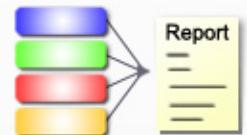


Protein Structure Validation Suite (PSVS)



PSVS report for dorh_rosettacm

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PSVS report for S_0003



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.): 372

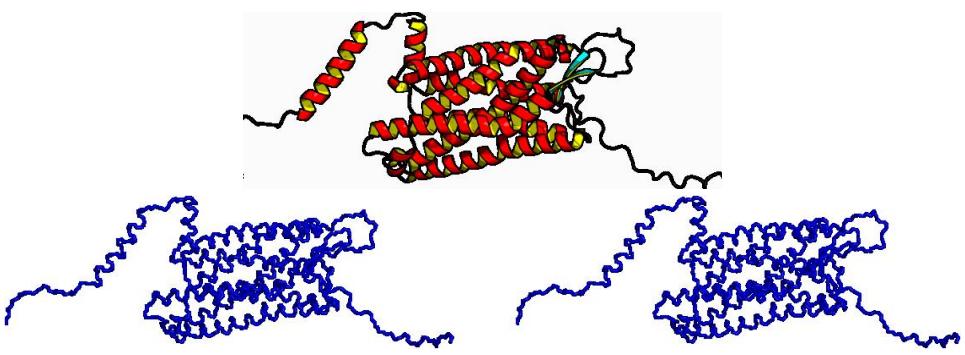
Organism:

SwissProt /
TrEMBL ID:

models: 1

Oligomerization: monomer

Molecular
weight: 40368



Secondary Structure Elements:

alpha helices:

beta strands:

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
93.5%	5.5%	0.3%	0.6%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobity

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
94.3%	3.8%	1.9%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
Raw score	0.03	0.13	0.19	0.15	0.00
Z-score ¹	-6.90	-2.15	1.06	0.89	1.53

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

Number of close contacts (within 2.2 Å): 0

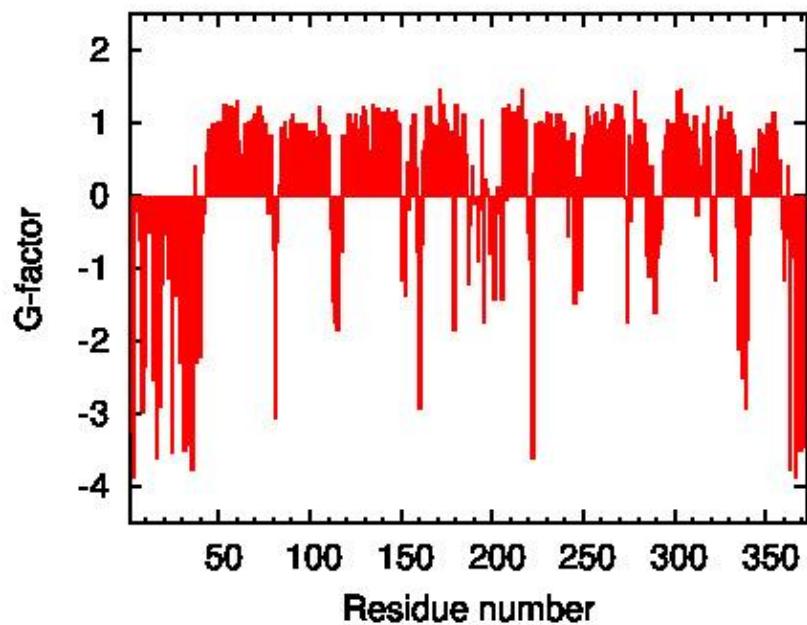
RMS deviation for bond angles: 1.8 °

RMS deviation for bond lengths: 0.013 Å

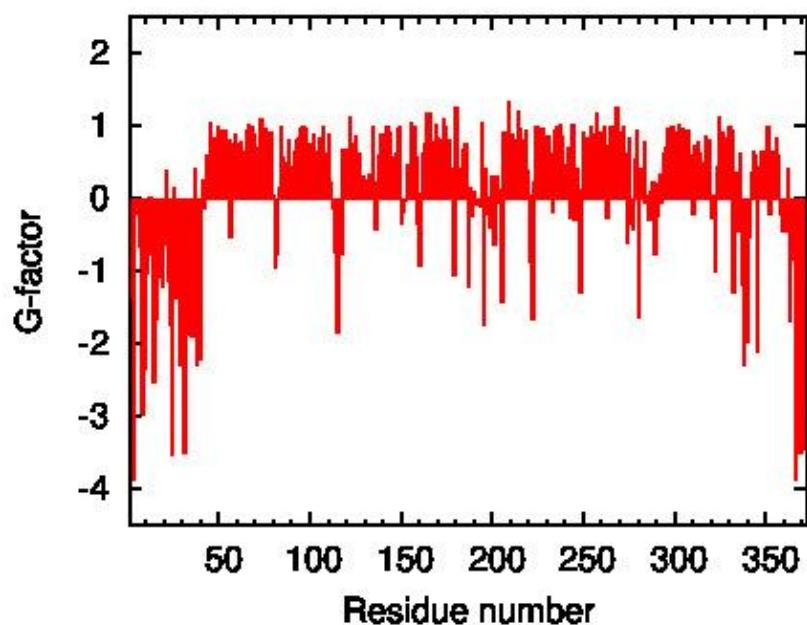
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

³Selected residues: all

Procheck G-factor for phi-psi

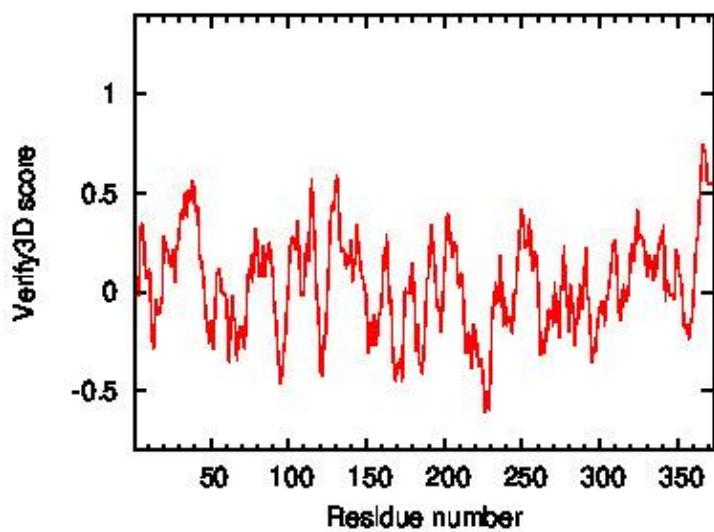


Procheck G-factor for all dihedral angles

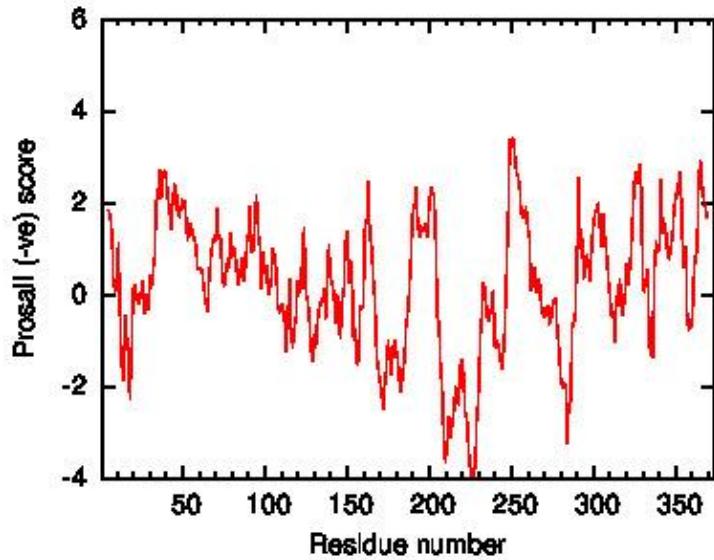


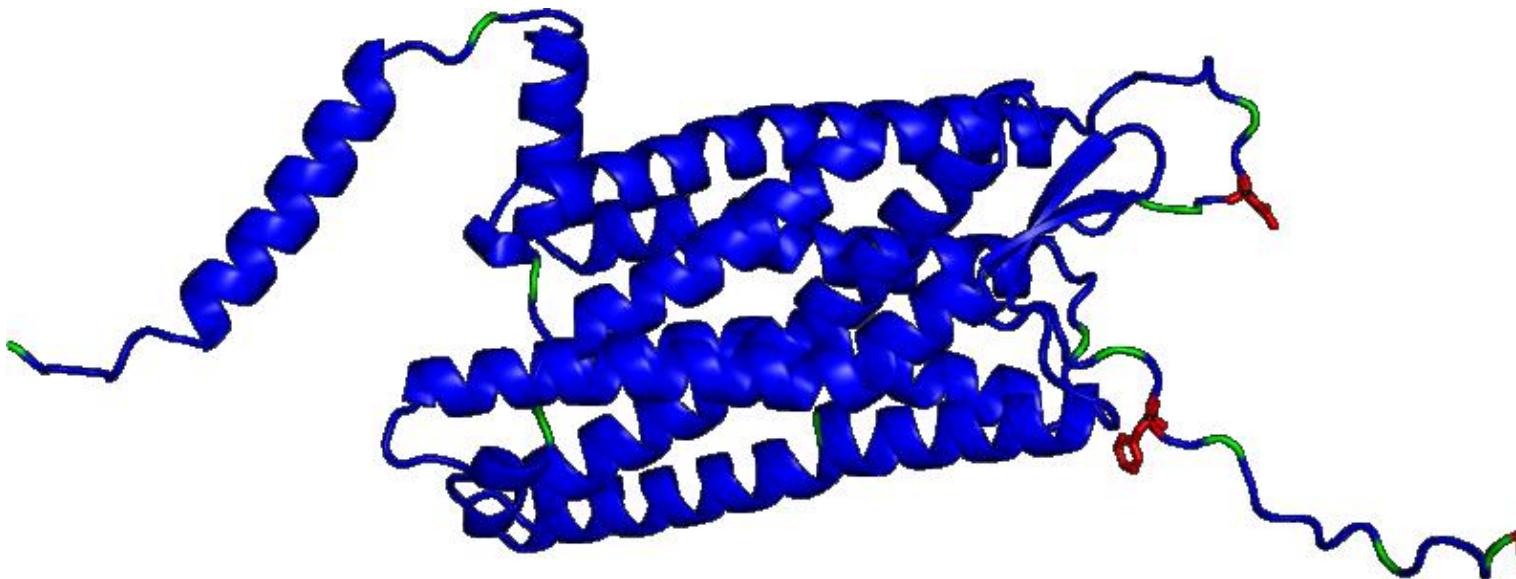
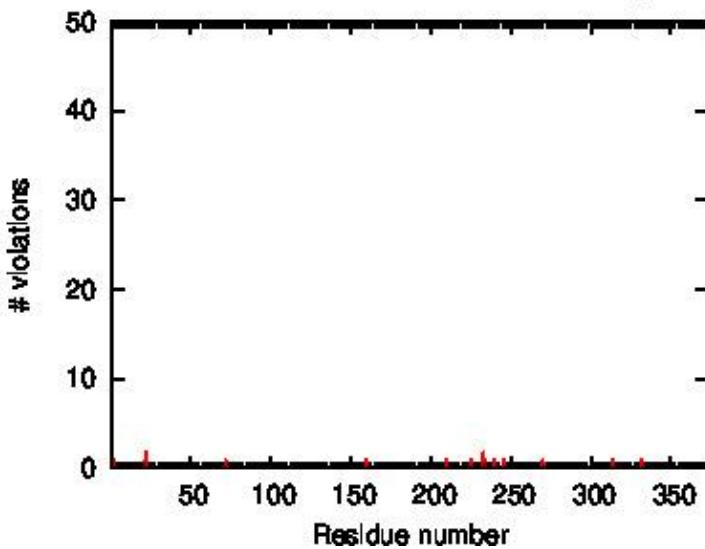
PSVS Software Environment

Verify3D score over window of 7 residues



ProsaII (-ve) score over window of 7 residues



Residual VdW violations from MolProbity**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
5. Sippl MJ, "Recognition of errors in three-dimensional structures of proteins". *Proteins* 1993, 17:355-362
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

PSVS Software Environment

8. Laskowski RA et al "PROCHECK: a program to check the stereochemical quality of protein structures". *J Appl Cryst* 1993, 26:283-291
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
13. Richardson DC, Richardson J S, "The kinemage: a tool for scientific communication". *Prot Sci* 1992, 1(1):3-9
14. Guntärt 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)	0.19	N/A	1.06
Procheck G-factor ^e (all dihedral angles)	0.15	N/A	0.89
Verify3D	0.03	0.0000	-6.90
ProsaII (-ve)	0.13	0.0000	-2.15
MolProbity clashscore	0.00	0.0000	1.53
Ramachandran Plot Summary from Procheck			
Most favoured regions	93.5%		
Additionally allowed regions	5.5%		
Generously allowed regions	0.3%		
Disallowed regions	0.6%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	94.3%		
Allowed regions	3.8%		
Disallowed regions	1.9%		

^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 dorh_rosettacm by PSVS

Output from PDBStat

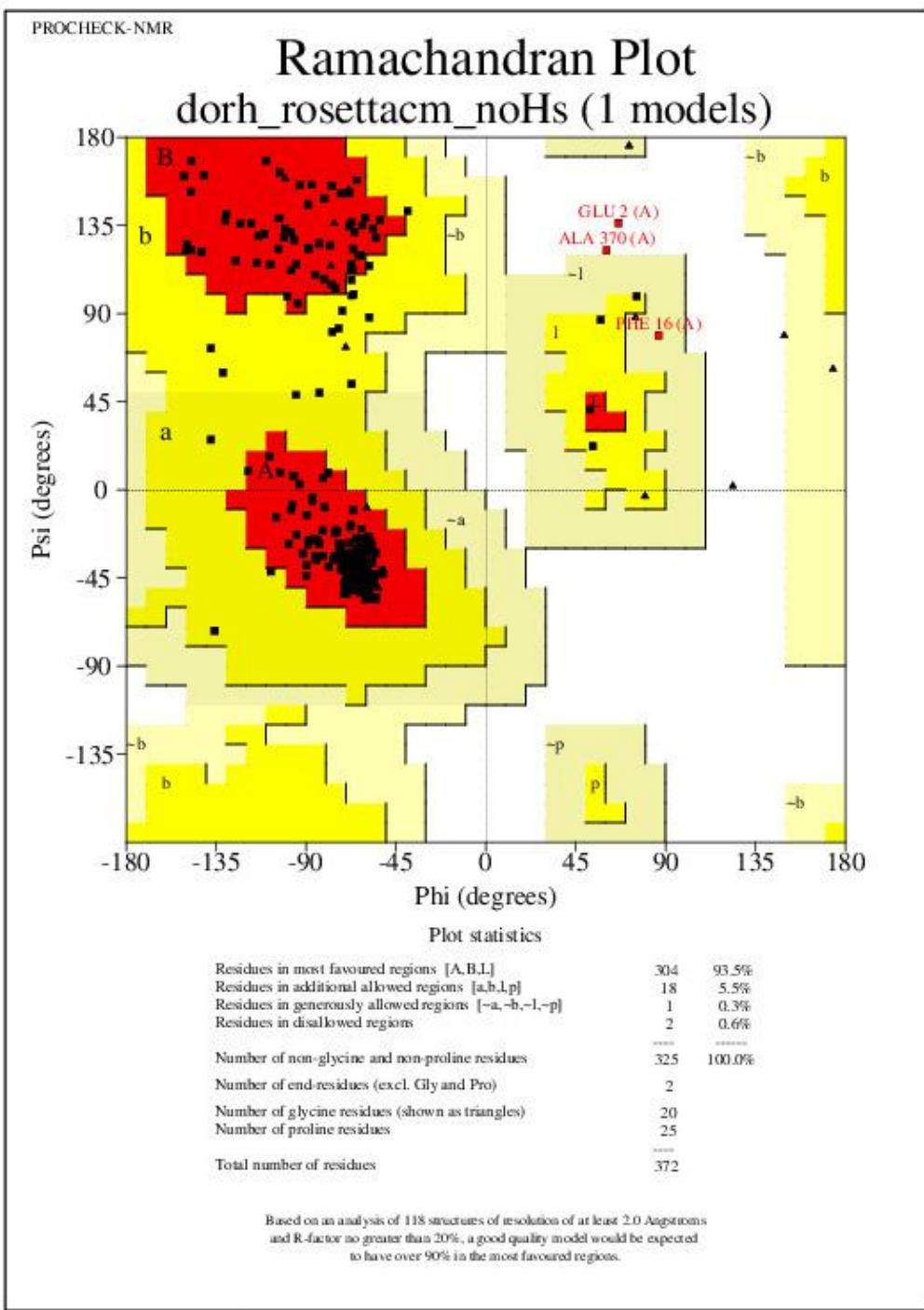
Output from PROCHECK

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   >>>-----+
| |
| dorh_rosettacm_noHs_000.rin    0.0                                372 residues |
| |
*| Ramachandran plot:    93.5% core      5.5% allow      0.3% gener     0.6% disall |
| |
*| All Ramachandrans:    15 labelled residues (out of 370) |
+| Chil-chi2 plots:        4 labelled residues (out of 186) |
```

JPEG image for all model Ramachandran Plot



dorh_rosettaclm_noHs_01_ramachand.ps

Residue Properties for all models

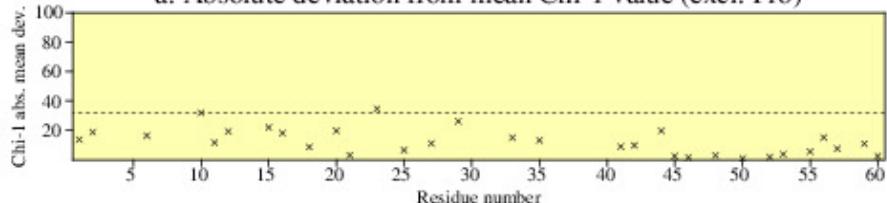
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

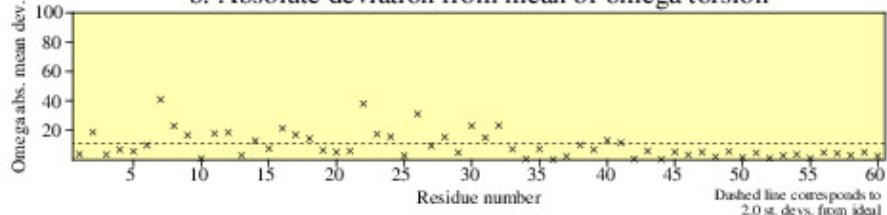
Page 1

Residue properties dorh_rosettacm_noHs (1 models)

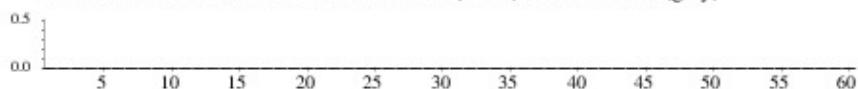
a. Absolute deviation from mean Chi-1 value (excl. Pro)



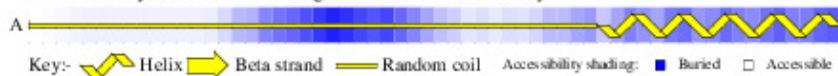
b. Absolute deviation from mean of omega torsion



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



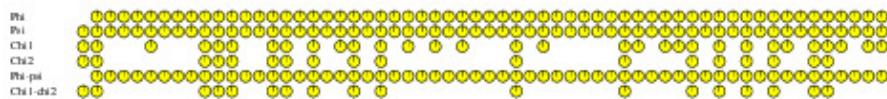
d. Secondary structure & average estimated accessibility



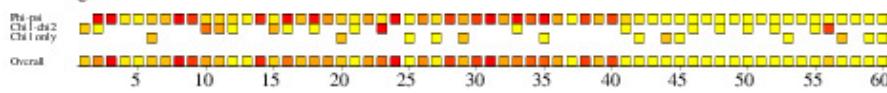
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



dorh_rosettacm_noHs_10_residprop.ps

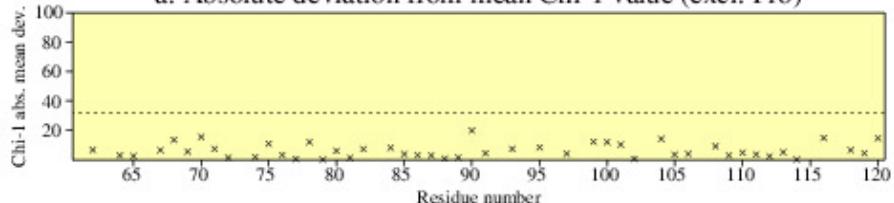
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

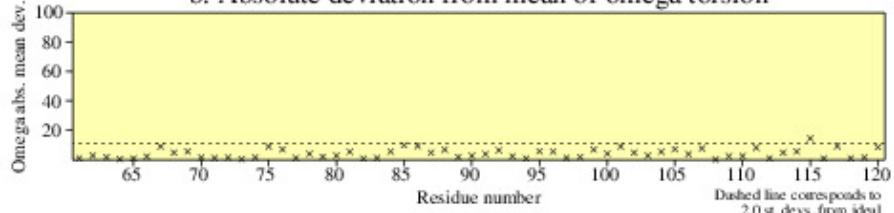
Page 2

Residue properties dorh_rosettacm_noHs (1 models)

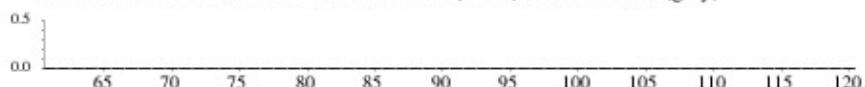
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



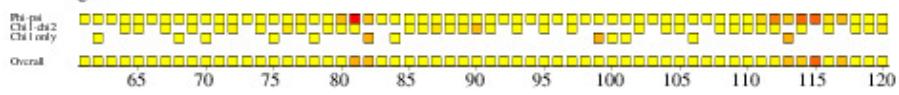
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



dorh_rosettacm_noHs_10_residprop.ps

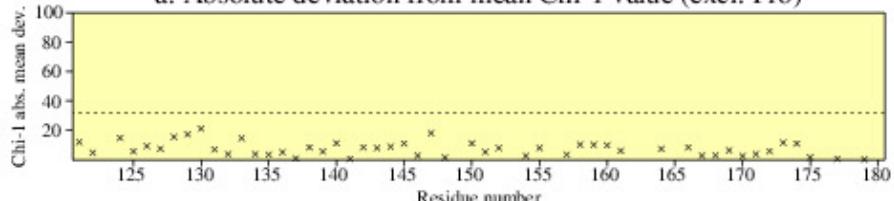
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

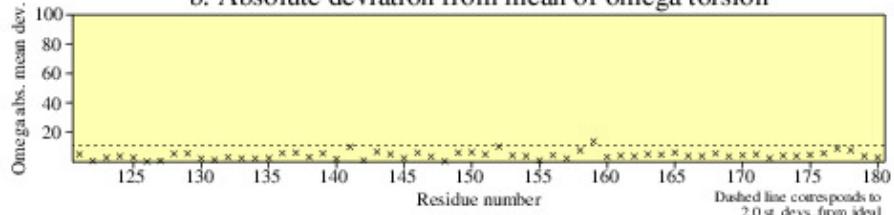
Page 3

Residue properties dorh_rosettacm_noHs (1 models)

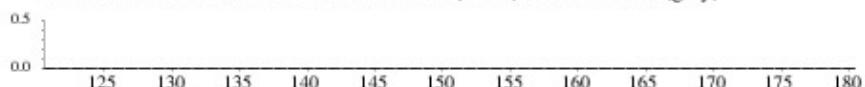
a. Absolute deviation from mean Chi-1 value (excl. Pro)



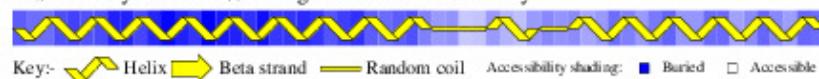
b. Absolute deviation from mean of omega torsion



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



dorh_rosettacm_noHs_10_residprop.ps

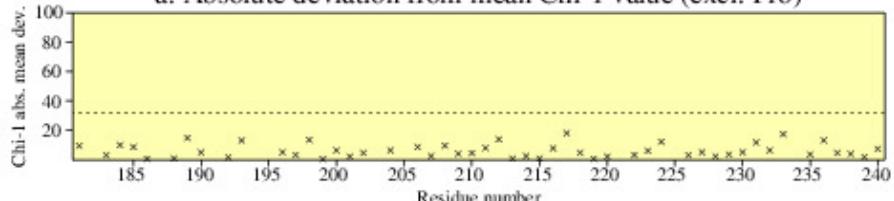
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

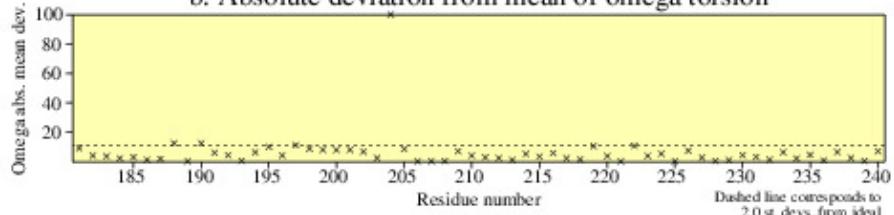
Page 4

Residue properties dorh_rosettacm_noHs (1 models)

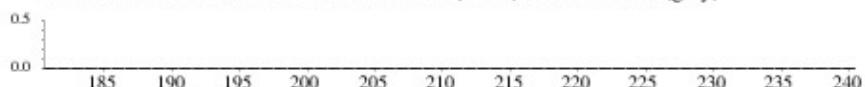
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



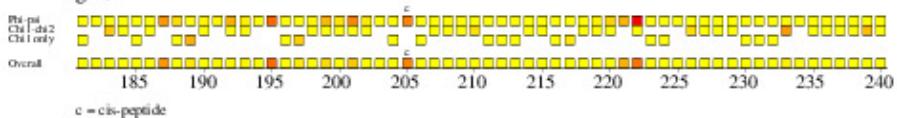
e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



dorh_rosettacm_noHs_10_residprop.ps

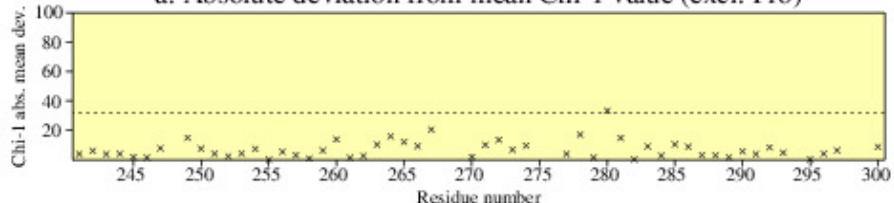
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

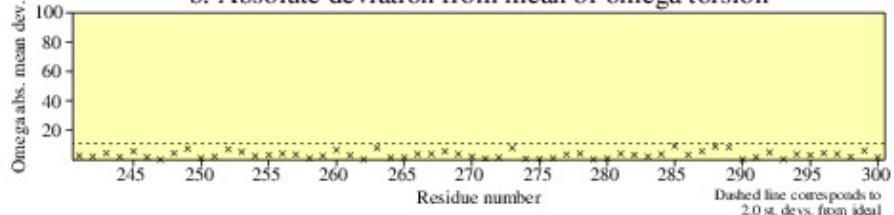
Page 5

Residue properties dorh_rosettacm_noHs (1 models)

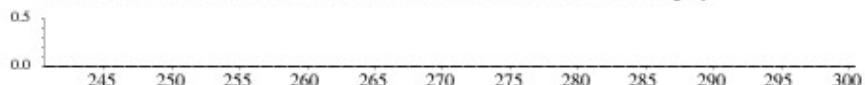
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



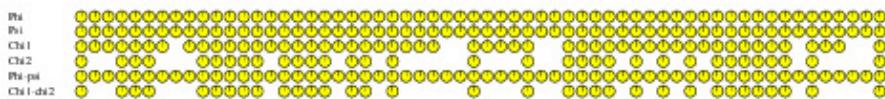
d. Secondary structure & average estimated accessibility



e. Sequence & average estimated accessibilities



f. Circular variances



g. G-factors



dorh_rosettacm_noHs_10_residprop.ps

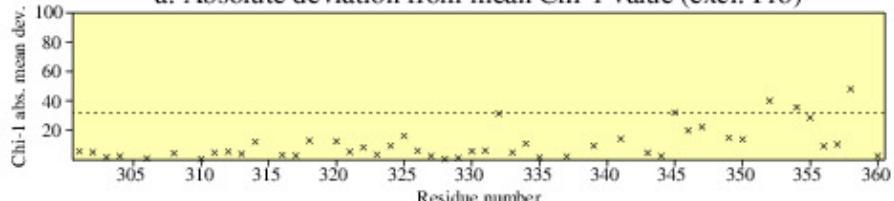
JPEG for all model Residue Properties - page \$num_n

PROCHECK-NMR

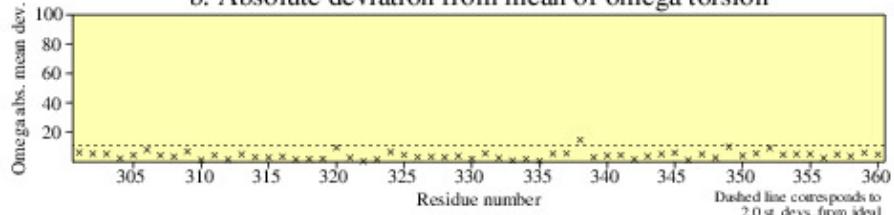
Page 6

Residue properties dorh_rosettacm_noHs (1 models)

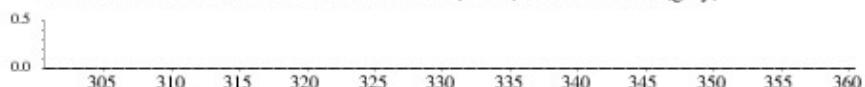
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

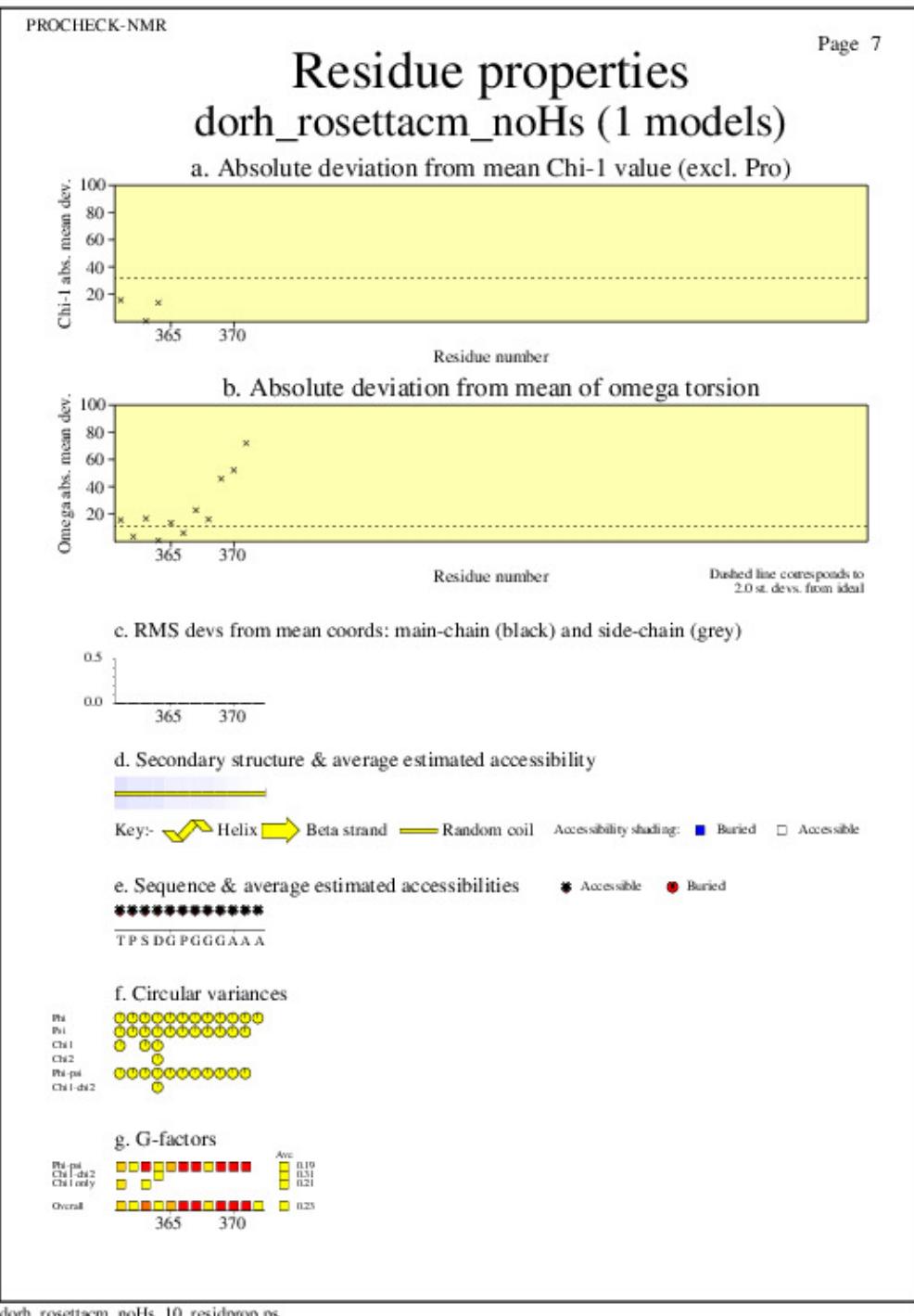


g. G-factors



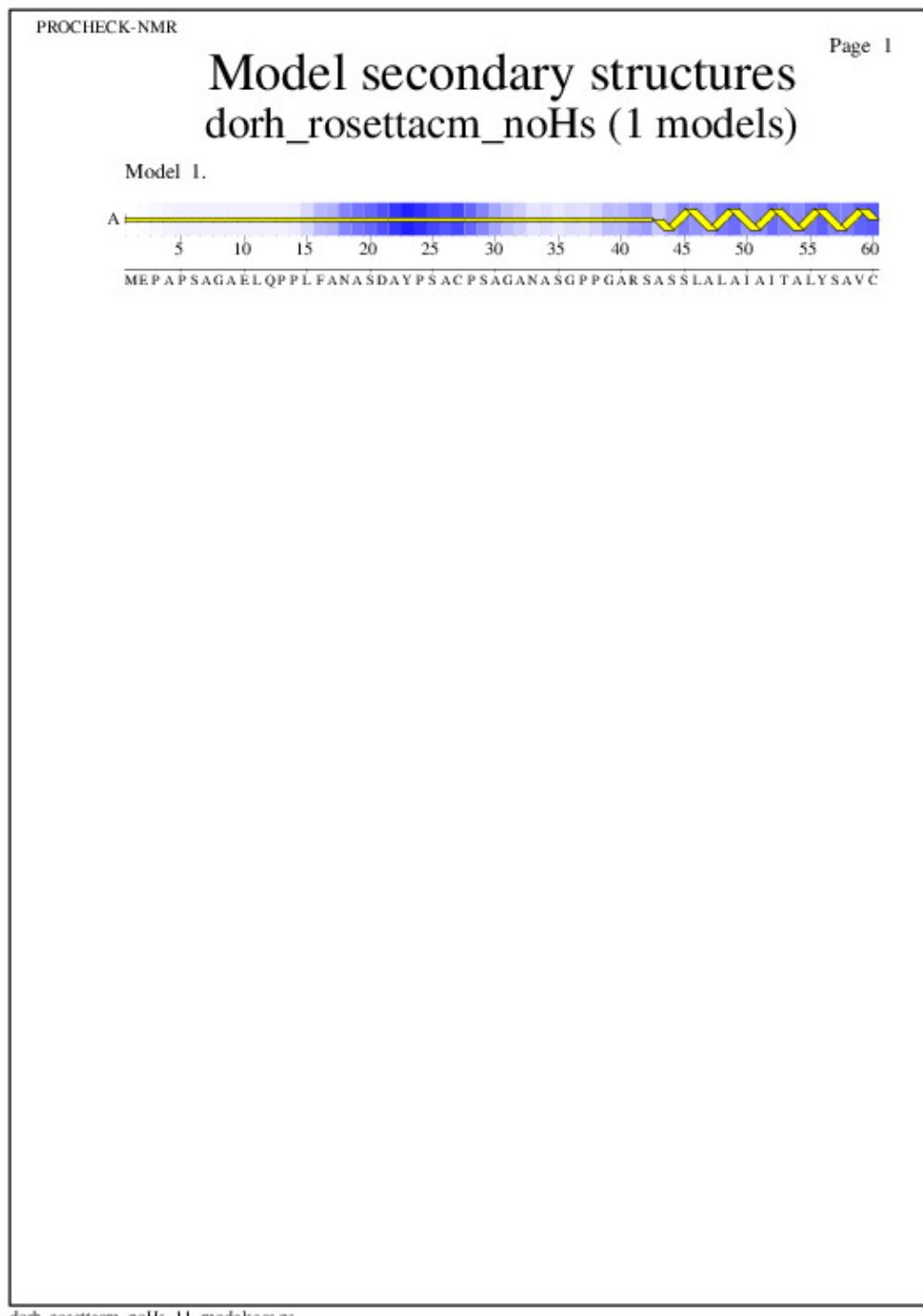
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JPEG for all model Residue Properties - page \$num_n

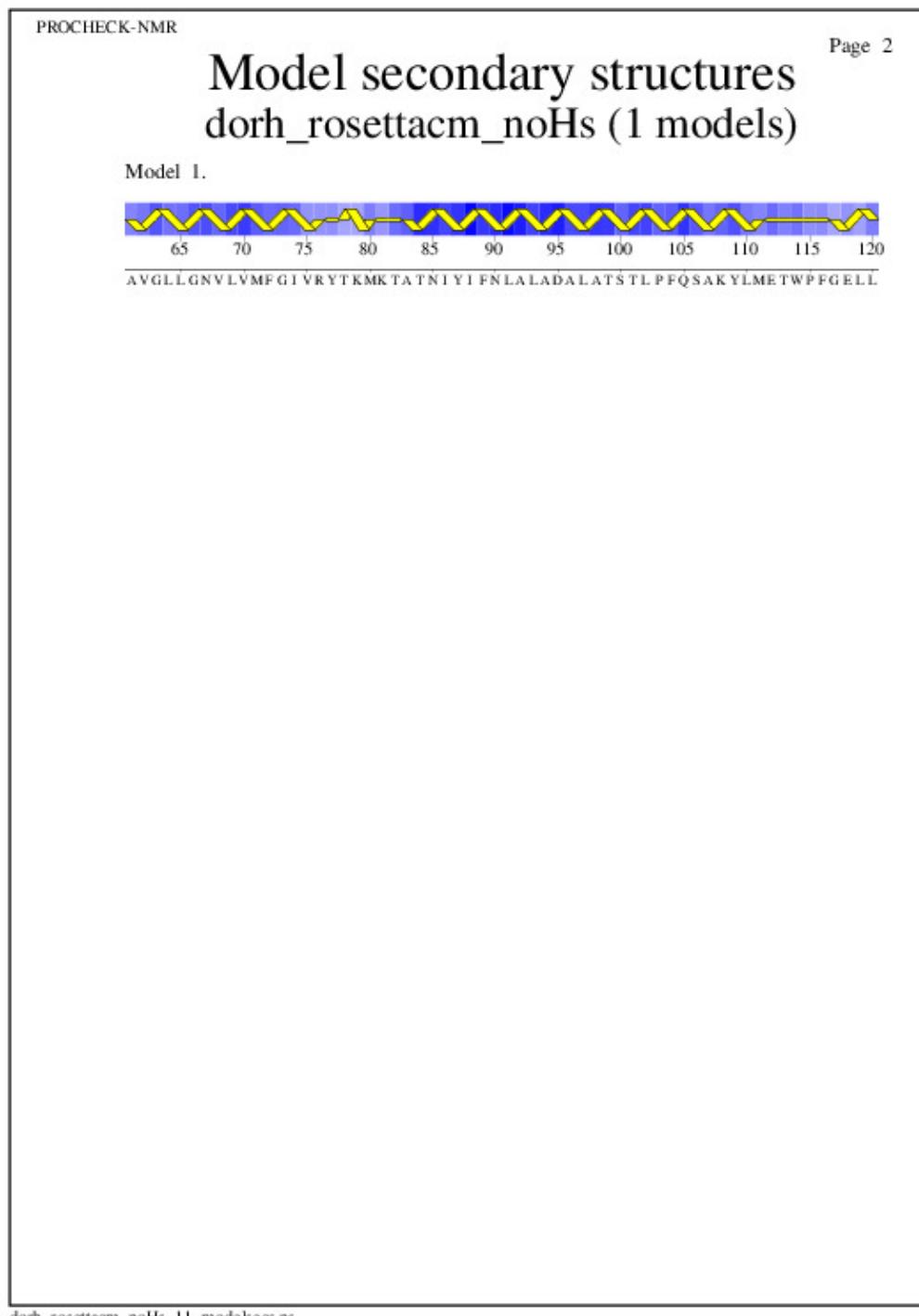


Model Secondary Structures from Procheck

JPEG for Model Secondary Structures - page \$num_n

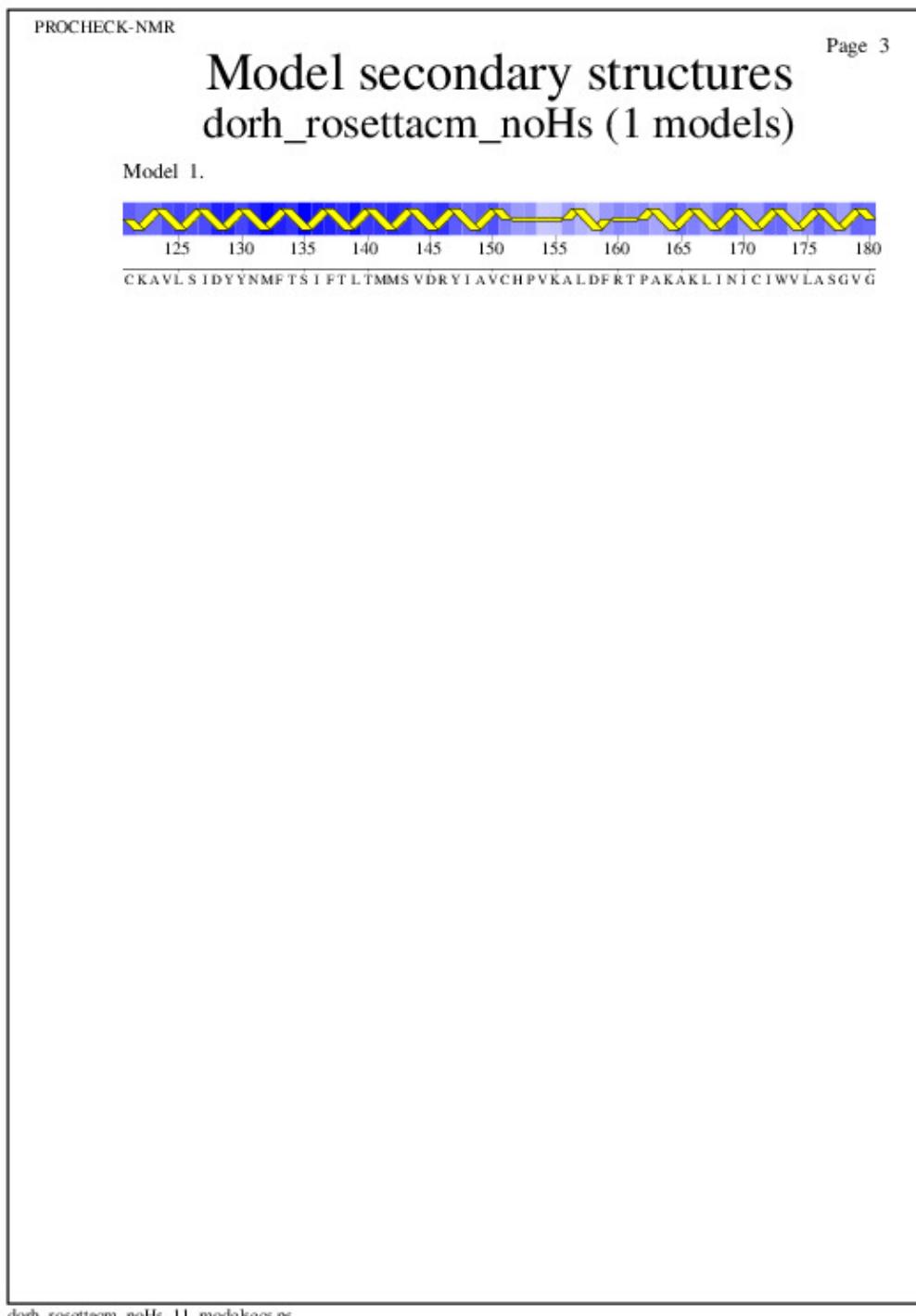


JPEG for Model Secondary Structures - page \$num_n

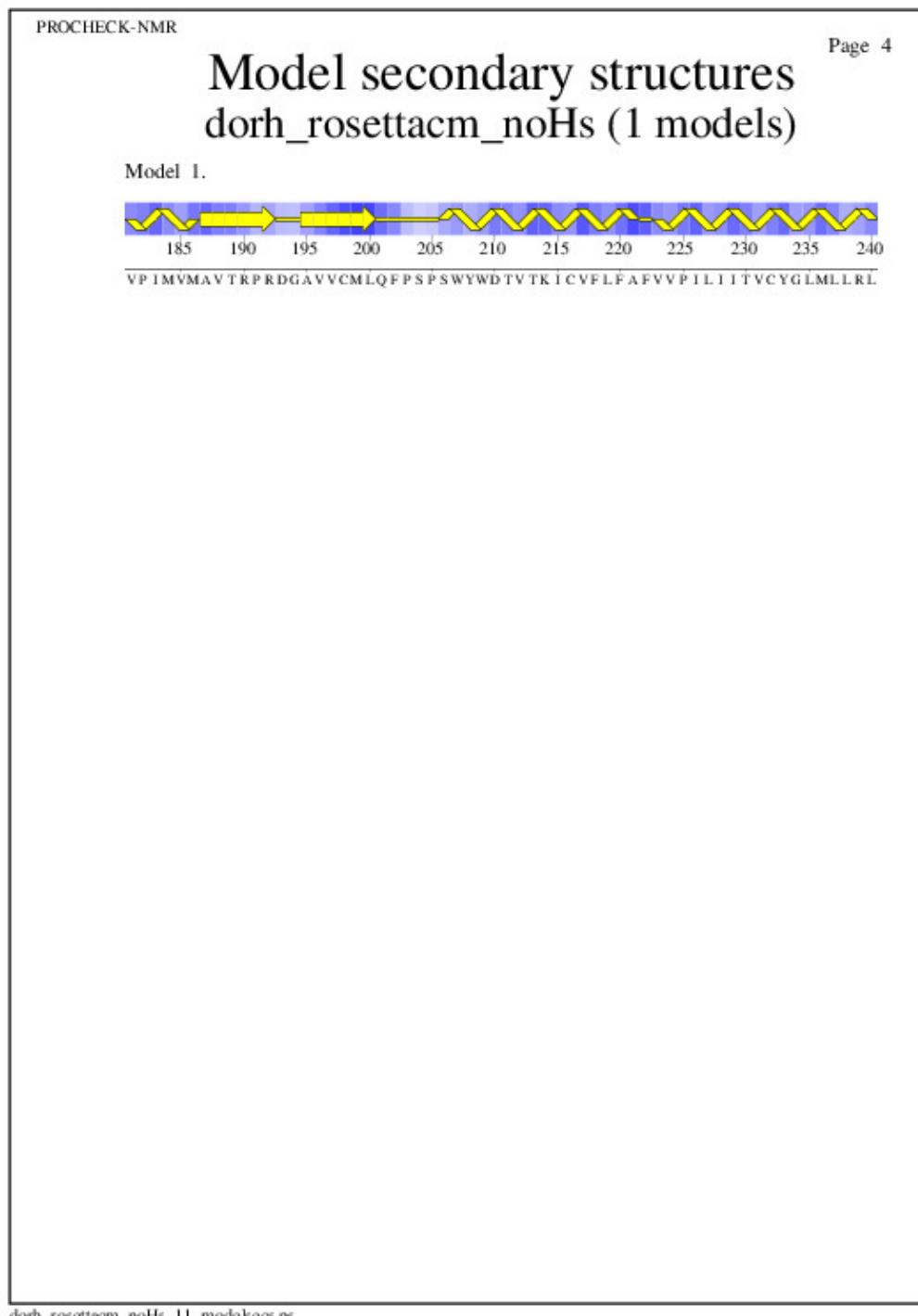


dorh_rosettaclm_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n

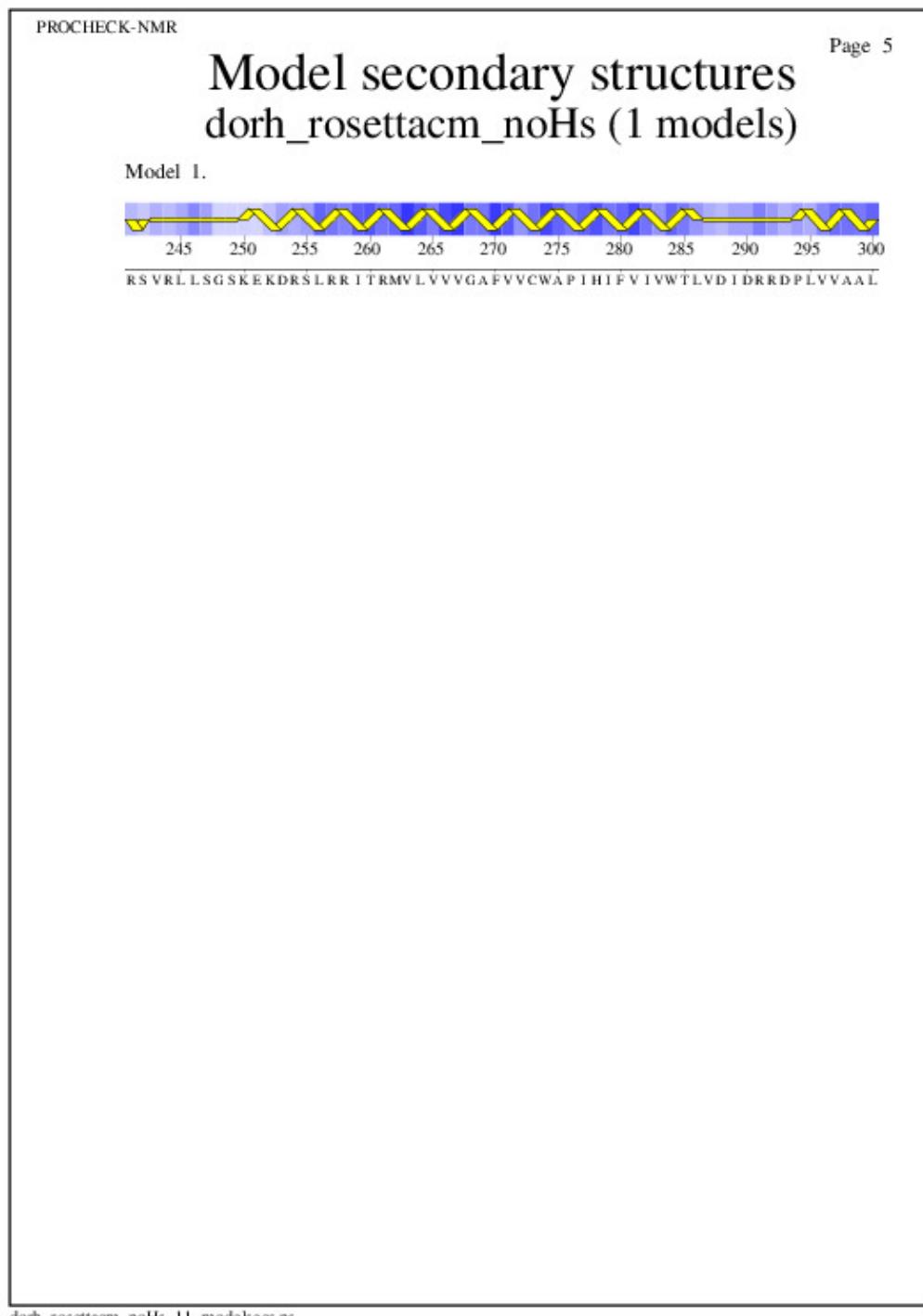


JPEG for Model Secondary Structures - page \$num_n

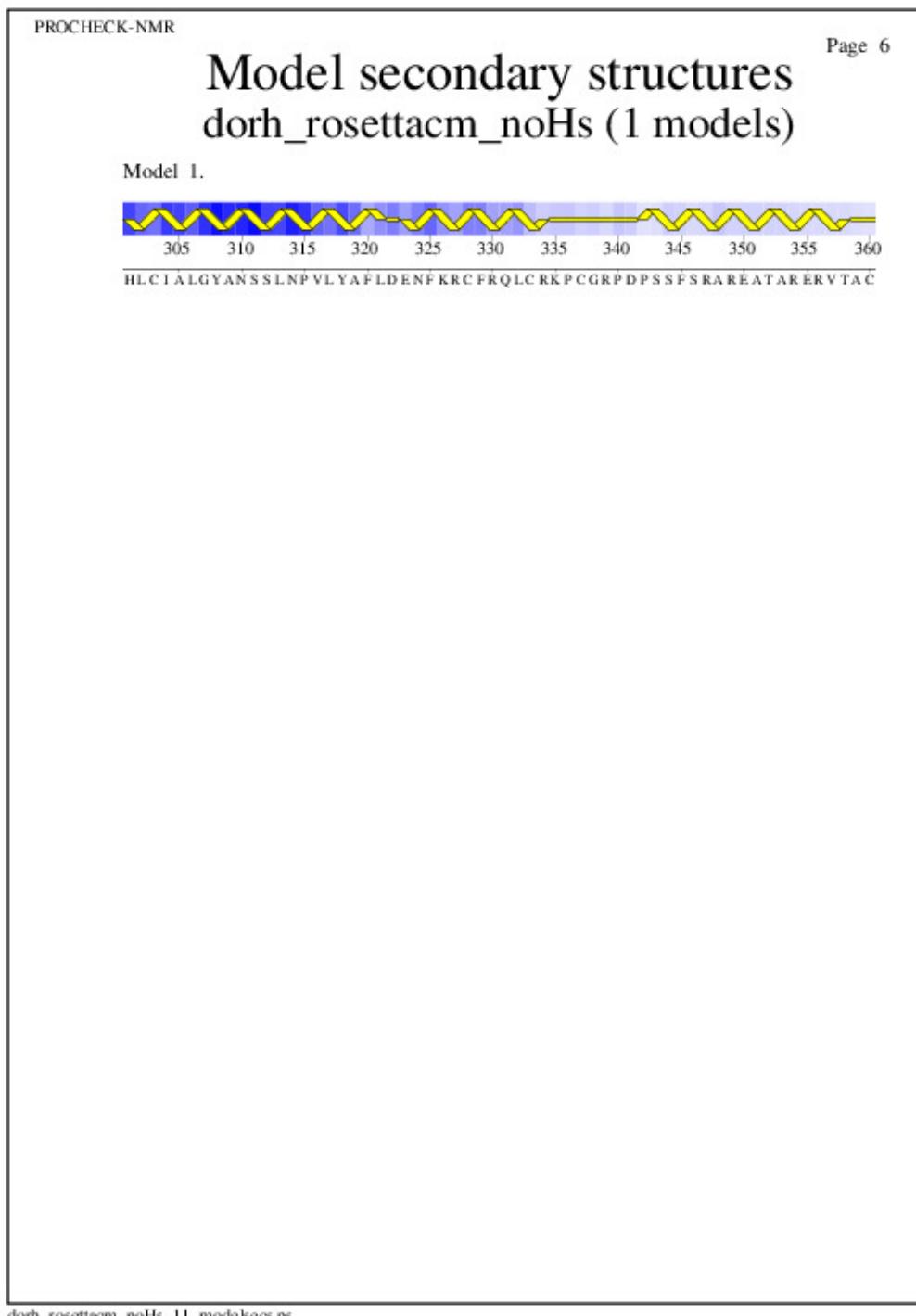


dorh_rosettaclm_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n

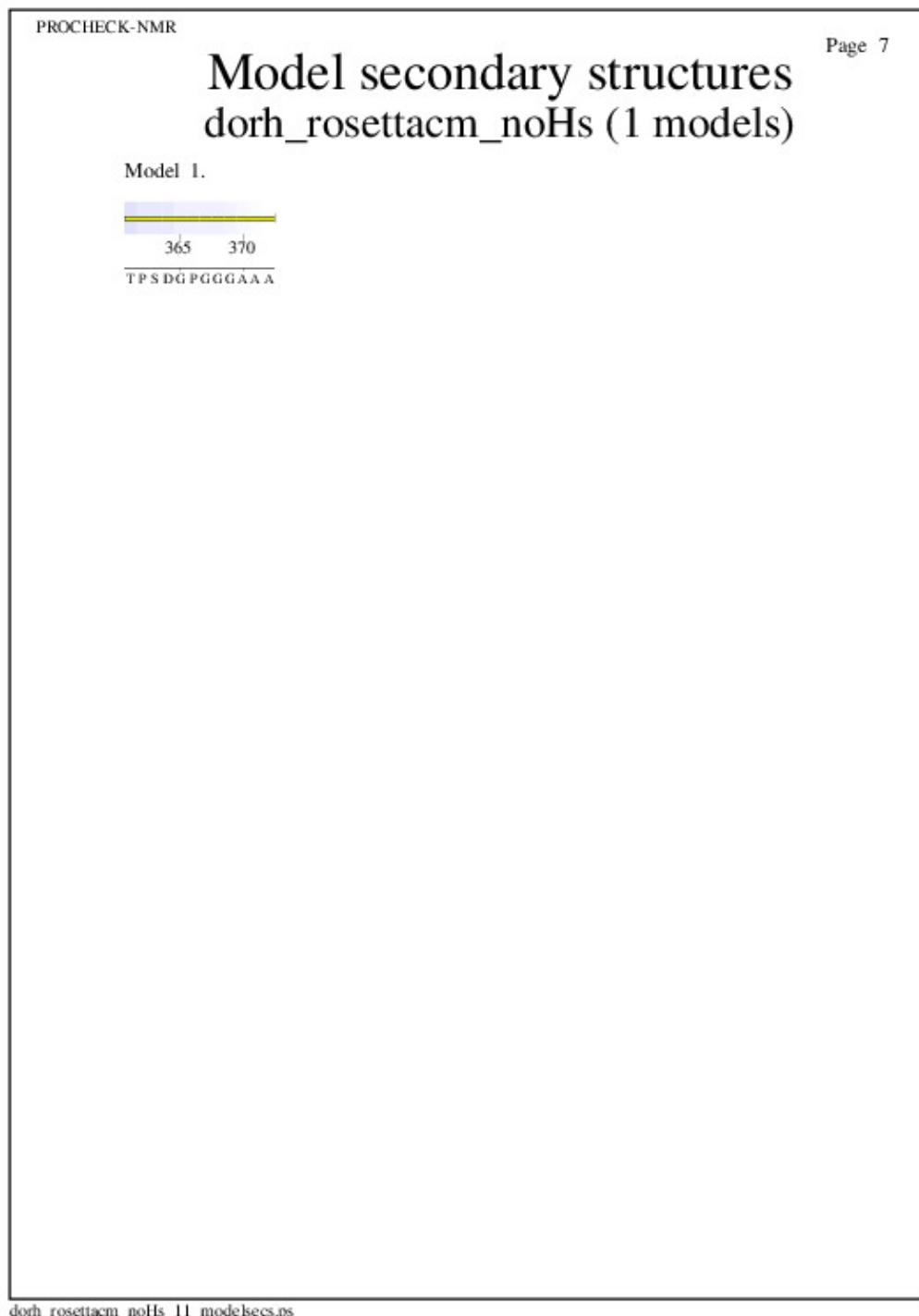


JPEG for Model Secondary Structures - page \$num_n



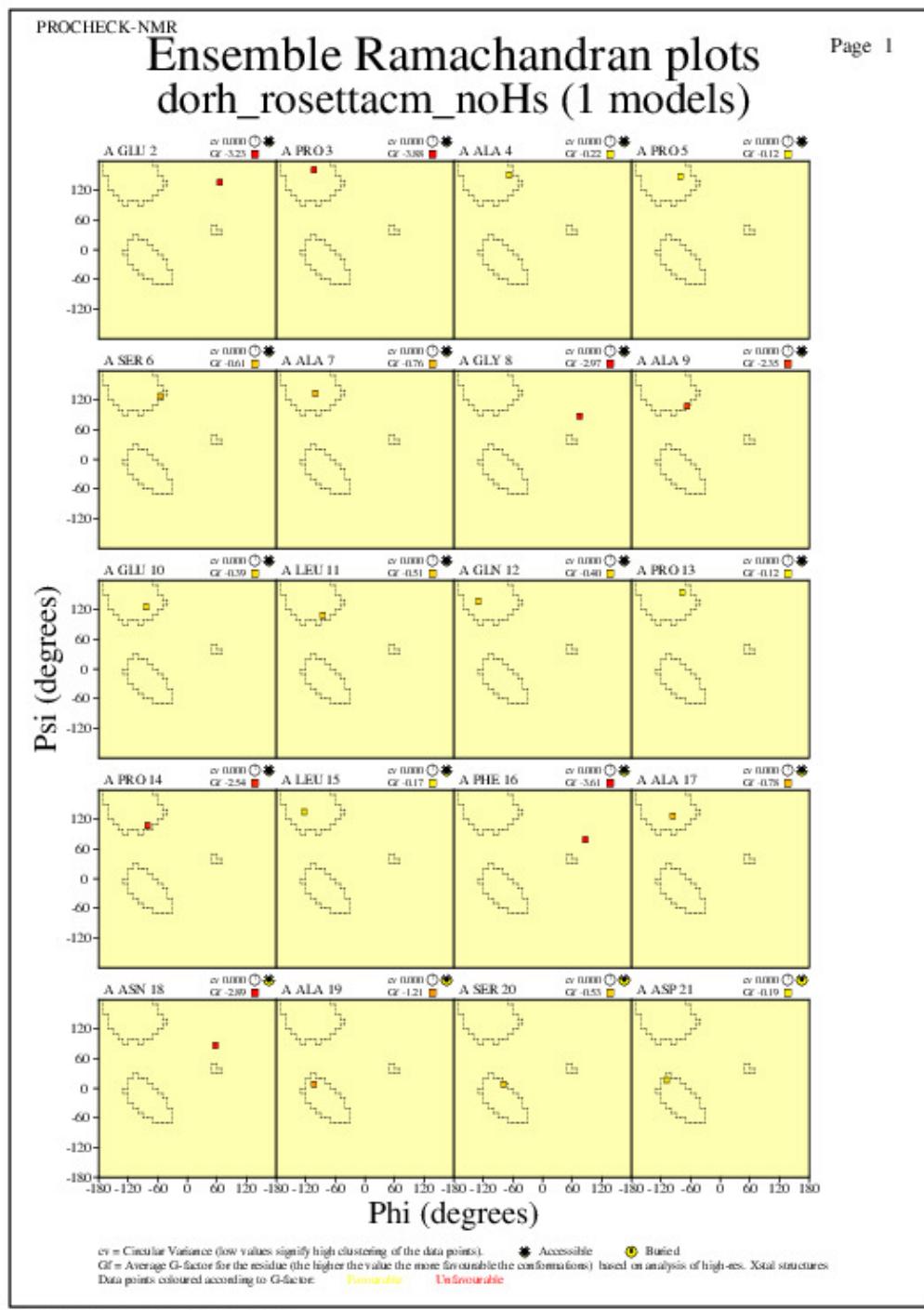
dorh_rosettaclm_noHs_11_modsecs.ps

JPEG for Model Secondary Structures - page \$num_n

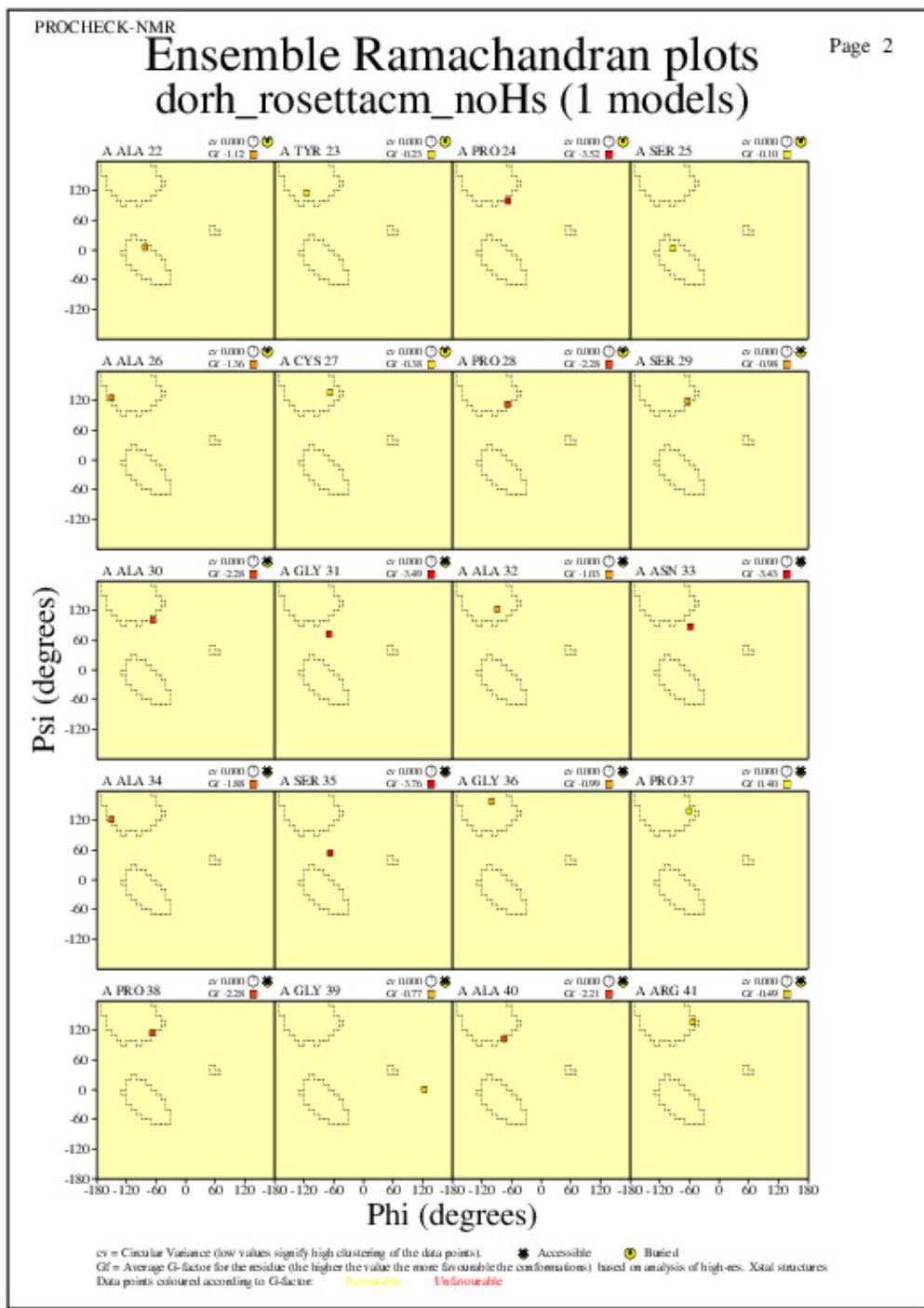


Ramachandran Plots for each residue

JPEG for residue Ramachandran Plots - page \$num_n

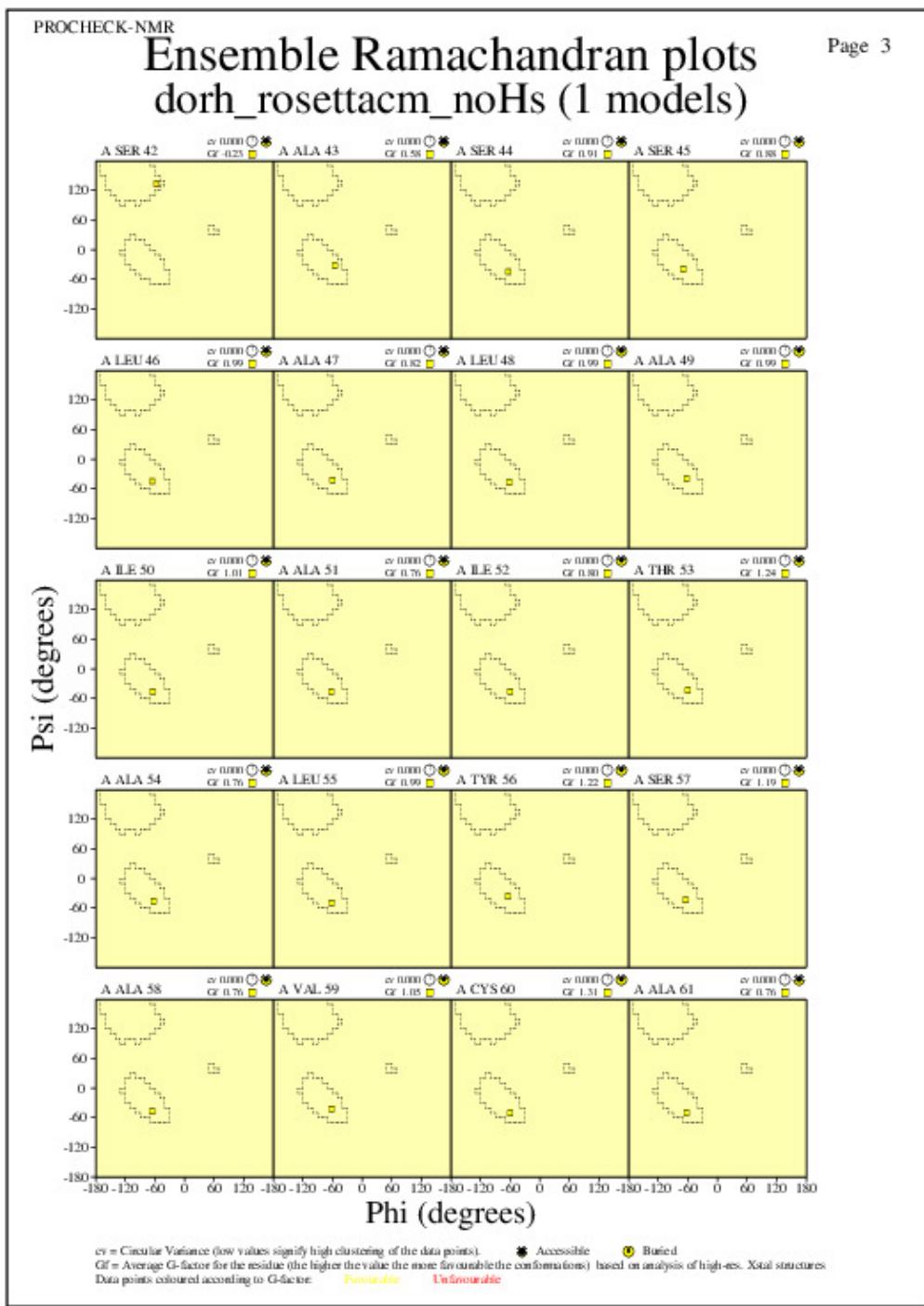


JPEG for residue Ramachandran Plots - page \$num_n



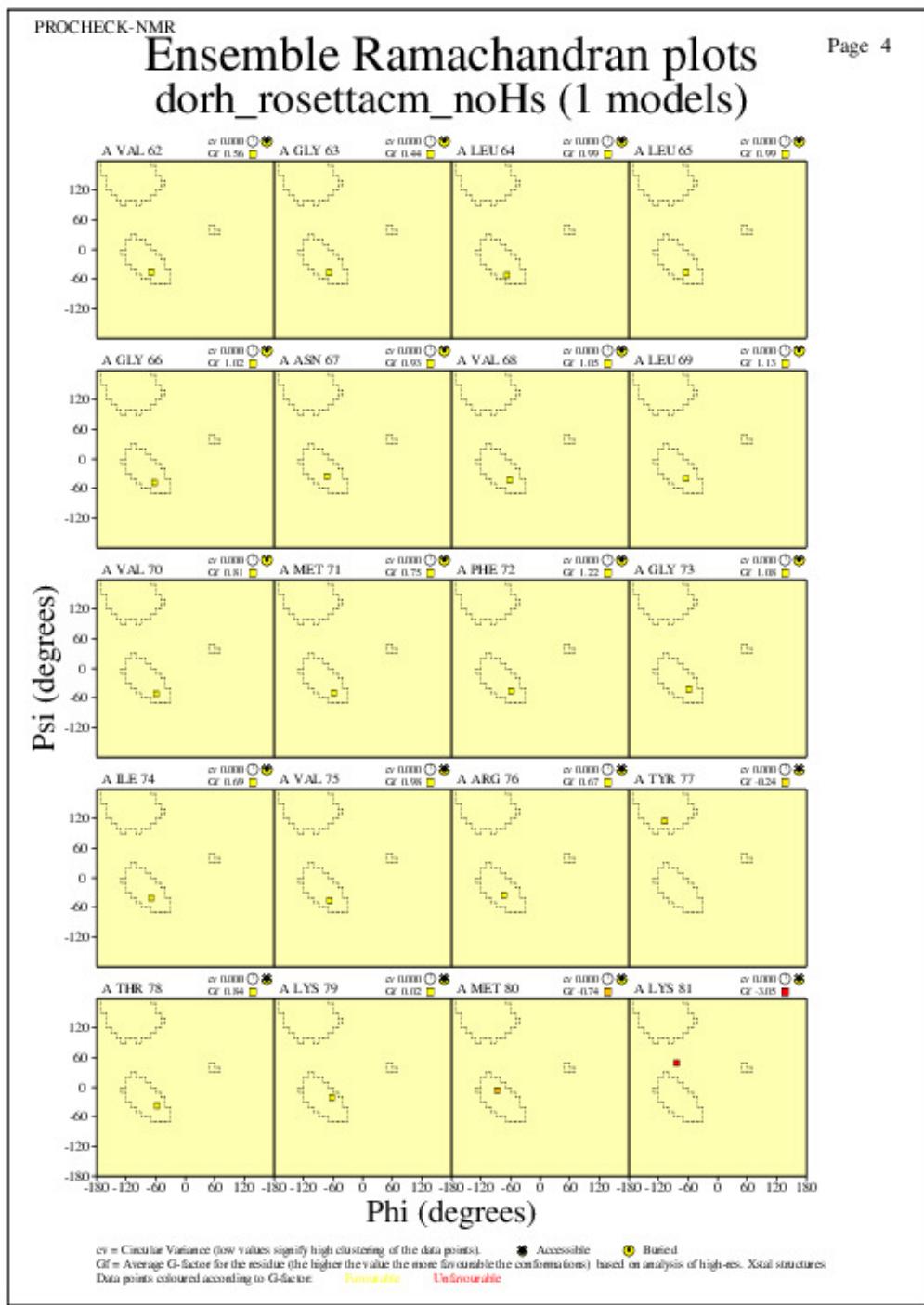
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



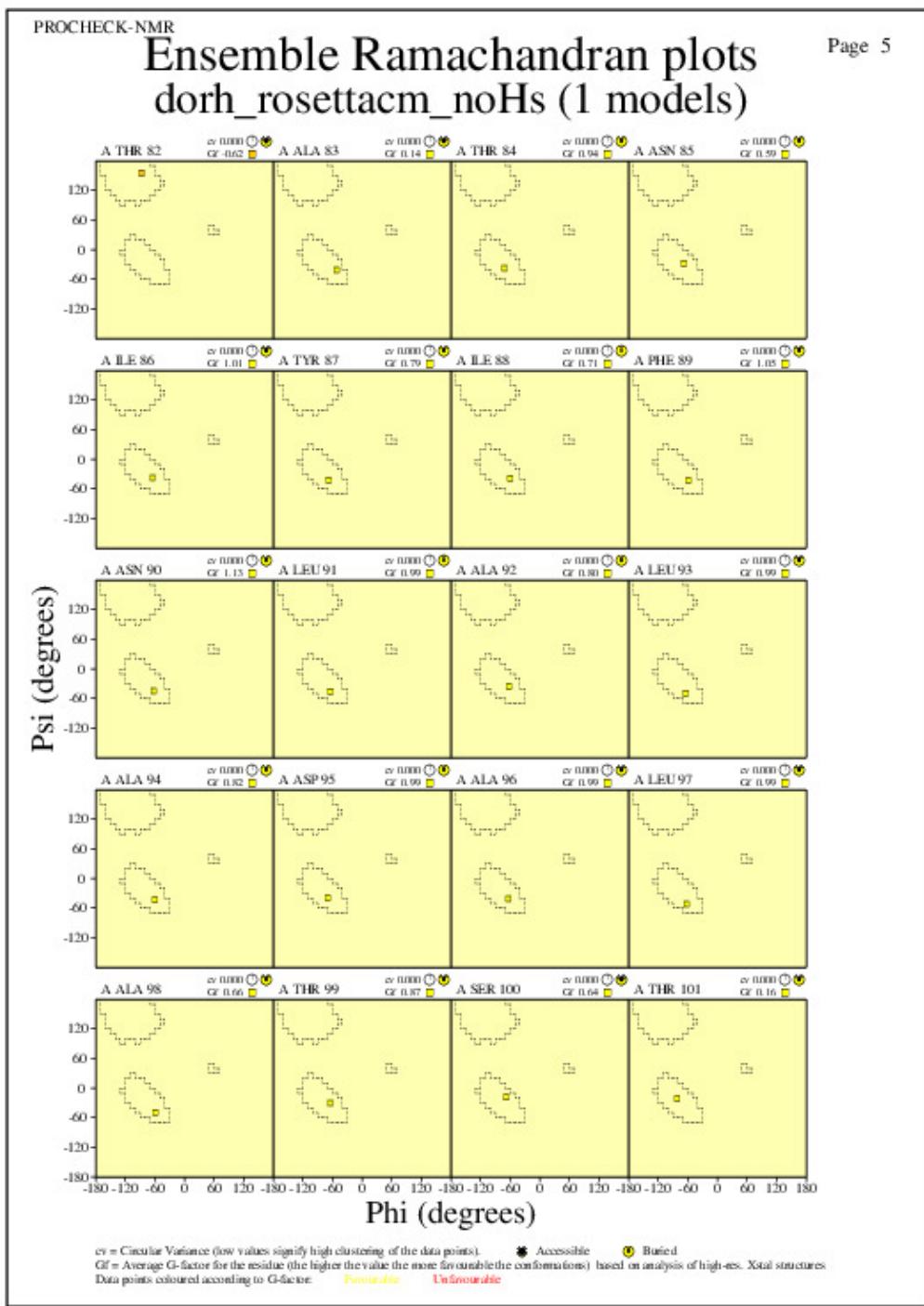
dorh_rosettacm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



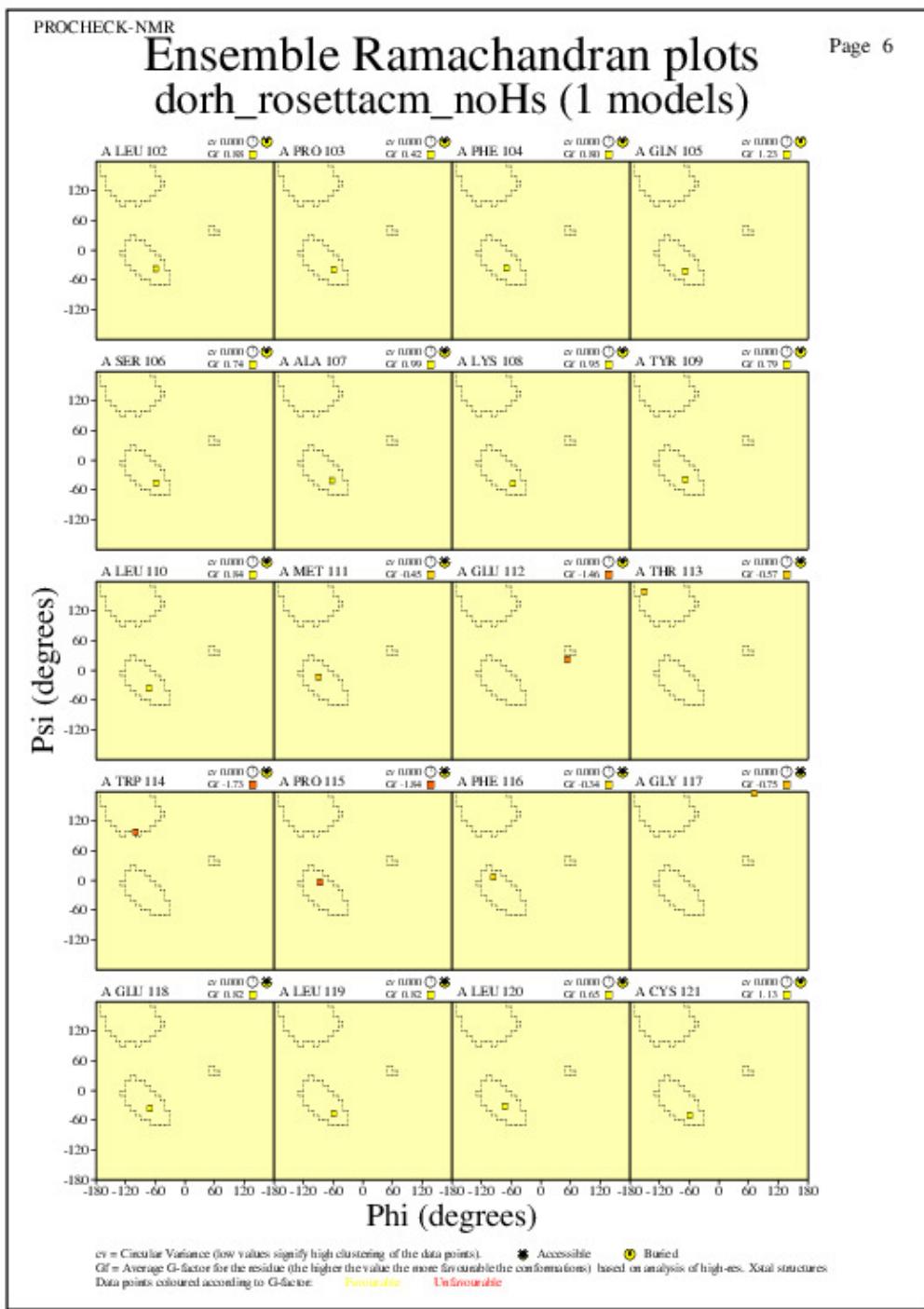
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



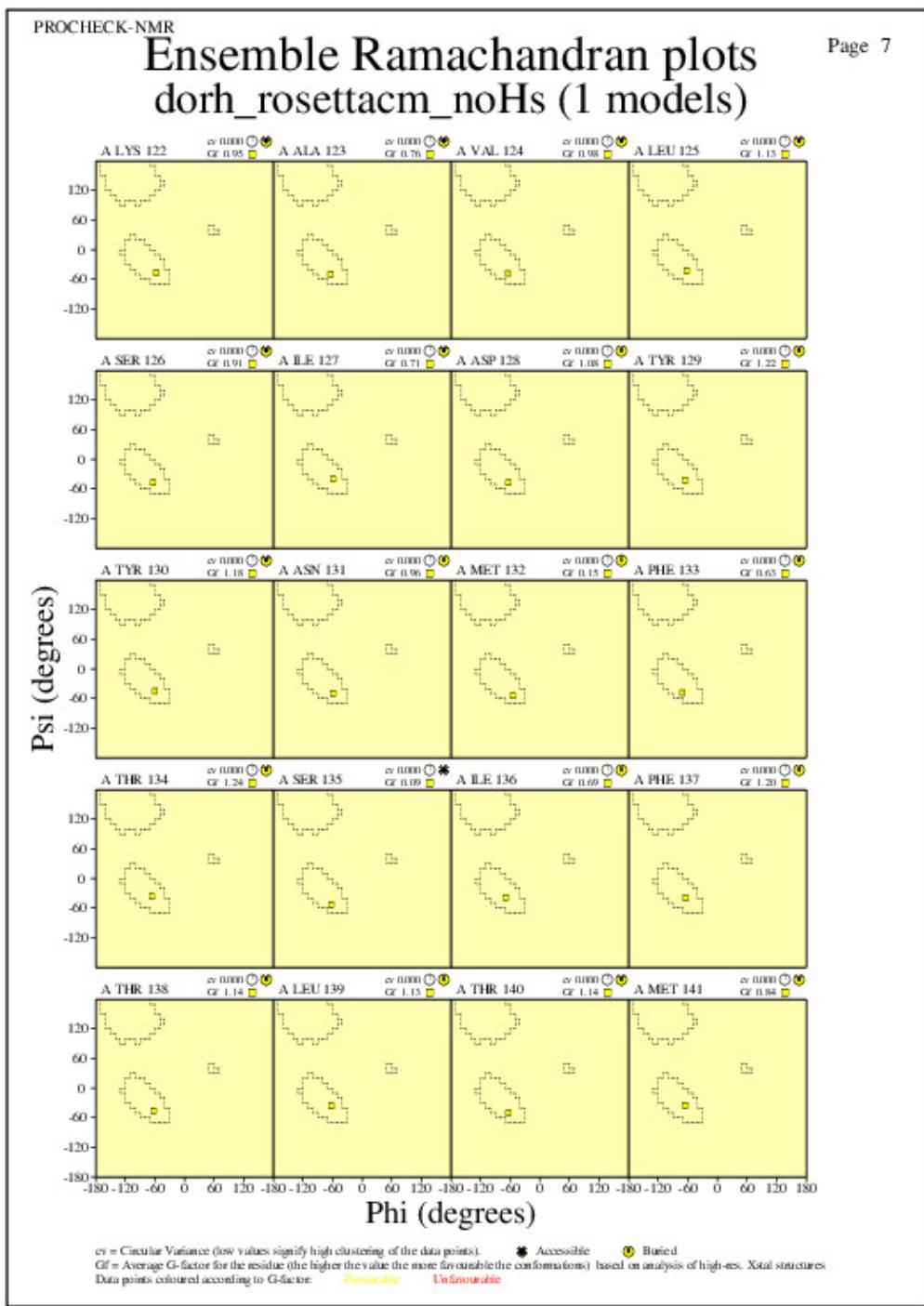
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



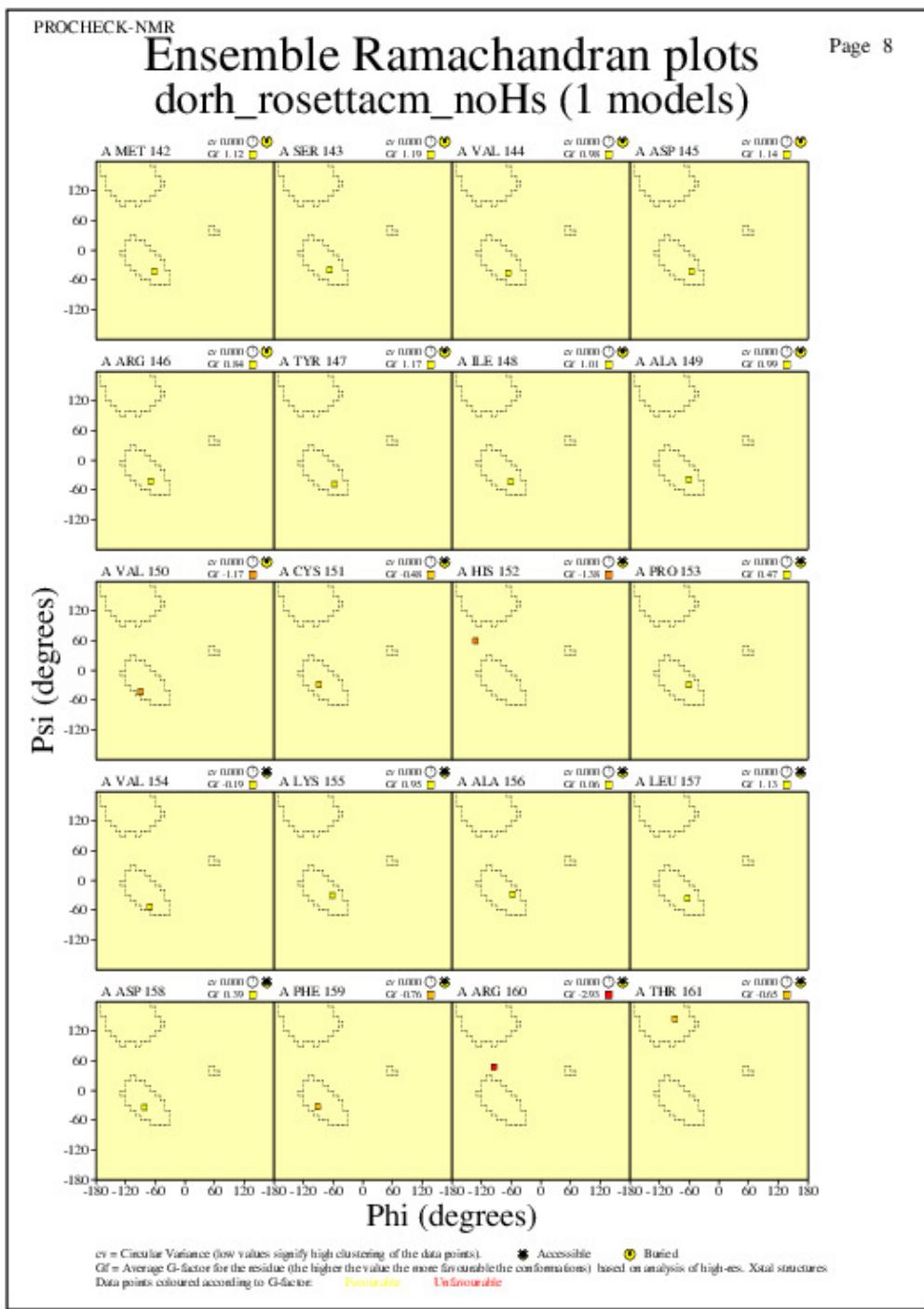
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



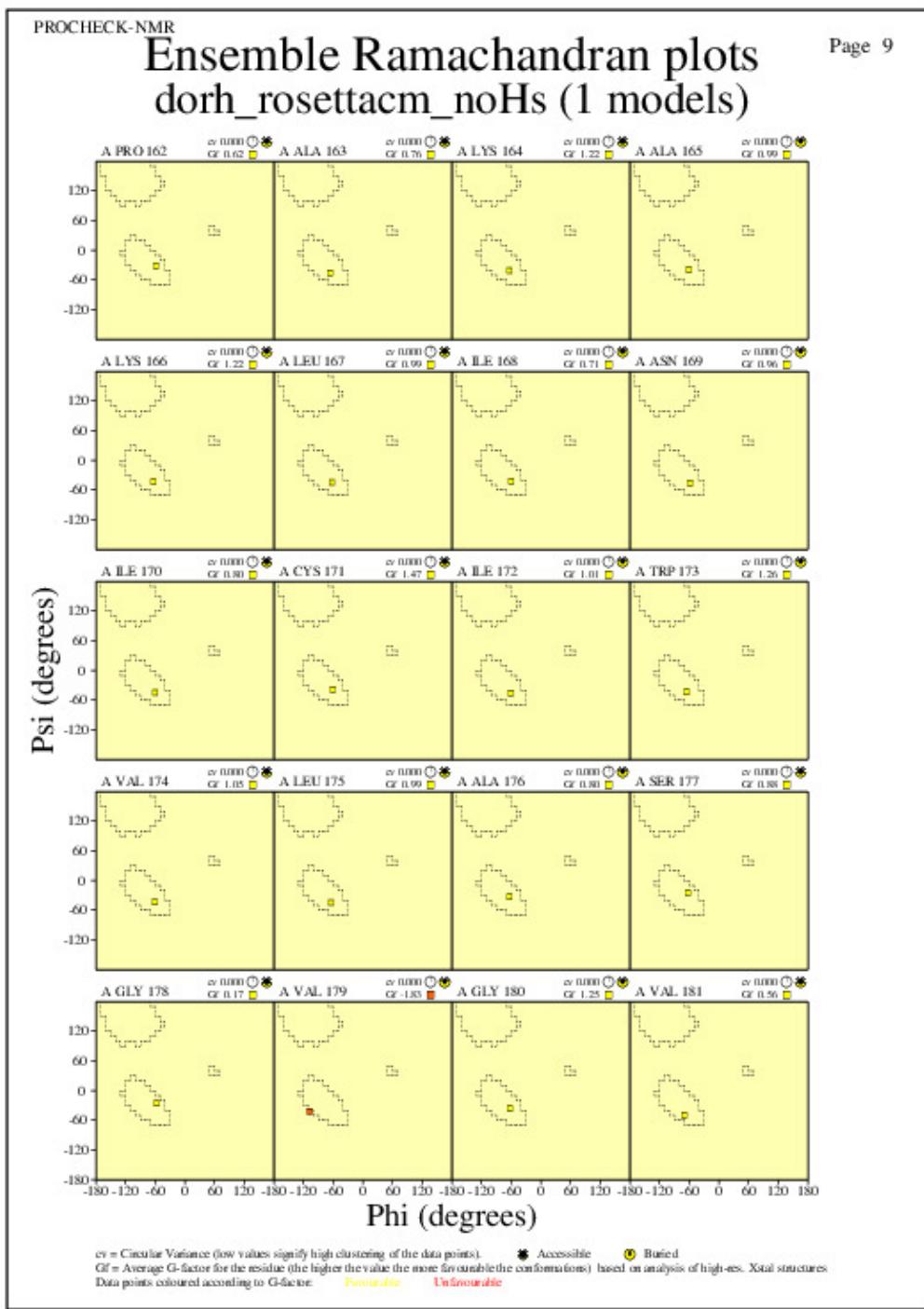
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



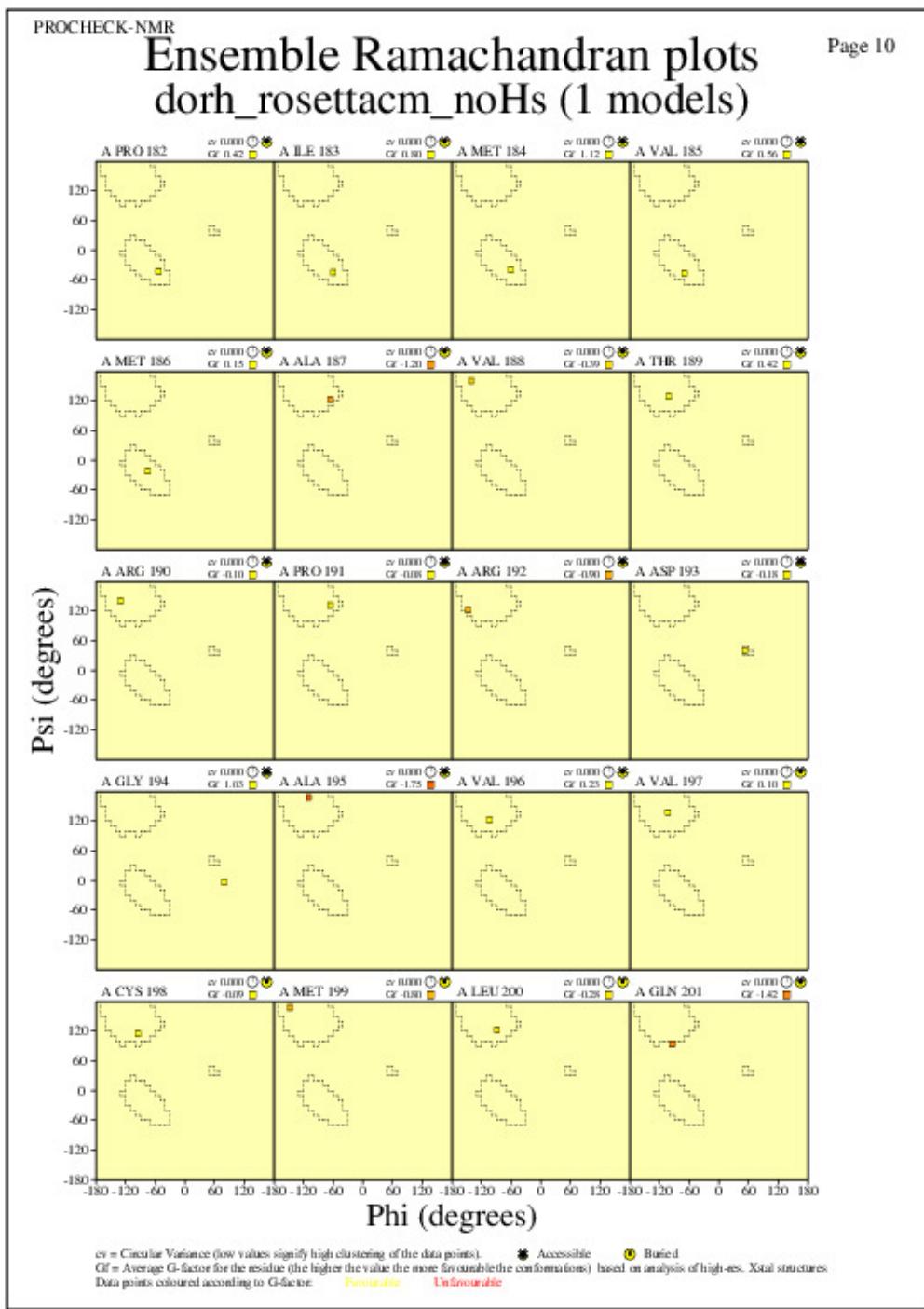
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



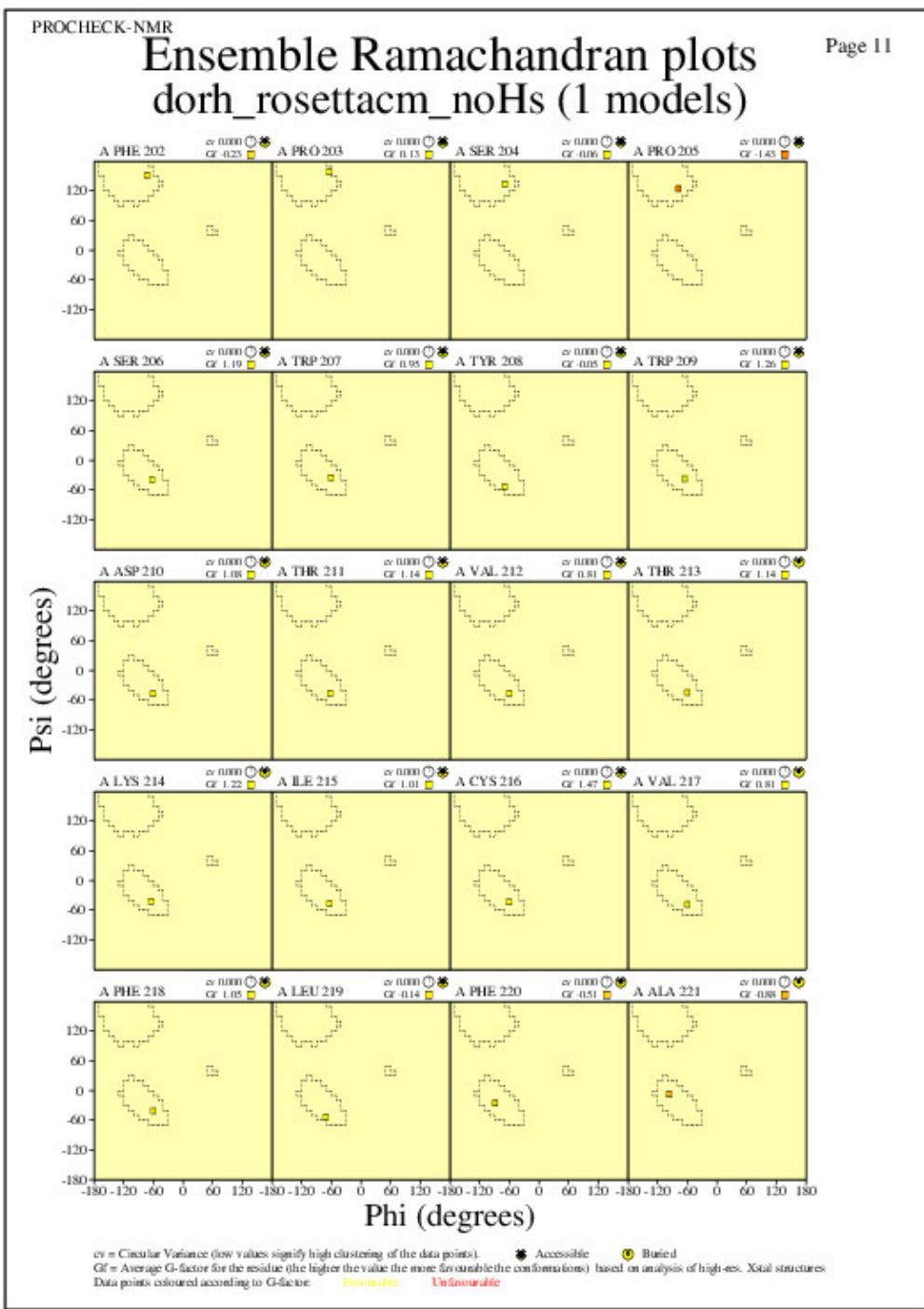
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



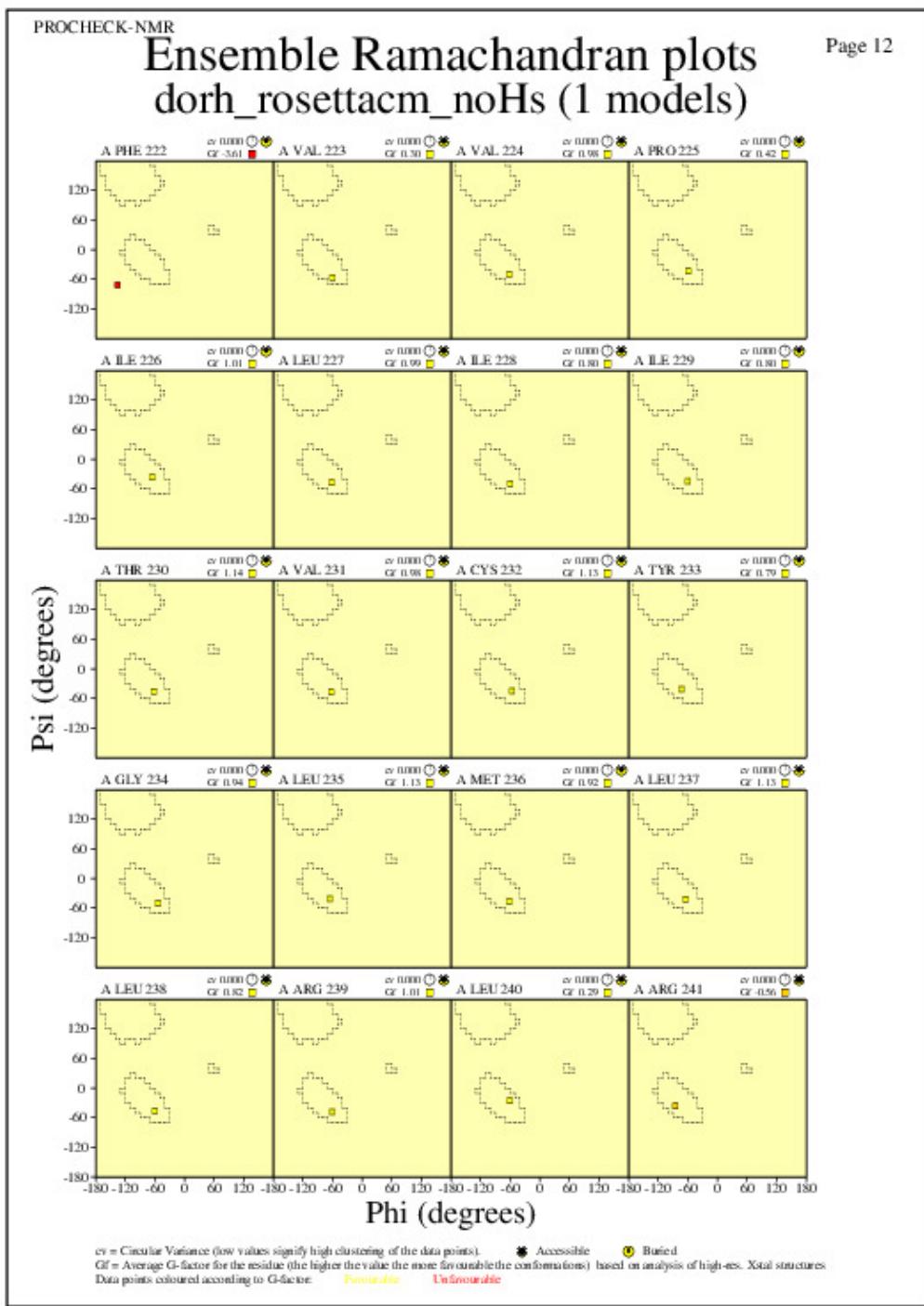
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



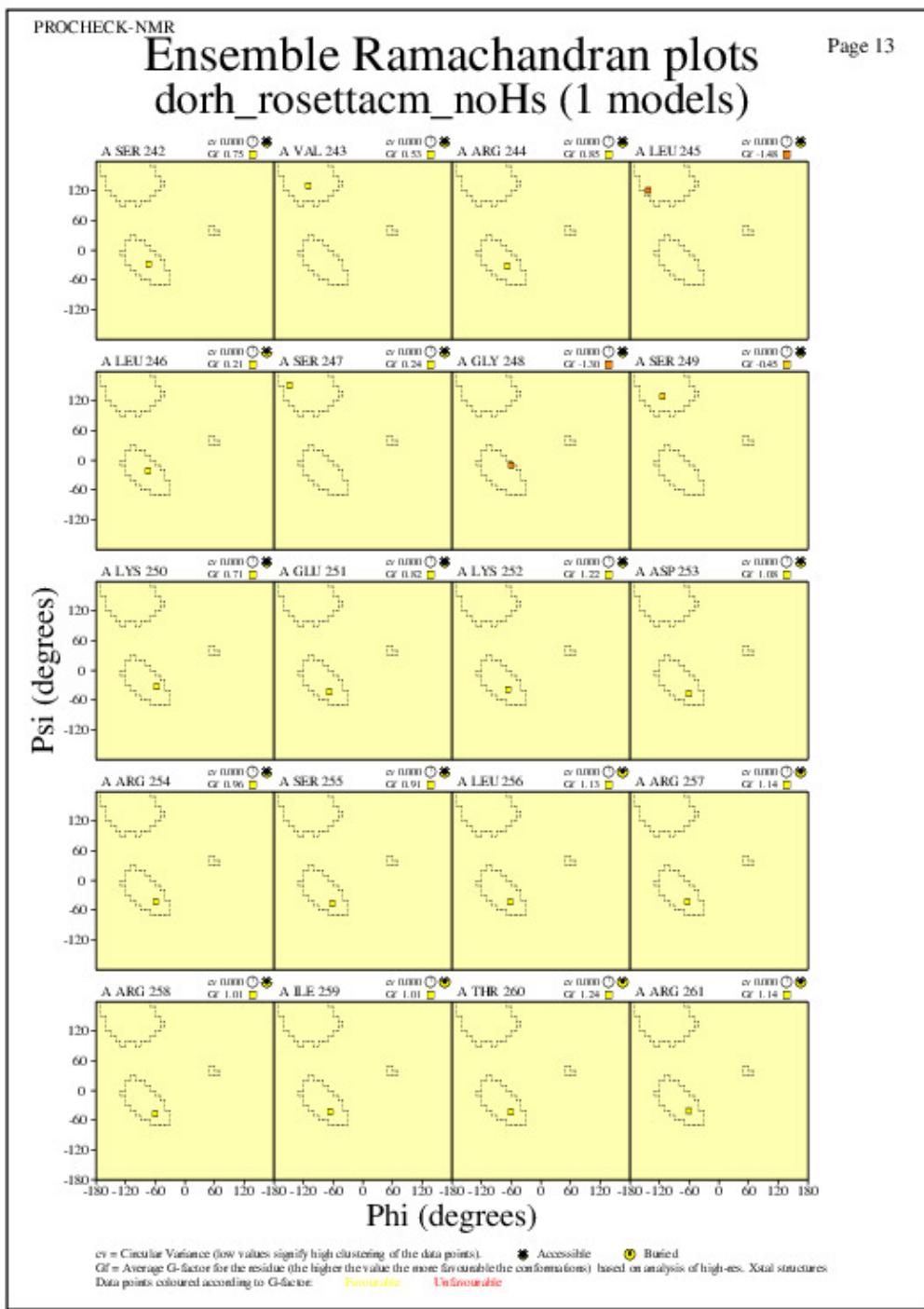
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



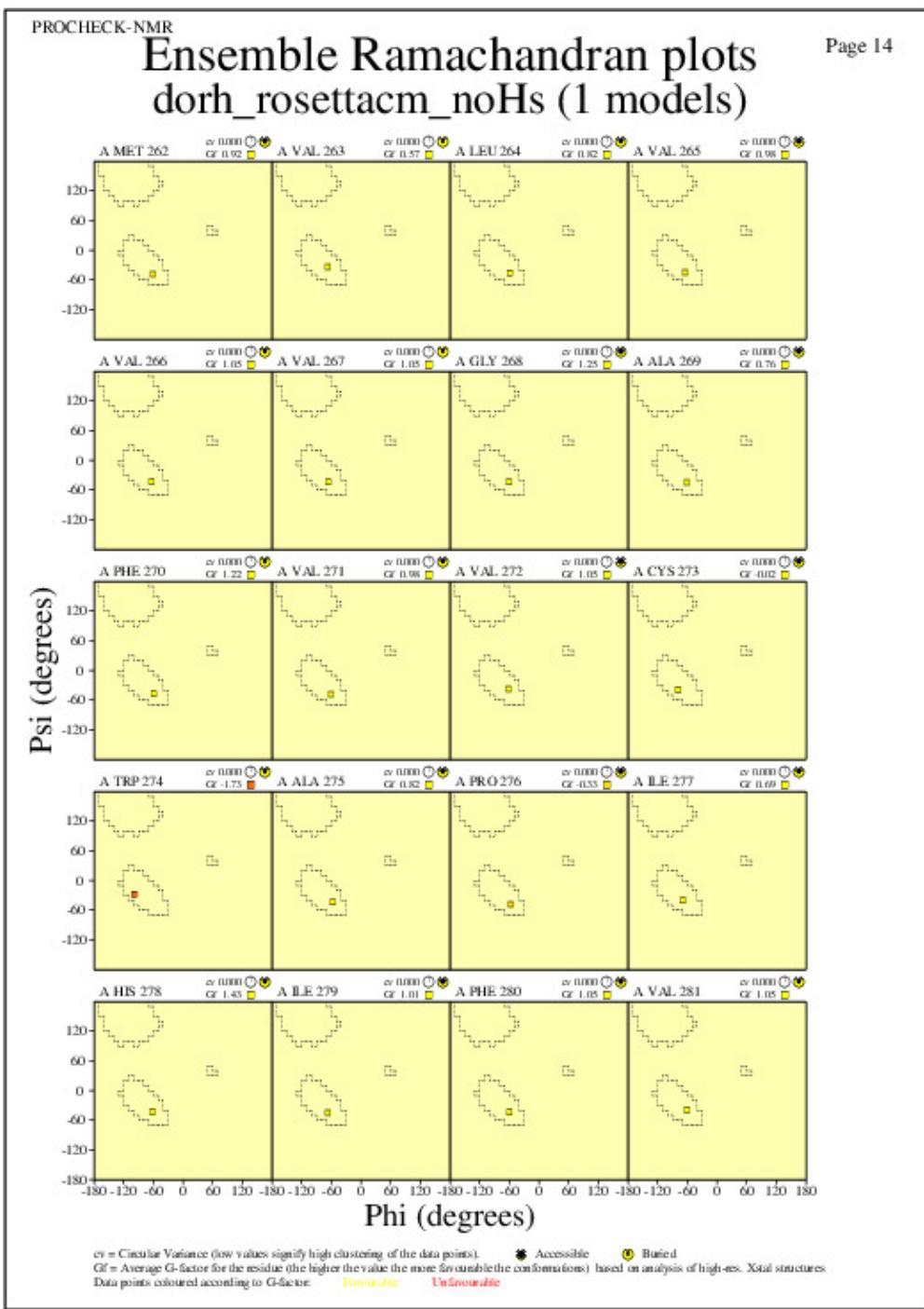
dorh_rosettacm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



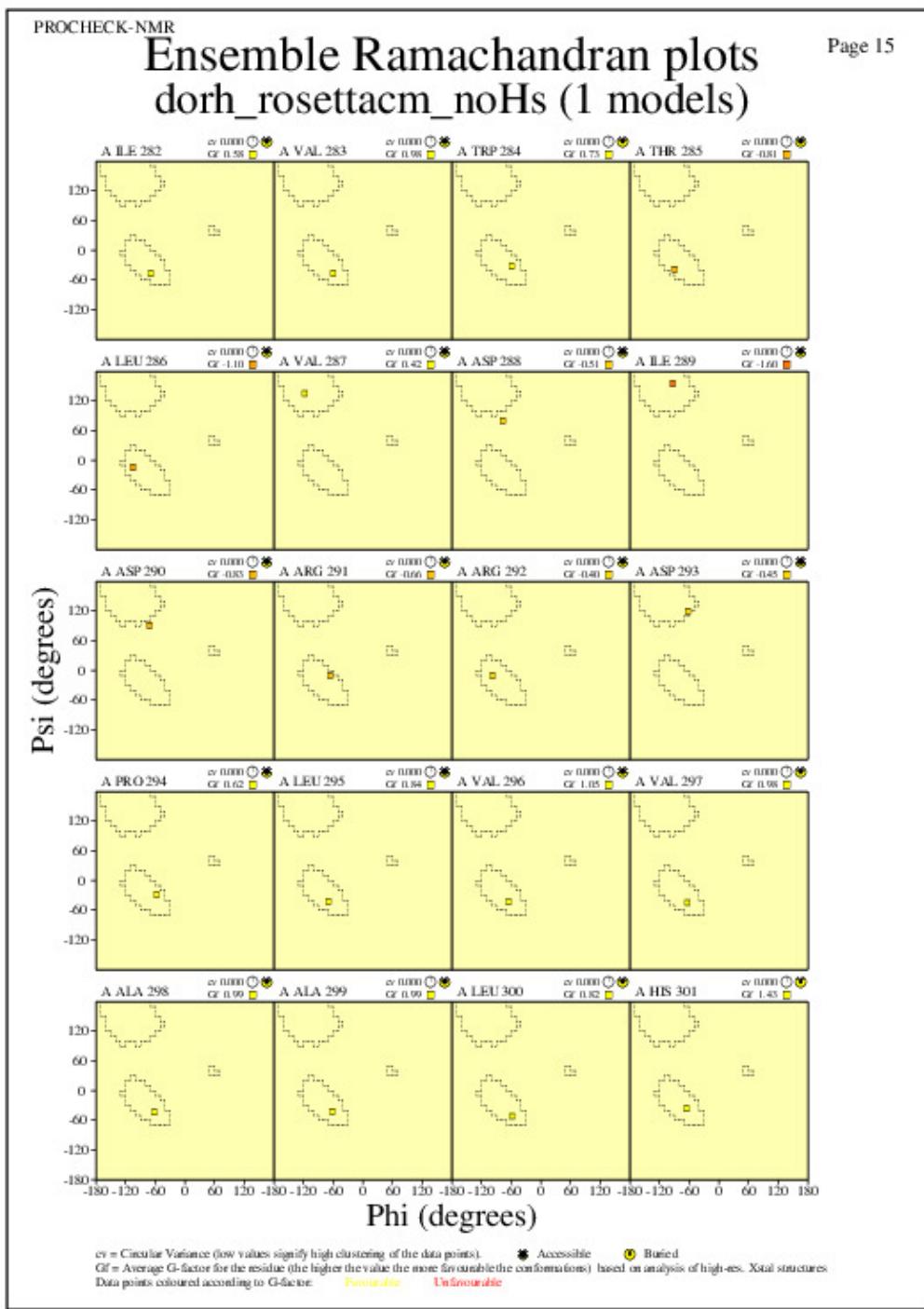
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n

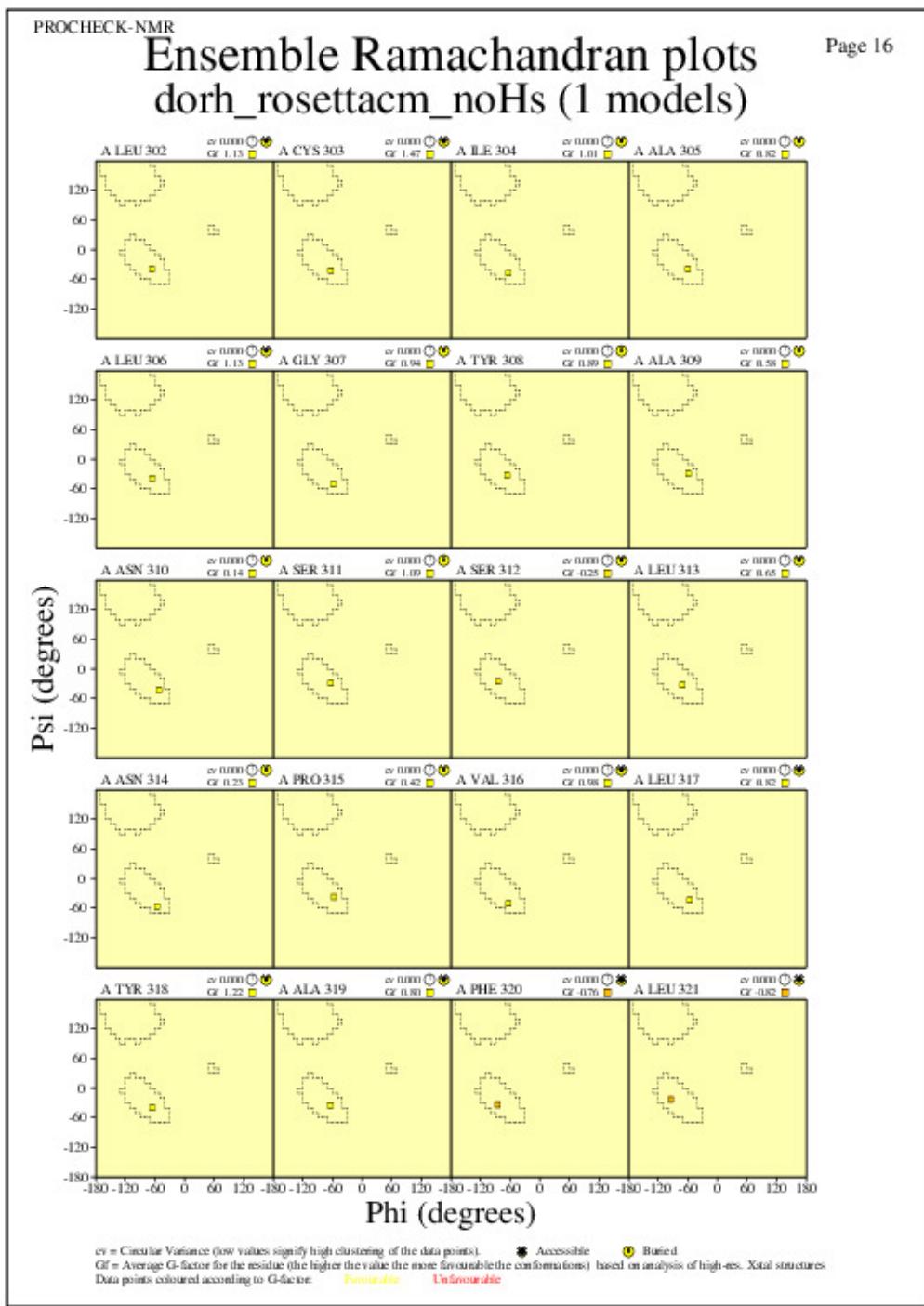


dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n

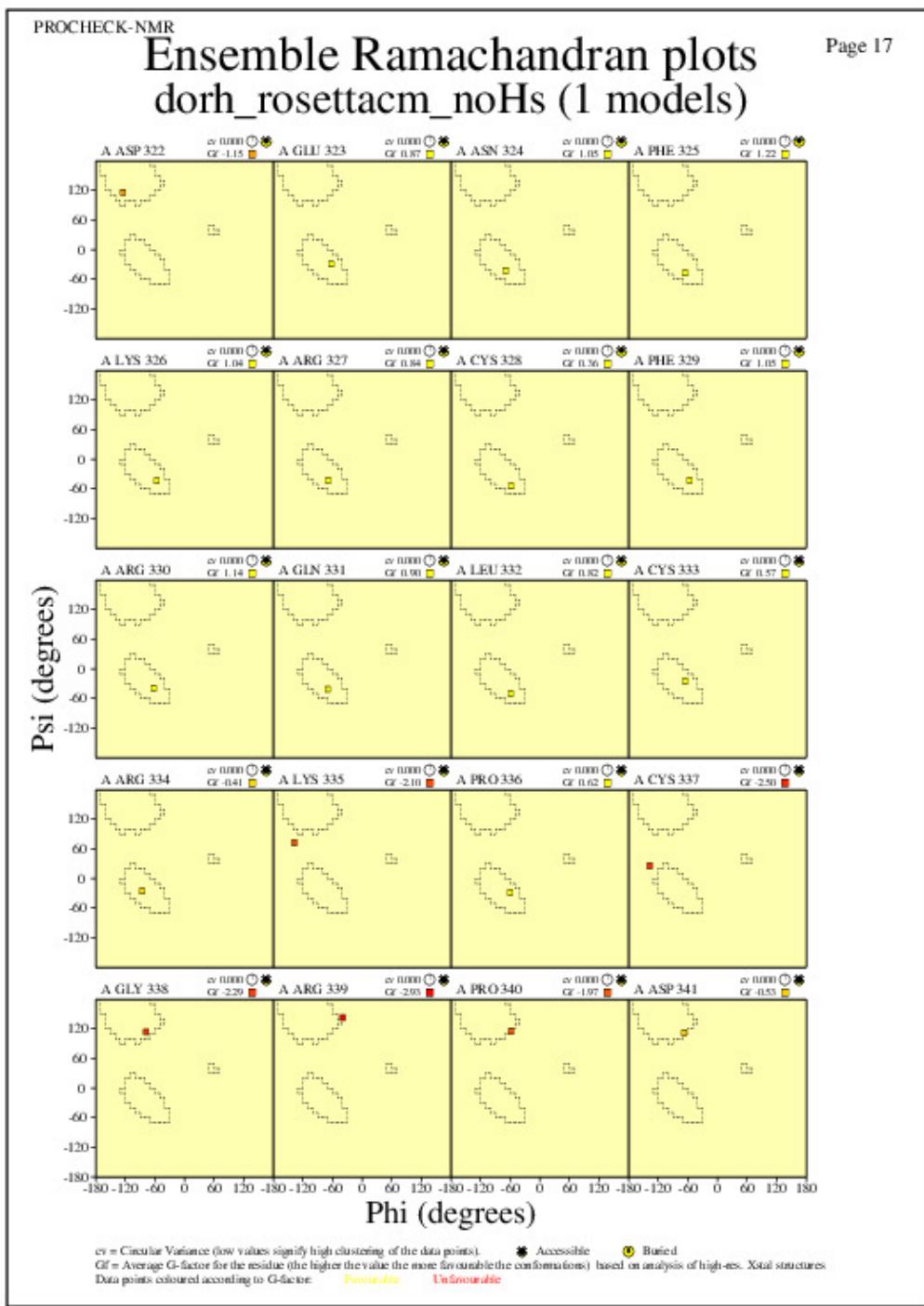


JPEG for residue Ramachandran Plots - page \$num_n



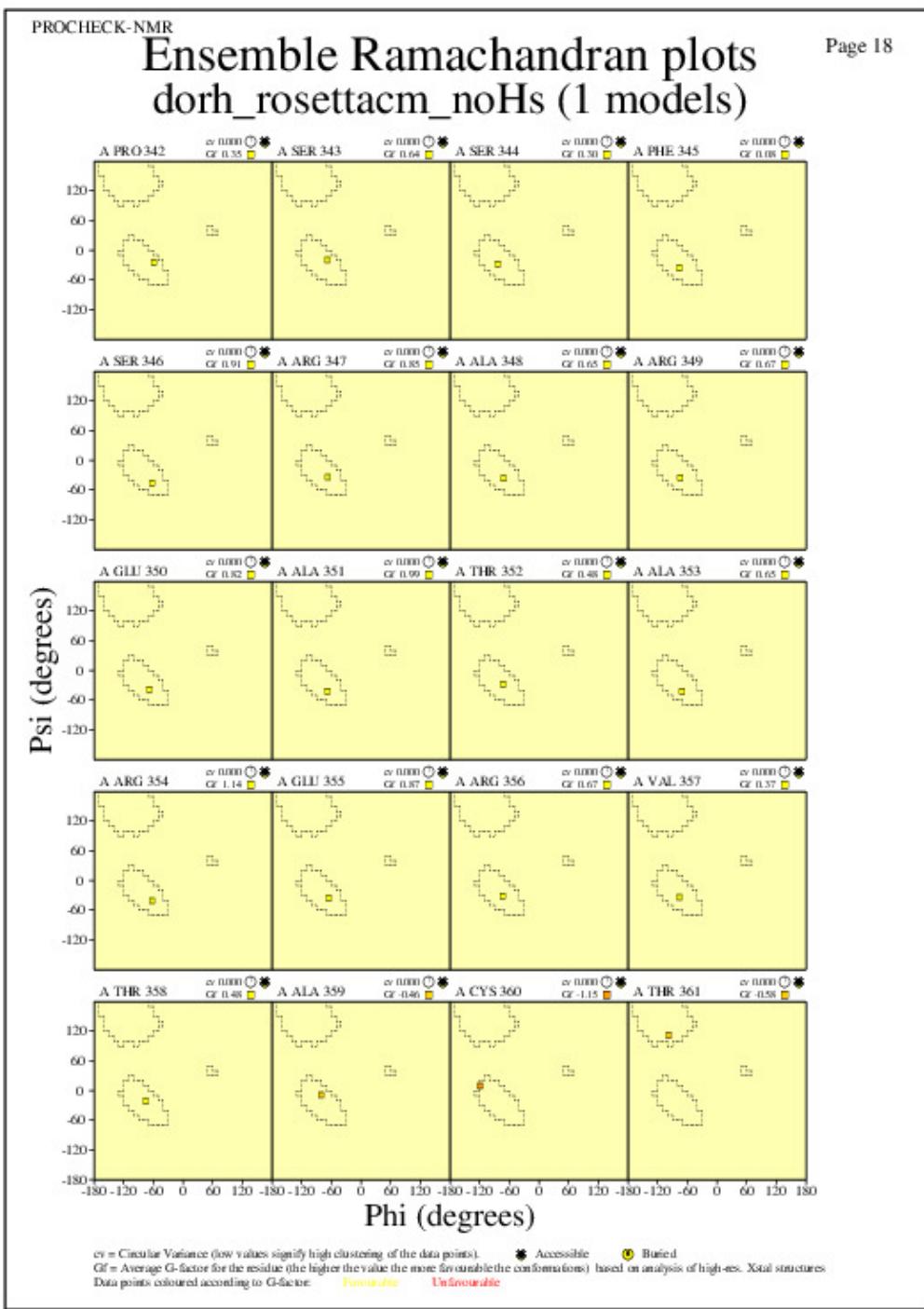
dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n

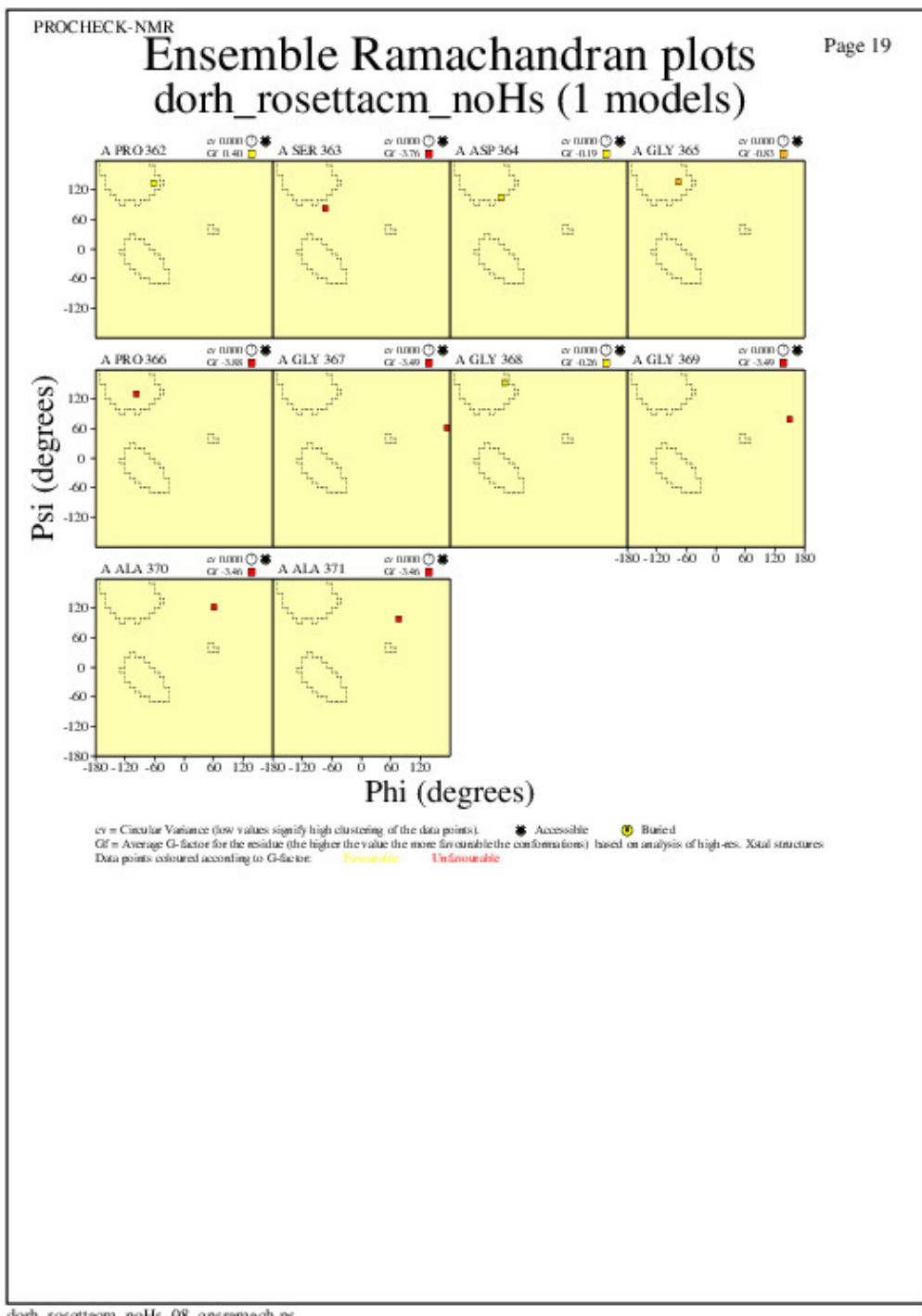


dorh_rosettaclm_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page \$num_n



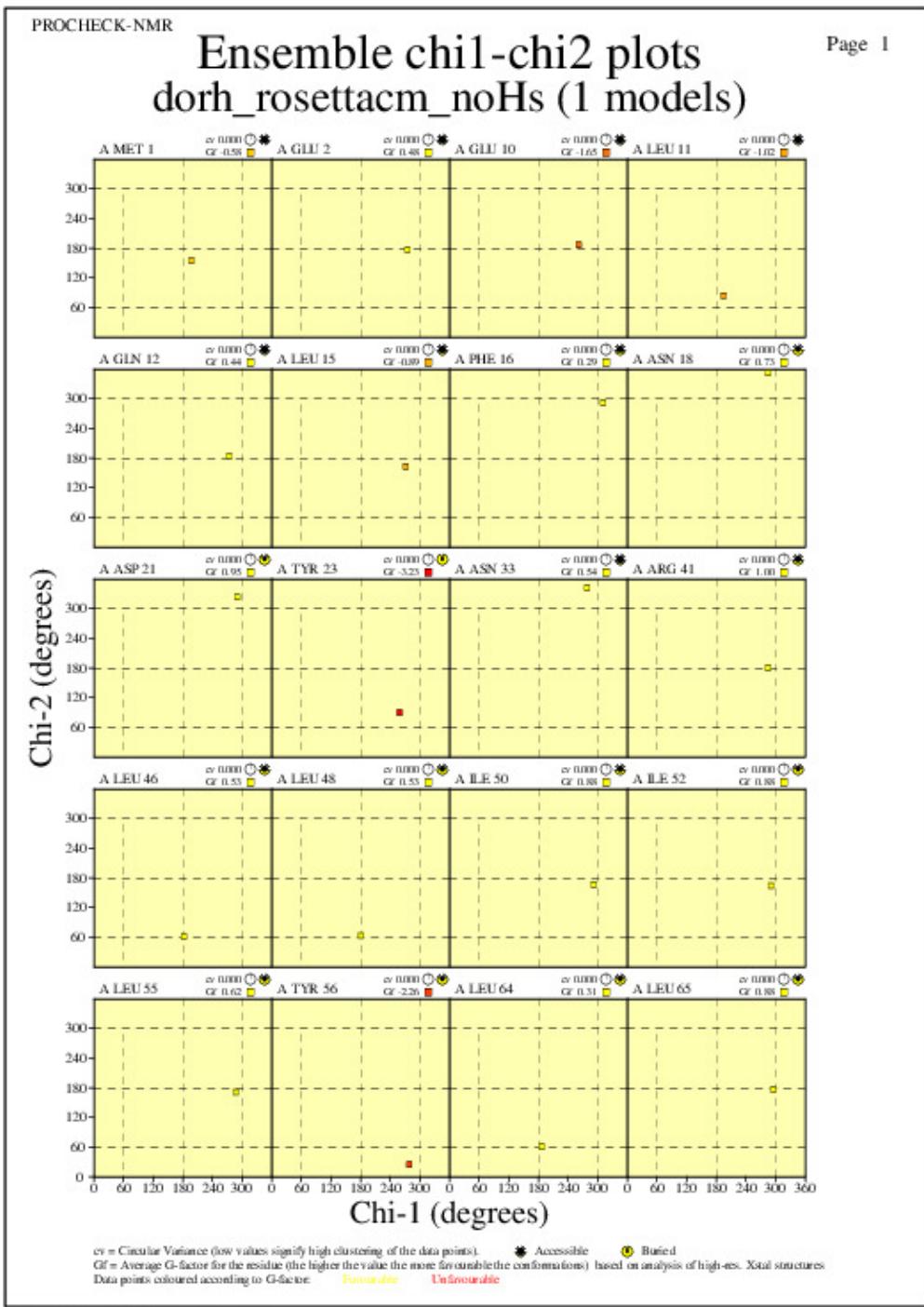
JPEG for residue Ramachandran Plots - page \$num_n



Ramachandran analysis for each residue from Molprobit

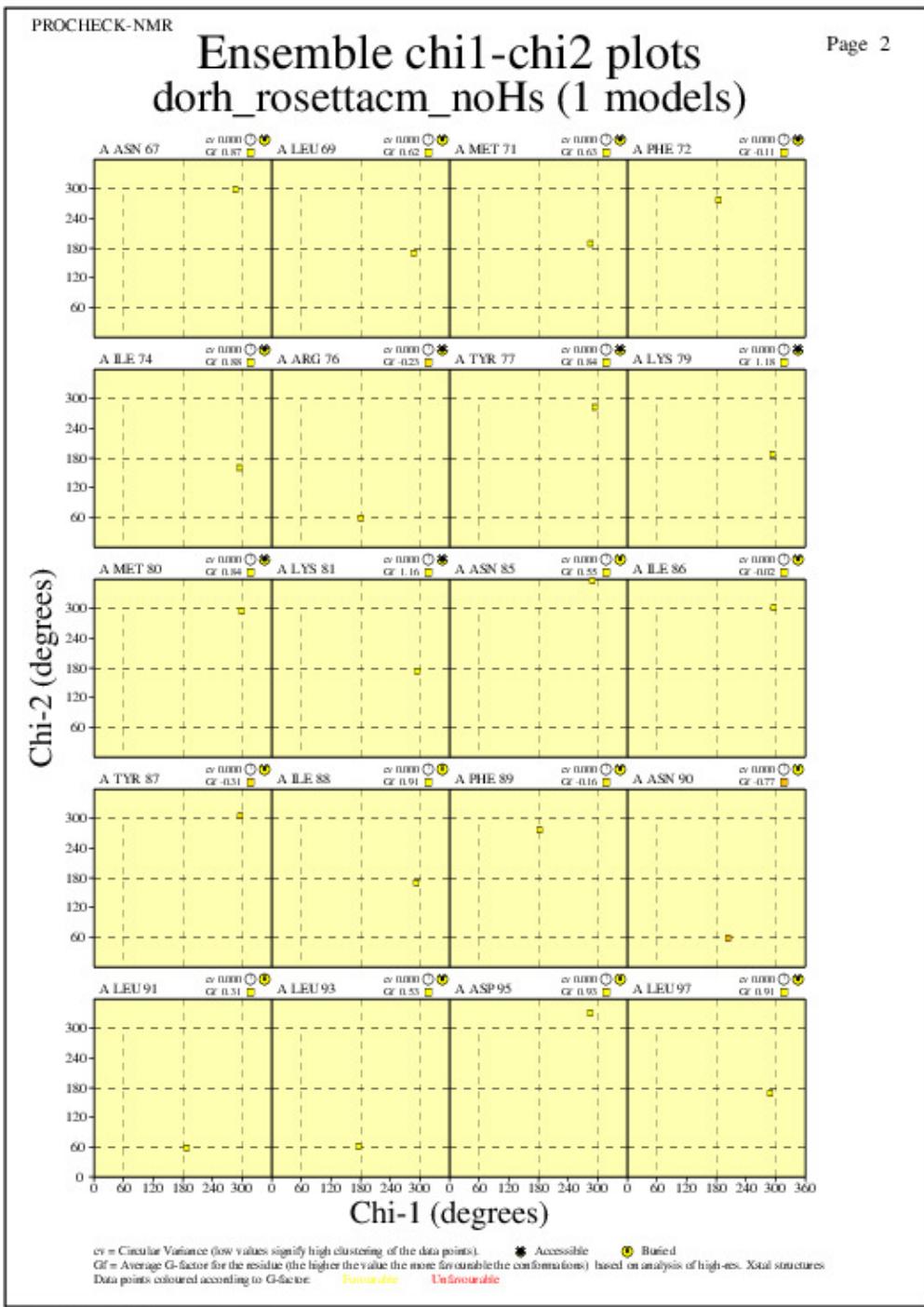
Chi1-Chi2 Plots for each residue

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



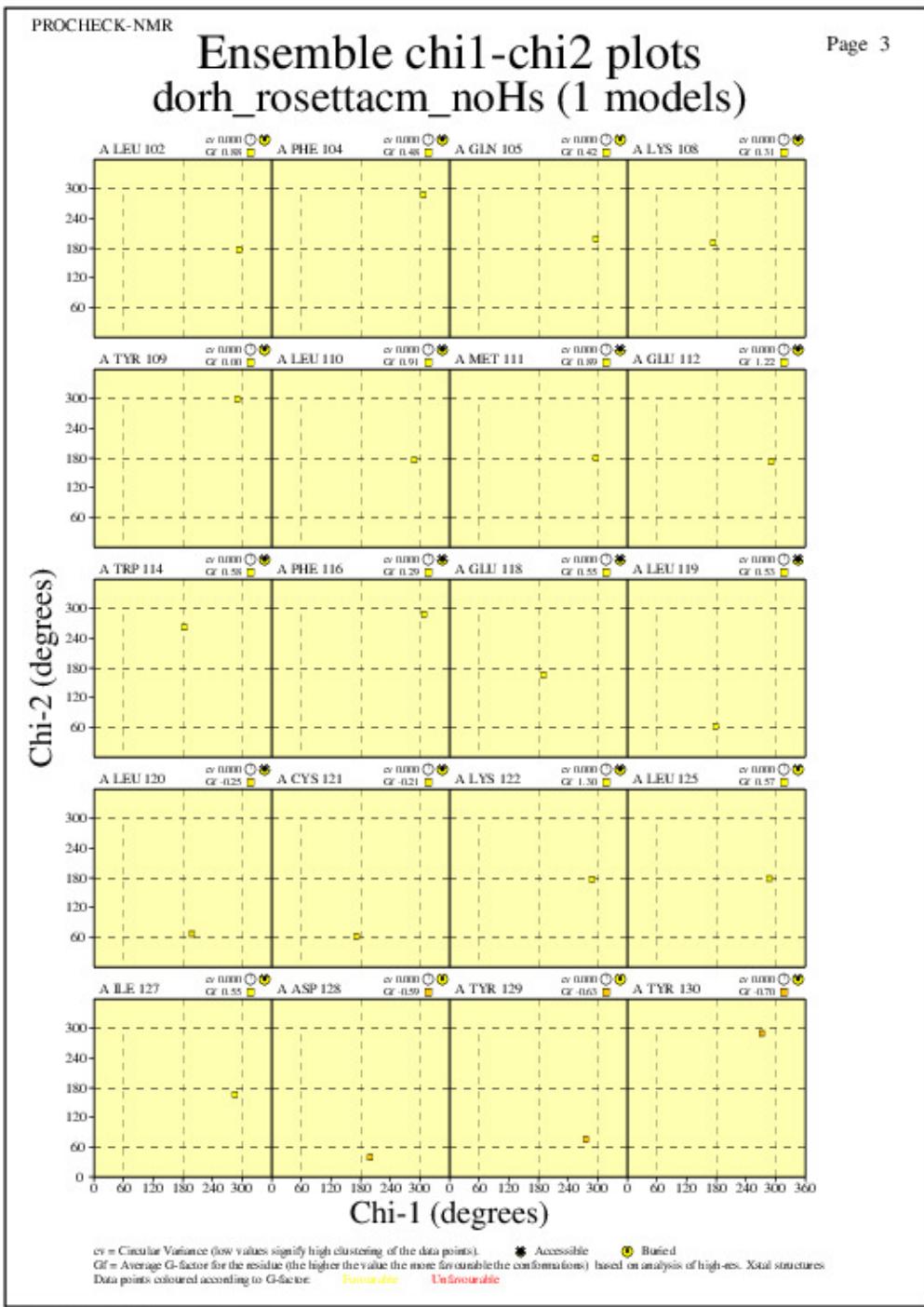
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



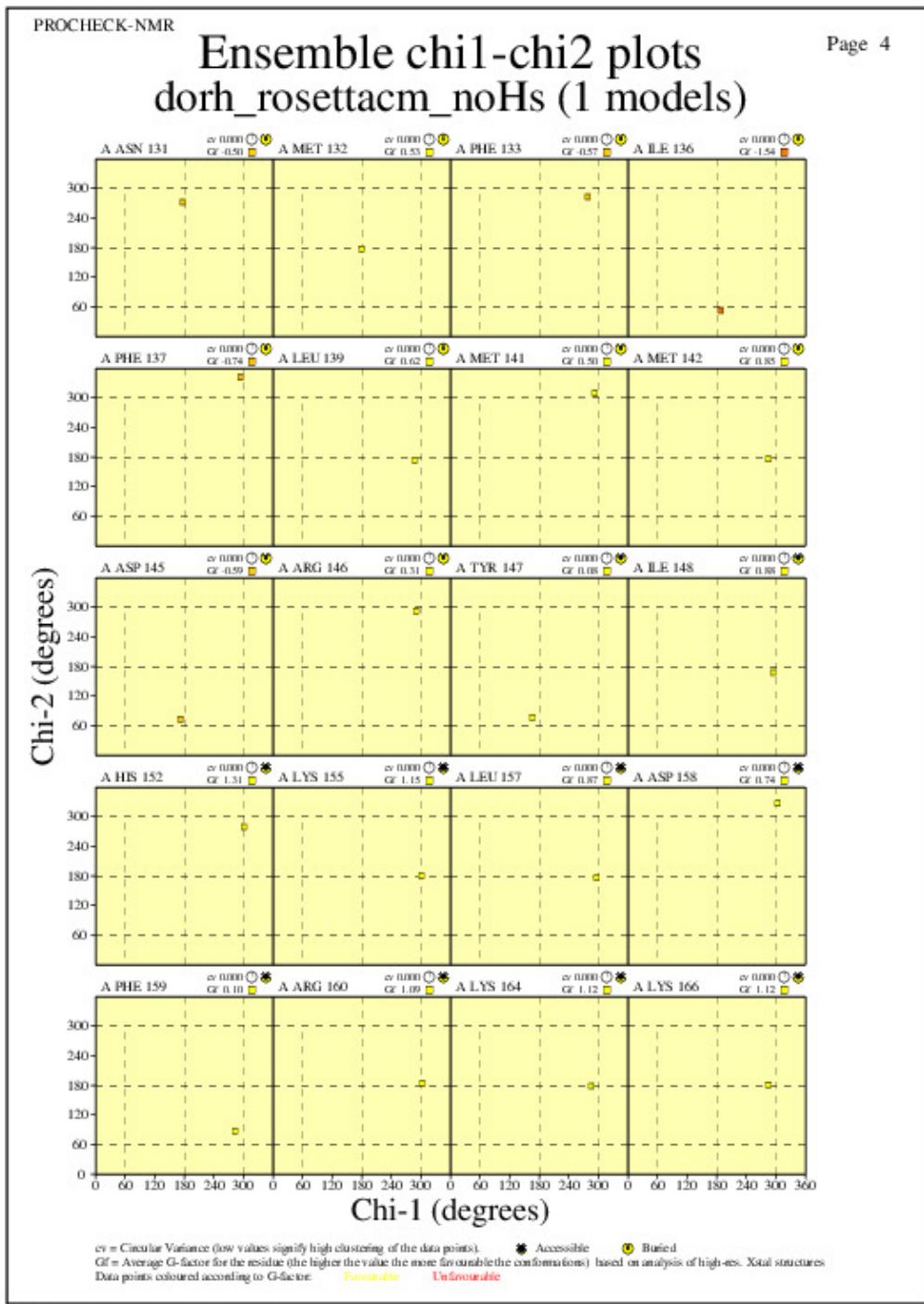
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



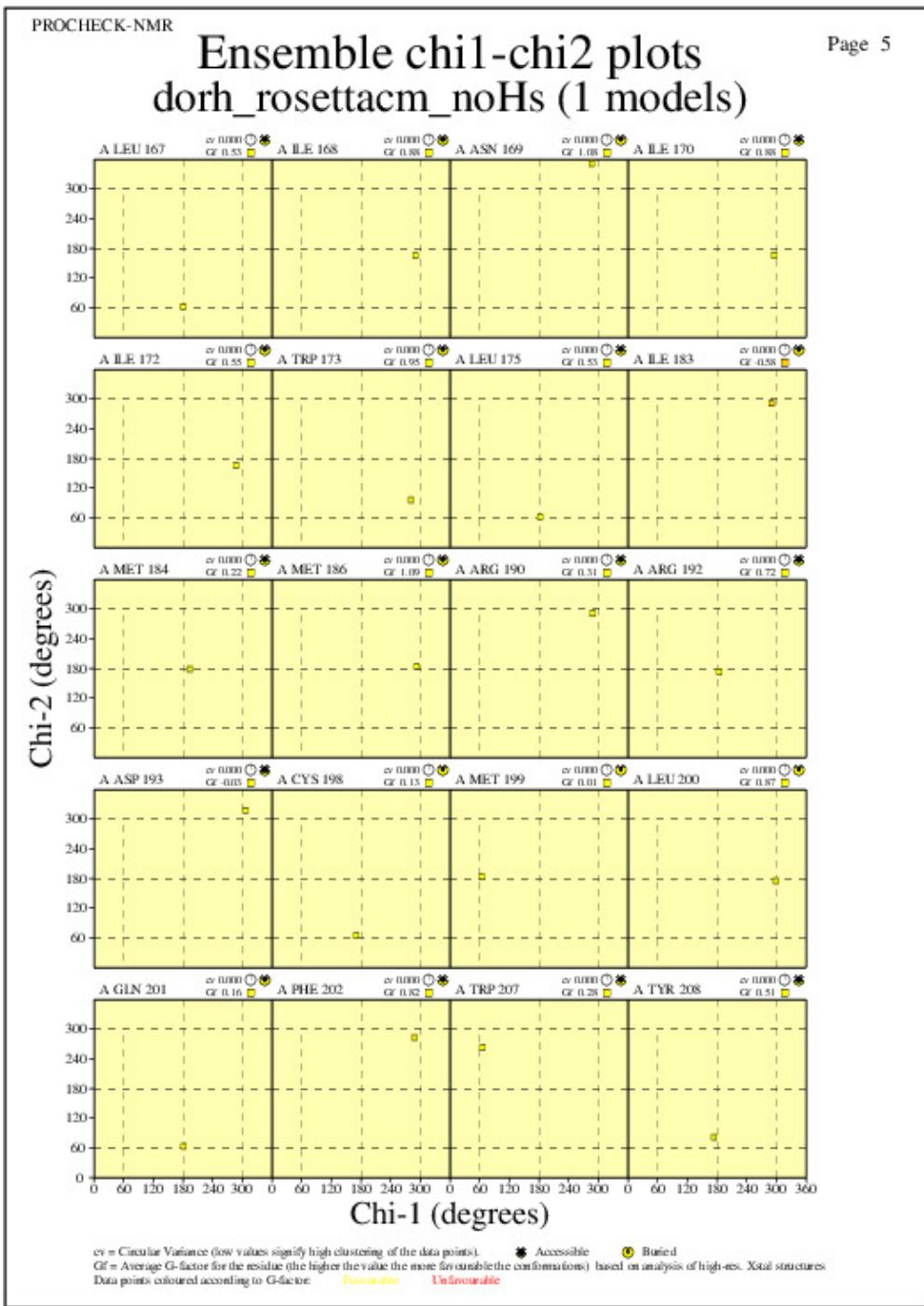
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



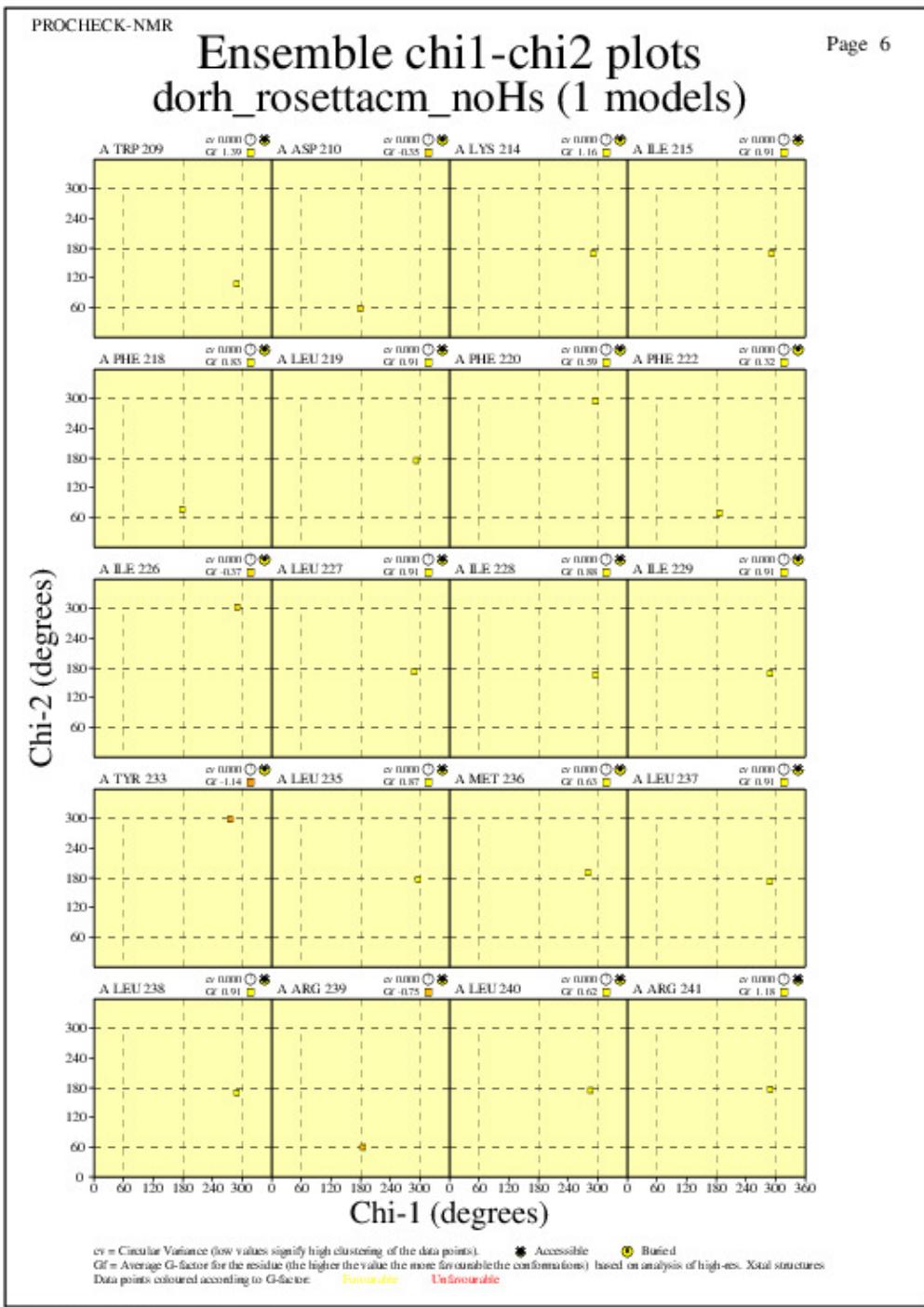
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



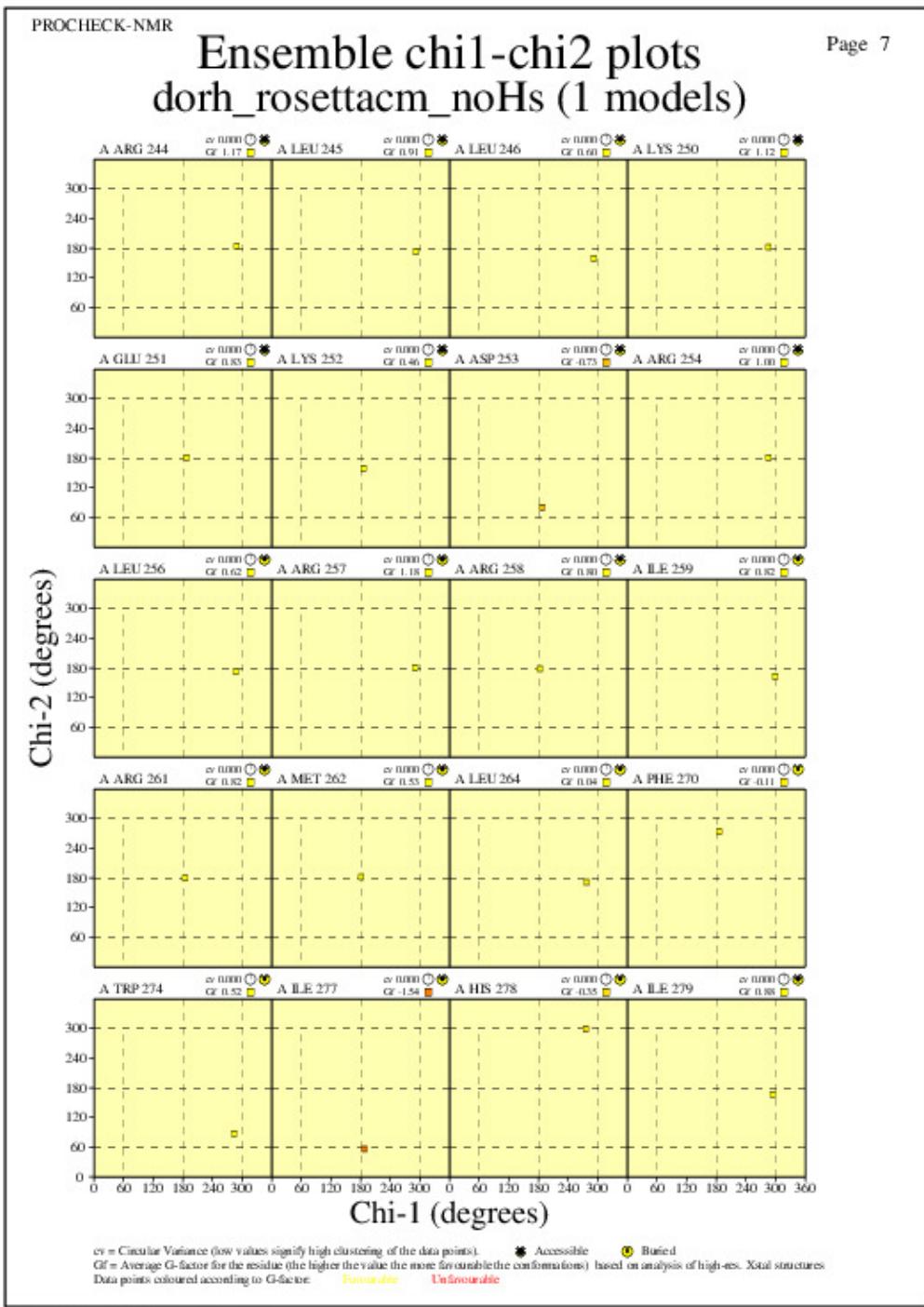
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



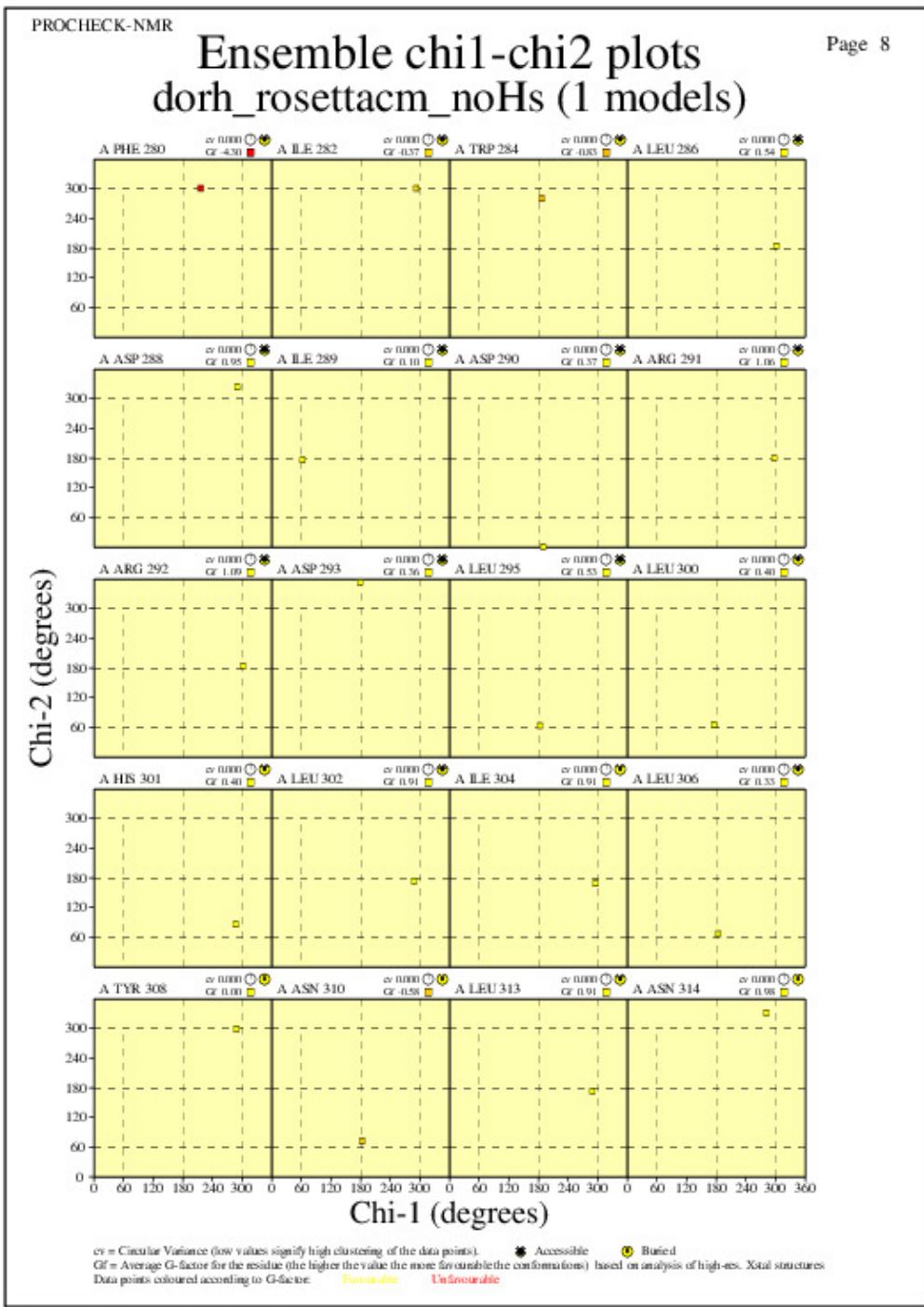
dorh_rosettacm_noHs_09_enschi1ch2.ps

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



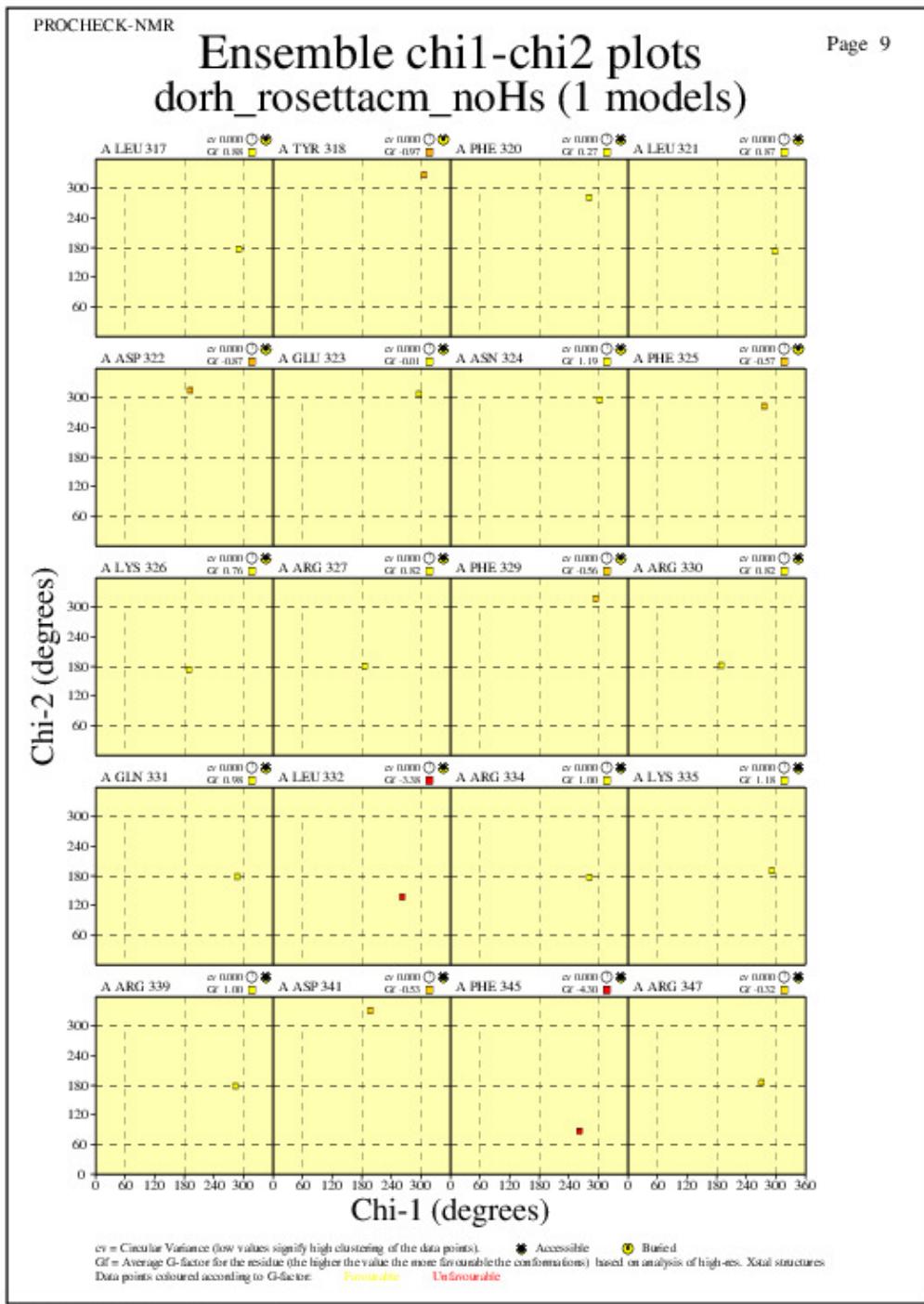
dorh_rosettacm_noHs_09_enschi1ch2.ps

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

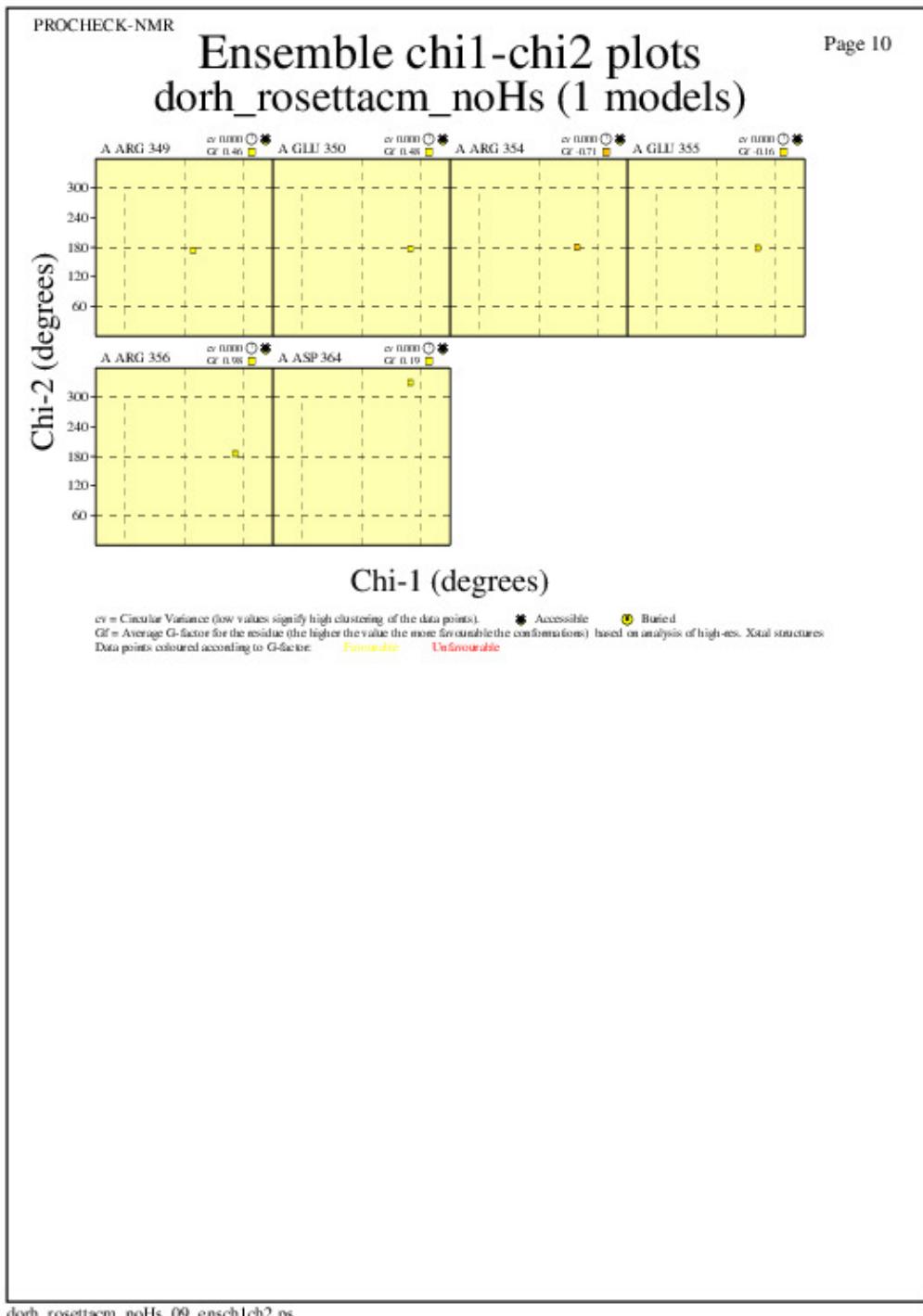


dorh_rosettacm_noHs_09_enschi1ch2.ps

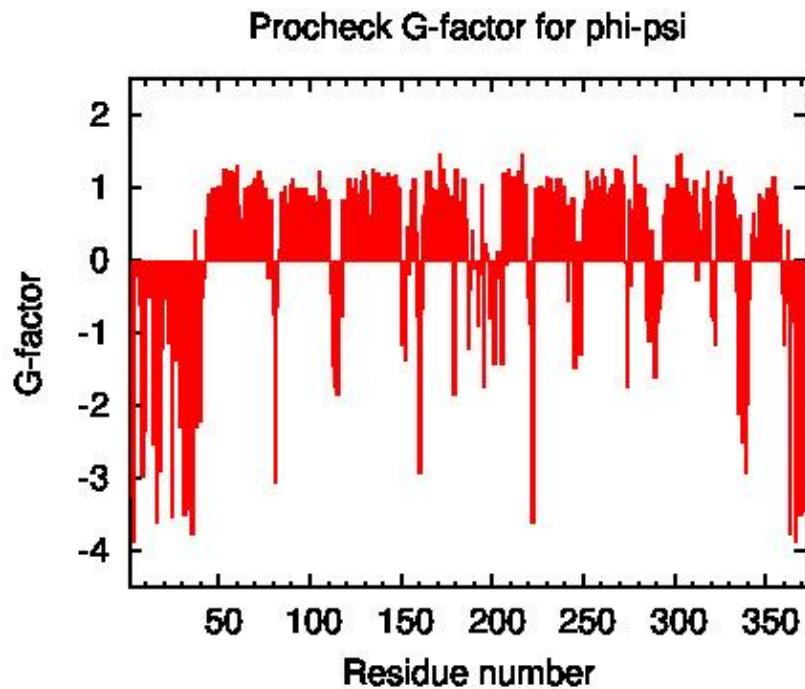
JPEG for residue Chi1-Chi2 Plots - page \$num_n



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
2      -3.23
3      -3.88
4      -0.22
5      -0.12
6      -0.61
7      -0.76
8      -2.97
9      -2.35
10     -0.39
11     -0.51
12     -0.40
13     -0.12
14     -2.54
15     -0.17
16     -3.61
17     -0.78
18     -2.89
19     -1.21
20     -0.53
21     -0.19
22     -1.12
23     -0.23
24     -3.52
25     -0.10
26     -1.36
27     -0.38
28     -2.28
29     -0.98
30     -2.28
31     -3.49
```

PSVS Software Environment

32	-1.03
33	-3.43
34	-1.88
35	-3.76
36	-0.99
37	0.40
38	-2.28
39	-0.77
40	-2.21
41	-0.49
42	-0.23
43	0.58
44	0.91
45	0.88
46	0.99
47	0.82
48	0.99
49	0.99
50	1.01
51	0.76
52	0.80
53	1.24
54	0.76
55	0.99
56	1.22
57	1.19
58	0.76
59	1.05
60	1.31
61	0.76
62	0.56
63	0.44
64	0.99
65	0.99
66	1.02
67	0.93
68	1.05
69	1.13
70	0.81
71	0.75
72	1.22
73	1.08
74	0.69
75	0.98
76	0.67
77	-0.24
78	0.84
79	0.02
80	-0.74
81	-3.05
82	-0.62
83	0.14
84	0.94
85	0.59
86	1.01
87	0.79
88	0.71
89	1.05
90	1.13
91	0.99
92	0.80
93	0.99

PSVS Software Environment

94	0.82
95	0.99
96	0.99
97	0.99
98	0.66
99	0.87
100	0.64
101	0.16
102	0.88
103	0.42
104	0.80
105	1.23
106	0.74
107	0.99
108	0.95
109	0.79
110	0.84
111	-0.45
112	-1.46
113	-0.57
114	-1.73
115	-1.84
116	-0.34
117	-0.75
118	0.82
119	0.82
120	0.65
121	1.13
122	0.95
123	0.76
124	0.98
125	1.13
126	0.91
127	0.71
128	1.08
129	1.22
130	1.18
131	0.96
132	0.15
133	0.63
134	1.24
135	0.09
136	0.69
137	1.20
138	1.14
139	1.13
140	1.14
141	0.84
142	1.12
143	1.19
144	0.98
145	1.14
146	0.84
147	1.17
148	1.01
149	0.99
150	-1.17
151	-0.48
152	-1.38
153	0.47
154	-0.19
155	0.95

PSVS Software Environment

156	0.06
157	1.13
158	0.39
159	-0.76
160	-2.93
161	-0.65
162	0.62
163	0.76
164	1.22
165	0.99
166	1.22
167	0.99
168	0.71
169	0.96
170	0.80
171	1.47
172	1.01
173	1.26
174	1.05
175	0.99
176	0.80
177	0.88
178	0.17
179	-1.83
180	1.25
181	0.56
182	0.42
183	0.80
184	1.12
185	0.56
186	0.15
187	-1.20
188	-0.39
189	0.42
190	-0.10
191	-0.08
192	-0.90
193	-0.18
194	1.03
195	-1.75
196	0.23
197	0.10
198	-0.09
199	-0.80
200	-0.28
201	-1.42
202	-0.23
203	0.13
204	-0.06
205	-1.43
206	1.19
207	0.95
208	-0.05
209	1.26
210	1.08
211	1.14
212	0.81
213	1.14
214	1.22
215	1.01
216	1.47
217	0.81

PSVS Software Environment

218	1.05
219	-0.14
220	-0.51
221	-0.88
222	-3.61
223	0.30
224	0.98
225	0.42
226	1.01
227	0.99
228	0.80
229	0.80
230	1.14
231	0.98
232	1.13
233	0.79
234	0.94
235	1.13
236	0.92
237	1.13
238	0.82
239	1.01
240	0.29
241	-0.56
242	0.75
243	0.53
244	0.85
245	-1.48
246	0.21
247	0.24
248	-1.30
249	-0.45
250	0.71
251	0.82
252	1.22
253	1.08
254	0.96
255	0.91
256	1.13
257	1.14
258	1.01
259	1.01
260	1.24
261	1.14
262	0.92
263	0.57
264	0.82
265	0.98
266	1.05
267	1.05
268	1.25
269	0.76
270	1.22
271	0.98
272	1.05
273	-0.02
274	-1.73
275	0.82
276	-0.33
277	0.69
278	1.43
279	1.01

PSVS Software Environment

280	1.05
281	1.05
282	0.58
283	0.98
284	0.73
285	-0.81
286	-1.10
287	0.42
288	-0.51
289	-1.60
290	-0.83
291	-0.66
292	-0.40
293	-0.45
294	0.62
295	0.84
296	1.05
297	0.98
298	0.99
299	0.99
300	0.82
301	1.43
302	1.13
303	1.47
304	1.01
305	0.82
306	1.13
307	0.94
308	0.89
309	0.58
310	0.14
311	1.09
312	-0.25
313	0.65
314	0.23
315	0.42
316	0.98
317	0.82
318	1.22
319	0.80
320	-0.76
321	-0.82
322	-1.15
323	0.87
324	1.05
325	1.22
326	1.04
327	0.84
328	0.36
329	1.05
330	1.14
331	0.90
332	0.82
333	0.57
334	-0.41
335	-2.10
336	0.62
337	-2.50
338	-2.29
339	-2.93
340	-1.97
341	-0.53

```

342      0.35
343      0.64
344      0.30
345      0.08
346      0.91
347      0.85
348      0.65
349      0.67
350      0.82
351      0.99
352      0.48
353      0.65
354      1.14
355      0.87
356      0.67
357      0.37
358      0.48
359      -0.46
360      -1.15
361      -0.58
362      0.40
363      -3.76
364      -0.19
365      -0.83
366      -3.88
367      -3.49
368      -0.26
369      -3.49
370      -3.46
371      -3.46
#Reported_Model_Average 0.188
#Overall_Average_Reported      0.188

```

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

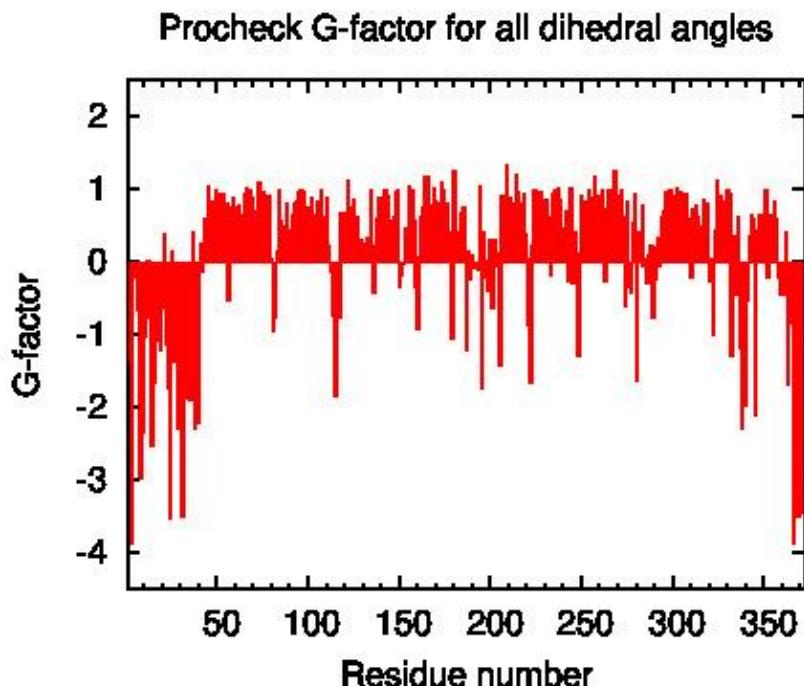


Table of Procheck G-factors for all dihedrals for ordered residues

```
#alldih_gfactor
#Residue\Model  average
1      -0.58
2      -1.37
3      -3.88
4      -0.22
5      -0.12
6      -0.66
7      -0.76
8      -2.97
9      -2.35
10     -1.02
11     -0.77
12     0.02
13     -0.12
14     -2.54
15     -0.53
16     -1.66
17     -0.78
18     -1.08
19     -1.21
20     -0.62
21     0.38
22     -1.12
23     -1.73
24     -3.52
25     0.14
26     -1.36
27     -0.12
28     -2.28
29     -0.85
30     -2.28
31     -3.49
32     -1.03
33     -1.45
34     -1.88
35     -1.89
36     -0.99
37     0.40
38     -2.28
39     -0.77
40     -2.21
41     0.25
42     -0.13
43     0.58
44     0.10
45     1.04
46     0.76
47     0.82
48     0.76
49     0.99
50     0.94
51     0.76
52     0.84
53     0.94
54     0.76
55     0.81
56     -0.52
57     0.24
58     0.76
```

PSVS Software Environment

59	0.89
60	0.72
61	0.76
62	0.77
63	0.44
64	0.65
65	0.94
66	1.02
67	0.90
68	0.98
69	0.88
70	0.65
71	0.69
72	0.55
73	1.08
74	0.78
75	0.95
76	0.22
77	0.30
78	0.91
79	0.60
80	0.05
81	-0.94
82	-0.75
83	0.14
84	1.00
85	0.57
86	0.50
87	0.24
88	0.81
89	0.44
90	0.18
91	0.65
92	0.80
93	0.76
94	0.82
95	0.96
96	0.99
97	0.95
98	0.66
99	0.00
100	0.76
101	0.10
102	0.88
103	0.42
104	0.64
105	0.82
106	0.55
107	0.99
108	0.63
109	0.40
110	0.88
111	0.22
112	-0.12
113	-0.73
114	-0.58
115	-1.84
116	-0.03
117	-0.75
118	0.68
119	0.67
120	0.20

PSVS Software Environment

121	0.46
122	1.12
123	0.76
124	0.37
125	0.85
126	0.10
127	0.63
128	0.25
129	0.30
130	0.24
131	0.23
132	0.34
133	0.03
134	1.00
135	0.23
136	-0.43
137	0.23
138	0.59
139	0.88
140	0.71
141	0.67
142	0.98
143	0.24
144	0.92
145	0.27
146	0.57
147	0.63
148	0.95
149	0.99
150	-0.34
151	-0.18
152	-0.03
153	0.47
154	0.28
155	1.05
156	0.06
157	1.00
158	0.57
159	-0.33
160	-0.92
161	0.06
162	0.62
163	0.76
164	1.17
165	0.99
166	1.17
167	0.76
168	0.79
169	1.02
170	0.84
171	0.80
172	0.78
173	1.10
174	0.98
175	0.76
176	0.80
177	0.42
178	0.17
179	-1.04
180	1.25
181	0.35
182	0.42

PSVS Software Environment

183	0.11
184	0.67
185	0.74
186	0.62
187	-1.20
188	0.14
189	-0.23
190	0.10
191	-0.08
192	-0.09
193	-0.10
194	1.03
195	-1.75
196	0.41
197	-0.22
198	0.02
199	-0.39
200	0.30
201	-0.63
202	0.30
203	0.13
204	-0.05
205	-1.43
206	0.92
207	0.61
208	0.23
209	1.33
210	0.36
211	0.89
212	0.54
213	0.81
214	1.19
215	0.96
216	0.80
217	0.28
218	0.94
219	0.38
220	0.04
221	-0.88
222	-1.65
223	0.22
224	0.98
225	0.42
226	0.32
227	0.95
228	0.84
229	0.85
230	0.81
231	0.86
232	0.63
233	-0.18
234	0.94
235	1.00
236	0.78
237	1.02
238	0.86
239	0.13
240	0.46
241	0.31
242	0.70
243	-0.27
244	1.01

PSVS Software Environment

245	-0.29
246	0.41
247	0.11
248	-1.30
249	-0.58
250	0.91
251	0.83
252	0.84
253	0.17
254	0.98
255	0.44
256	0.88
257	1.16
258	0.90
259	0.92
260	0.76
261	0.98
262	0.73
263	-0.26
264	0.43
265	0.98
266	0.72
267	0.40
268	1.25
269	0.76
270	0.55
271	0.92
272	0.98
273	0.63
274	-0.61
275	0.82
276	-0.33
277	-0.43
278	0.54
279	0.94
280	-1.63
281	0.40
282	0.11
283	0.79
284	-0.05
285	0.03
286	-0.28
287	0.09
288	0.22
289	-0.75
290	-0.23
291	0.20
292	0.34
293	-0.05
294	0.62
295	0.69
296	0.96
297	0.95
298	0.99
299	0.99
300	0.61
301	0.92
302	1.02
303	0.80
304	0.96
305	0.82
306	0.73

PSVS Software Environment

307	0.94
308	0.44
309	0.58
310	-0.22
311	0.73
312	0.06
313	0.78
314	0.61
315	0.42
316	0.48
317	0.85
318	0.13
319	0.80
320	-0.25
321	0.03
322	-1.01
323	0.43
324	1.12
325	0.33
326	0.90
327	0.83
328	0.25
329	0.25
330	0.98
331	0.94
332	-1.28
333	0.35
334	0.30
335	-0.46
336	0.62
337	-1.19
338	-2.29
339	-0.96
340	-1.97
341	-0.53
342	0.35
343	0.65
344	0.59
345	-2.11
346	0.44
347	0.26
348	0.65
349	0.56
350	0.65
351	0.99
352	-0.20
353	0.65
354	0.21
355	0.35
356	0.82
357	0.59
358	-0.20
359	-0.46
360	-0.14
361	-0.44
362	0.40
363	-1.69
364	0.00
365	-0.83
366	-3.88
367	-3.49
368	-0.26

```

369      -3.49
370      -3.46
371      -3.46
372       0.00
#Reported_Model_Average 0.149
#Overall_Average_Reported      0.149

```

Output from Verify3D

Verify3D Score over a window of \$winsize_s residues

JPEG image for Verify3D Score

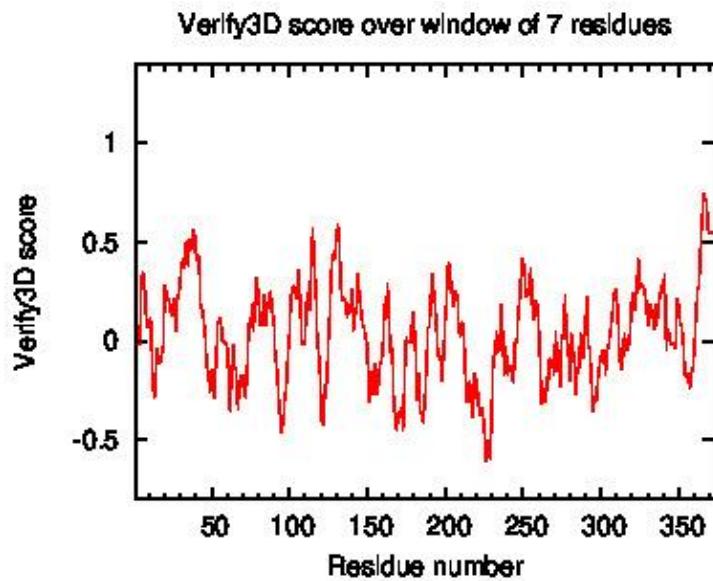


Table of Verify3D scores for ordered residues across all models

#verify3d	#Residue\Model	only_model
1		-1.30
2		0.04
3		0.25
4		0.14
5		0.25
6		0.34
7		0.14
8		1.10
9		0.14
10		0.04
11		-1.14
12		-0.03
13		0.44
14		0.25
15		-0.68
16		-0.84
17		0.14
18		0.41
19		-0.25
20		0.17
21		0.51

PSVS Software Environment

22	-0.25
23	1.25
24	-0.11
25	0.17
26	-0.25
27	-0.35
28	0.44
29	0.34
30	0.14
31	1.10
32	0.14
33	0.41
34	0.14
35	0.34
36	1.10
37	0.25
38	0.25
39	1.10
40	0.14
41	0.71
42	0.34
43	0.14
44	0.34
45	0.17
46	-0.68
47	0.14
48	0.29
49	-0.25
50	-0.94
51	0.14
52	-0.54
53	0.08
54	0.14
55	-0.68
56	1.25
57	0.34
58	0.14
59	-0.40
60	-0.81
61	0.14
62	-0.74
63	1.10
64	-0.68
65	-1.14
66	1.10
67	0.09
68	-0.74
69	-0.68
70	-0.40
71	0.23
72	-0.84
73	1.10
74	-0.54
75	-0.80
76	0.24
77	1.25
78	0.08
79	-0.10
80	0.23
81	0.47
82	0.08
83	-0.25

PSVS Software Environment

84	0.08
85	0.51
86	-0.54
87	1.25
88	-0.54
89	0.71
90	0.09
91	0.29
92	-0.25
93	-0.68
94	-0.25
95	-0.83
96	-0.25
97	-0.68
98	-0.25
99	0.08
100	0.17
101	0.08
102	0.29
103	0.44
104	0.71
105	0.10
106	0.17
107	-0.25
108	0.08
109	1.25
110	-0.68
111	-0.83
112	0.28
113	0.08
114	1.12
115	0.44
116	0.71
117	1.10
118	0.28
119	-1.14
120	-0.68
121	-0.81
122	0.08
123	-0.25
124	-0.40
125	0.29
126	0.17
127	-0.54
128	0.51
129	1.25
130	1.25
131	0.09
132	0.23
133	0.71
134	0.08
135	0.17
136	-0.54
137	0.71
138	0.08
139	0.29
140	0.08
141	0.23
142	0.23
143	0.17
144	-0.74
145	0.51

PSVS Software Environment

146	0.71
147	1.25
148	-0.54
149	-0.25
150	-0.40
151	-0.81
152	0.20
153	0.44
154	-0.80
155	0.47
156	-0.25
157	-1.14
158	0.23
159	-0.84
160	0.71
161	0.08
162	0.44
163	0.14
164	0.47
165	-0.25
166	0.47
167	-0.68
168	-0.94
169	0.51
170	-1.63
171	-0.35
172	-0.54
173	1.12
174	-0.80
175	-0.68
176	-0.25
177	0.17
178	1.10
179	-0.74
180	1.10
181	-0.74
182	0.44
183	-0.54
184	-0.83
185	-0.80
186	0.23
187	-0.25
188	-0.74
189	0.08
190	0.24
191	0.25
192	0.71
193	0.23
194	1.10
195	-0.25
196	-0.74
197	-0.40
198	-0.81
199	0.23
200	0.29
201	0.25
202	0.71
203	0.44
204	0.34
205	0.44
206	0.17
207	-0.42

PSVS Software Environment

208	-0.43
209	1.12
210	0.51
211	0.08
212	-0.74
213	0.08
214	0.08
215	-0.94
216	-0.35
217	-0.40
218	0.71
219	-0.68
220	-0.84
221	-0.25
222	0.71
223	-0.74
224	-0.74
225	-0.11
226	-0.54
227	-0.68
228	-0.94
229	-0.54
230	0.08
231	-0.80
232	-0.81
233	1.25
234	1.10
235	-0.68
236	0.23
237	-0.68
238	-0.68
239	0.71
240	0.29
241	-0.41
242	0.34
243	-0.74
244	-0.41
245	-0.68
246	0.29
247	0.17
248	1.10
249	0.17
250	0.47
251	0.04
252	0.47
253	0.51
254	-0.41
255	0.34
256	0.29
257	0.71
258	0.71
259	-0.94
260	0.08
261	0.24
262	0.23
263	-0.40
264	-0.68
265	-0.74
266	-0.40
267	-0.40
268	1.10
269	-0.25

PSVS Software Environment

270	0.71
271	-0.74
272	-0.80
273	-0.81
274	1.12
275	-0.25
276	0.44
277	-0.54
278	1.04
279	-0.94
280	0.71
281	-0.40
282	-0.54
283	-0.74
284	1.12
285	0.08
286	-0.68
287	-0.74
288	0.51
289	-0.54
290	0.51
291	0.71
292	-0.41
293	0.51
294	0.25
295	-1.14
296	-0.74
297	-0.74
298	-0.25
299	0.14
300	0.29
301	1.04
302	-0.68
303	-0.35
304	-0.54
305	-0.25
306	-0.68
307	1.10
308	1.25
309	-0.25
310	0.09
311	0.17
312	0.17
313	-0.68
314	0.09
315	-0.11
316	-0.74
317	0.29
318	1.25
319	-0.25
320	-0.84
321	0.29
322	0.51
323	0.28
324	0.41
325	0.71
326	0.47
327	0.24
328	-0.81
329	0.71
330	0.24
331	0.25

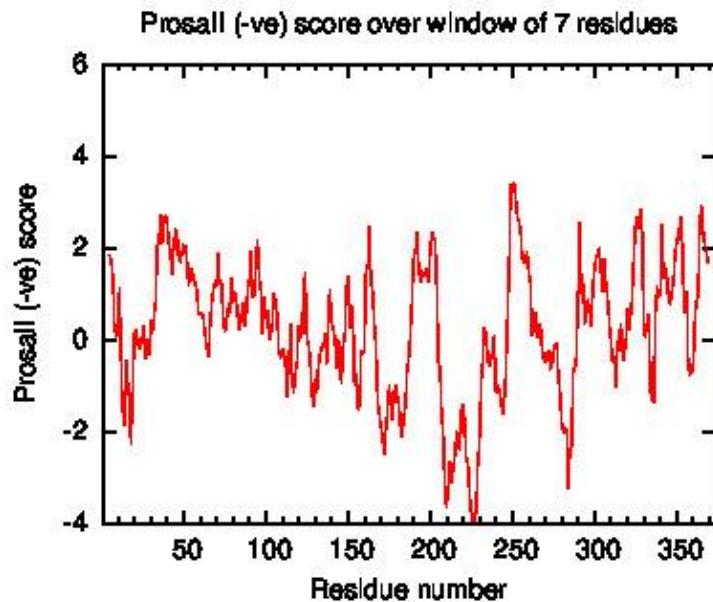
PSVS Software Environment

```
332      0.29
333     -0.35
334      0.24
335     -0.10
336      0.44
337     -0.35
338      1.10
339     -0.41
340      0.44
341      0.51
342      0.25
343      0.17
344      0.34
345     -1.63
346      0.34
347      0.24
348      0.14
349      0.24
350      0.28
351      0.14
352      0.08
353      0.14
354     -0.41
355      0.04
356     -0.41
357     -0.80
358      0.08
359      0.14
360     -0.35
361      0.08
362      0.25
363      0.34
364      0.23
365      1.10
366      0.25
367      1.10
368      1.10
369      1.10
370      0.14
371      0.14
372      0.00
#Reported_Model_Average 0.031
#Overall_Average_Reported      0.031
```

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
1      -1.30
2       0.04
3       0.25
4       0.14
5       0.25
6       0.34
7       0.14
8       1.10
9       0.14
10      0.04
11      -1.14
12      -0.03
13      0.44
14      0.25
15      -0.68
16      -0.84
17      0.14
18      0.41
19      -0.25
20      0.17
21      0.51
22      -0.25
23      1.25
24      -0.11
25      0.17
26      -0.25
27      -0.35
28      0.44
29      0.34
30      0.14
31      1.10
32      0.14
33      0.41
34      0.14
35      0.34
```

PSVS Software Environment

36	1.10
37	0.25
38	0.25
39	1.10
40	0.14
41	0.71
42	0.34
43	0.14
44	0.34
45	0.17
46	-0.68
47	0.14
48	0.29
49	-0.25
50	-0.94
51	0.14
52	-0.54
53	0.08
54	0.14
55	-0.68
56	1.25
57	0.34
58	0.14
59	-0.40
60	-0.81
61	0.14
62	-0.74
63	1.10
64	-0.68
65	-1.14
66	1.10
67	0.09
68	-0.74
69	-0.68
70	-0.40
71	0.23
72	-0.84
73	1.10
74	-0.54
75	-0.80
76	0.24
77	1.25
78	0.08
79	-0.10
80	0.23
81	0.47
82	0.08
83	-0.25
84	0.08
85	0.51
86	-0.54
87	1.25
88	-0.54
89	0.71
90	0.09
91	0.29
92	-0.25
93	-0.68
94	-0.25
95	-0.83
96	-0.25
97	-0.68

PSVS Software Environment

98	-0.25
99	0.08
100	0.17
101	0.08
102	0.29
103	0.44
104	0.71
105	0.10
106	0.17
107	-0.25
108	0.08
109	1.25
110	-0.68
111	-0.83
112	0.28
113	0.08
114	1.12
115	0.44
116	0.71
117	1.10
118	0.28
119	-1.14
120	-0.68
121	-0.81
122	0.08
123	-0.25
124	-0.40
125	0.29
126	0.17
127	-0.54
128	0.51
129	1.25
130	1.25
131	0.09
132	0.23
133	0.71
134	0.08
135	0.17
136	-0.54
137	0.71
138	0.08
139	0.29
140	0.08
141	0.23
142	0.23
143	0.17
144	-0.74
145	0.51
146	0.71
147	1.25
148	-0.54
149	-0.25
150	-0.40
151	-0.81
152	0.20
153	0.44
154	-0.80
155	0.47
156	-0.25
157	-1.14
158	0.23
159	-0.84

PSVS Software Environment

160	0.71
161	0.08
162	0.44
163	0.14
164	0.47
165	-0.25
166	0.47
167	-0.68
168	-0.94
169	0.51
170	-1.63
171	-0.35
172	-0.54
173	1.12
174	-0.80
175	-0.68
176	-0.25
177	0.17
178	1.10
179	-0.74
180	1.10
181	-0.74
182	0.44
183	-0.54
184	-0.83
185	-0.80
186	0.23
187	-0.25
188	-0.74
189	0.08
190	0.24
191	0.25
192	0.71
193	0.23
194	1.10
195	-0.25
196	-0.74
197	-0.40
198	-0.81
199	0.23
200	0.29
201	0.25
202	0.71
203	0.44
204	0.34
205	0.44
206	0.17
207	-0.42
208	-0.43
209	1.12
210	0.51
211	0.08
212	-0.74
213	0.08
214	0.08
215	-0.94
216	-0.35
217	-0.40
218	0.71
219	-0.68
220	-0.84
221	-0.25

PSVS Software Environment

222	0.71
223	-0.74
224	-0.74
225	-0.11
226	-0.54
227	-0.68
228	-0.94
229	-0.54
230	0.08
231	-0.80
232	-0.81
233	1.25
234	1.10
235	-0.68
236	0.23
237	-0.68
238	-0.68
239	0.71
240	0.29
241	-0.41
242	0.34
243	-0.74
244	-0.41
245	-0.68
246	0.29
247	0.17
248	1.10
249	0.17
250	0.47
251	0.04
252	0.47
253	0.51
254	-0.41
255	0.34
256	0.29
257	0.71
258	0.71
259	-0.94
260	0.08
261	0.24
262	0.23
263	-0.40
264	-0.68
265	-0.74
266	-0.40
267	-0.40
268	1.10
269	-0.25
270	0.71
271	-0.74
272	-0.80
273	-0.81
274	1.12
275	-0.25
276	0.44
277	-0.54
278	1.04
279	-0.94
280	0.71
281	-0.40
282	-0.54
283	-0.74

PSVS Software Environment

284	1.12
285	0.08
286	-0.68
287	-0.74
288	0.51
289	-0.54
290	0.51
291	0.71
292	-0.41
293	0.51
294	0.25
295	-1.14
296	-0.74
297	-0.74
298	-0.25
299	0.14
300	0.29
301	1.04
302	-0.68
303	-0.35
304	-0.54
305	-0.25
306	-0.68
307	1.10
308	1.25
309	-0.25
310	0.09
311	0.17
312	0.17
313	-0.68
314	0.09
315	-0.11
316	-0.74
317	0.29
318	1.25
319	-0.25
320	-0.84
321	0.29
322	0.51
323	0.28
324	0.41
325	0.71
326	0.47
327	0.24
328	-0.81
329	0.71
330	0.24
331	0.25
332	0.29
333	-0.35
334	0.24
335	-0.10
336	0.44
337	-0.35
338	1.10
339	-0.41
340	0.44
341	0.51
342	0.25
343	0.17
344	0.34
345	-1.63

```
346      0.34
347      0.24
348      0.14
349      0.24
350      0.28
351      0.14
352      0.08
353      0.14
354      -0.41
355      0.04
356      -0.41
357      -0.80
358      0.08
359      0.14
360      -0.35
361      0.08
362      0.25
363      0.34
364      0.23
365      1.10
366      0.25
367      1.10
368      1.10
369      1.10
370      0.14
371      0.14
372      0.00
#Reported_Model_Average 0.031
#Overall_Average_Reported      0.031
```

Output from MolProbity

VdW violations from MAGE

JPEG image for MAGE VdW violation

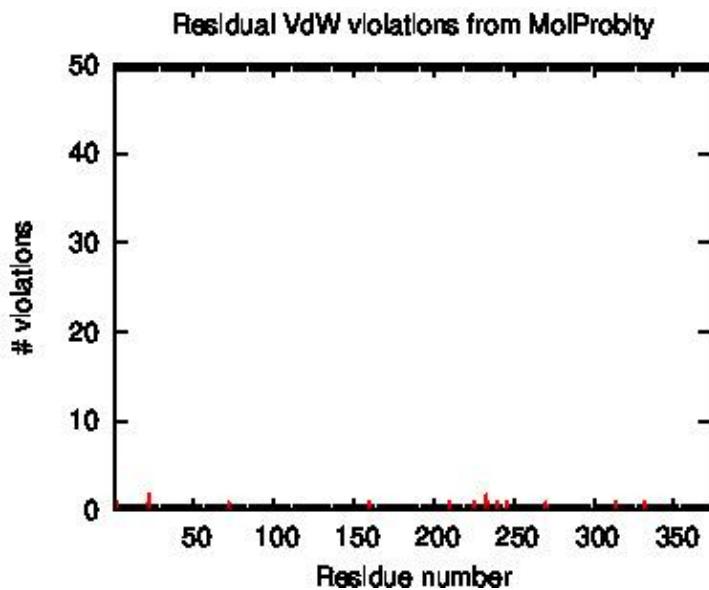


Table of MAGE VdW violations for ordered residues across all models

```
#mage_clash
#Residue\Model  only_model
1.000  0
2.000  1
3.000  0
4.000  0
5.000  0
6.000  0
7.000  0
8.000  0
9.000  0
10.000 0
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 0
20.000 0
21.000 0
22.000 2
23.000 0
24.000 0
25.000 0
26.000 0
27.000 0
28.000 0
29.000 0
30.000 0
31.000 0
32.000 0
33.000 0
34.000 0
35.000 0
36.000 0
37.000 0
38.000 0
39.000 0
40.000 0
41.000 0
42.000 0
43.000 0
44.000 0
45.000 0
46.000 0
47.000 0
48.000 0
49.000 0
50.000 0
51.000 0
52.000 0
53.000 0
54.000 0
55.000 0
56.000 0
57.000 0
58.000 0
```

PSVS Software Environment

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 1
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 0
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
106.000 0
107.000 0
108.000 0
109.000 0
110.000 0
111.000 0
112.000 0
113.000 0
114.000 0
115.000 0
116.000 0
117.000 0
118.000 0
119.000 0
120.000 0

PSVS Software Environment

121.000 0
122.000 0
123.000 0
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 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 0
154.000 0
155.000 0
156.000 0
157.000 0
158.000 0
159.000 0
160.000 1
161.000 0
162.000 0
163.000 0
164.000 0
165.000 0
166.000 0
167.000 0
168.000 0
169.000 0
170.000 0
171.000 0
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

PSVS Software Environment

183.000 0
184.000 0
185.000 0
186.000 0
187.000 0
188.000 0
189.000 0
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 0
210.000 1
211.000 0
212.000 0
213.000 0
214.000 0
215.000 0
216.000 0
217.000 0
218.000 0
219.000 0
220.000 0
221.000 0
222.000 0
223.000 0
224.000 0
225.000 1
226.000 0
227.000 0
228.000 0
229.000 0
230.000 0
231.000 0
232.000 0
233.000 2
234.000 0
235.000 0
236.000 0
237.000 0
238.000 0
239.000 0
240.000 1
241.000 0
242.000 0
243.000 0
244.000 0

PSVS Software Environment

245.000 0
246.000 1
247.000 0
248.000 0
249.000 0
250.000 0
251.000 0
252.000 0
253.000 0
254.000 0
255.000 0
256.000 0
257.000 0
258.000 0
259.000 0
260.000 0
261.000 0
262.000 0
263.000 0
264.000 0
265.000 0
266.000 0
267.000 0
268.000 0
269.000 0
270.000 1
271.000 0
272.000 0
273.000 0
274.000 0
275.000 0
276.000 0
277.000 0
278.000 0
279.000 0
280.000 0
281.000 0
282.000 0
283.000 0
284.000 0
285.000 0
286.000 0
287.000 0
288.000 0
289.000 0
290.000 0
291.000 0
292.000 0
293.000 0
294.000 0
295.000 0
296.000 0
297.000 0
298.000 0
299.000 0
300.000 0
301.000 0
302.000 0
303.000 0
304.000 0
305.000 0
306.000 0

PSVS Software Environment

307.000 0
308.000 0
309.000 0
310.000 0
311.000 0
312.000 0
313.000 0
314.000 1
315.000 0
316.000 0
317.000 0
318.000 0
319.000 0
320.000 0
321.000 0
322.000 0
323.000 0
324.000 0
325.000 0
326.000 0
327.000 0
328.000 0
329.000 0
330.000 0
331.000 0
332.000 1
333.000 0
334.000 0
335.000 0
336.000 0
337.000 0
338.000 0
339.000 0
340.000 0
341.000 0
342.000 0
343.000 0
344.000 0
345.000 0
346.000 0
347.000 0
348.000 0
349.000 0
350.000 0
351.000 0
352.000 0
353.000 0
354.000 0
355.000 0
356.000 0
357.000 0
358.000 0
359.000 0
360.000 0
361.000 0
362.000 0
363.000 0
364.000 0
365.000 0
366.000 0
367.000 0
368.000 0

PSVS Software Environment

```
369.000 0
370.000 0
371.000 0
372.000 0
#Reported_Model_Average 0.038
#Overall_Average_Reported      0.038
```

List of bad contacts calculated by MAGE

5750 A 240 LEU CD2	A 246 LEU 1HD1	-0.846	82
5750 A 246 LEU 1HD1	A 240 LEU 3HD2	-0.648	82
5750 A 72 PHE CD1	A 332 LEU 1HD2	-0.818	91
5750 A 332 LEU 1HD2	A 72 PHE CE1	-0.560	91
5750 A 214 LYS 1HE	A 22 ALA 3HB	-0.583	91
5750 A 214 LYS CE	A 22 ALA 3HB	-0.531	91
5750 A 214 LYS 2HE	A 210 ASP OD1	-0.460	91
5750 A 224 VAL HB	A 225 PRO 2HD	-0.474	95
5750 A 264 LEU 1HD2	A 233 TYR CD1	-0.432	87
5750 A 263 VAL 2HG1	A 233 TYR OH	-0.402	87
5750 A 315 PRO 2HD	A 314 ASN 1HB	-0.415	88
5750 A 136 ILE 3HD1	A 270 PHE CE1	-0.403	94
5750 A 146 ARG NH2	A 160 ARG 2HH2	-0.403	90
5750 A 3 PRO 2HD	A 2 GLU HA	-0.400	42

Output from PDB validation software

Summary from PDB validation

Apr. 17, 17:23:13 2022

Greetings,

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

The following checks were made on :

DISTANCES AND ANGLES

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

==> The following solvent molecules are further away than 3.5 Angstroms from macromolecule atoms which are available for hydrogen bonding in the asymmetric unit.

none

The coordinates for water molecules which could be translated back into the asymmetric unit are listed. If you do not indicate otherwise we will replace the solvent coordinates in the entry with the ones below:

none

==> Close contacts in same asymmetric unit. Distances smaller than 2.2 Angstroms are considered as close contacts.

PSVS Software Environment

none

==> Close contacts based on crystal symmetry. Distances smaller than 2.2 Angstroms are considered as close contacts.

none

==> 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

All covalent bonds lie within a 6.0*RMSD range about the standard dictionary values.

*** 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
11.5	ALA	A	370	N	-	CA	-	C	122.7	111.2

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 and there are no incorrect carbon chiral centers. Some of O1P and O2P atoms do not follow the convention defined in the standard IUBMB nomenclature (Liebecq, C. Compendium of Biochemical Nomenclature and Related Documents, 2nd ed.; Portland Press: London and Chapel Hill, 1992). If you do not indicate otherwise, we will switch the labels of O1P and O2P as shown below.

PSVS Software Environment

OTHER IMPORTANT ISSUES

==> Please check carefully REMARKS 3 and 200 and fill in the parameters as appropriate.

==> The following residues have extra atoms:

RES MOD#C SEQ	ATOMS
ALA(A 372)	O2

dorh_rosettacm.pdb: Missing KEYWDS records

dorh_rosettacm.pdb: Missing TITLE record