5860	M	394	TYR	CD2	M	59	ILE	C	-0.414	0
5860	M	34	PHE	CE2	M	119	GLU	CB	-0.412	0
5860	M	394	TYR	HD2	M	59	ILE	CB	-0.410	0
5860	M	394	TYR	OH	M	113	SER	CA	-0.410	0

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5860	M	116	TYR	2HB	M	394	TYR	CA	-0.409	0
5860	M	311	ILE	2HG2	M	63	TYR	CZ	-0.409	0
5860	M	116	TYR	CD2	M	393	GLY	CA	-0.408	0
5860	M	311	ILE	1HG2	M	391	ALA	CA	-0.405	0
5860	M	55	LEU	2HB	M	396	SER	N	-0.404	0
5860	M	308	HIS	CD2	M	304	VAL	C	-0.402	0
5860	M	53	LEU	HA	M	56	ALA	3HB	-0.401	0
5860	M	59	ILE	2HG2	M	394	TYR	HE2	-0.401	0
5860	M	391	ALA	3HB	M	112	GLN	CG	-0.401	0
5860	M	396	SER	OG	M	52	SER	2HB	-0.401	0
5860	M	122	PRO	N	M	122	PRO	CD	-1.433	0
5860	M	121	TRP	C	M	122	PRO	CD	-1.291	0
5860	M	121	TRP	O	M	122	PRO	CD	-0.989	0
5860	M	122	PRO	2HD	M	121	TRP	O	-0.926	0
5860	M	122	PRO	C	M	122	PRO	CD	-0.685	0
5860	M	122	PRO	C	M	122	PRO	1HD	-0.673	0
5860	M	122	PRO	1HD	M	123	PHE	N	-0.644	0
5860	M	121	TRP	C	M	122	PRO	2HD	-0.576	0
5860	M	123	PHE	N	M	122	PRO	CD	-0.510	0
5860	M	221	LYS	1HG	M	218	THR	O	-0.702	0
5860	M	221	LYS	1HD	M	225	PHE	CZ	-0.570	0
5860	M	289	ILE	CG1	M	225	PHE	CE1	-0.524	0
5860	M	225	PHE	CE1	M	289	ILE	1HG1	-0.501	0
5860	M	225	PHE	CZ	M	289	ILE	2HG1	-0.475	0
5860	M	221	LYS	1HG	M	218	THR	HA	-0.463	0
5860	M	218	THR	O	M	221	LYS	CG	-0.462	0
5860	M	25	ASN	CB	M	24	ALA	HA	-0.657	0
5860	M	24	ALA	HA	M	25	ASN	1HB	-0.433	0
5860	M	32	SER	O	M	115	LYS	NZ	-0.627	0
5860	M	153	ARG	NE	M	153	ARG	HA	-0.609	0
5860	M	153	ARG	HA	M	153	ARG	CZ	-0.466	0
5860	M	165	ASP	OD2	M	171	LYS	NZ	-0.513	0
5860	M	231	VAL	HB	M	232	PRO	2HD	-0.503	0
5860	M	229	PHE	C	M	232	PRO	1HD	-0.417	0
5860	M	232	PRO	CD	M	231	VAL	N	-0.415	0
5860	M	216	TRP	1HB	M	211	SER	2HB	-0.488	0
5860	M	209	PHE	2HB	M	216	TRP	2HB	-0.473	0
5860	M	210	PRO	1HD	M	209	PHE	HA	-0.404	0
5860	M	21	PRO	2HD	M	19	GLN	C	-0.476	0
5860	M	37	ALA	1HB	M	20	PRO	1HD	-0.440	0
5860	M	20	PRO	N	M	21	PRO	2HD	-0.430	0
5860	M	20	PRO	2HD	M	19	GLN	N	-0.419	0
5860	M	186	VAL	C	M	189	PRO	1HD	-0.474	0
5860	M	188	VAL	HB	M	189	PRO	2HD	-0.473	0
5860	M	152	ASP	OD2	M	91	THR	OG1	-0.470	0
5860	M	322	PRO	1HD	M	321	ASN	N	-0.469	0
5860	M	349	PRO	1HD	M	348	ASP	HA	-0.462	0
5860	M	347	PRO	O	M	349	PRO	2HD	-0.458	0
5860	M	106	THR	1HG2	M	70	GLY	2HA	-0.461	0
5860	M	282	ALA	3HB	M	283	PRO	2HD	-0.455	0
5860	M	283	PRO	CD	M	282	ALA	N	-0.431	0
5860	M	277	PHE	2HB	M	274	VAL	HA	-0.450	0
5860	M	362	GLU	1HB	M	369	PRO	2HD	-0.440	0
5860	M	145	THR	OG1	M	97	ASN	ND2	-0.438	0
5860	M	40	ASN	O	M	41	ALA	C	-0.438	0
5860	M	158	CYS	HA	M	246	ARG	1HG	-0.431	0
5860	M	194	ALA	3HB	M	129	LYS	HA	-0.427	0
5860	M	315	TYR	HH	M	135	ASP	CG	-0.422	0
5860	M	109	LEU	N	M	110	PRO	1HD	-0.420	0
5860	M	110	PRO	CD	M	109	LEU	N	-0.419	0
5860	M	9	GLU	N	M	10	PRO	CD	-0.406	0
5860	M	284	ILE	O	M	288	VAL	3HG2	-0.404	0

# Output from PDB validation software

## Summary from PDB validation

Apr. 22, 19:15:38 2022

[ Text modified to reflect that this was run under PSVS - Aneerban Bhattacharya: Dec 2005 ]

The following checks were made on :

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### CLOSE CONTACTS

==> Distances smaller than 2.2 Angstroms are considered as close contacts  
for heavy atoms, 1.6 Angstroms for hydrogens.

Chain	Atom	Res	Seq	Chain	Atom	Res	Seq	Symm_Code	Distance
A	CD2	TYR	116	-	B	CD2	TYR	5	( 1, 5, 5, 5)
A	OH	TYR	116	-	B	O	ALA	2	( 1, 5, 5, 5)
A	CD2	TYR	116	-	B	CE2	TYR	5	( 1, 5, 5, 5)
A	CD2	TYR	116	-	B	CG	TYR	5	( 1, 5, 5, 5)
A	OH	TYR	63	-	B	O	PHE	3	( 1, 5, 5, 5)
A	CB	TYR	116	-	B	CD1	TYR	5	( 1, 5, 5, 5)
A	O	VAL	304	-	A	CG	LEU	307	( 1, 5, 5, 5)
A	O	GLN	112	-	A	CD1	TYR	116	( 1, 5, 5, 5)
A	O	ALA	56	-	A	OG1	THR	60	( 1, 5, 5, 5)
A	OG1	THR	60	-	B	CD1	TYR	5	( 1, 5, 5, 5)

### DISTANCES AND ANGLES

We have checked your intra and intermolecular distances and angles with the procedures currently in place at PDB:

==> Bond and angle checks are performed by first computing the average rms error for all bonds and angles relative to standard values for nucleotide units [L. Clowney et al., Geometric Parameters in Nucleic Acids: Nitrogenous Bases, J.Am.Chem.Soc. 1996, 118, 509-518; A. Gelbin et al., Geometric Parameters in Nucleic Acids: Sugar and Phosphate Constituents, J.Am.Chem.Soc. 1996, 118, 519-529] and amino acid units [R.A. Engh and R. Huber, Accurate Bond and Angle Parameters for X-ray protein structure refinement, Acta Crystallogr. 1991, A47, 392-400]. Any bond or angle which deviates from the dictionary values by more than six times this computed rms error is identified as an outlier.

\*\*\* Covalent Bond Lengths:

The RMS deviation for covalent bonds relative to the standard dictionary is 0.013 Angstroms

The following table contains a list of the covalent bonds greater than 6.0\*RMSD.

## PSVS Software Environment

Deviation	Residue	Chain	Sequence	AT1	-	AT2	Bond	Dictionary
	Name	ID	Number				Distance	Value
-0.113	PRO	A	31	CD	-	N	1.360	1.473
-0.097	PRO	A	122	CB	-	CG	1.395	1.492
0.245	PRO	A	122	CD	-	N	1.718	1.473
-0.162	PRO	B	6	CD	-	N	1.311	1.473

\*\*\* Covalent Angle Values:

The RMS deviation for covalent angles relative to the standard dictionary is 1.8 degrees.

The following table contains a list of the covalent bond angles greater than 6.0\*RMSD.

Deviation	Residue	Chain	Sequence	AT1	-	AT2	-	AT3	Bond	Dictionary
	Name	ID	Number						Angle	Value
15.0	ASN	A	25	C	-	N	-	CA	136.7	121.7
33.0	ALA	A	39	C	-	N	-	CA	154.7	121.7
-30.4	PRO	A	122	CA	-	N	-	CD	81.6	112.0
44.4	PRO	A	122	C	-	N	-	CA	167.0	122.6
30.3	GLY	A	124	C	-	N	-	CA	150.9	120.6

### TORSION ANGLES

The torsion angle distributions have been checked. The postscript file of the conformation rings showing the torsion angle distributions will be sent in a separate E-mail message.

### CHIRALITY

The chirality has been checked. O1P, O2P, and hydrogen atoms which do not follow the convention defined in the IUBMB (Liebecq, C. Compendium of Biochemical Nomenclature and Related Documents, 2nd ed.; Portland Press: London and Chapel Hill, 1992) and IUPAC nomenclature (J.L. Markley, A. Bax, Y. Arata, C.W. Hilbers, R. Kaptein, B.D. Sykes, P.E. Wright and K. Wüthrich, Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids, Pure & Appl. Chem., Vol. 70, pp. 117–142, 1998) have been standardized. Any other stereochemical violations are listed below.

### OTHER IMPORTANT ISSUES

Final\_model\_1.pdb: Missing KEYWDS records

Final\_model\_1.pdb: Missing TITLE record