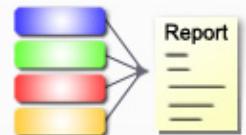


Protein Structure Validation Suite (PSVS)

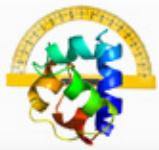


PSVS report for Final_refined_model

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PSVS report for Final_refined_model



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	Ghostsript 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

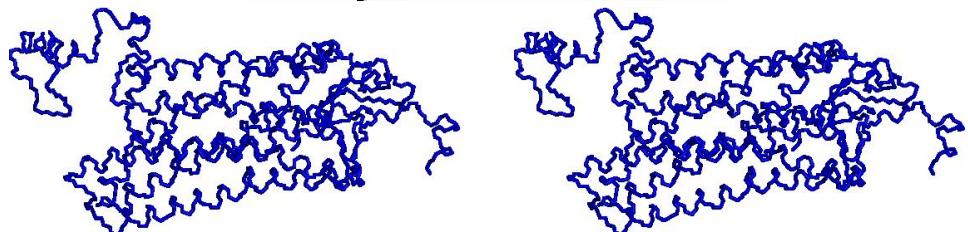
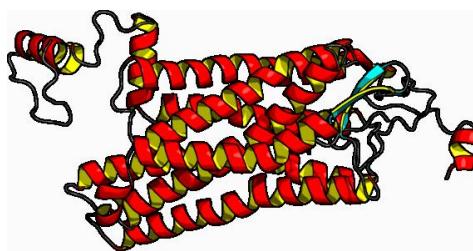
Organism:

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 residues³ 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 residues³ from Richardson Lab's Molprobity

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

92% 4.8% 3.2%

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity	Clashscore
---------	----------	---------------	---------------------------------	-----------------------------	------------	------------

Raw score	0.04	0.08	0.05	0.09	21.16
-----------	------	------	------	------	-------

Z-score ¹	-6.74	-2.36	0.51	0.53	-2.11
----------------------	-------	-------	------	------	-------

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

Number of close contacts (within 2.2 Å): 0

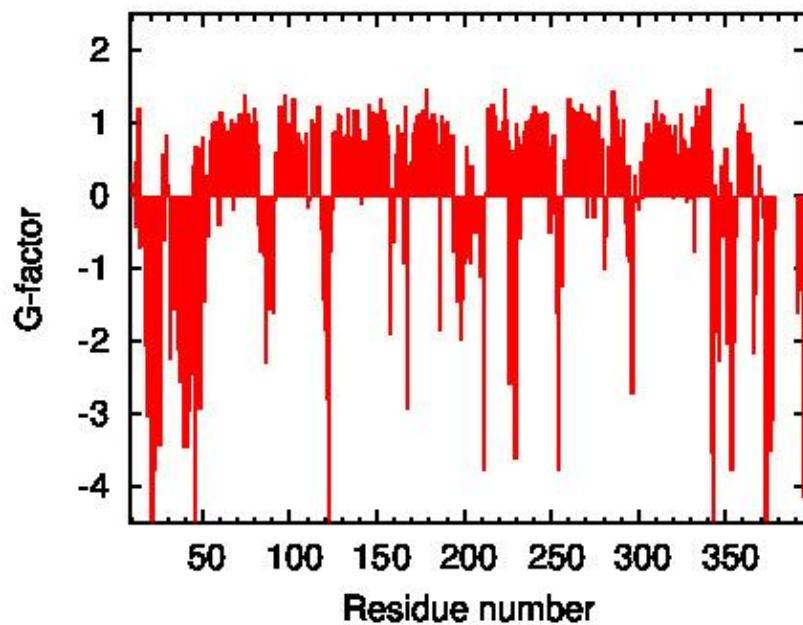
RMS deviation for bond angles: 1.8 °

RMS deviation for bond lengths: 0.012 Å

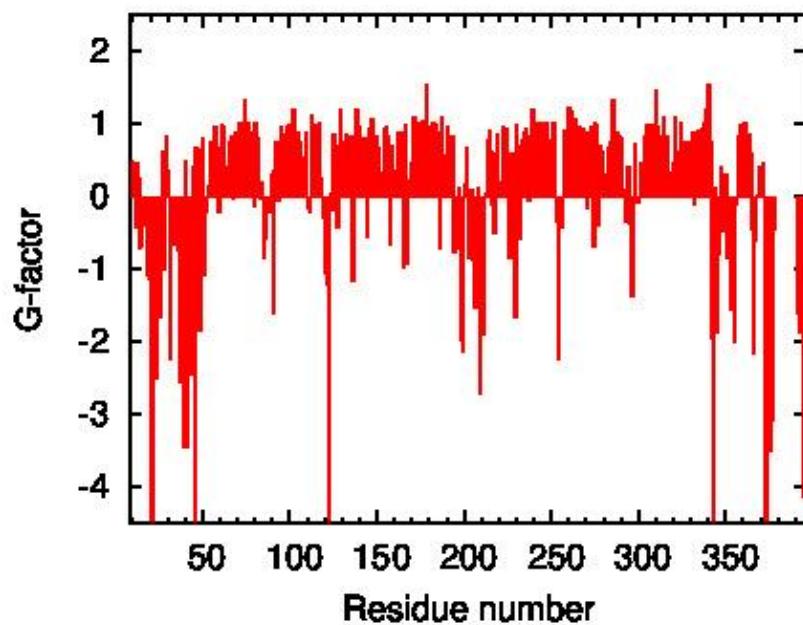
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

³Selected residues: all

Procheck G-factor for phi-psi

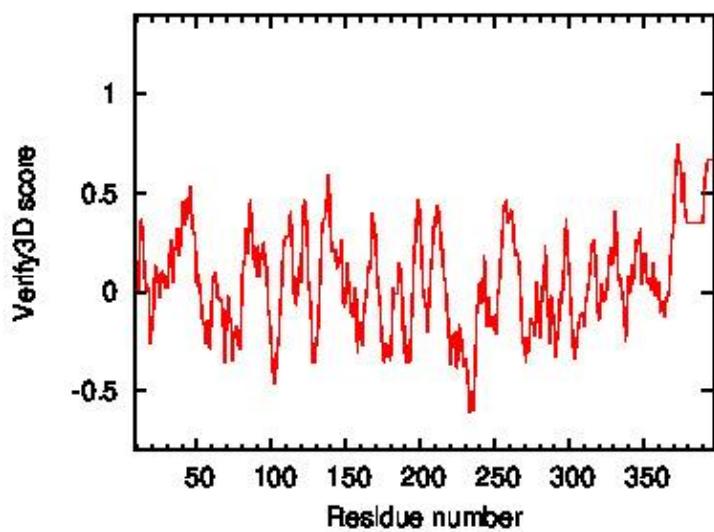


Procheck G-factor for all dihedral angles

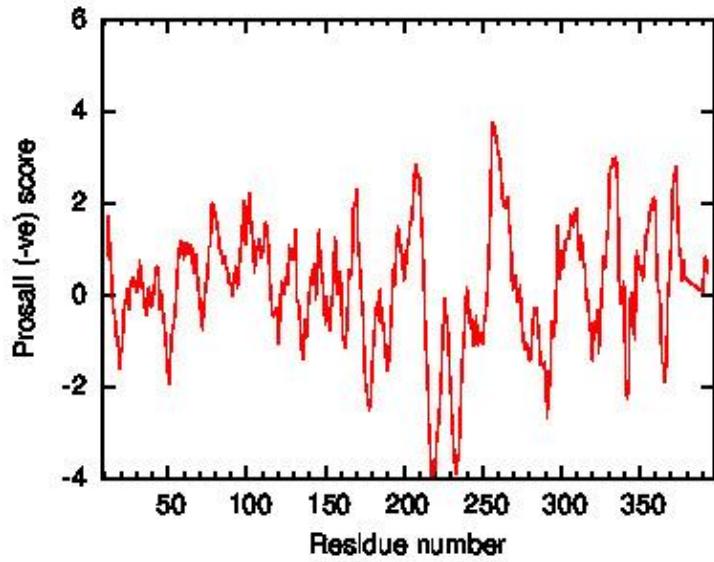


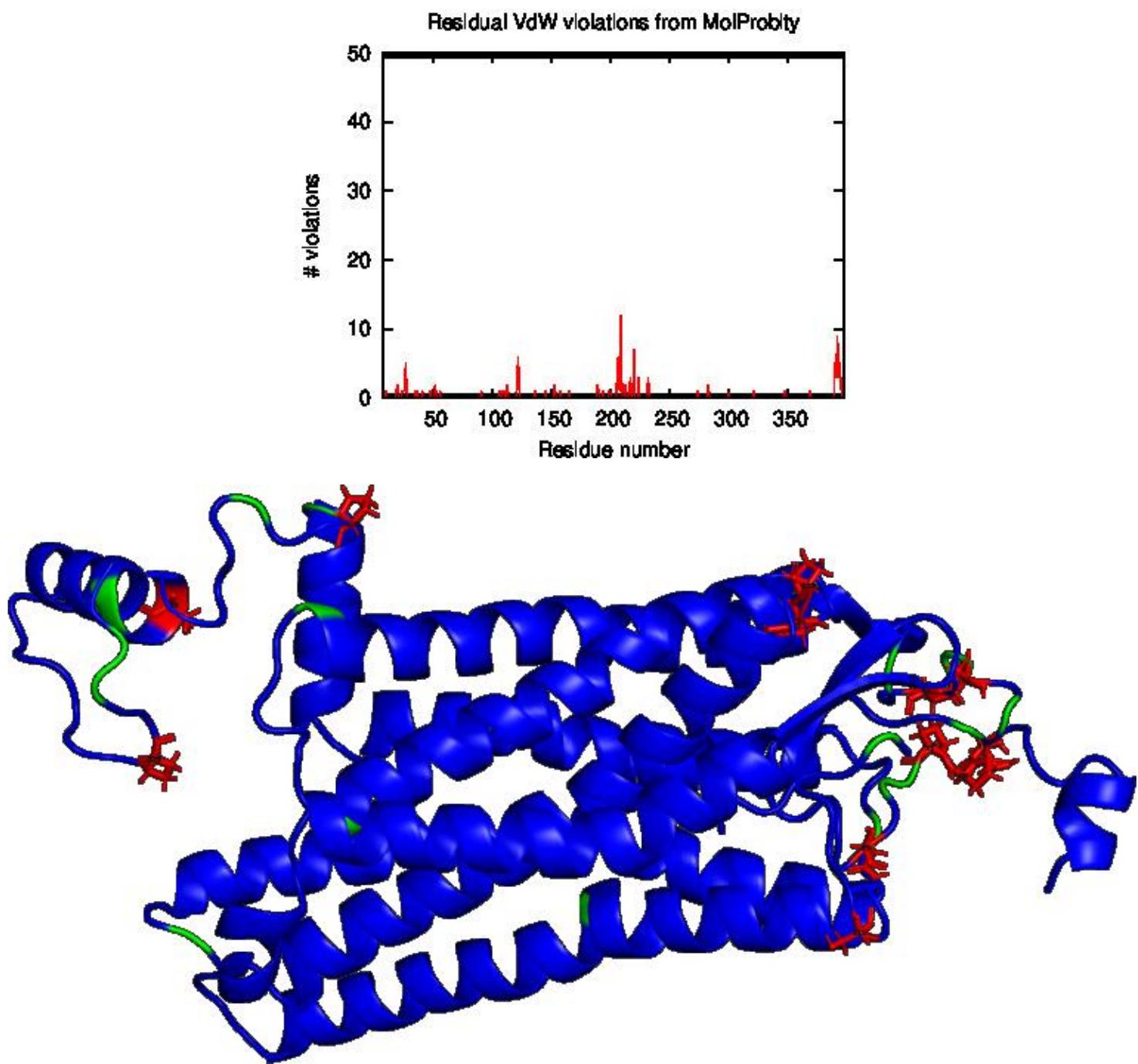
PSVS Software Environment

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:

1. Bhattacharya A, Tejero R and Montelione GT, "Evaluating protein structures determined by structural genomics consortia". *Proteins* 2007, 66:778-795
2. Tejero R, Snyder D, Mao B, Aramini JM and Montelione GT, "PDBStat: a universal restraint converter and restraint analysis software package for protein NMR". *J Biomol NMR* 2013, 56:337-351
3. Luthy R, Bowie JU and Eisenberg D, "Assessment of protein models with three-dimensional profiles". *Nature* 1992, 356:83-85
4. Bowie JU, Luthy R and Eisenberg D, "A Method to identify protein sequences that fold into a known three-dimensional structure". *Science* 1991, 253:164-169

PSVS Software Environment

5. Sippl MJ, "Recognition of errors in three-dimensional structures of proteins". *Proteins* 1993, 17:355-362
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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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9. Word JM et al, "Exploring steric constraints on protein mutations using MAGE / PROBE". *Prot Sci* 2000, 9:2251-2259
10. Word JM et al, "Asparagine and glutamine: using hydrogen atom contacts in the choice of side-chain amide orientation". *J Mol Biol* 1999, 285:1735-1747
11. Word JM et al, "Visualizing and quantifying molecular goodness-of-fit: small-probe contact dots with explicit hydrogens". *J Mol Biol* 1999, 285:1711-1733
12. Luthy R, McLachlan AD and Eisenberg D, "Secondary structure-based profiles: use of structure-conserving scoring tables in searching protein sequence databases for structural similarities". *Proteins* 1991, 18:229-239
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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 ^g
Procheck G-factor ^e (phi / psi only)	0.05	N/A	0.51
Procheck G-factor ^e (all dihedral angles)	0.09	N/A	0.53
Verify3D	0.04	0.0000	-6.74
ProsaII (-ve)	0.08	0.0000	-2.36
MolProbity clashscore	21.16	0.0000	-2.11
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	92%		
Allowed regions	4.8%		
Disallowed regions	3.2%		

^f Residues selected based on: all residues

Selected residue ranges: all

^g 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_refined_model by PSVS

Output from PDBStat

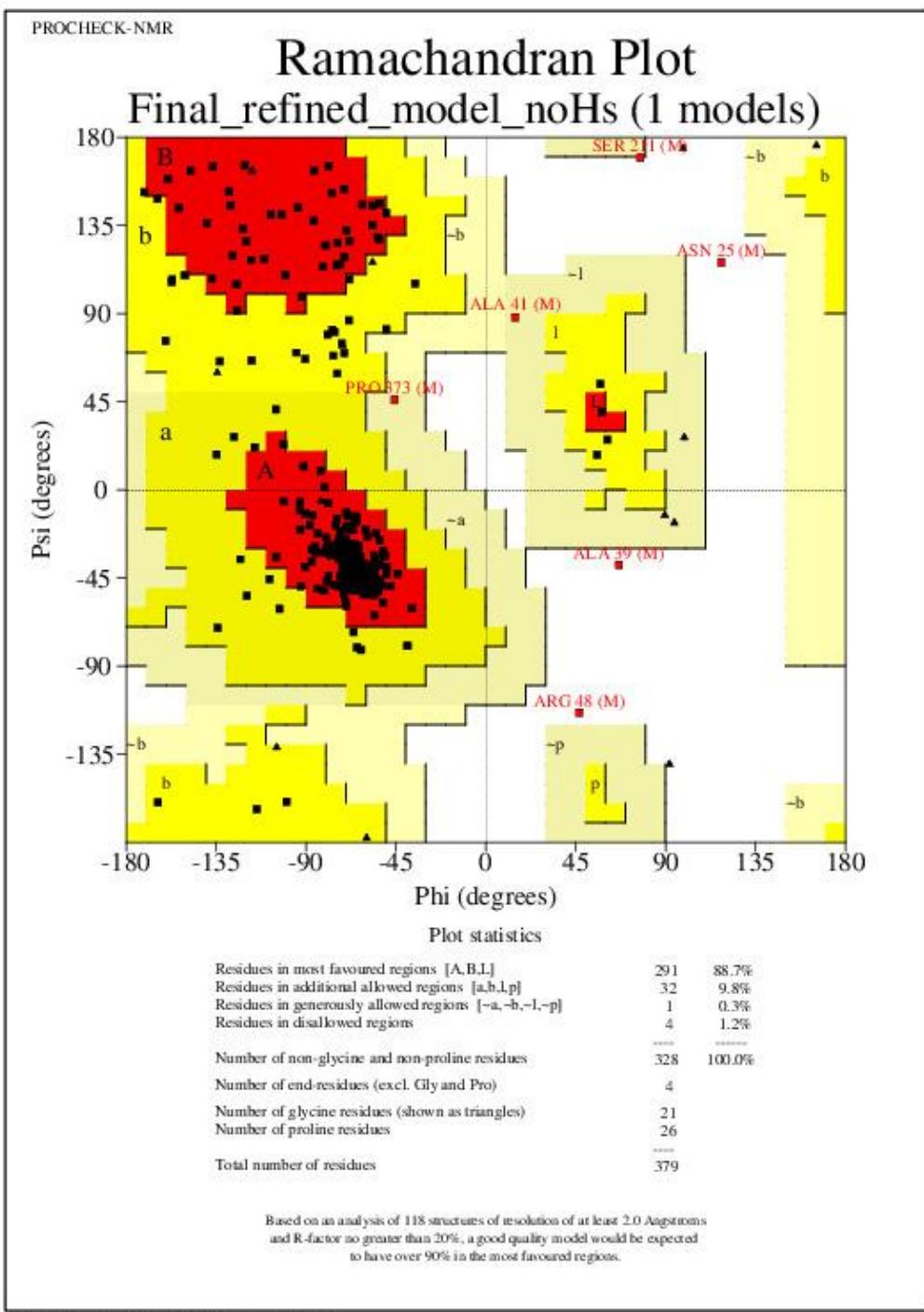
Output from PROCHECK

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_refined_model_noHs_000.rin     0.0                               379 residues |
|                                         |
*| Ramachandran plot:    88.7% core      9.8% allow      0.3% gener      1.2% disall |
|                                         |
*| All Ramachandrans:    20 labelled residues (out of 375)           |
+| Chil-chi2 plots:        3 labelled residues (out of 190)           |
```

JPEG image for all model Ramachandran Plot



Final_refined_model_noHs_01_ramachand.ps

Residue Properties for all models

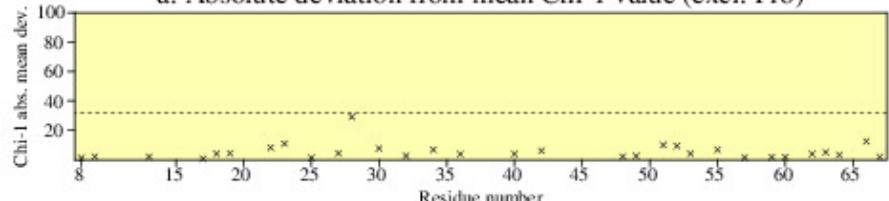
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

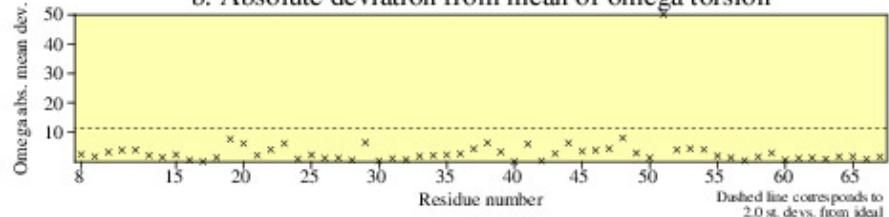
Page 1

Residue properties Final_refined_model_noHs (1 models)

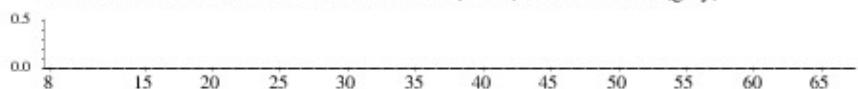
a. Absolute deviation from mean Chi-1 value (excl. Pro)



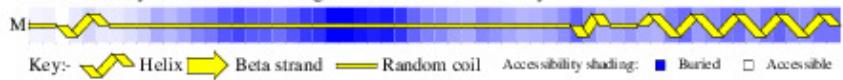
b. Absolute deviation from mean of omega torsion



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



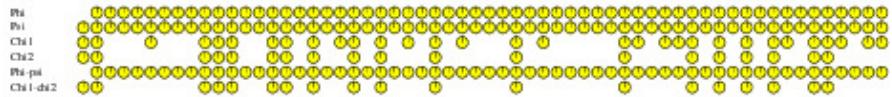
d. Secondary structure & average estimated accessibility



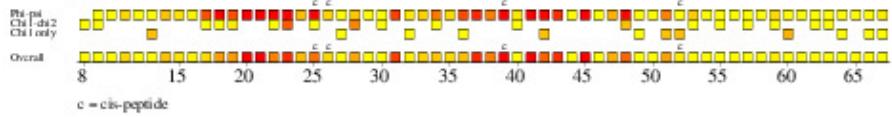
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



Final_refined_model_noHs_10_residprop.ps

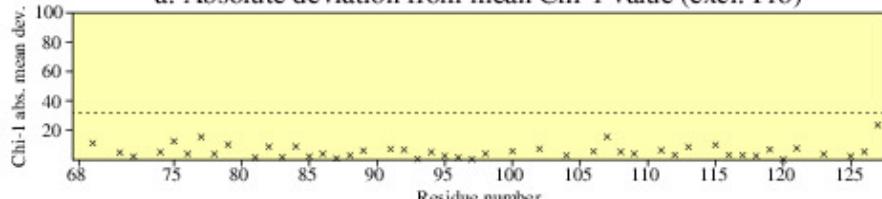
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

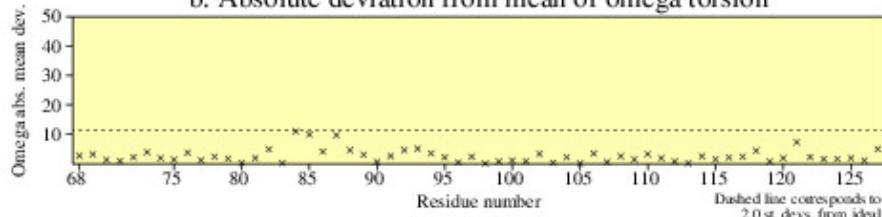
Page 2

Residue properties Final_refined_model_noHs (1 models)

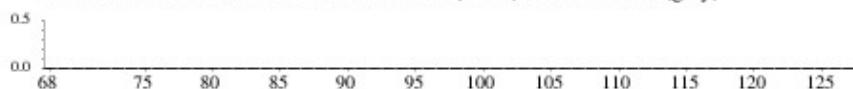
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



d. Secondary structure & average estimated accessibility



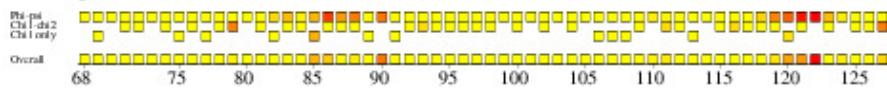
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



Final_refined_model_noHs_10_residprop.ps

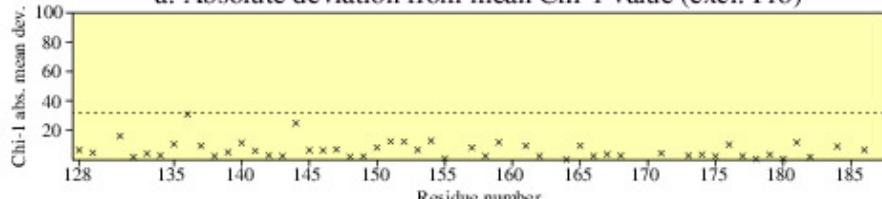
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

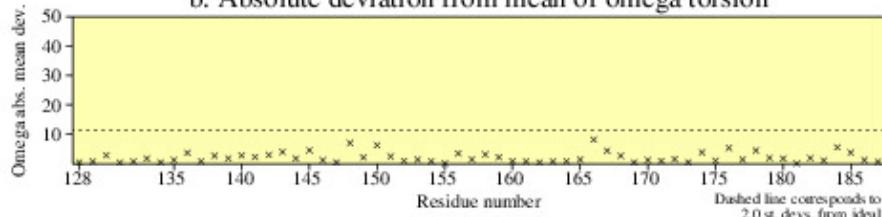
Page 3

Residue properties Final_refined_model_noHs (1 models)

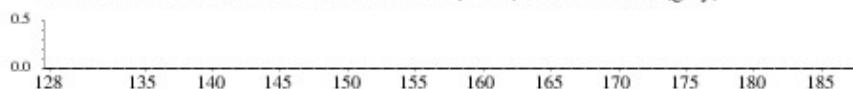
a. Absolute deviation from mean Chi-1 value (excl. Pro)



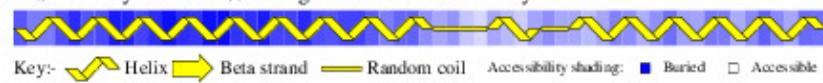
b. Absolute deviation from mean of omega torsion



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



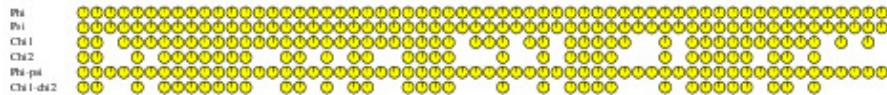
d. Secondary structure & average estimated accessibility



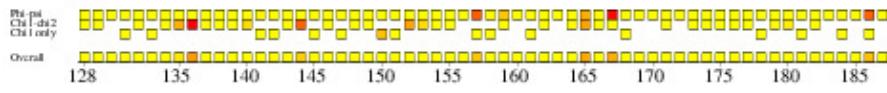
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



Final_refined_model_noHs_10_residprop.ps

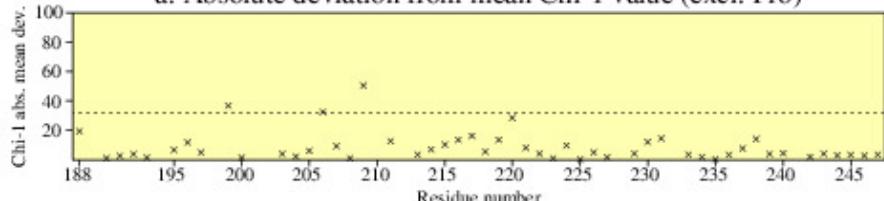
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

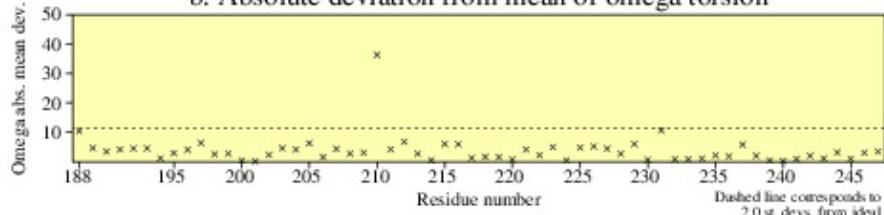
Page 4

Residue properties Final_refined_model_noHs (1 models)

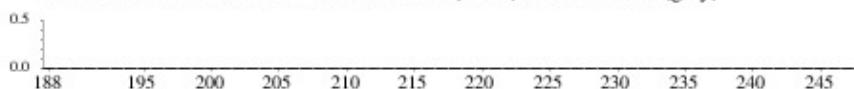
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



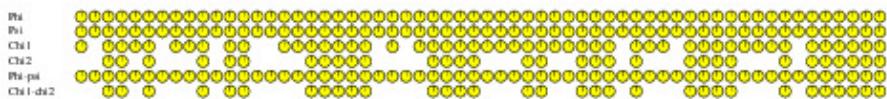
d. Secondary structure & average estimated accessibility



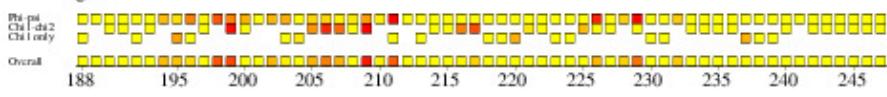
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



Final_refined_model_noHs_10_residprop.ps

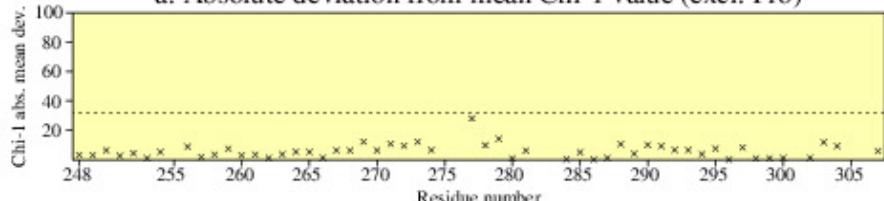
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

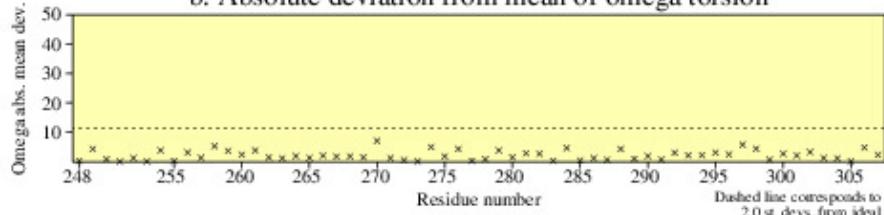
Page 5

Residue properties Final_refined_model_noHs (1 models)

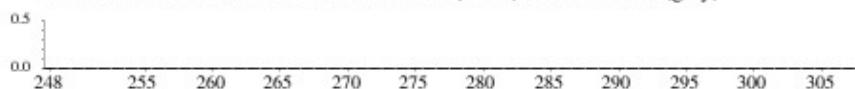
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



d. Secondary structure & average estimated accessibility



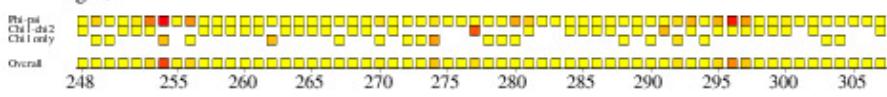
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



Final_refined_model_noHs_10_residprop.ps

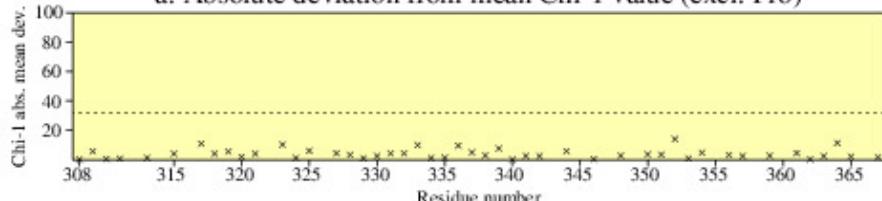
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

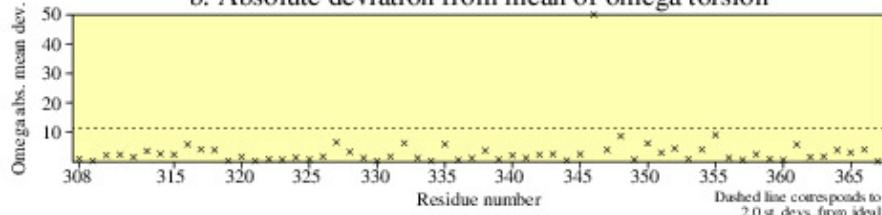
Page 6

Residue properties Final_refined_model_noHs (1 models)

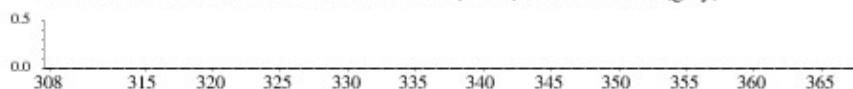
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



d. Secondary structure & average estimated accessibility



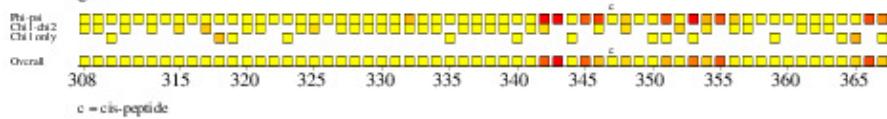
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



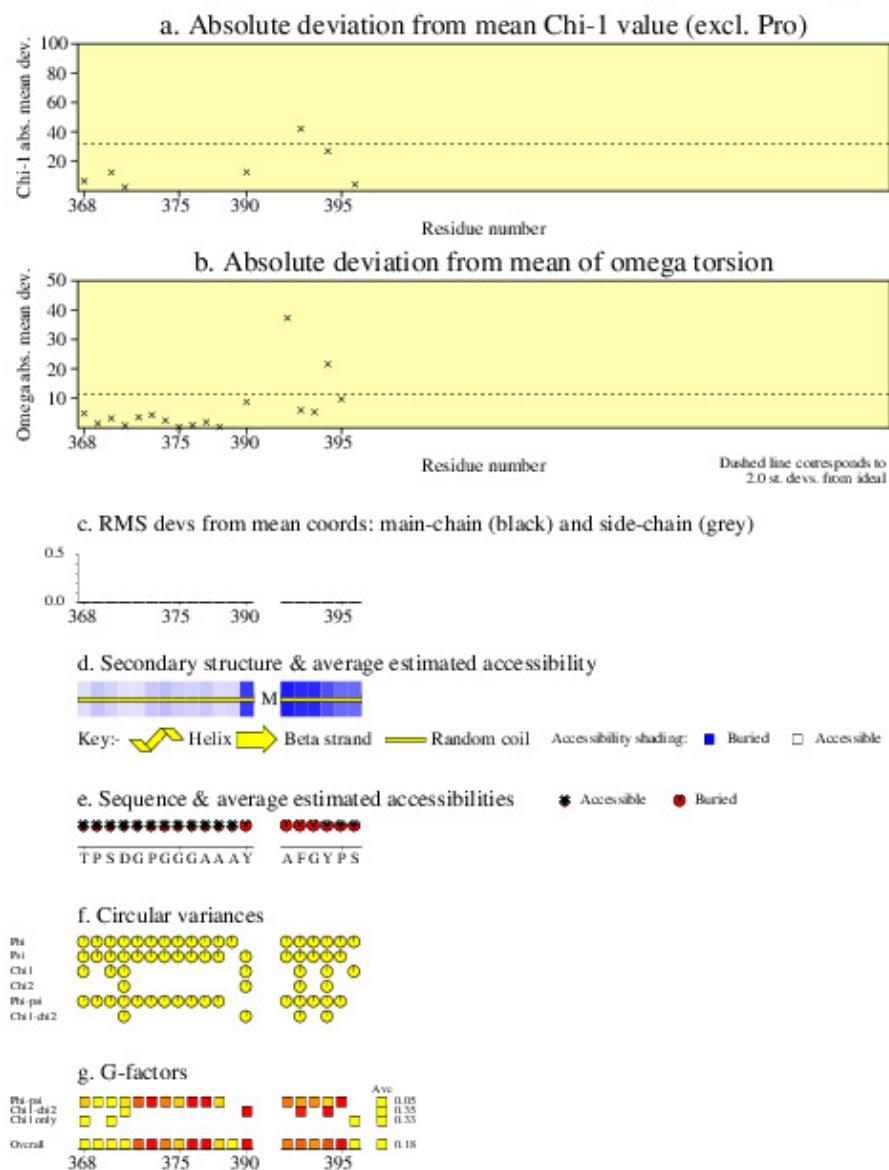
Final_refined_model_noHs_10_residprop.ps

JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

Page 7

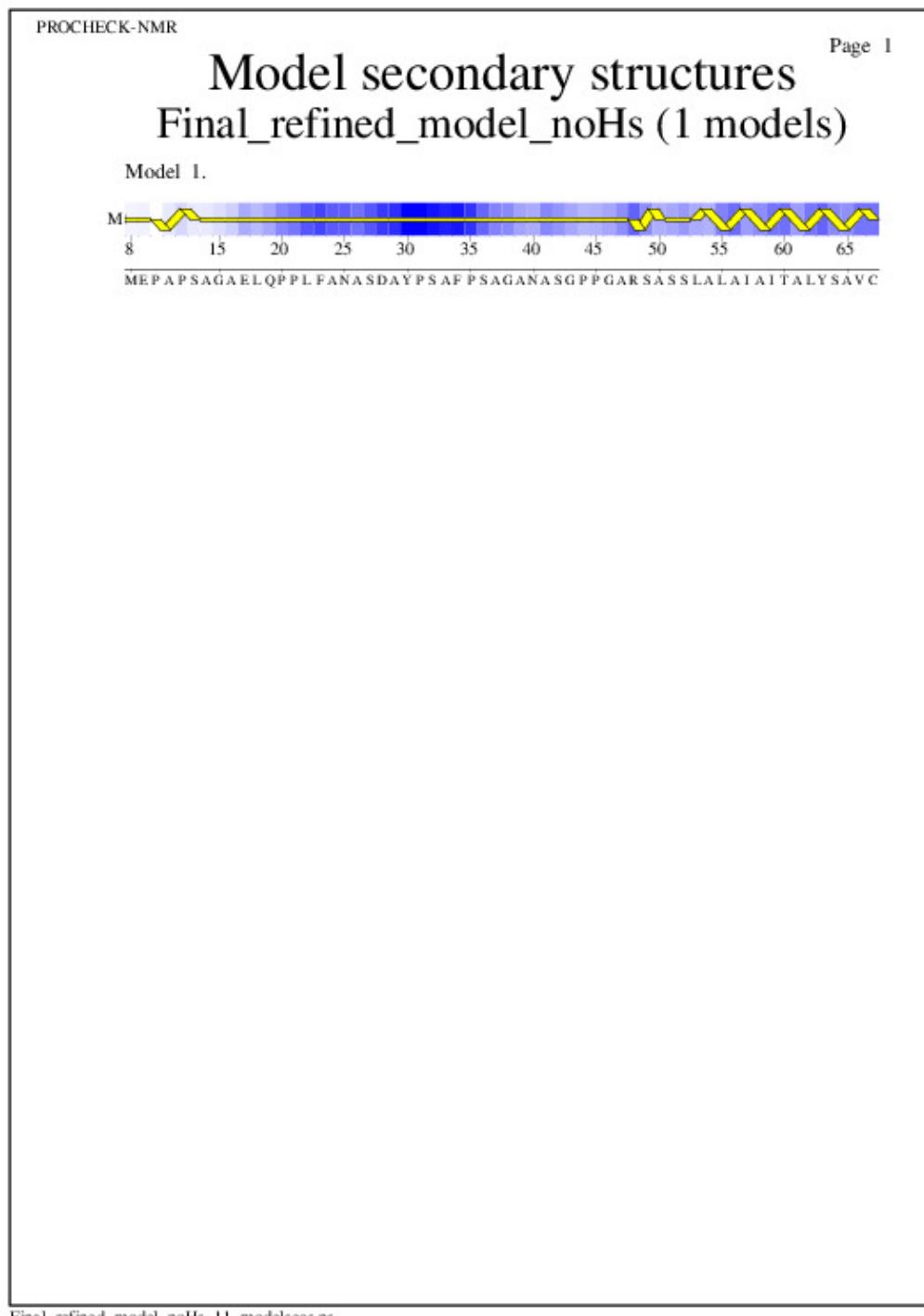
Residue properties Final_refined_model_noHs (1 models)



Final_refined_model_noHs_10_residprop.ps

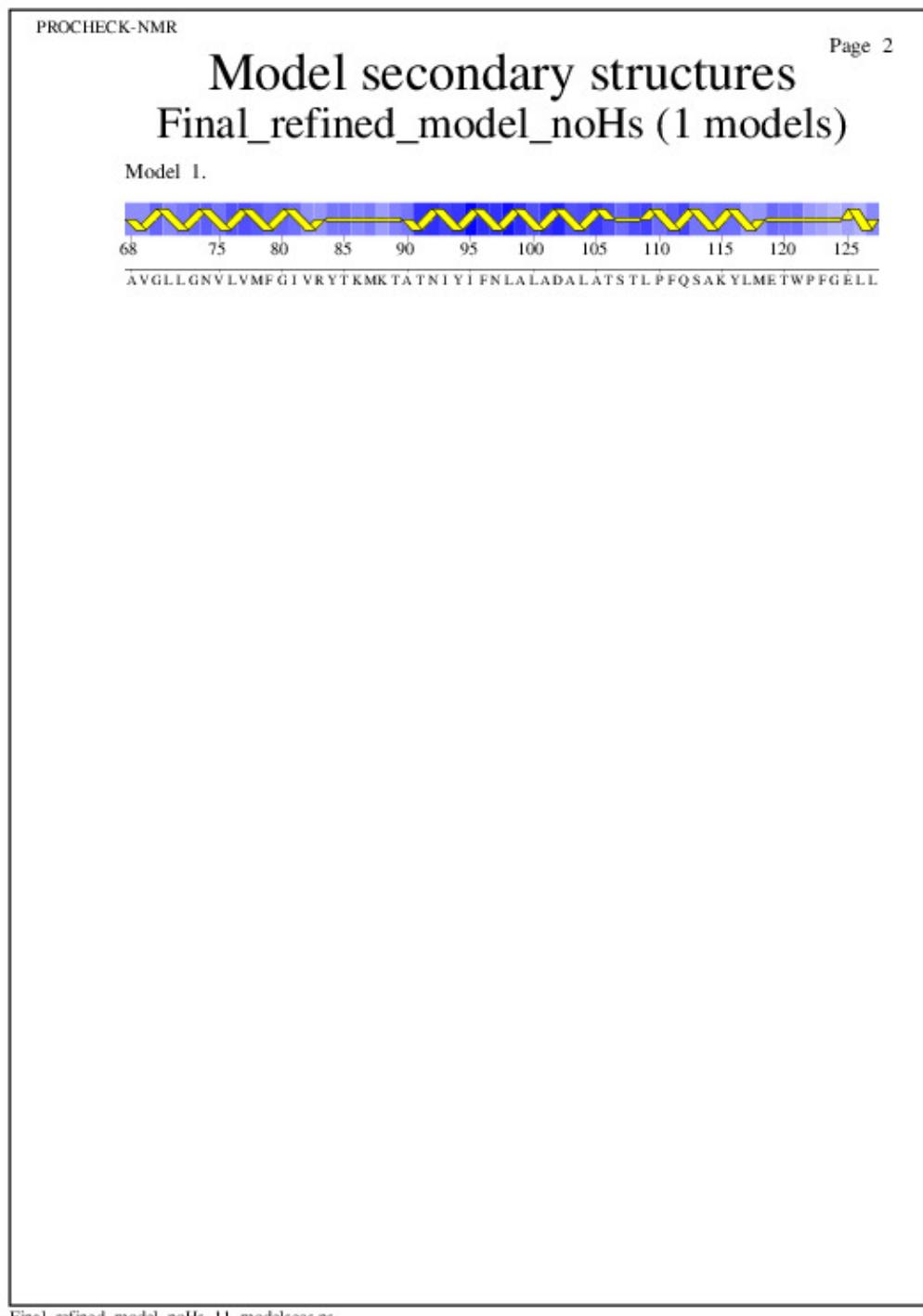
Model Secondary Structures from Procheck

JPEG for Model Secondary Structures - page \$num_n



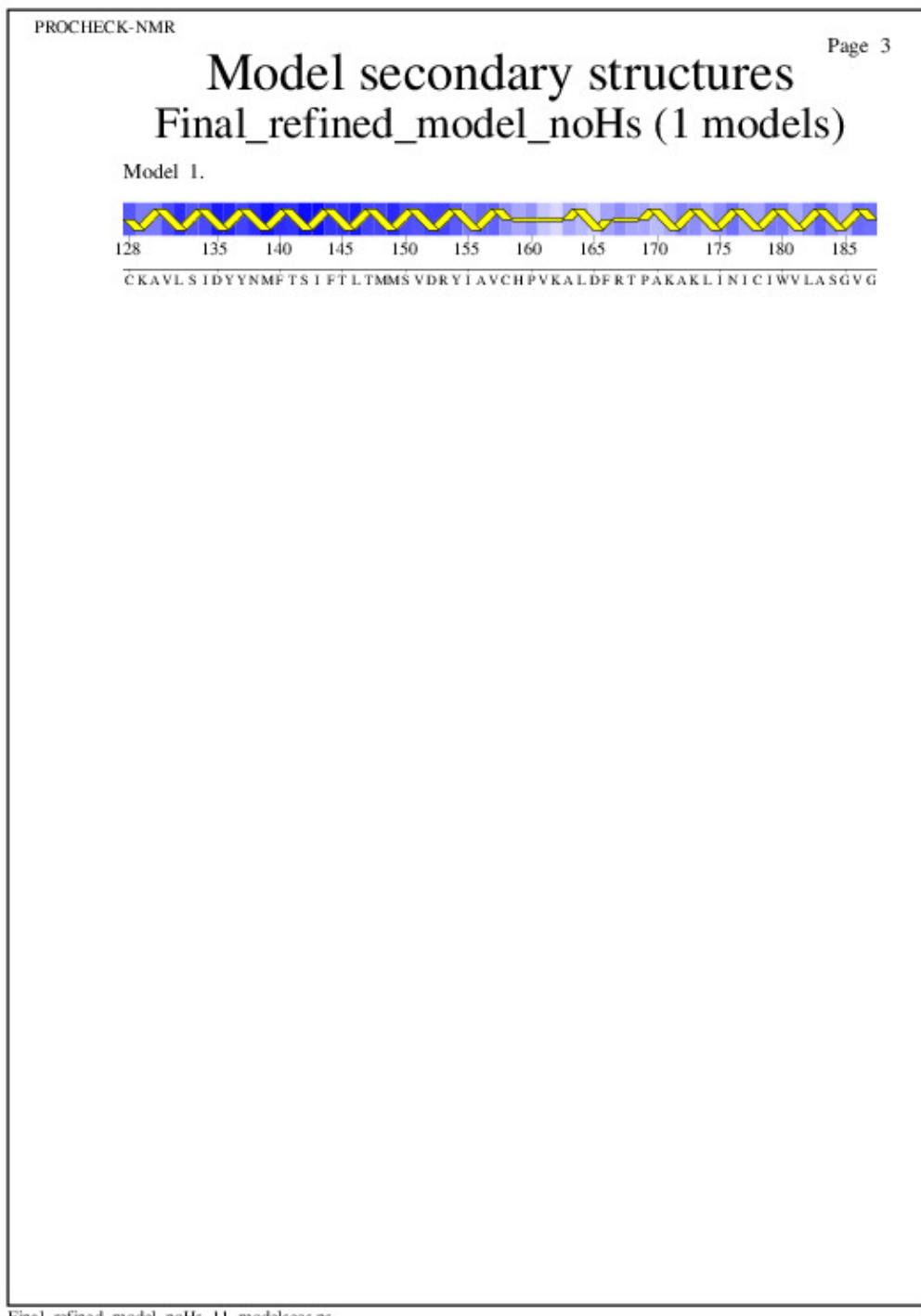
Final_refined_model_noHs_11_modelsecs.ps

JPEG for Model Secondary Structures - page \$num_n



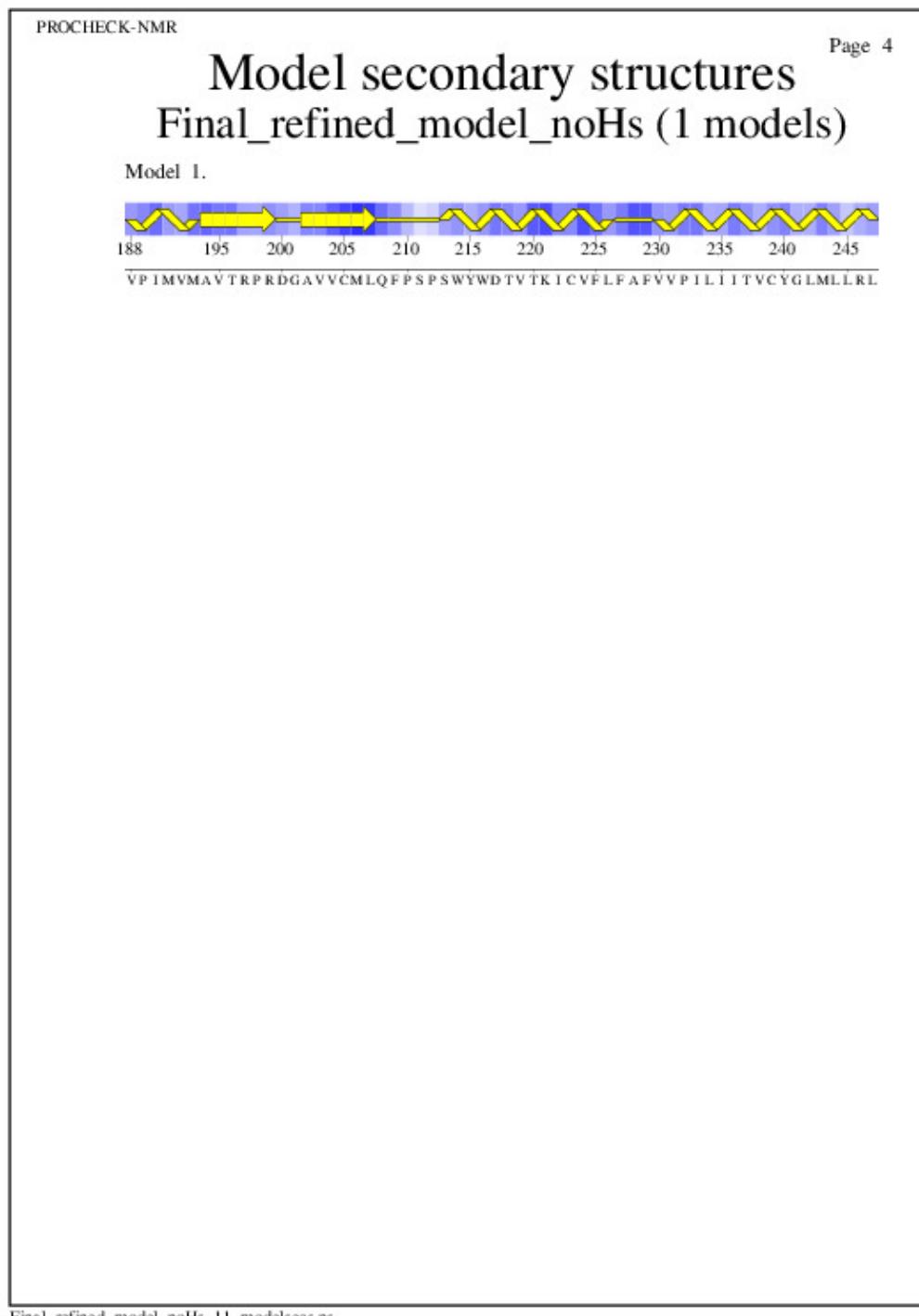
Final_refined_model_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n



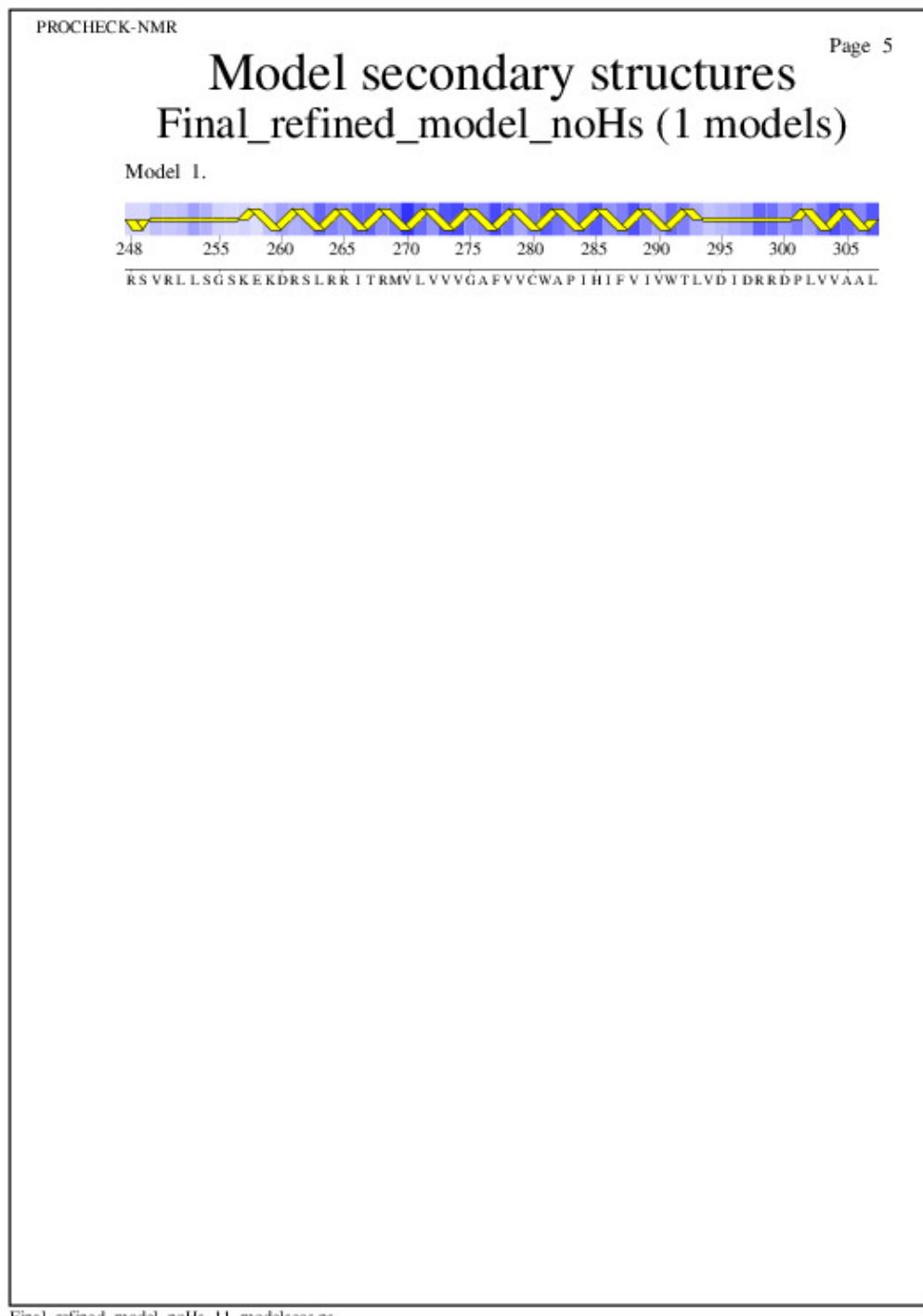
Final_refined_model_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n



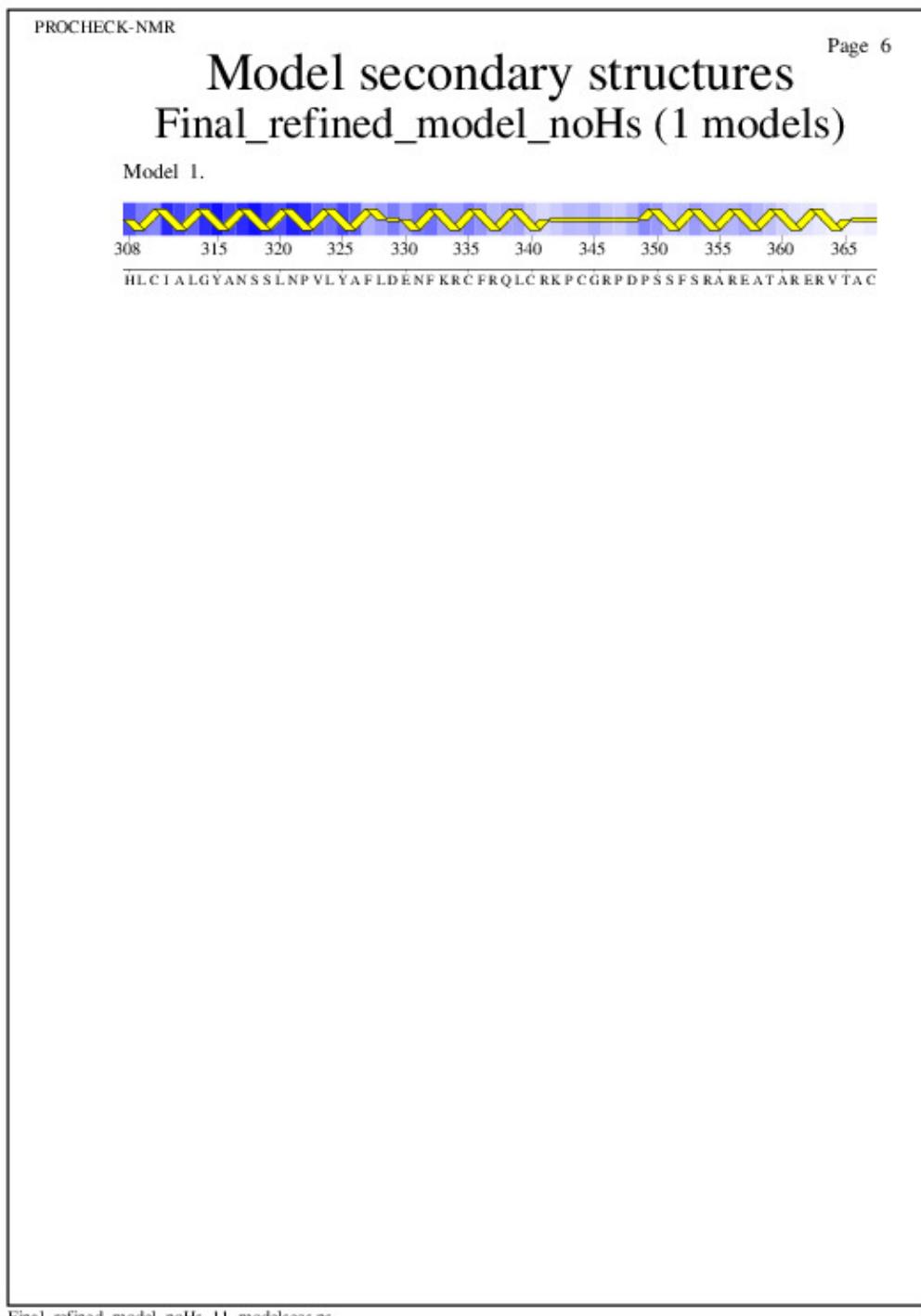
Final_refined_model_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n



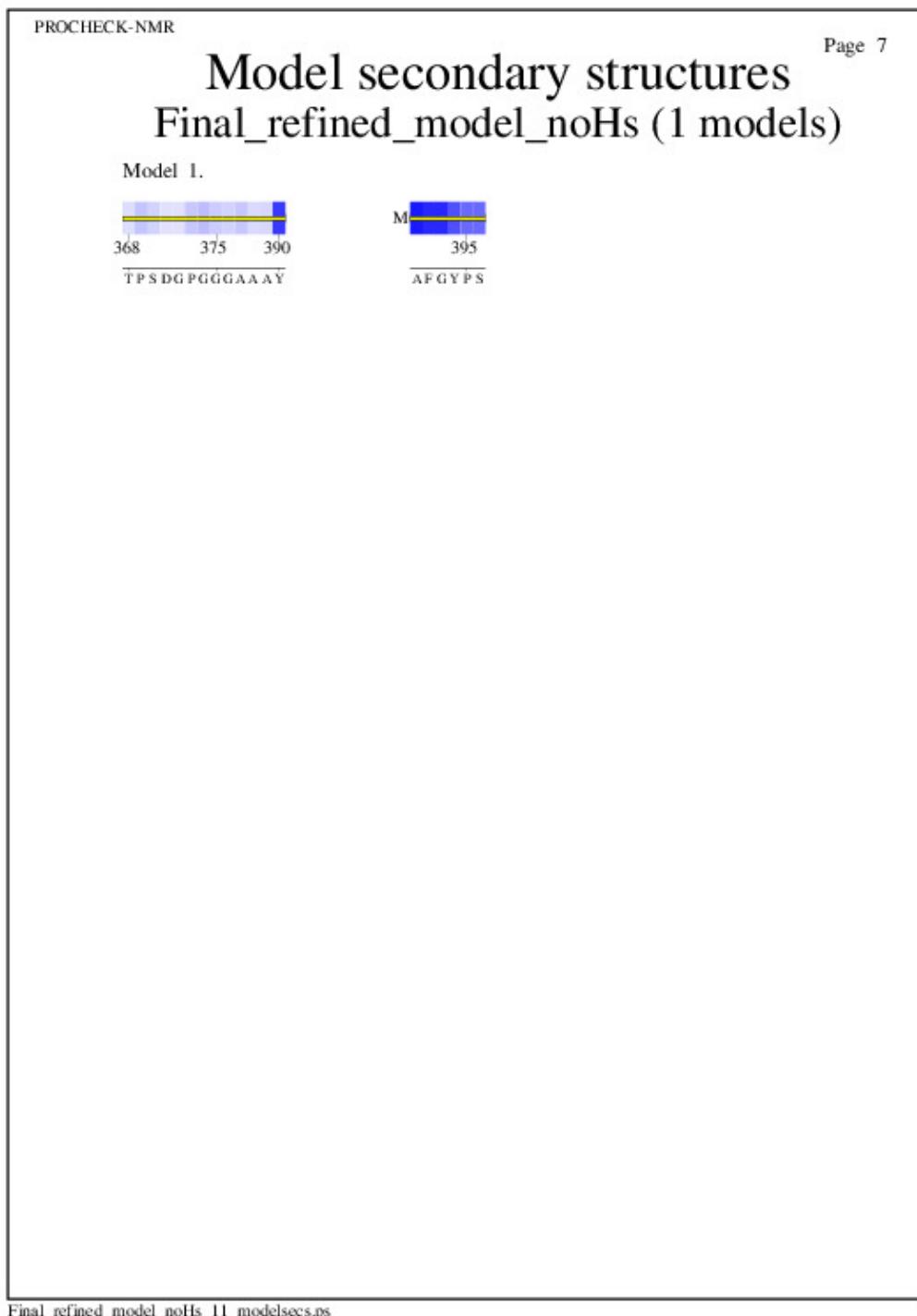
Final_refined_model_noHs_11_modelsecs.ps

JPEG for Model Secondary Structures - page \$num_n



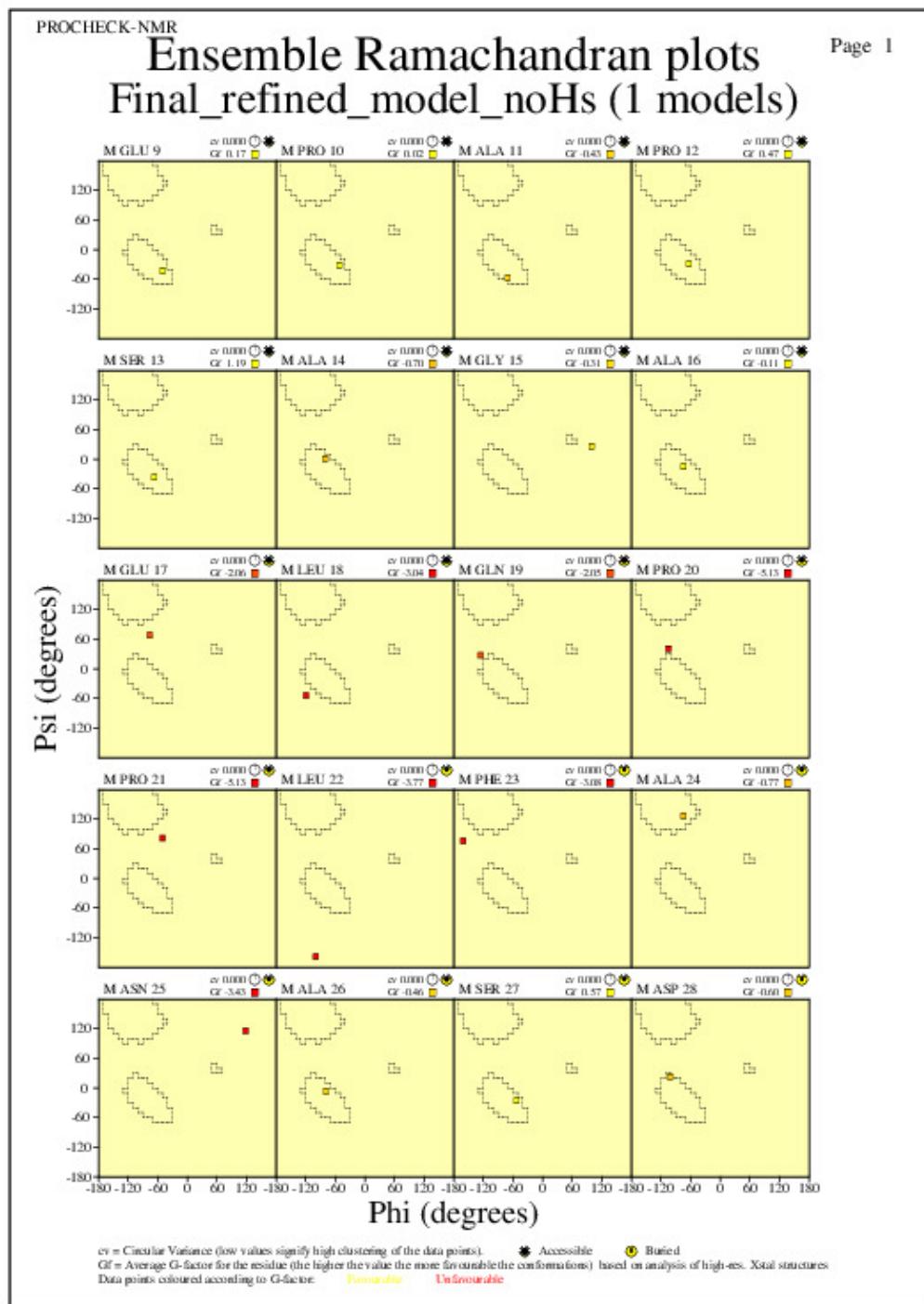
Final_refined_model_noHs_11_modelsecs.ps

JPEG for Model Secondary Structures - page \$num_n



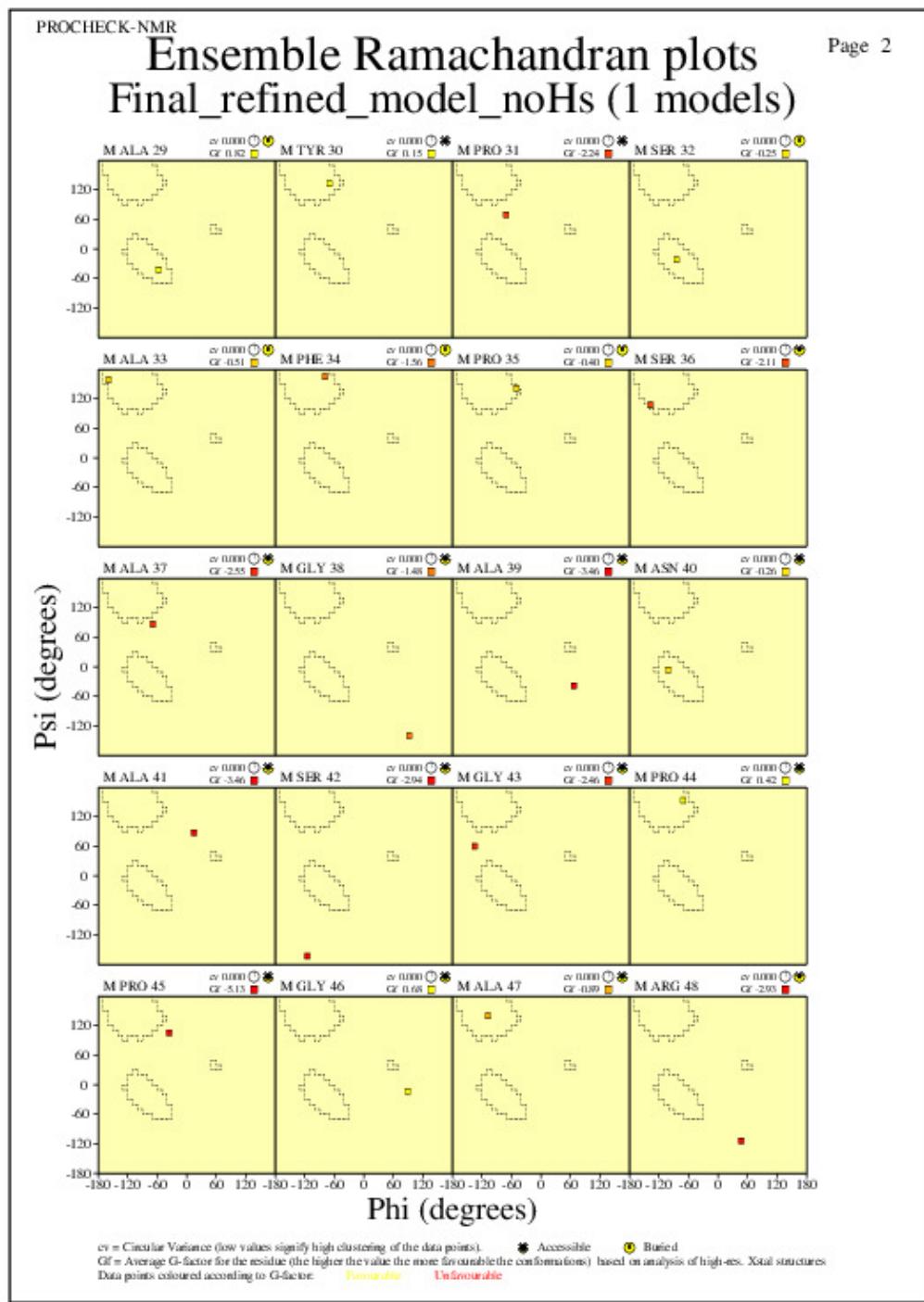
Ramachandran Plots for each residue

JPEG for residue Ramachandran Plots - page \$num_n



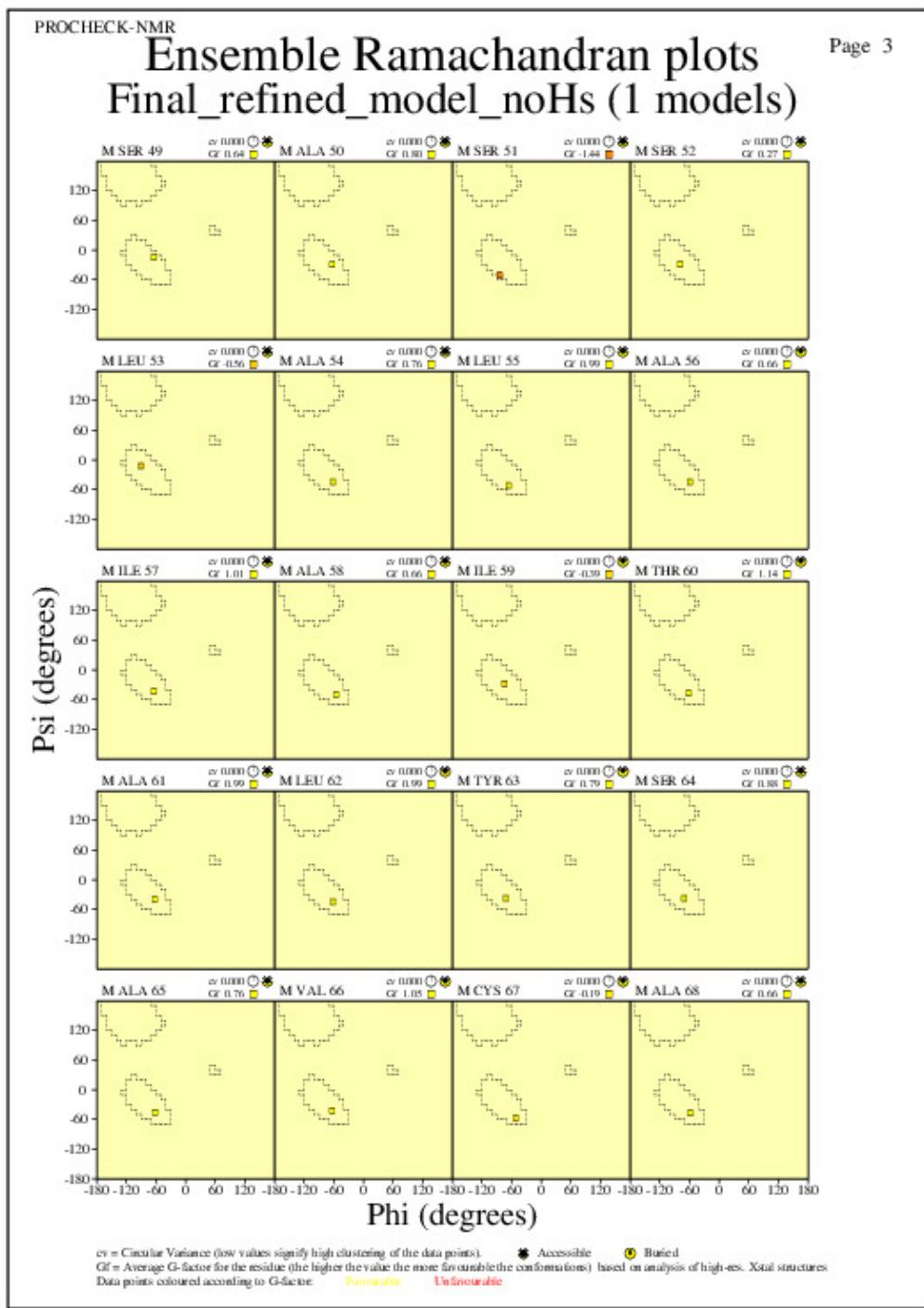
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



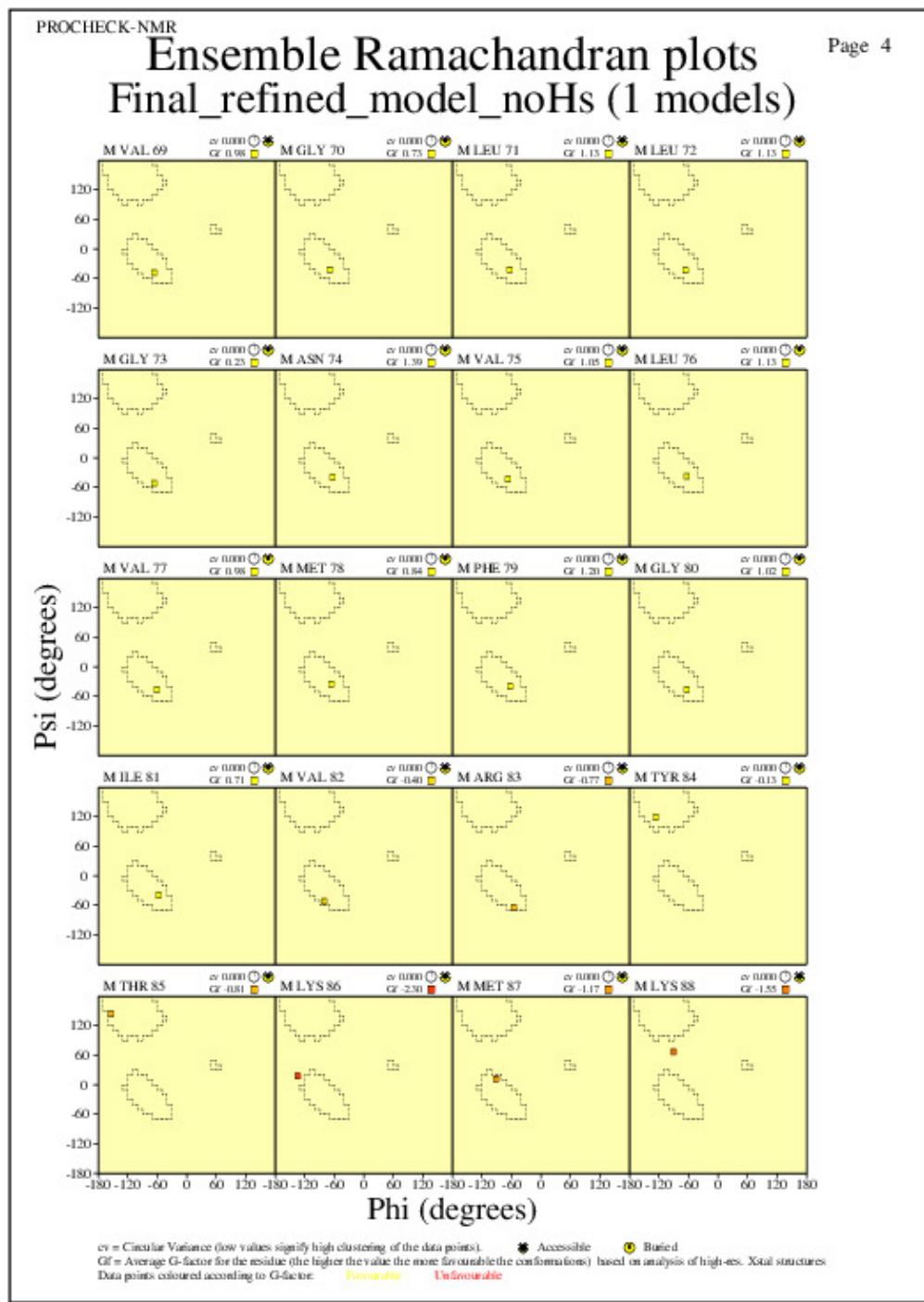
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



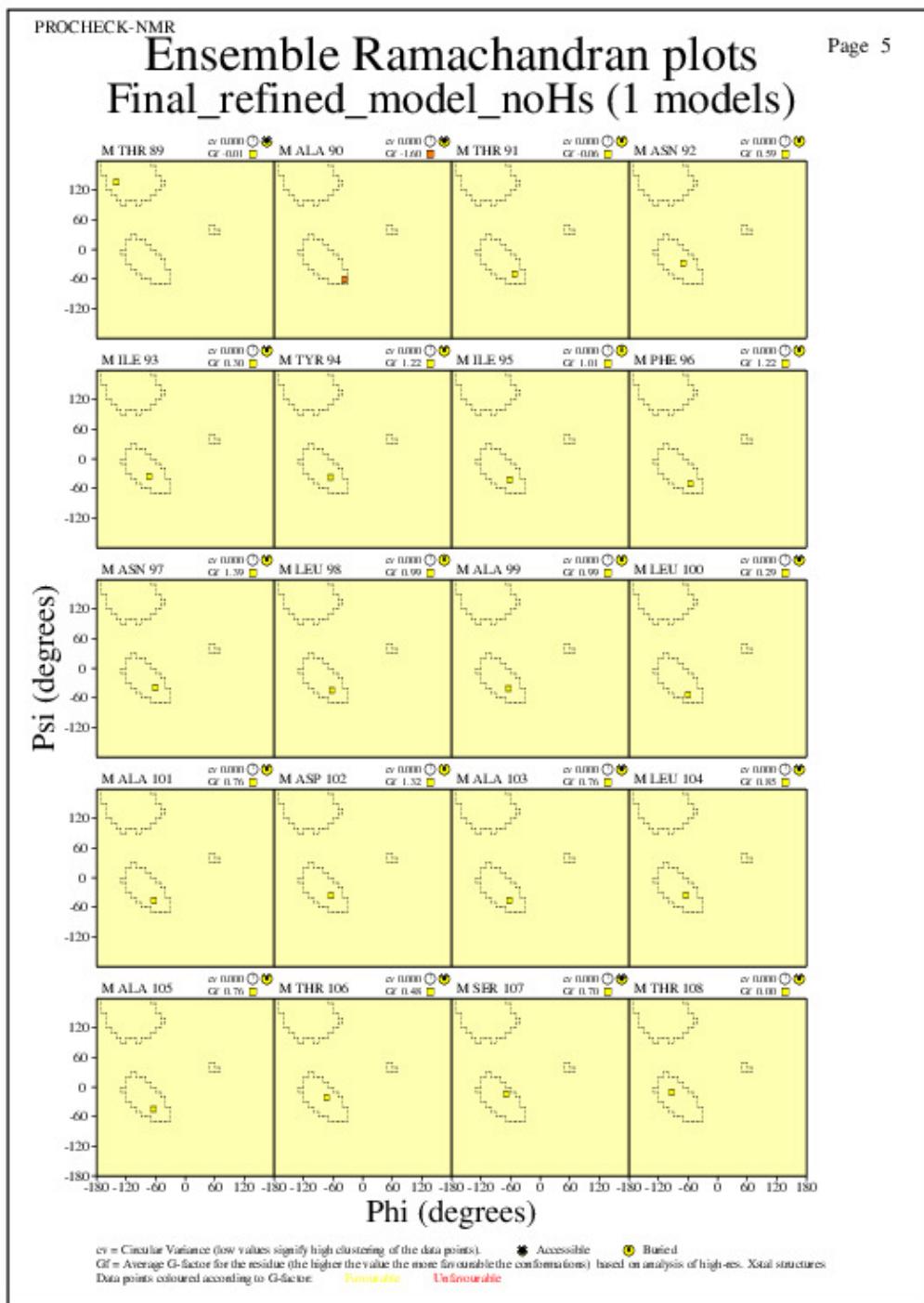
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



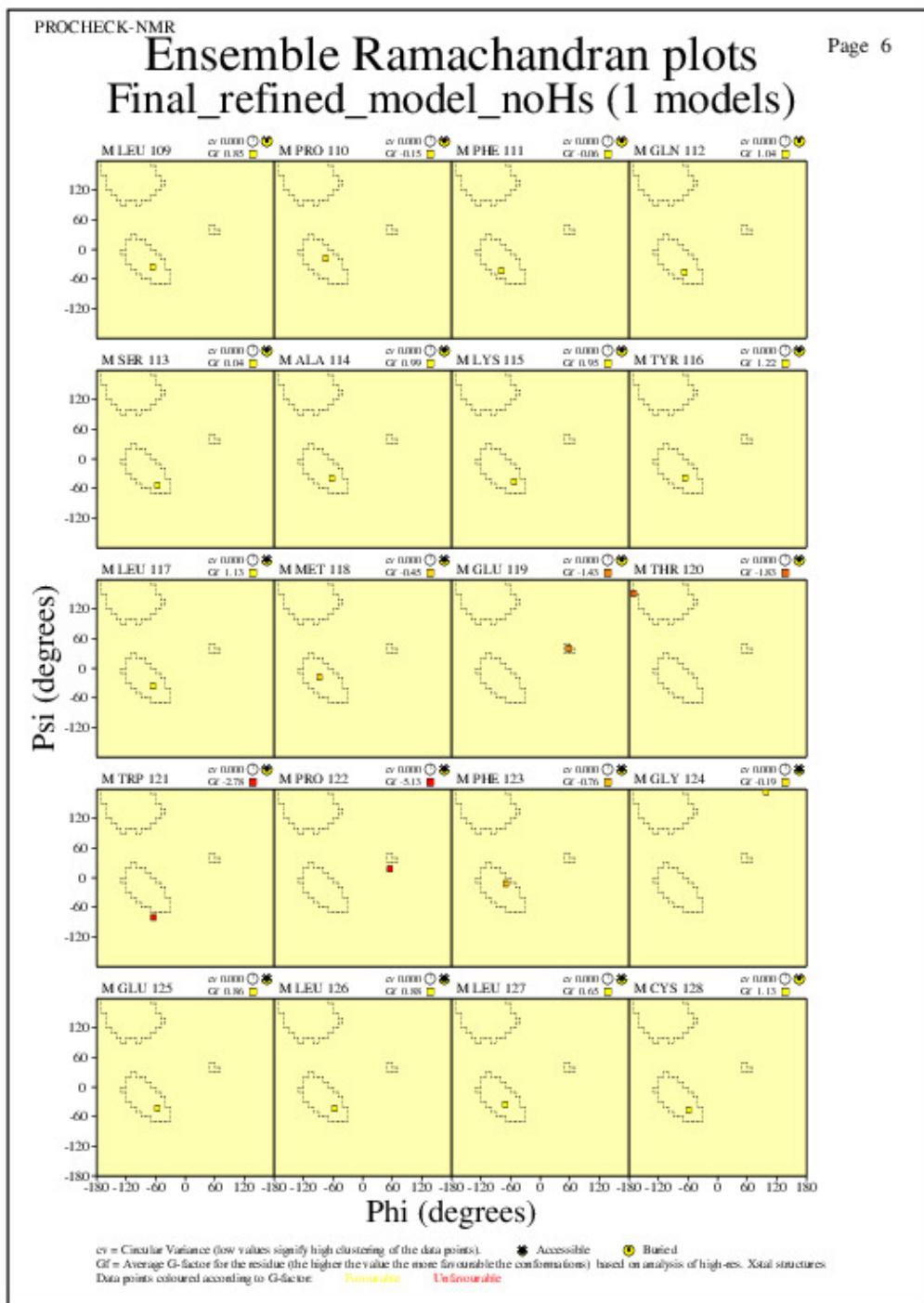
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



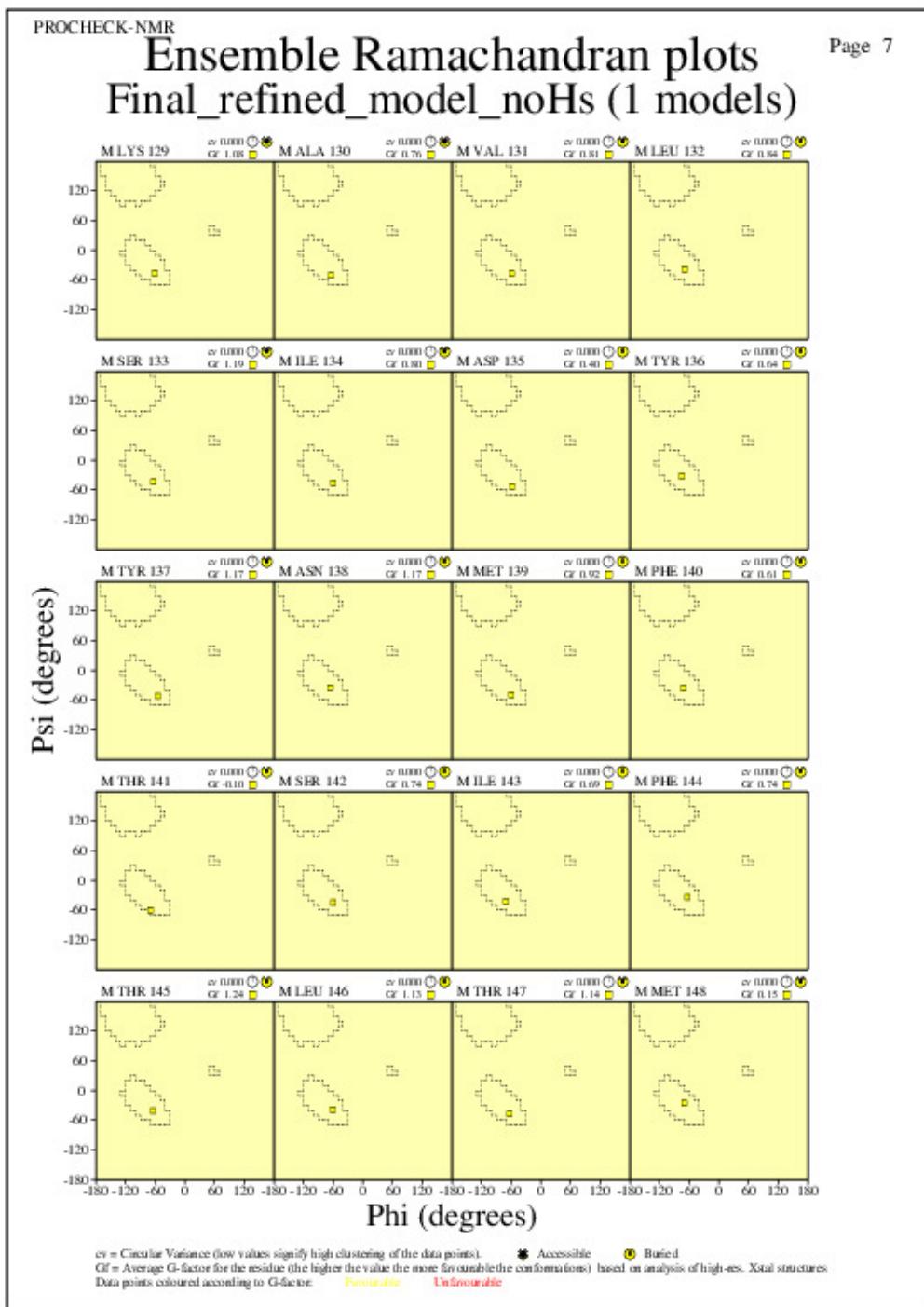
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



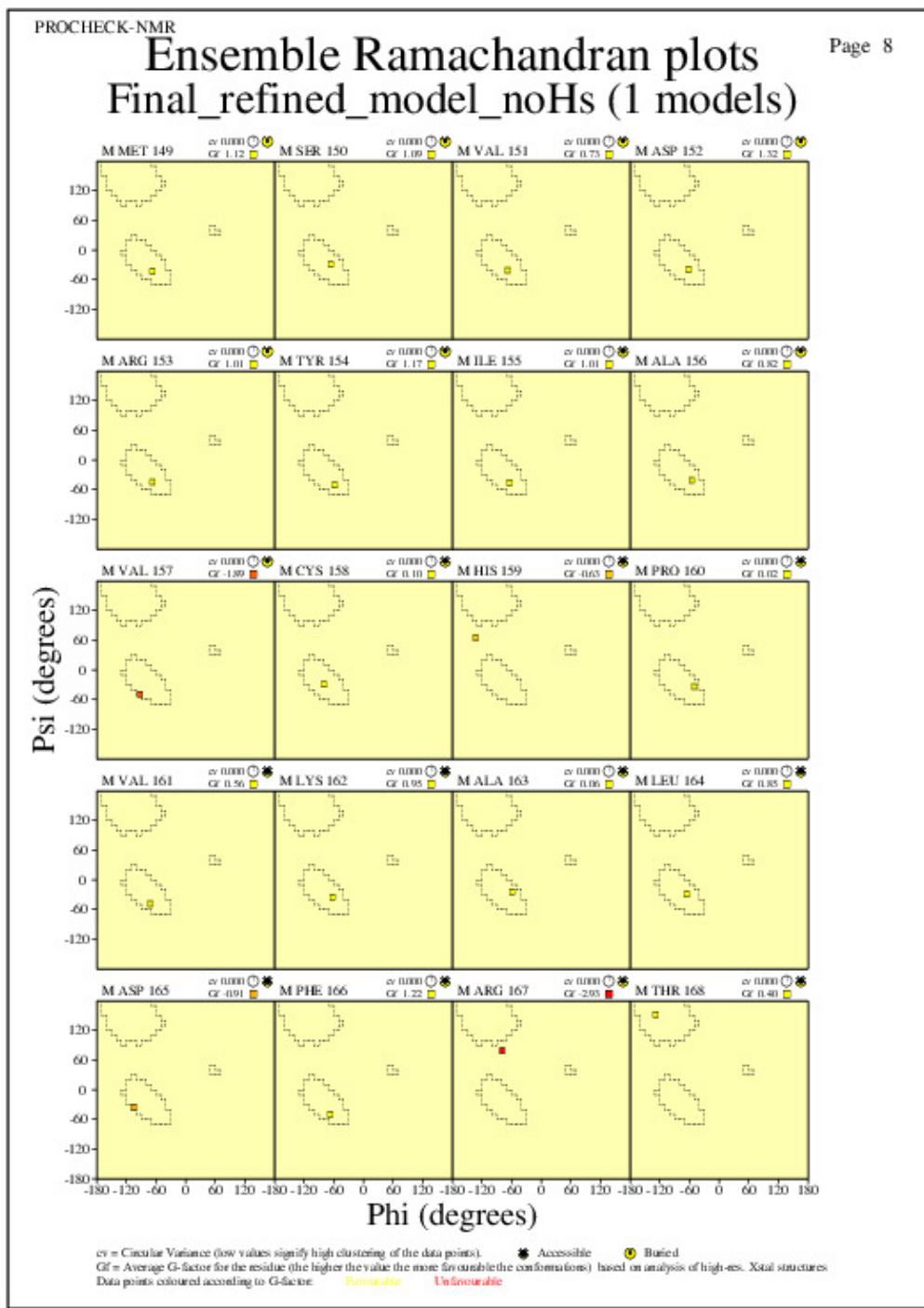
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



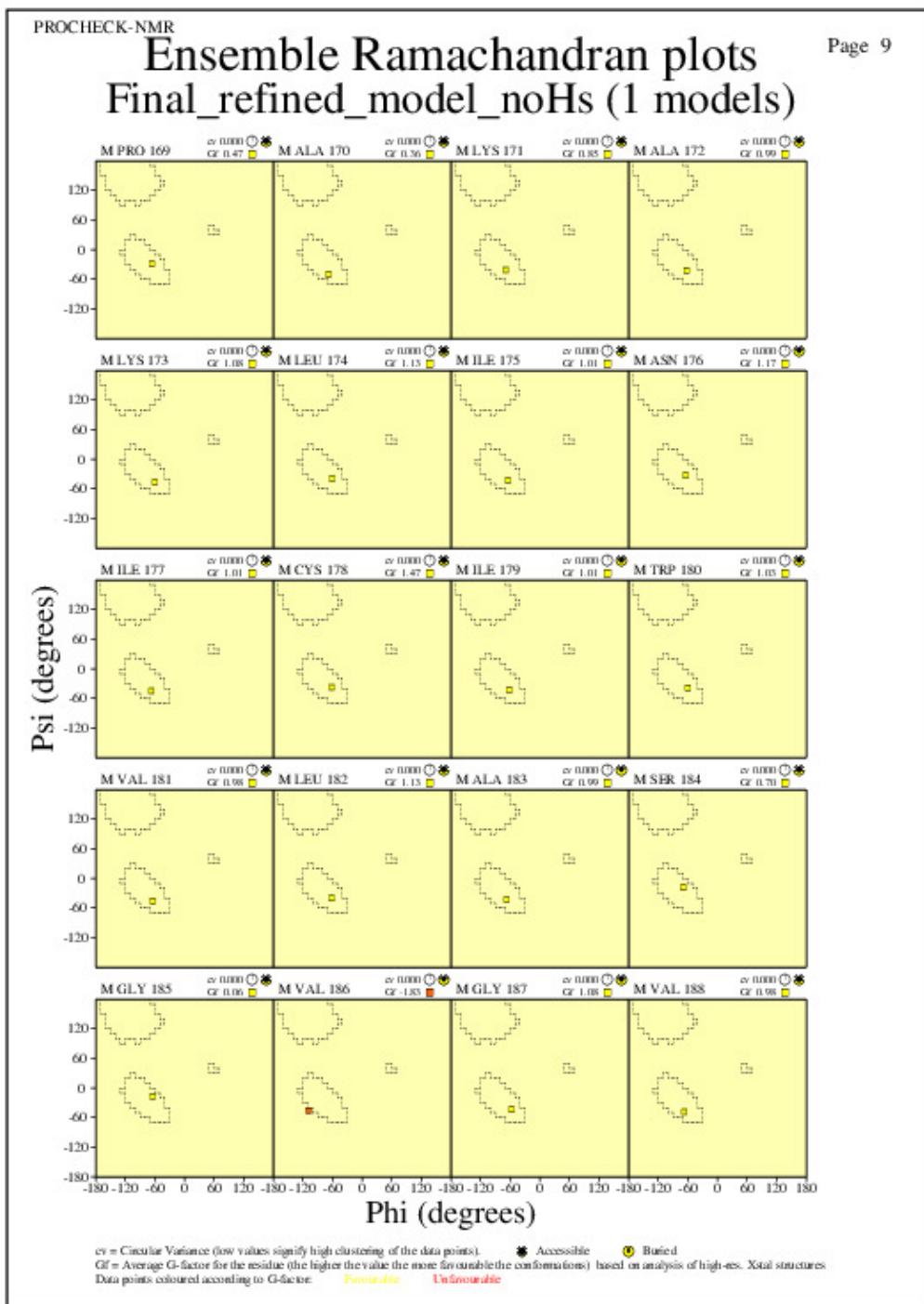
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



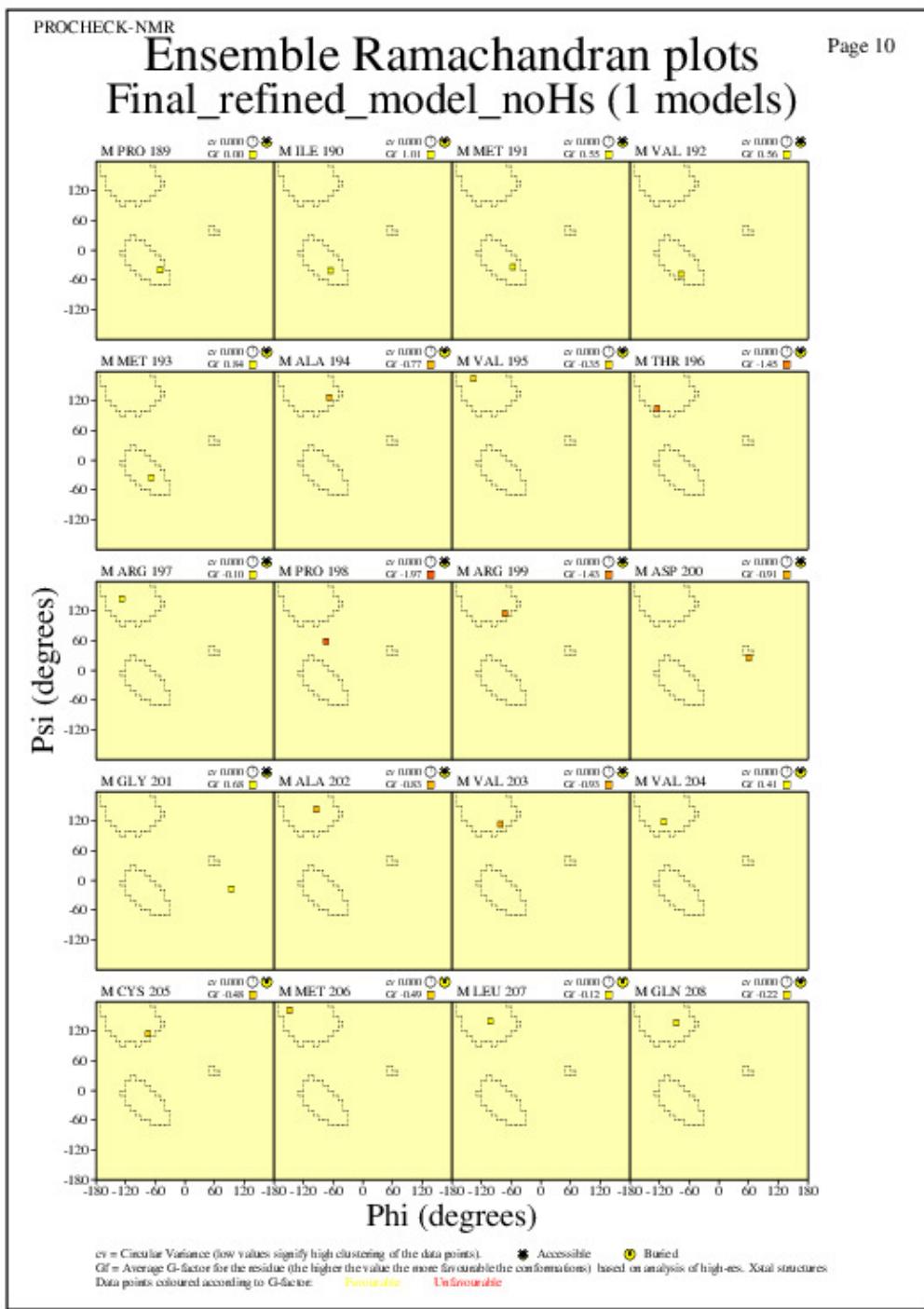
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



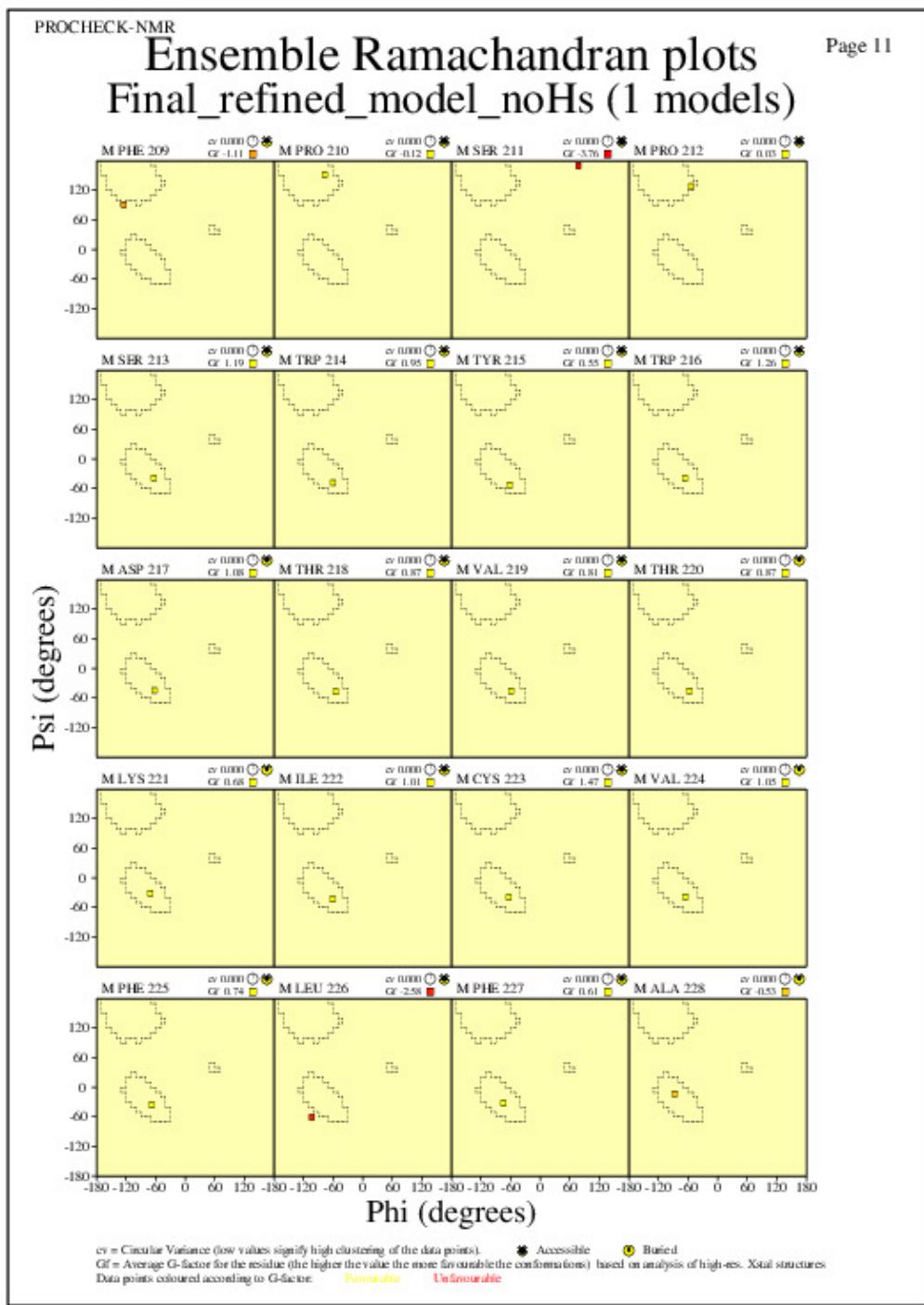
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



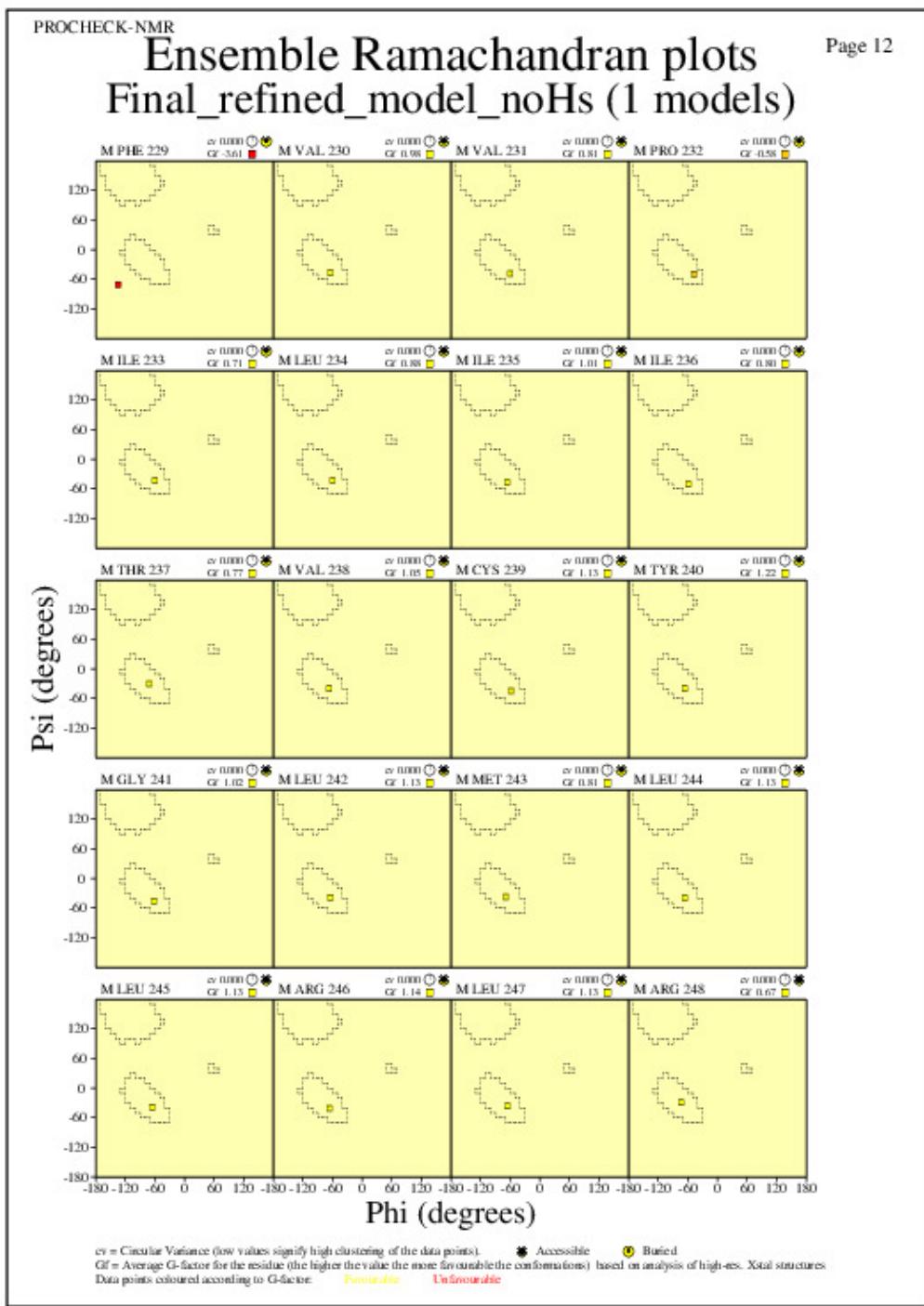
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



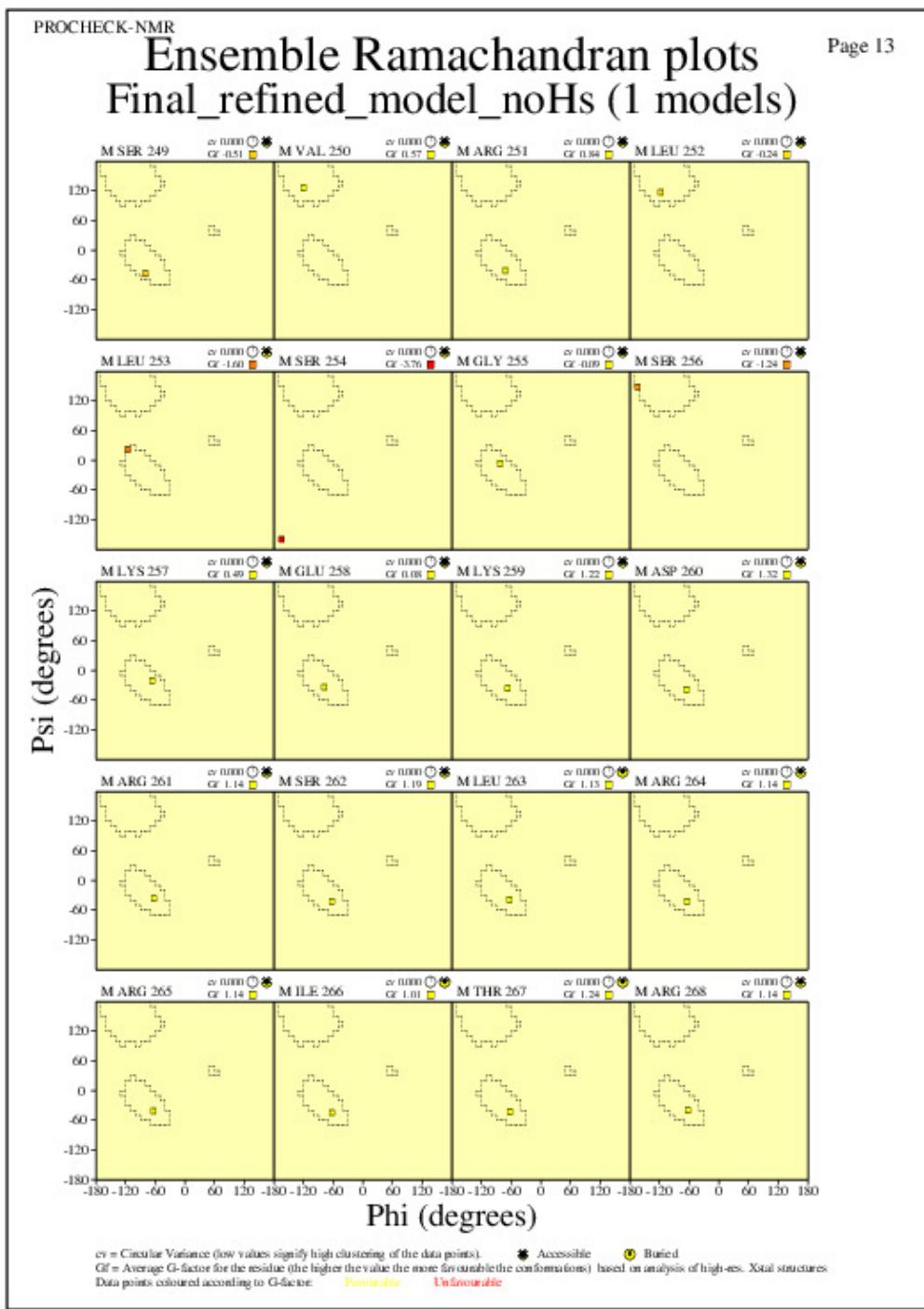
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



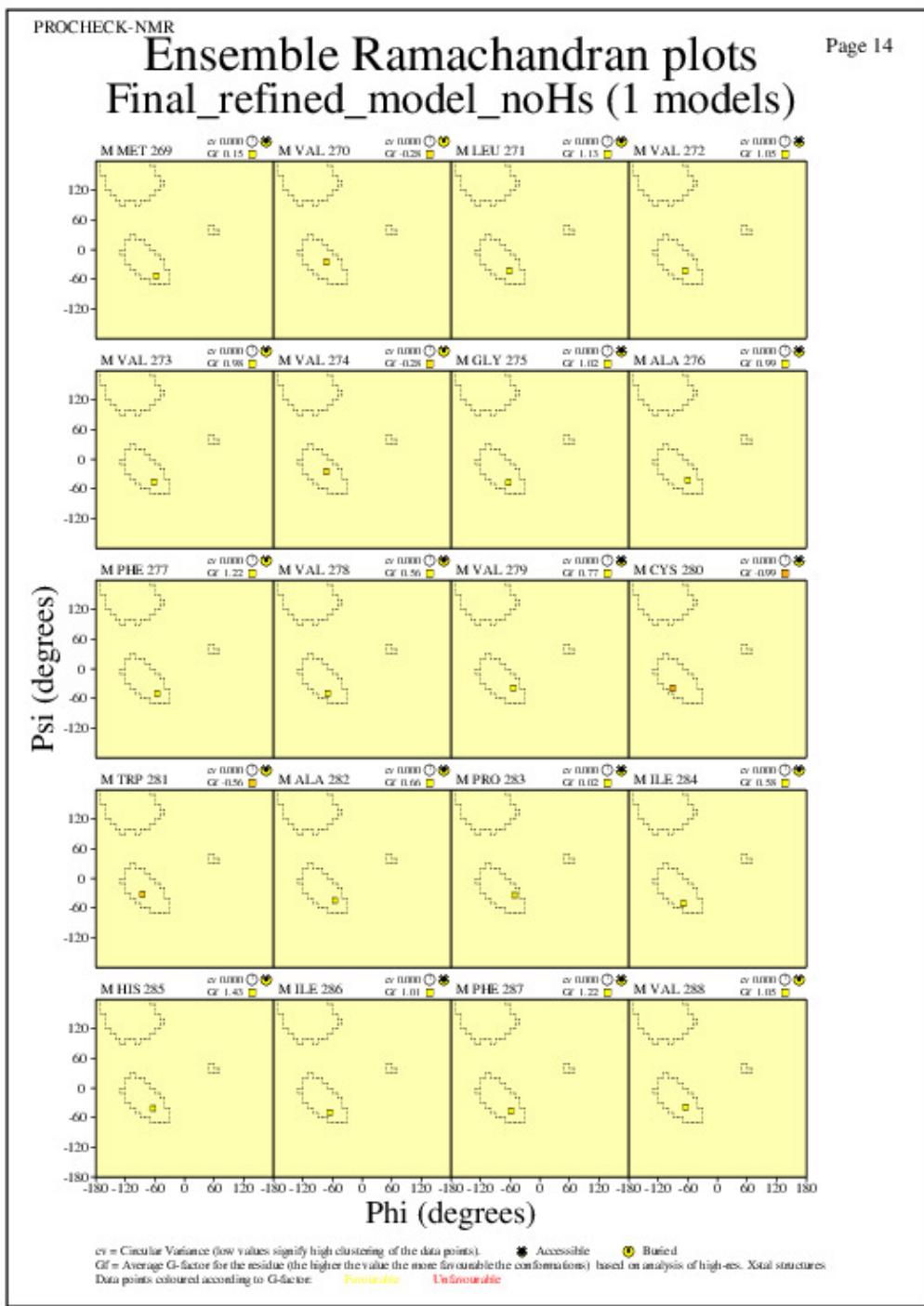
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



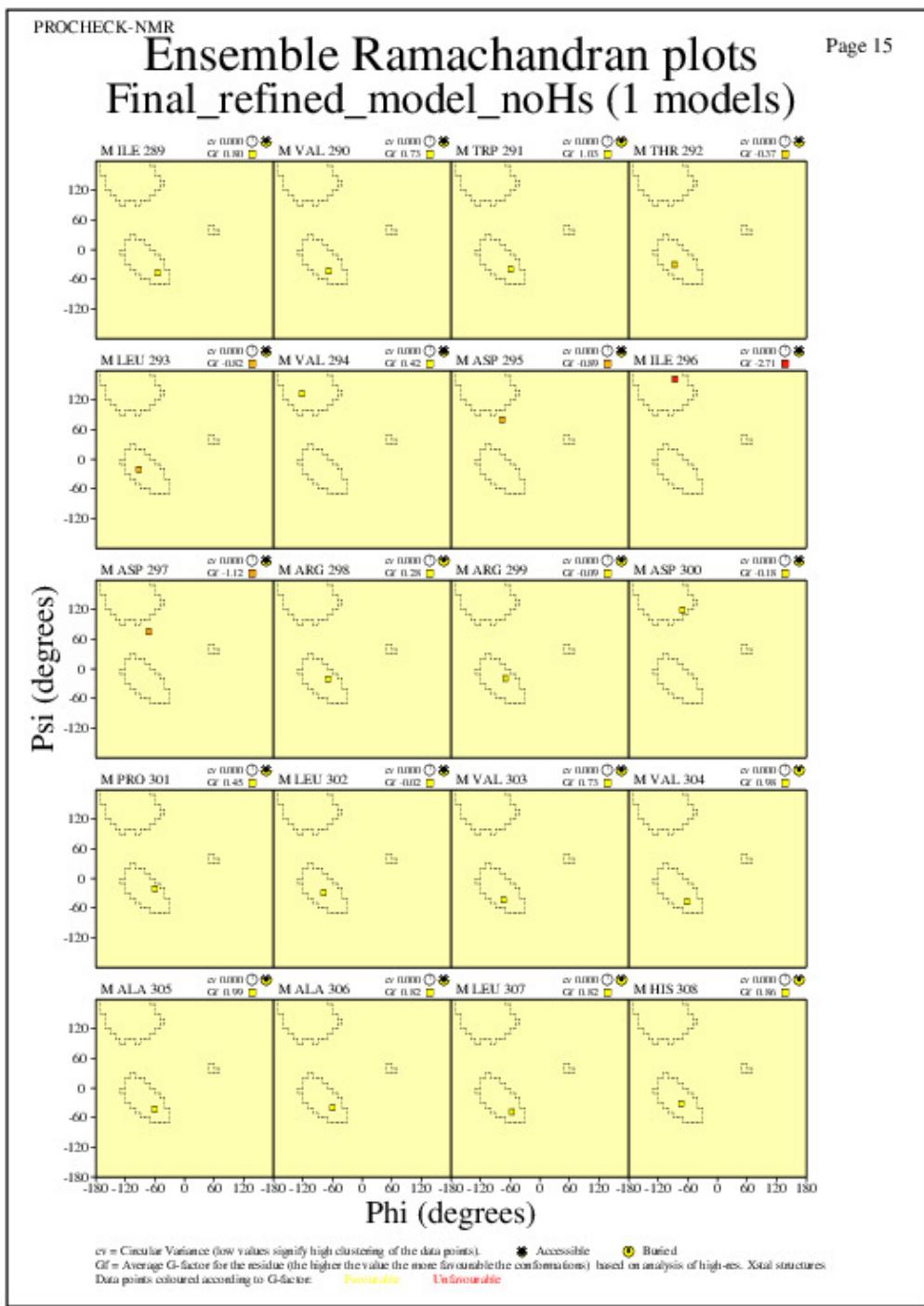
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



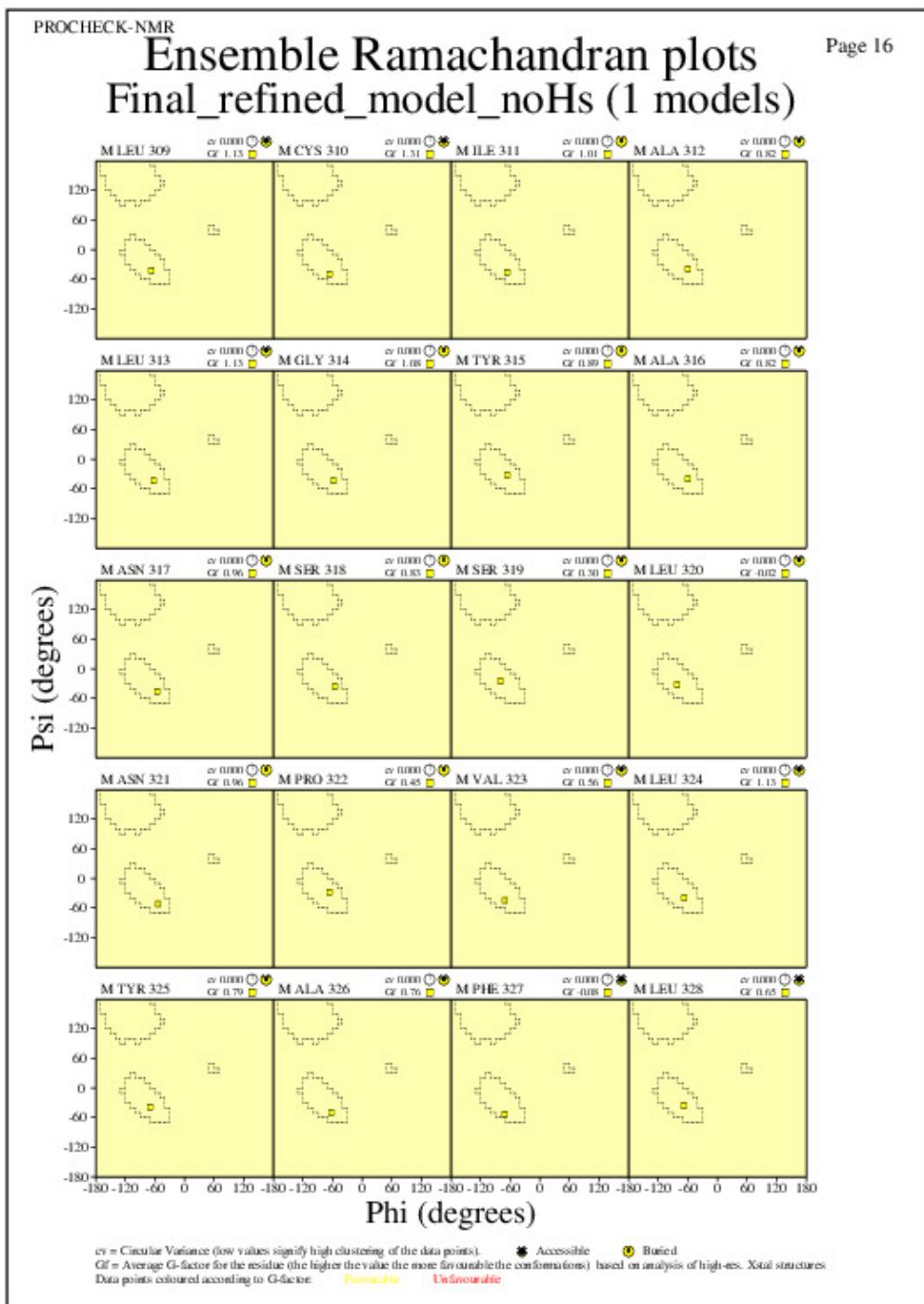
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



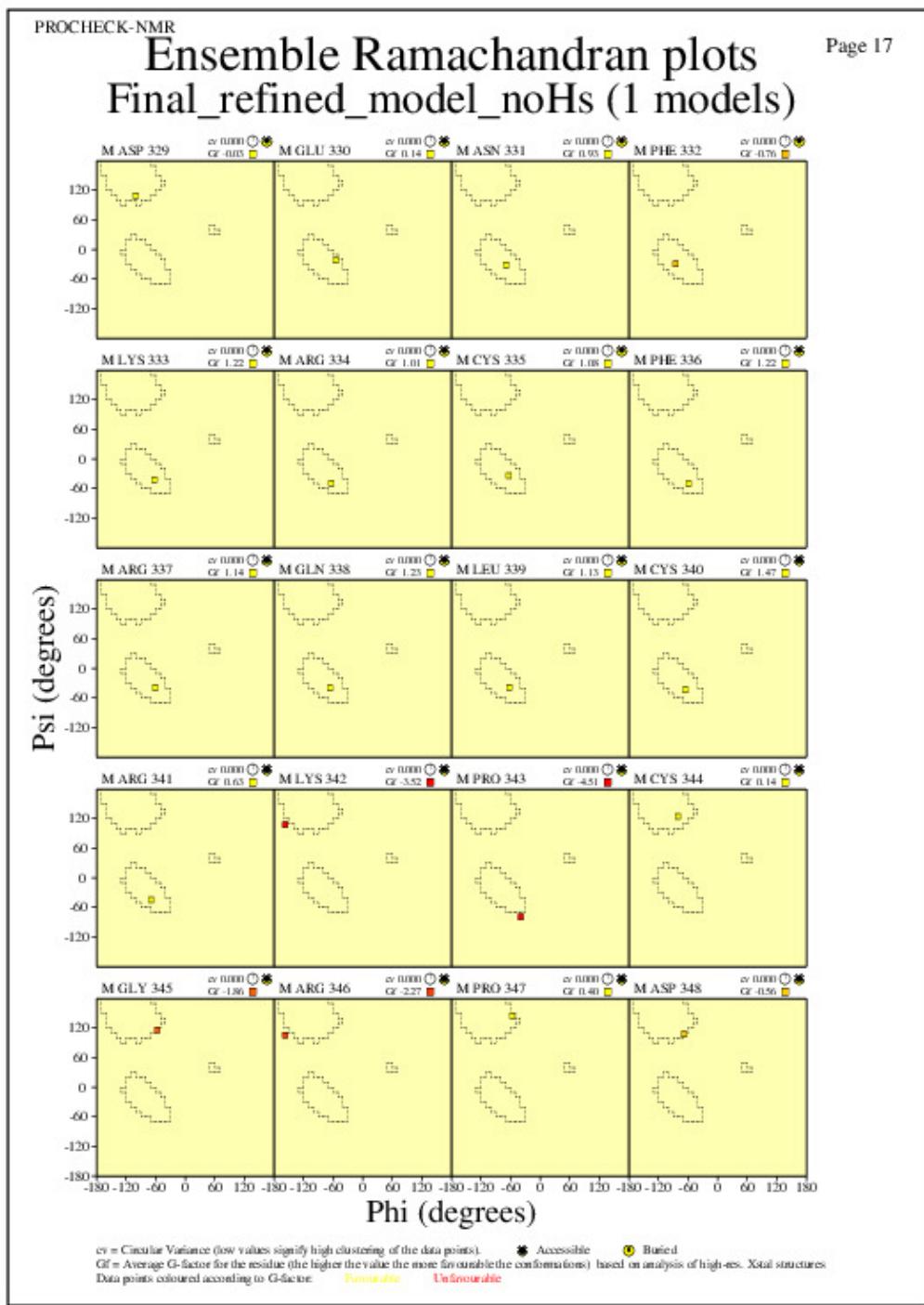
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



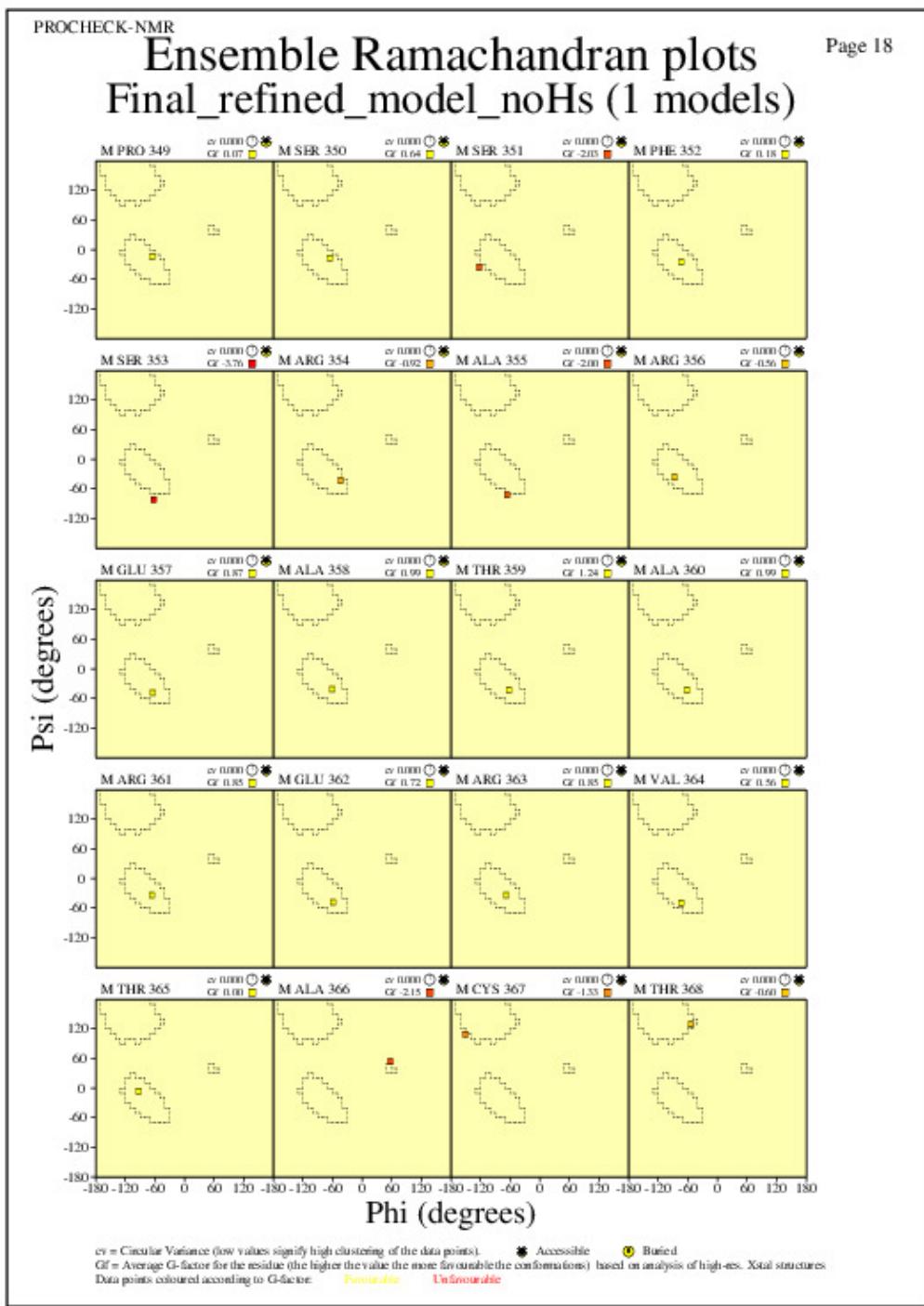
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



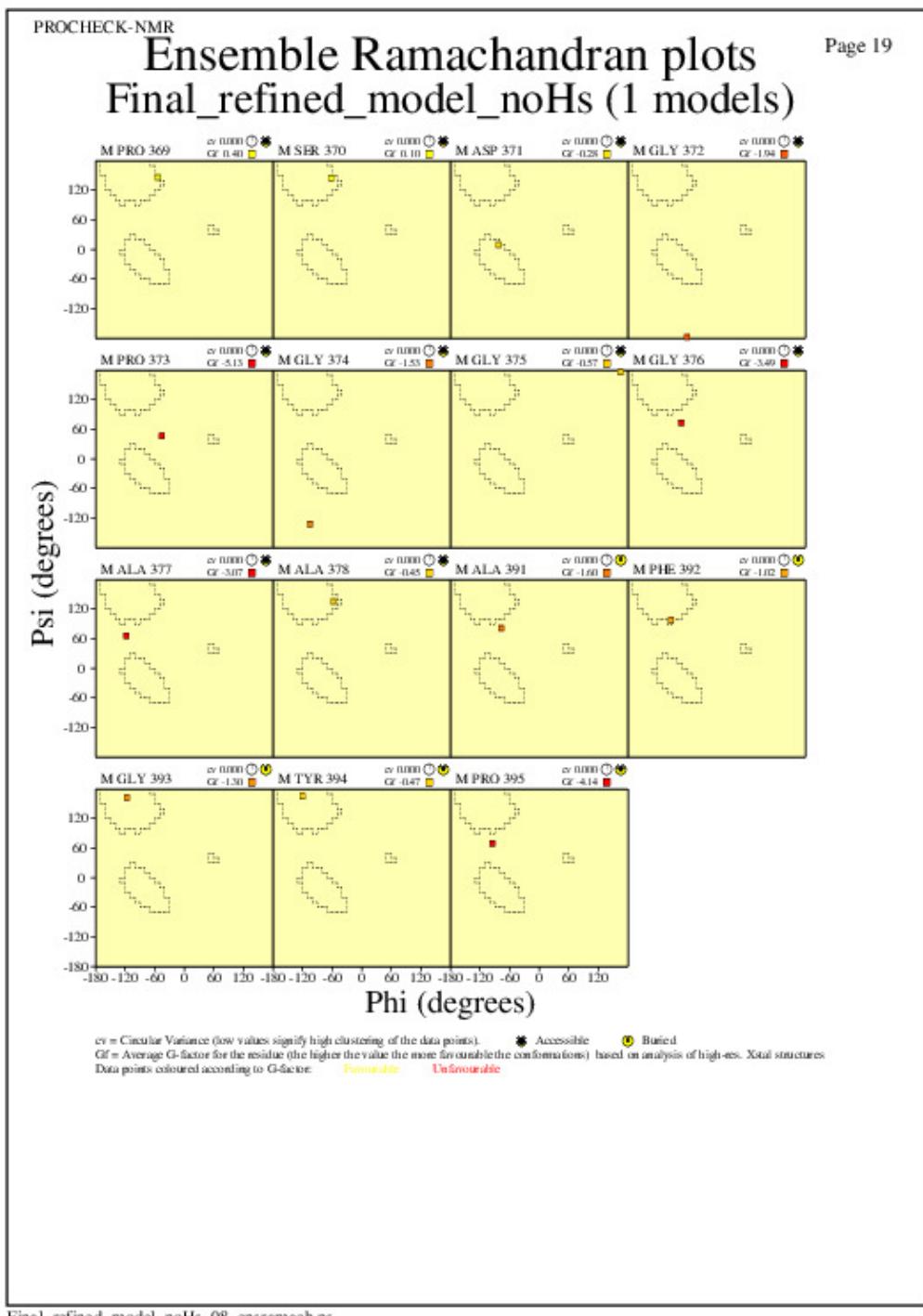
Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



Final_refined_model_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n

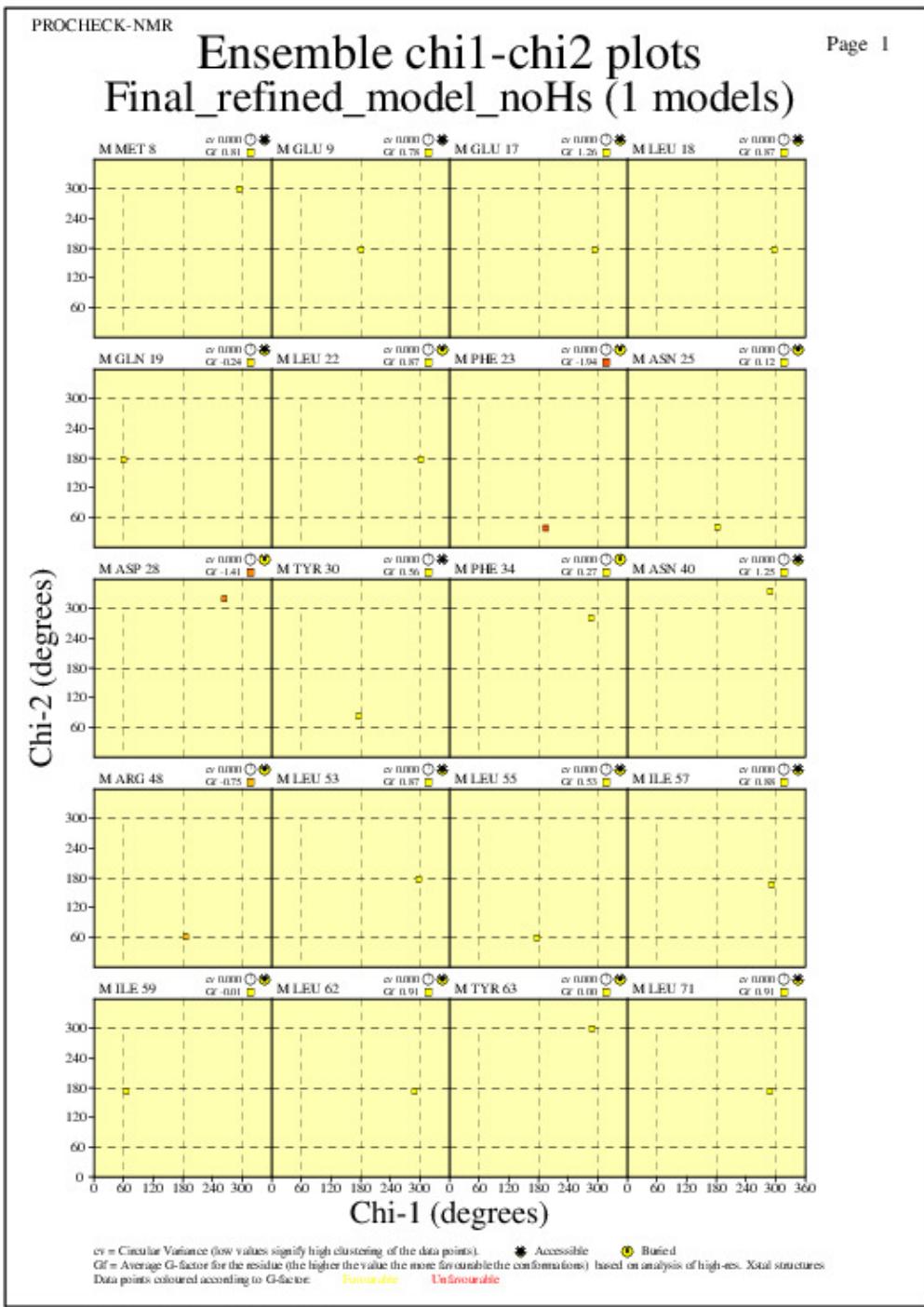


Final_refined_model_noHs_08_ensramach.ps

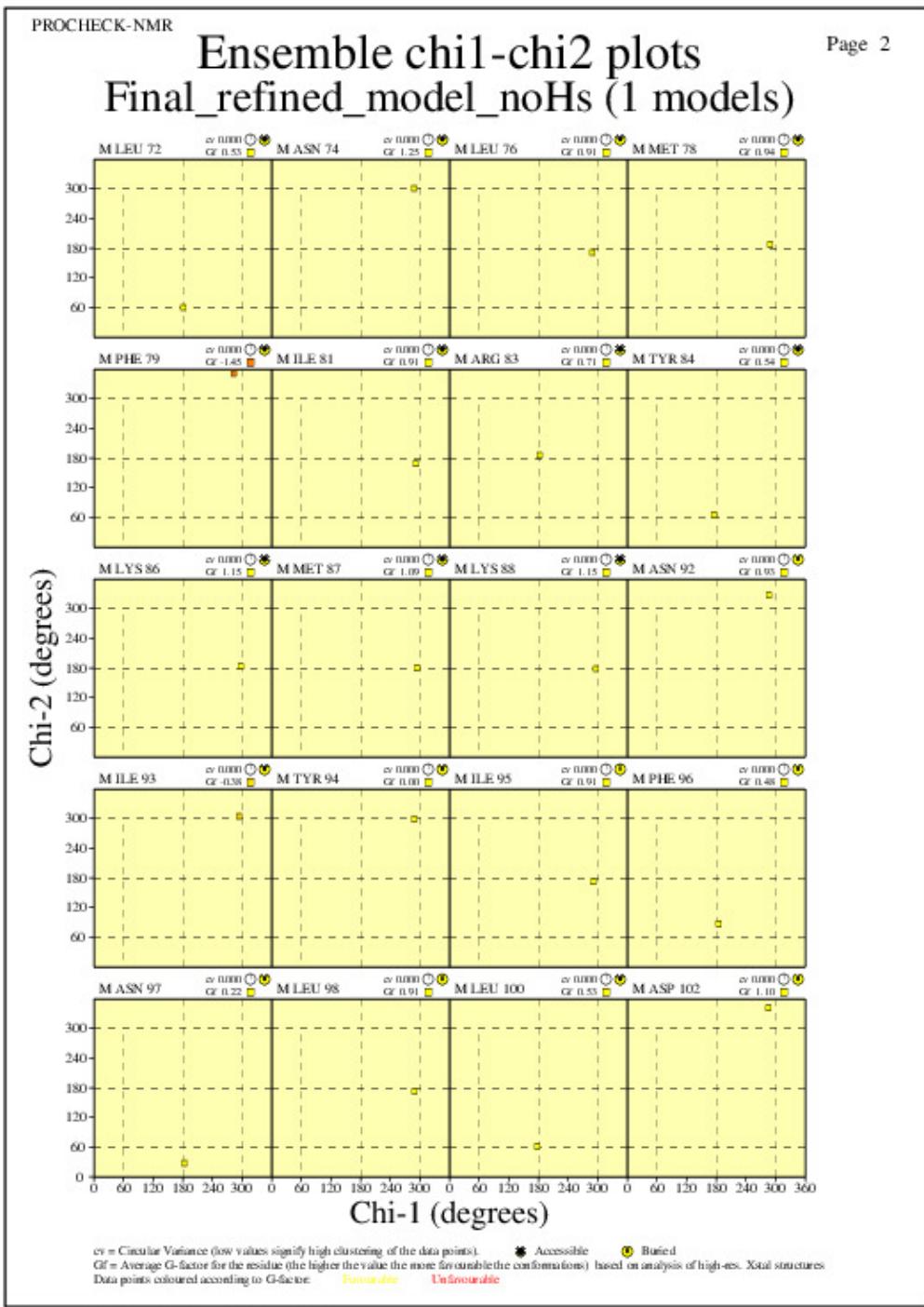
Ramachandran analysis for each residue from Molprobit

Chi1-Chi2 Plots for each residue

JPEG for residue Chi1-Chi2 Plots - page \$num_n

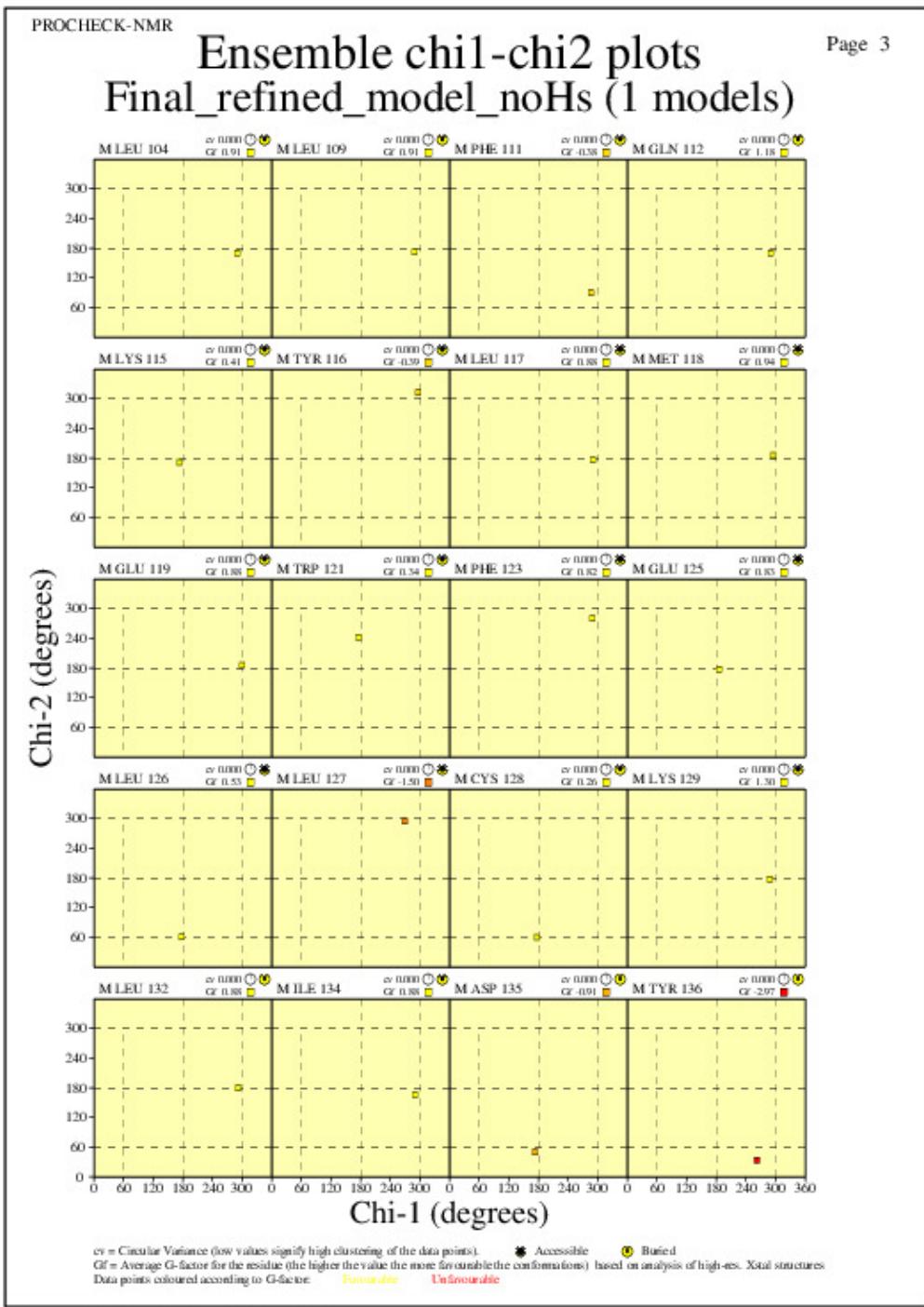


JPEG for residue Chi1-Chi2 Plots - page \$num_n



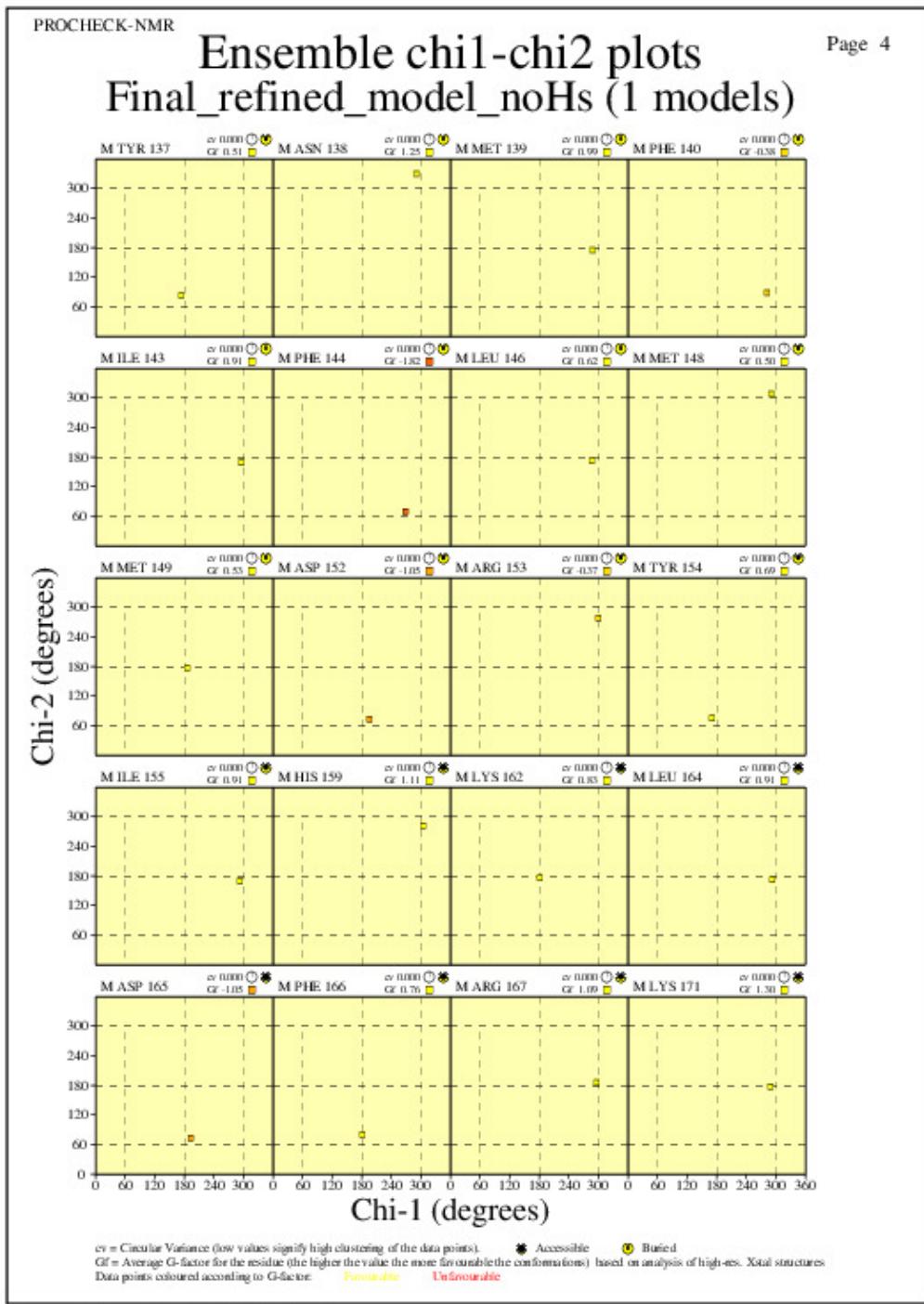
Final_refined_model_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n



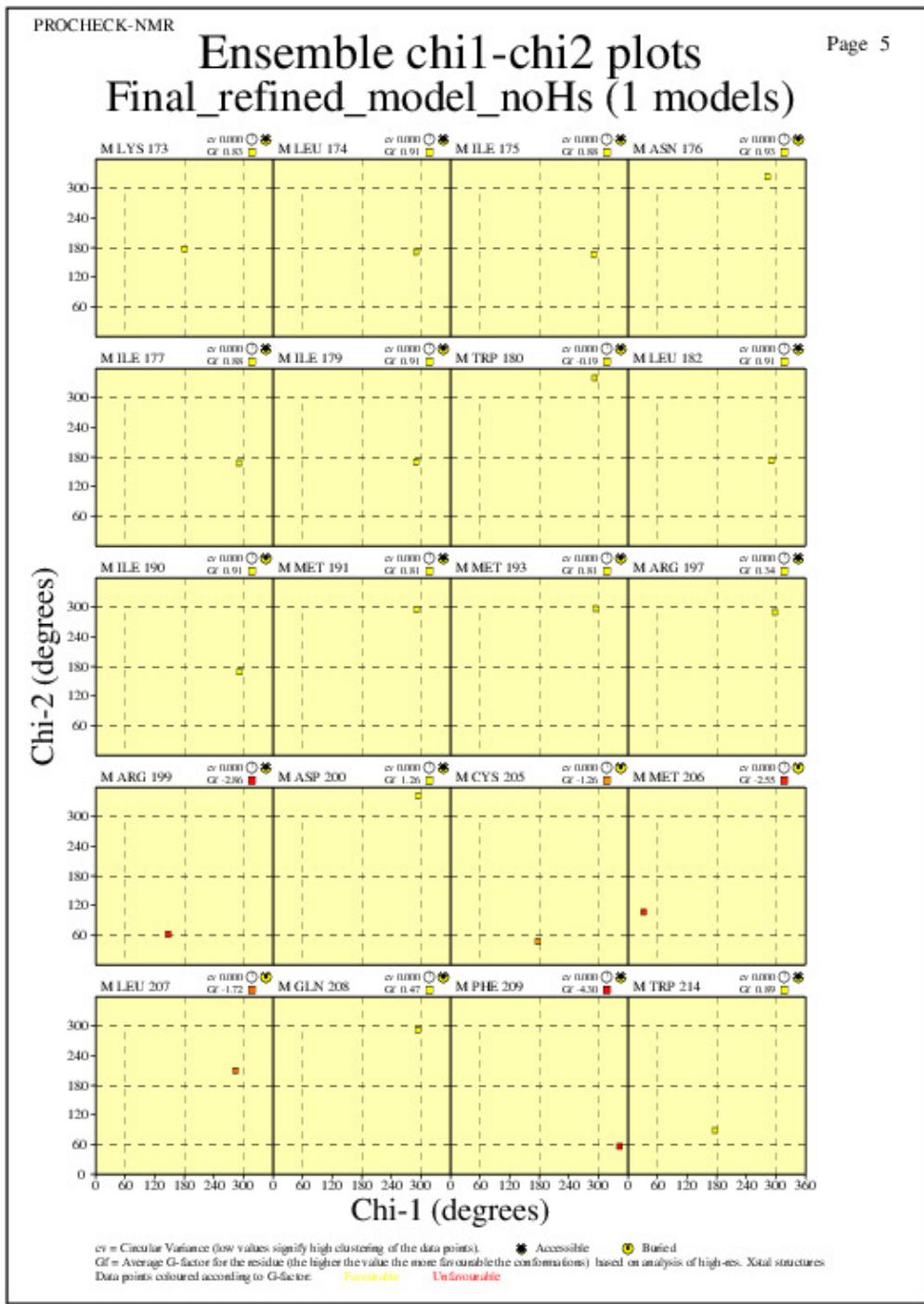
Final_refined_model_noHs_09_enschi2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n



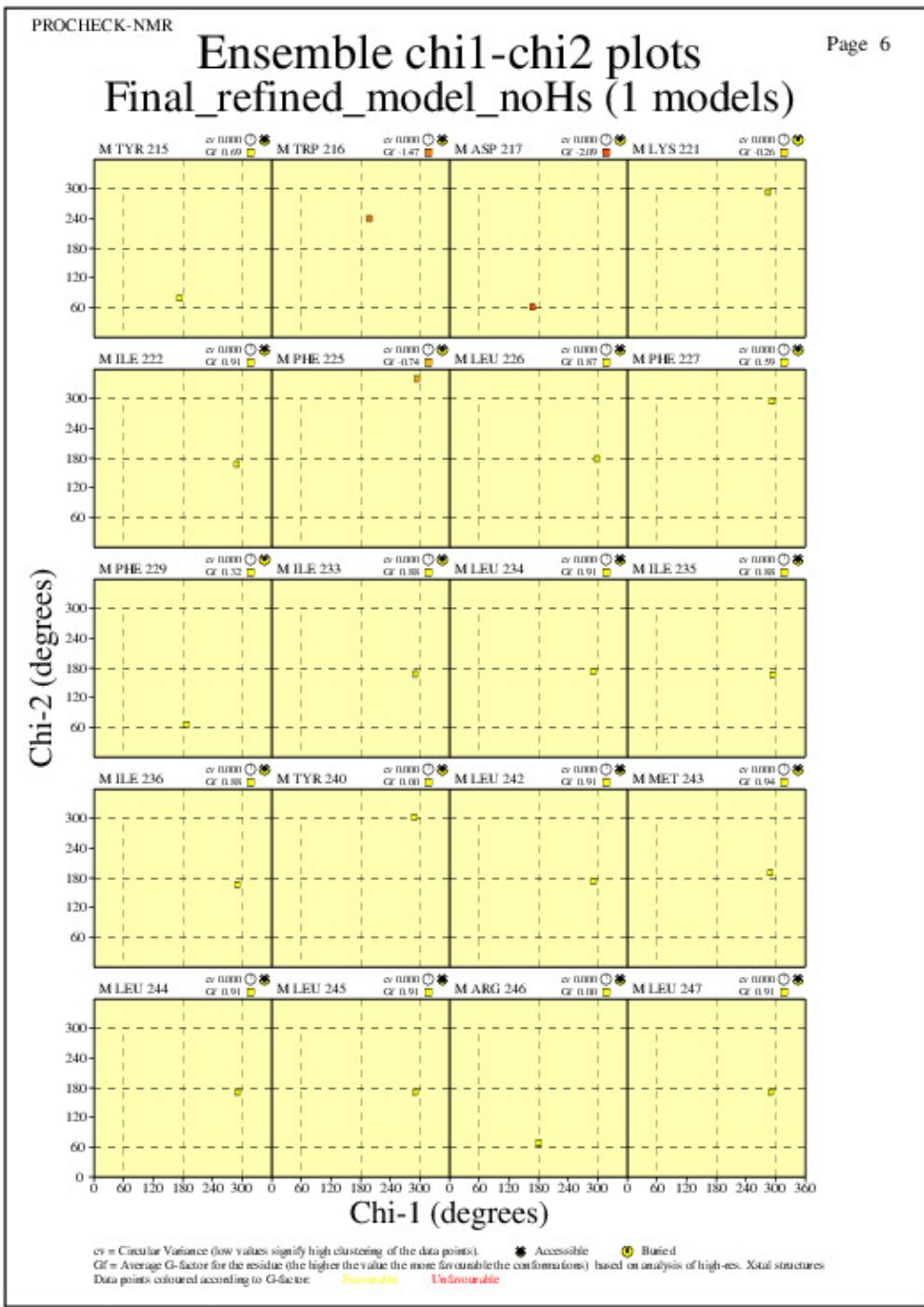
Final_refined_model_noHs_09_enschi2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n

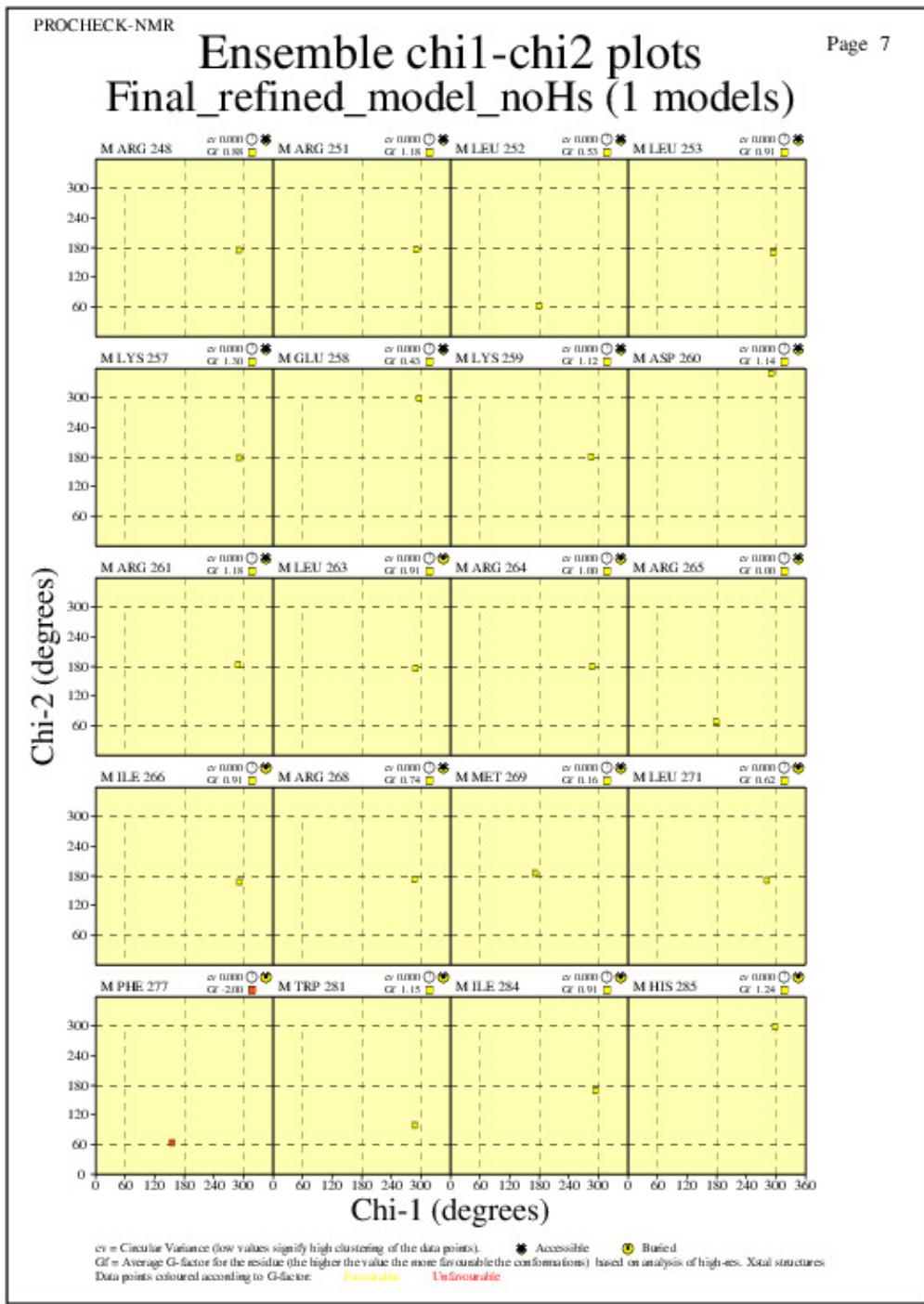


Final_refined_model_noHs_09_enschi2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n

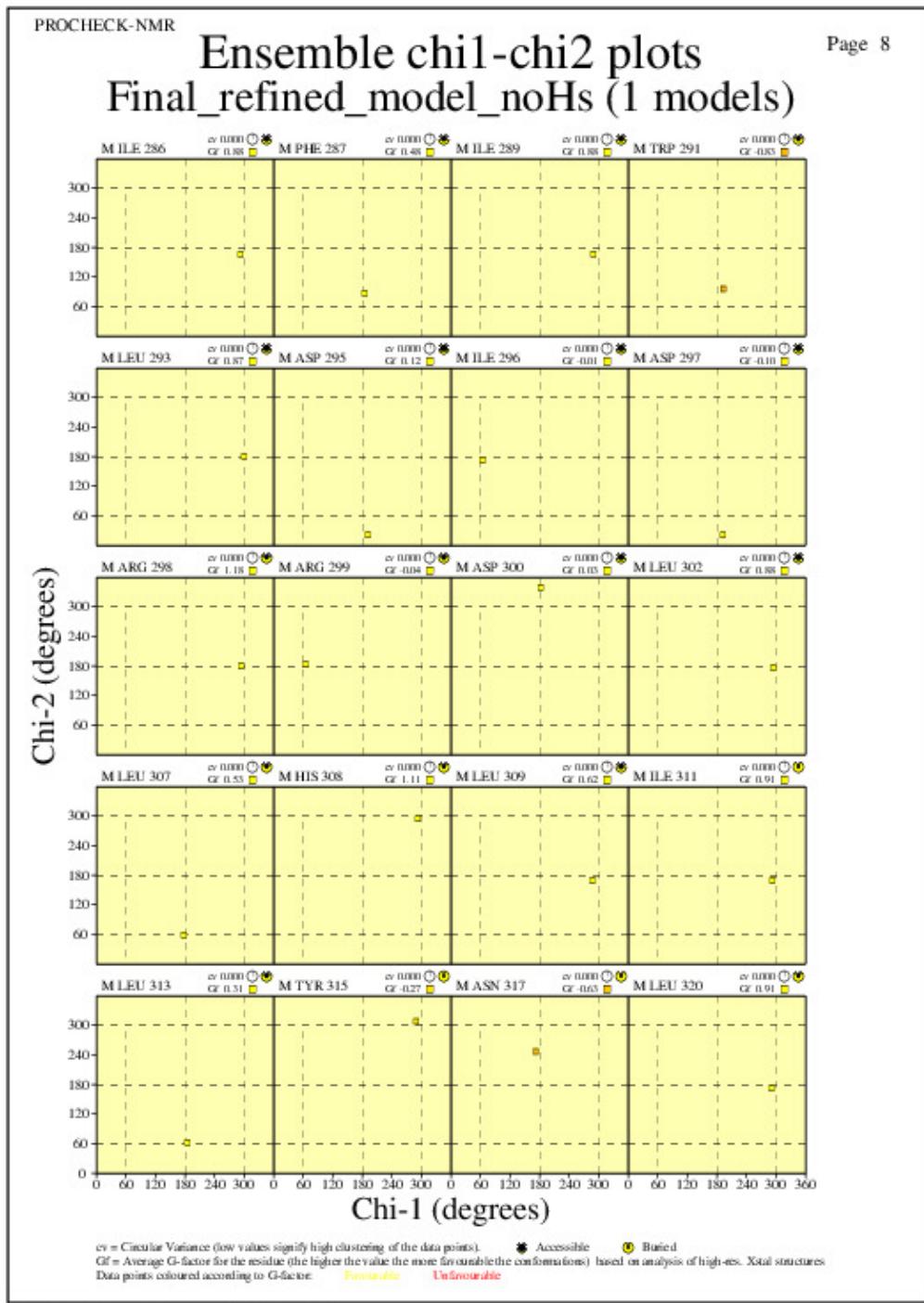


JPEG for residue Chi1-Chi2 Plots - page \$num_n



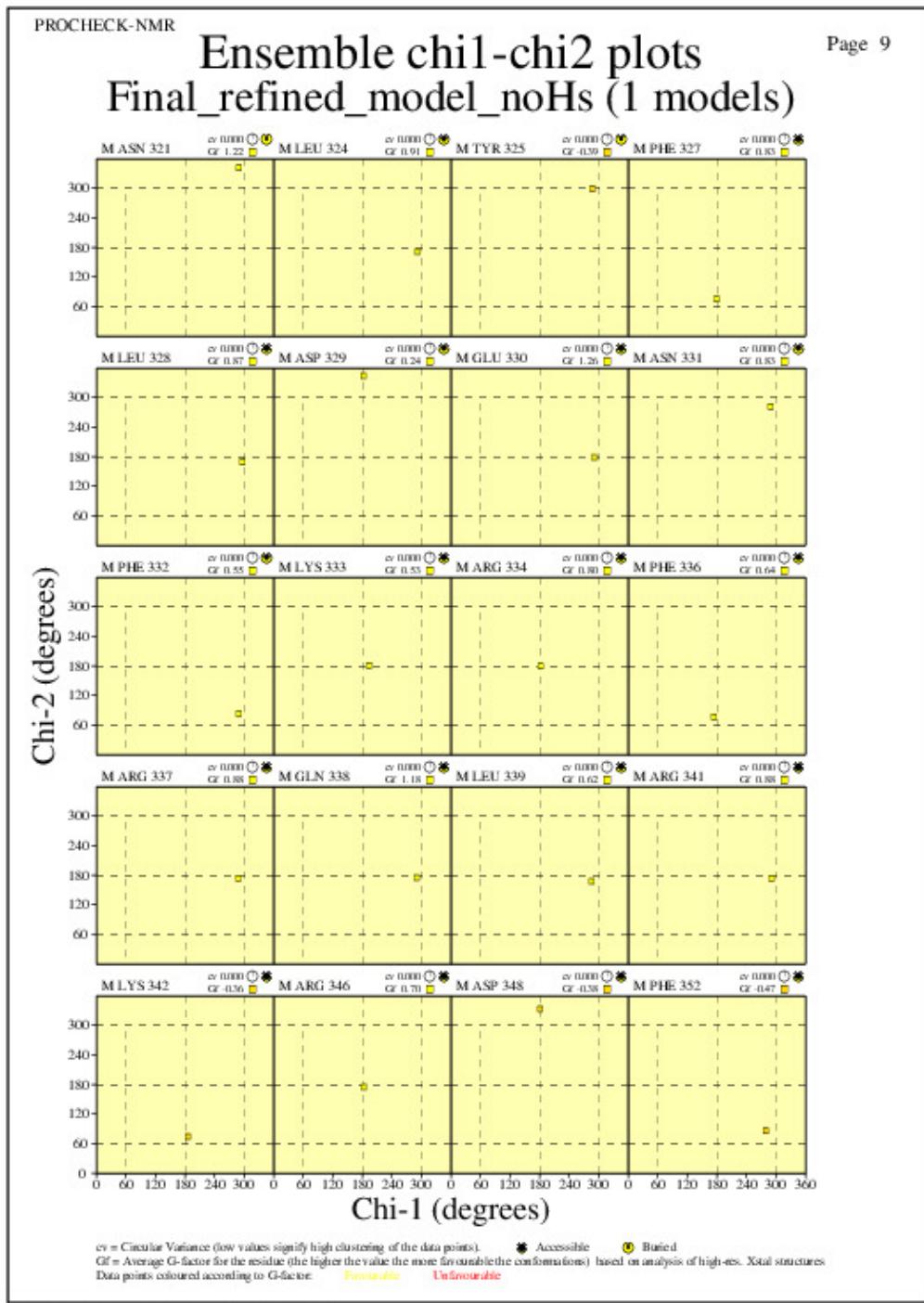
Final_refined_model_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n



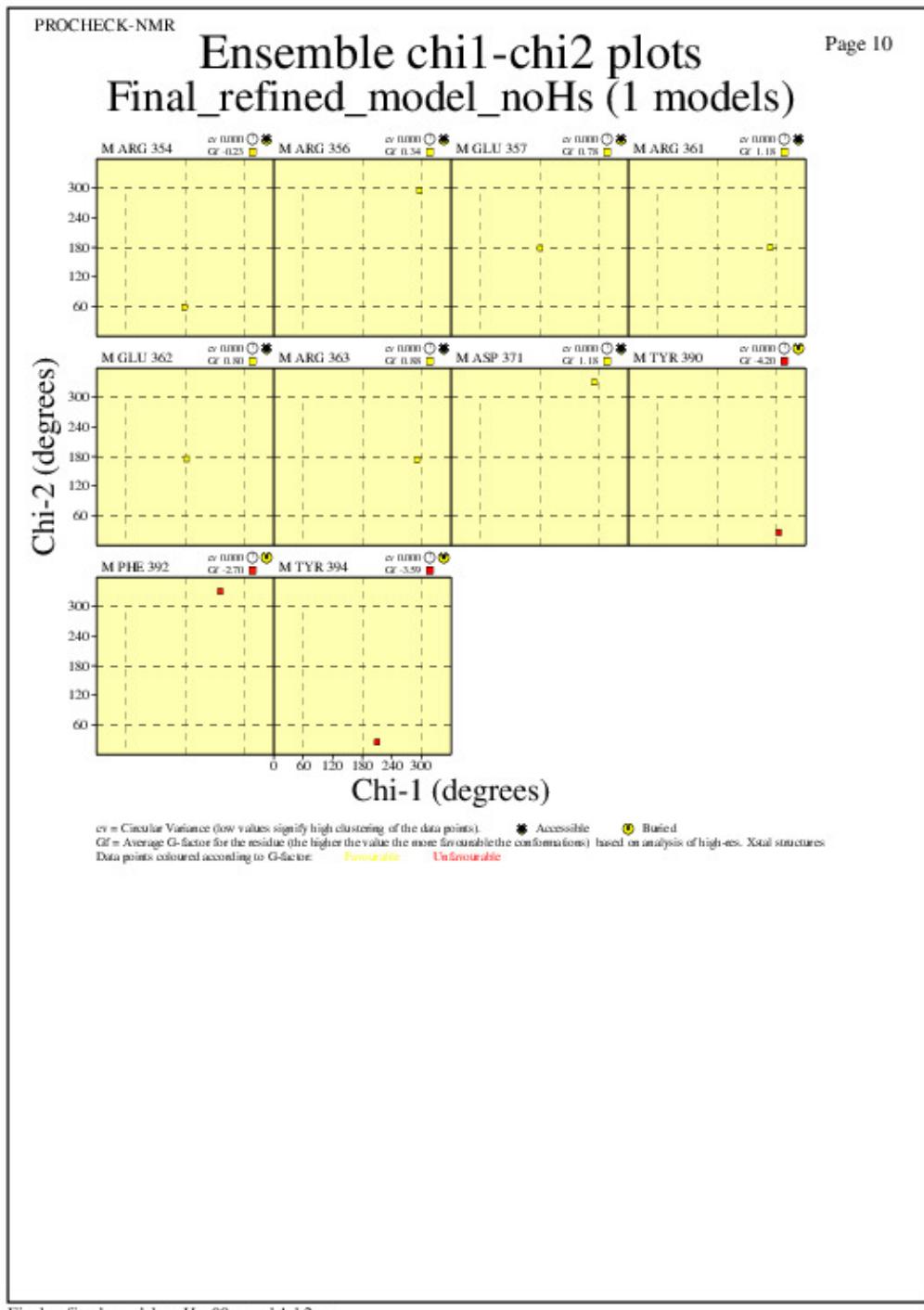
Final_refined_model_noHs_09_enschi2.ps

JPEG for residue Chi1-Chi2 Plots - page \$num_n

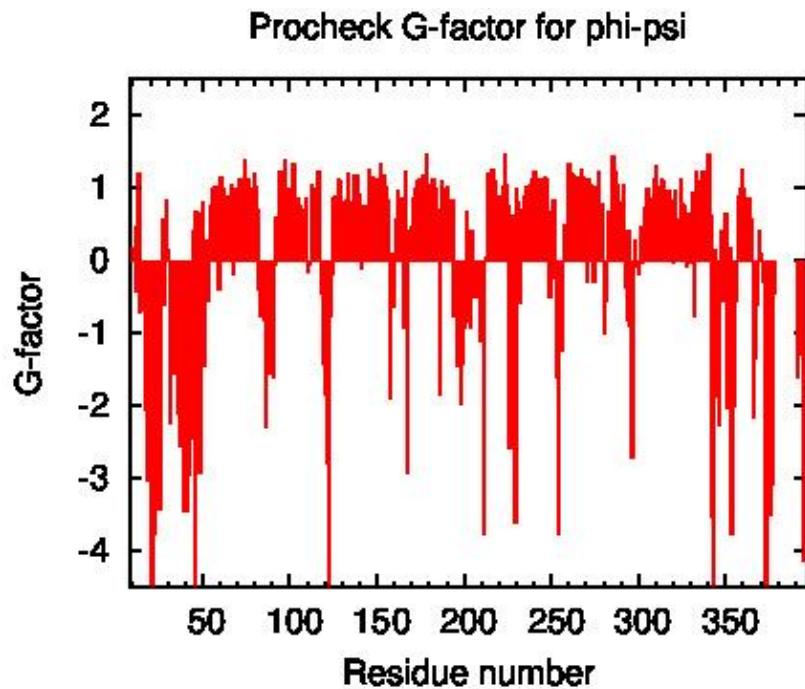


Final_refined_model_noHs_09_ensch1ch2.ps

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

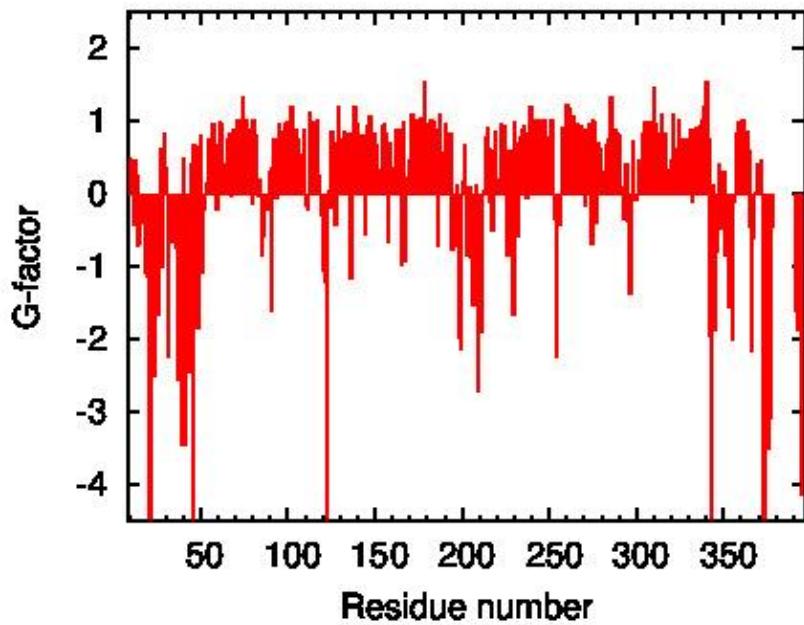
287	1.22
288	1.05
289	0.80
290	0.73
291	1.03
292	-0.37
293	-0.82
294	0.42
295	-0.89
296	-2.71
297	-1.12
298	0.28
299	-0.09
300	-0.18
301	0.45
302	-0.02
303	0.73
304	0.98
305	0.99
306	0.82
307	0.82
308	0.86
309	1.13
310	1.31
311	1.01
312	0.82
313	1.13
314	1.08
315	0.89
316	0.82
317	0.96
318	0.83
319	0.30
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     -1.60
392     -1.02
393     -1.30
394     -0.47
395     -4.14
#Reported_Model_Average 0.054
#Overall_Average_Reported      0.054
```

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     0.61
28     -1.01
29     0.82
30     0.35
31     -2.24
32     -0.14
33     -0.51
34     -0.65
35     -0.40
36     -0.73
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	-1.84
49	0.65
50	0.80
51	-1.08
52	-0.22
53	0.15
54	0.76
55	0.76
56	0.66
57	0.95
58	0.66
59	-0.20
60	0.13
61	0.99
62	0.95
63	0.40
64	0.42
65	0.76
66	0.82
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	0.85
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	0.32
109	0.88
110	-0.15
111	-0.22
112	1.11
113	0.00
114	0.99
115	0.68
116	0.42
117	1.01
118	0.25
119	-0.28
120	-1.06
121	-1.22
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	0.70
132	0.86
133	0.78
134	0.84
135	-0.26
136	-1.17
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	-0.65
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	0.88
185	0.06
186	-0.71
187	1.08
188	0.56
189	0.00
190	0.96
191	0.68
192	0.69
193	0.83
194	-0.77
195	-0.72
196	-0.41
197	0.12
198	-1.97
199	-2.14
200	0.18
201	0.68
202	-0.83
203	-0.17
204	0.08
205	-0.87
206	-1.52
207	-0.92
208	0.12
209	-2.71
210	-0.12
211	-1.89
212	0.03
213	0.78
214	0.92
215	0.62
216	-0.11
217	-0.51
218	0.58
219	0.86
220	-0.01
221	0.21
222	0.96
223	0.80
224	0.93
225	0.00
226	-0.85

PSVS Software Environment

227	0.60
228	-0.53
229	-1.65
230	0.98
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	0.15
281	0.29
282	0.66
283	0.02
284	0.74
285	1.34
286	0.94
287	0.85
288	0.89

PSVS Software Environment

289	0.84
290	0.80
291	0.10
292	-0.33
293	0.03
294	0.41
295	-0.38
296	-1.36
297	-0.61
298	0.73
299	-0.07
300	-0.07
301	0.45
302	0.43
303	0.82
304	0.69
305	0.99
306	0.82
307	0.67
308	0.98
309	0.88
310	1.45
311	0.96
312	0.82
313	0.72
314	1.08
315	0.31
316	0.82
317	0.17
318	0.06
319	0.34
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	0.10
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

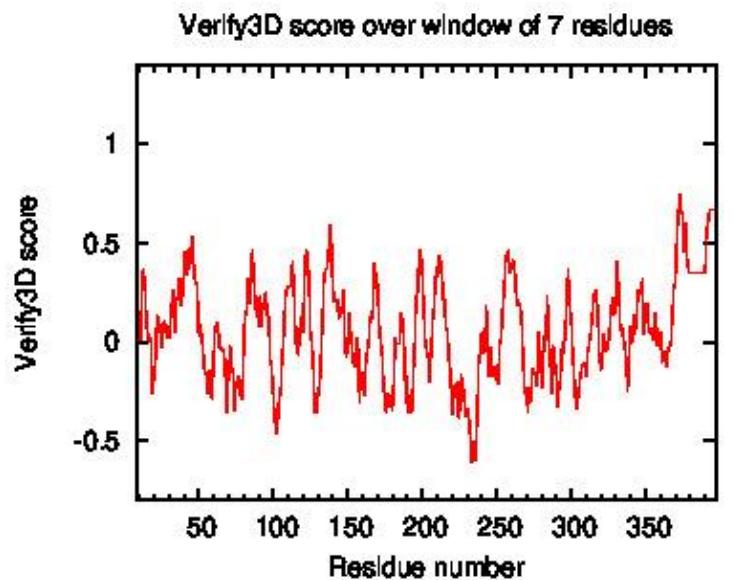
PSVS Software Environment

```
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      0.58
365      -0.44
366      -2.15
367      -0.60
368      0.02
369      0.40
370      0.04
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      -4.20
391      -1.60
392      -1.86
393      -1.30
394      -2.03
395      -4.14
396      0.66
#Reported_Model_Average 0.089
#Overall_Average_Reported      0.089
```

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     -0.83
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	0.17
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	0.51
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	0.71
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	-0.83
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

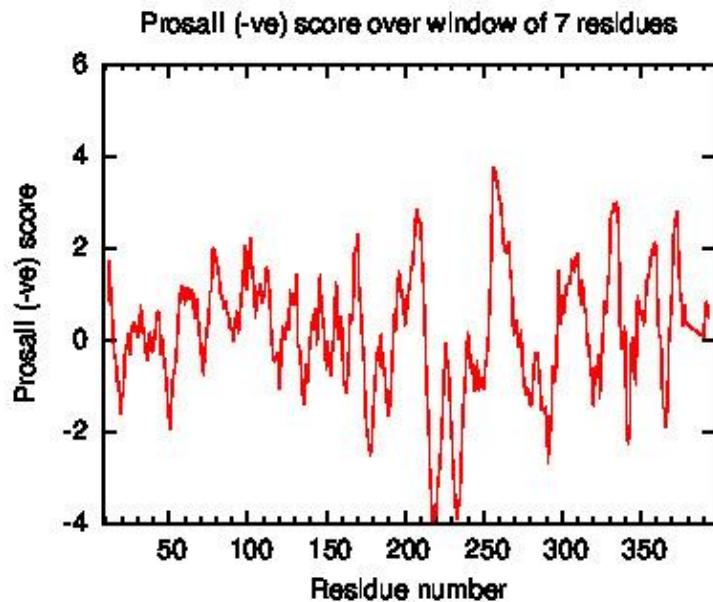
292	0.08
293	-0.68
294	-0.74
295	0.23
296	-0.54
297	0.51
298	0.71
299	0.71
300	0.51
301	0.44
302	-1.14
303	-0.74
304	-0.74
305	-0.25
306	-0.25
307	0.29
308	1.04
309	-0.68
310	-0.35
311	-0.54
312	-0.25
313	-0.68
314	1.10
315	1.25
316	-0.25
317	0.09
318	0.17
319	0.17
320	-0.68
321	0.09
322	-0.11
323	-0.74
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      0.44
396      0.17
#Reported_Model_Average 0.043
#Overall_Average_Reported      0.043
```

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     -0.83
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	0.17
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	0.51
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	0.71
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	-0.83
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	-0.74
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      0.44
396      0.17
#Reported_Model_Average 0.043
#Overall_Reported          0.043
```

Output from MolProbit

VdW violations from MAGE

JPEG image for MAGE VdW violation

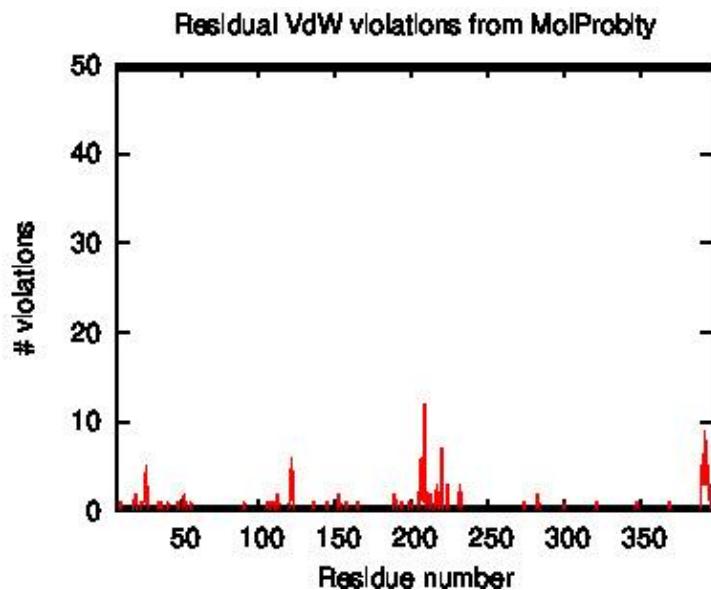


Table of MAGE VdW violations for ordered residues across all models

```
#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 1
20.000 2
21.000 0
22.000 0
23.000 0
24.000 1
25.000 1
26.000 1
27.000 5
28.000 0
29.000 0
30.000 0
31.000 0
32.000 0
33.000 0
34.000 0
35.000 1
36.000 0
37.000 1
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 0
50.000 0
51.000 0
52.000 2
53.000 0
54.000 0
55.000 0
56.000 1
57.000 0
58.000 0
59.000 0
60.000 0
61.000 0
62.000 0
63.000 0
64.000 0
65.000 0
66.000 0
67.000 0
68.000 0
69.000 0
70.000 0
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 0
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 1
107.000 0
108.000 0
109.000 1
110.000 1
111.000 0
112.000 0
113.000 2
114.000 0
115.000 0
116.000 0
117.000 0
118.000 0
119.000 0
120.000 0
121.000 2
122.000 6
123.000 1
124.000 0
125.000 0
126.000 0
127.000 0
128.000 0
129.000 0
130.000 0
131.000 0
132.000 0
133.000 0
134.000 0
135.000 0
136.000 1
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 1
146.000 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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PSVS Software Environment

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#Overall_Average_Reported      0.319

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List of bad contacts calculated by MAGE

5860	M	122	PRO	N	M	122	PRO	CD	-1.433	0
5860	M	122	PRO	CD	M	121	TRP	C	-1.291	0
5860	M	121	TRP	O	M	122	PRO	CD	-0.988	0
5860	M	122	PRO	2HD	M	121	TRP	O	-0.929	0
5860	M	122	PRO	CD	M	122	PRO	C	-0.686	0
5860	M	122	PRO	C	M	122	PRO	1HD	-0.676	0
5860	M	122	PRO	1HD	M	123	PHE	N	-0.645	0
5860	M	121	TRP	C	M	122	PRO	2HD	-0.574	0
5860	M	123	PHE	N	M	122	PRO	CD	-0.511	0
5860	M	392	PHE	HD2	M	207	LEU	1HB	-0.789	0
5860	M	209	PHE	CD2	M	392	PHE	CD2	-0.775	0
5860	M	209	PHE	CE1	M	207	LEU	O	-0.774	0
5860	M	390	TYR	N	M	390	TYR	HD1	-0.753	0
5860	M	392	PHE	CD1	M	217	ASP	HA	-0.753	0

PSVS Software Environment

5860	M	27	SER	HA	M	209	PHE	CE2	-0.743	0
5860	M	395	PRO	CD	M	394	TYR	CD1	-0.729	0
5860	M	206	MET	C	M	206	MET	2HE	-0.720	0
5860	M	209	PHE	CE2	M	392	PHE	CD2	-0.712	0
5860	M	209	PHE	N	M	209	PHE	CD1	-0.695	0
5860	M	27	SER	CB	M	209	PHE	CZ	-0.686	0
5860	M	392	PHE	HD2	M	207	LEU	CB	-0.672	0
5860	M	390	TYR	CD1	M	390	TYR	N	-0.666	0
5860	M	27	SER	1HB	M	209	PHE	CZ	-0.639	0
5860	M	136	TYR	CE2	M	224	VAL	1HG2	-0.608	0
5860	M	209	PHE	CD2	M	392	PHE	CE2	-0.594	0
5860	M	217	ASP	OD2	M	26	ALA	1HB	-0.589	0
5860	M	392	PHE	CD1	M	220	THR	1HG2	-0.589	0
5860	M	392	PHE	CE1	M	217	ASP	HA	-0.589	0
5860	M	395	PRO	2HD	M	394	TYR	CD1	-0.587	0
5860	M	392	PHE	HA	M	207	LEU	1HB	-0.586	0
5860	M	27	SER	O	M	393	GLY	C	-0.585	0
5860	M	209	PHE	CZ	M	27	SER	CA	-0.568	0
5860	M	207	LEU	CB	M	392	PHE	CD2	-0.567	0
5860	M	390	TYR	HA	M	190	ILE	CG1	-0.565	0
5860	M	209	PHE	1HB	M	213	SER	HA	-0.564	0
5860	M	207	LEU	CD1	M	390	TYR	2HB	-0.560	0
5860	M	392	PHE	CB	M	217	ASP	OD1	-0.559	0
5860	M	207	LEU	O	M	209	PHE	CZ	-0.558	0
5860	M	27	SER	1HB	M	209	PHE	CE1	-0.556	0
5860	M	27	SER	CB	M	209	PHE	CE1	-0.550	0
5860	M	395	PRO	1HD	M	394	TYR	CD1	-0.548	0
5860	M	392	PHE	CE1	M	220	THR	CB	-0.546	0
5860	M	394	TYR	CD1	M	209	PHE	HE1	-0.532	0
5860	M	206	MET	2HE	M	206	MET	O	-0.530	0
5860	M	390	TYR	1HB	M	220	THR	1HG2	-0.528	0
5860	M	190	ILE	1HG1	M	390	TYR	HA	-0.523	0
5860	M	136	TYR	CZ	M	391	ALA	HA	-0.506	0
5860	M	207	LEU	HG	M	391	ALA	O	-0.505	0
5860	M	27	SER	1HB	M	394	TYR	CG	-0.501	0
5860	M	199	ARG	1HB	M	395	PRO	1HB	-0.486	0
5860	M	395	PRO	O	M	199	ARG	NE	-0.484	0
5860	M	27	SER	O	M	393	GLY	CA	-0.478	0
5860	M	209	PHE	H	M	209	PHE	HD1	-0.459	0
5860	M	394	TYR	1HB	M	27	SER	C	-0.458	0
5860	M	220	THR	CG2	M	392	PHE	CD1	-0.455	0
5860	M	392	PHE	CD2	M	207	LEU	2HB	-0.453	0
5860	M	206	MET	C	M	206	MET	CE	-0.446	0
5860	M	217	ASP	1HB	M	209	PHE	CD2	-0.446	0
5860	M	392	PHE	CE1	M	220	THR	HB	-0.444	0
5860	M	220	THR	HG1	M	392	PHE	HE1	-0.443	0
5860	M	27	SER	HA	M	209	PHE	CZ	-0.440	0
5860	M	206	MET	1HB	M	206	MET	3HE	-0.437	0
5860	M	392	PHE	CD1	M	220	THR	CB	-0.436	0
5860	M	392	PHE	CD1	M	220	THR	HB	-0.436	0
5860	M	217	ASP	OD1	M	392	PHE	2HB	-0.435	0
5860	M	28	ASP	CG	M	394	TYR	2HB	-0.434	0
5860	M	195	VAL	CG2	M	206	MET	SD	-0.433	0
5860	M	393	GLY	O	M	207	LEU	N	-0.433	0
5860	M	207	LEU	2HB	M	392	PHE	CE2	-0.430	0
5860	M	209	PHE	CD2	M	392	PHE	CG	-0.429	0
5860	M	394	TYR	CD1	M	27	SER	1HB	-0.428	0
5860	M	394	TYR	CG	M	27	SER	CB	-0.428	0
5860	M	394	TYR	CG	M	395	PRO	1HD	-0.425	0
5860	M	27	SER	OG	M	213	SER	1HB	-0.423	0
5860	M	390	TYR	O	M	220	THR	1HG2	-0.423	0
5860	M	206	MET	1HB	M	393	GLY	O	-0.421	0

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5860 M 136 TYR CE2	M 224 VAL CG2	-0.417	0
5860 M 207 LEU CD1	M 391 ALA N	-0.415	0
5860 M 209 PHE CE1	M 27 SER OG	-0.411	0
5860 M 136 TYR CZ	M 224 VAL 1HG2	-0.410	0
5860 M 199 ARG 2HD	M 200 ASP N	-0.410	0
5860 M 207 LEU 2HD1	M 390 TYR C	-0.410	0
5860 M 391 ALA HA	M 136 TYR CE1	-0.406	0
5860 M 210 PRO 1HD	M 209 PHE HA	-0.405	0
5860 M 25 ASN CB	M 24 ALA HA	-0.657	0
5860 M 24 ALA HA	M 25 ASN 1HB	-0.434	0
5860 M 153 ARG HA	M 153 ARG NE	-0.605	0
5860 M 153 ARG HA	M 153 ARG CZ	-0.463	0
5860 M 188 VAL HB	M 189 PRO 2HD	-0.596	0
5860 M 186 VAL C	M 189 PRO 1HD	-0.473	0
5860 M 51 SER 1HB	M 52 SER HA	-0.543	0
5860 M 49 SER N	M 48 ARG 2HG	-0.429	0
5860 M 49 SER HA	M 52 SER 1HB	-0.417	0
5860 M 171 LYS NZ	M 165 ASP OD2	-0.511	0
5860 M 231 VAL HB	M 232 PRO 2HD	-0.501	0
5860 M 229 PHE C	M 232 PRO 1HD	-0.418	0
5860 M 231 VAL N	M 232 PRO CD	-0.415	0
5860 M 60 THR 3HG2	M 113 SER 1HB	-0.494	0
5860 M 109 LEU N	M 110 PRO 1HD	-0.420	0
5860 M 110 PRO CD	M 109 LEU N	-0.420	0
5860 M 110 PRO HA	M 113 SER 2HB	-0.402	0
5860 M 211 SER 2HB	M 216 TRP 1HB	-0.488	0
5860 M 21 PRO 2HD	M 19 GLN C	-0.477	0
5860 M 20 PRO 1HD	M 37 ALA 1HB	-0.440	0
5860 M 21 PRO 2HD	M 20 PRO N	-0.431	0
5860 M 19 GLN N	M 20 PRO 2HD	-0.421	0
5860 M 322 PRO 1HD	M 321 ASN N	-0.470	0
5860 M 152 ASP OD2	M 91 THR OG1	-0.469	0
5860 M 349 PRO 1HD	M 348 ASP HA	-0.461	0
5860 M 70 GLY 2HA	M 106 THR 1HG2	-0.461	0
5860 M 349 PRO 2HD	M 347 PRO O	-0.456	0
5860 M 301 PRO 1HD	M 300 ASP HA	-0.456	0
5860 M 282 ALA 3HB	M 283 PRO 2HD	-0.455	0
5860 M 282 ALA N	M 283 PRO CD	-0.431	0
5860 M 277 PHE 2HB	M 274 VAL HA	-0.450	0
5860 M 362 GLU 1HB	M 369 PRO 2HD	-0.439	0
5860 M 97 ASN ND2	M 145 THR OG1	-0.439	0
5860 M 40 ASN O	M 41 ALA C	-0.438	0
5860 M 246 ARG 1HG	M 158 CYS HA	-0.433	0
5860 M 129 LYS HA	M 194 ALA 3HB	-0.427	0
5860 M 9 GLU N	M 10 PRO CD	-0.406	0
5860 M 34 PHE 2HB	M 35 PRO 1HD	-0.405	0
5860 M 193 MET SD	M 208 GLN O	-0.405	0
5860 M 53 LEU HA	M 56 ALA 3HB	-0.401	0

Output from PDB validation software

Summary from PDB validation

Apr. 23, 17:34:40 2022

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

The following checks were made on :

PSVS Software Environment

CLOSE CONTACTS

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

none

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 0.012 Angstroms

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

Deviation	Residue	Chain	Sequence	AT1	-	AT2	Bond	Dictionary
	Name	ID	Number				Distance	Value
-0.096	PRO	A	122	CB	-	CG	1.396	1.492
0.245	PRO	A	122	CD	-	N	1.718	1.473
0.122	PRO	B	6	CD	-	N	1.595	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
-30.5	PRO	A	122	CA	-	N	-	CD	81.5	112.0

PSVS Software Environment

44.4	PRO	A	122	C	-	N	-	CA	167.0	122.6
30.3	GLY	A	124	C	-	N	-	CA	150.9	120.6
-12.7	PRO	B	6	CA	-	N	-	CD	99.3	112.0

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_refined_model.pdb: Missing KEYWDS records

Final_refined_model.pdb: Missing TITLE record