

Protein Structure Validation Suite (PSVS)

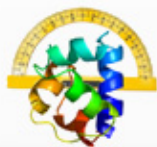


PSVS report for DocfISIRT1CathB

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PSVS report for DocfISIRT1CathB



Protein Structure Validation Suite
(PSVS)



Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdostat	PdbStat-5.9 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-1.0
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4
MolMol	Version 2K.2

MolProbit 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:

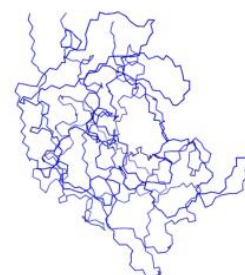
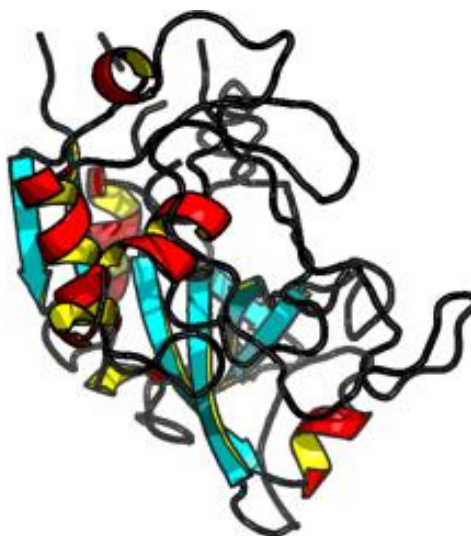
PERL	Version 5.8.0
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9
gnuplot	Version 3.7 patchlevel 3
jpegtopnm	year 2000
pnmcrop	year 2000
pnmtojpeg	year 2000

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.): 252
Organism:
SwissProt /
TrEMBL ID:
models: 2
Oligomerization: 5 mer
Molecular weight: 27606



Secondary Structure Elements:

Inter-chain break(s) between 66 & 77, 77 & 88, 256 & 267, 267 & 278

alpha helices: 7A-10A, 29A-44A, 56A-62A, 76A-85A, 157A-167A

beta strands: 5A-6A, 195A-209A, 170A-177A, 247A-248A, 151A-152A, 212A-218A, 230A-234A

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	6.9 Å	5.8 Å	6.9 Å
All heavy atoms	7.2 Å	6.6 Å	7.2 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
79.0%	19.6%	0.8%	0.6%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
90%	7.6%	2.4%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
-Raw score	0.40	0.43	-0.62	-0.50	19.95

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*Z-score*¹ -0.96 -0.91 -2.12 -2.96 -1.90

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

Number of close contacts (within 2.2 Å): 0

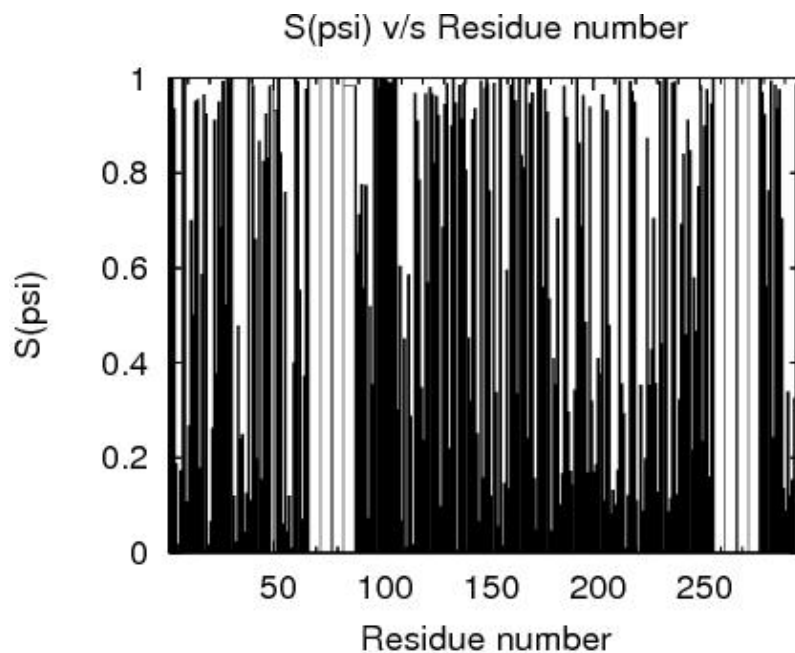
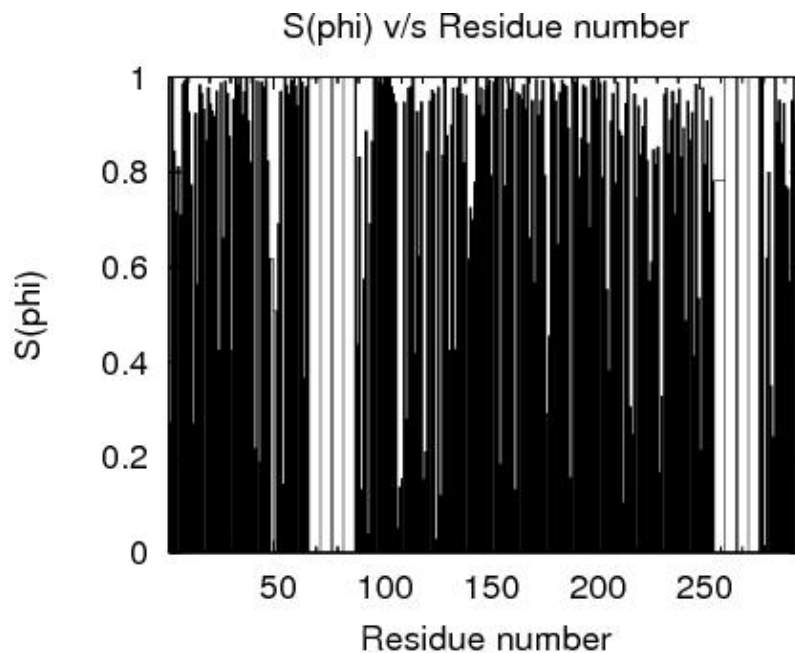
RMS deviation for bond angles: 2.4 °

RMS deviation for bond lengths: 0.014 Å

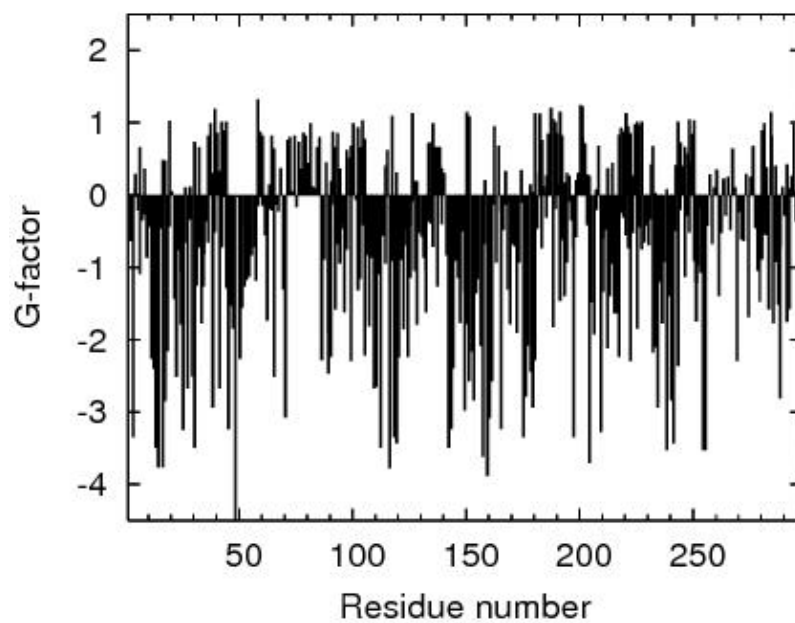
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28; a positive value indicates a 'better' score

²Order residues: HASH(0xd7f490)

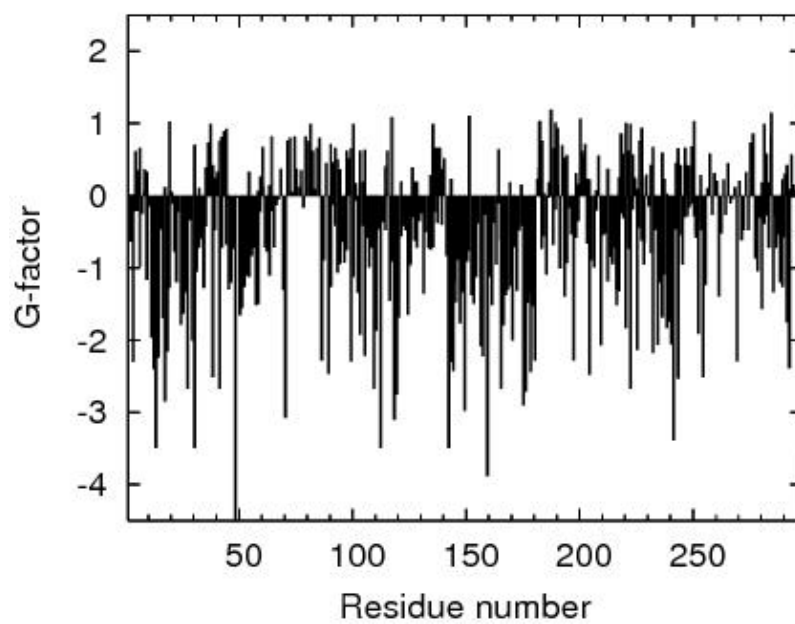
³Selected residues: all



Procheck G-factor for phi-psi

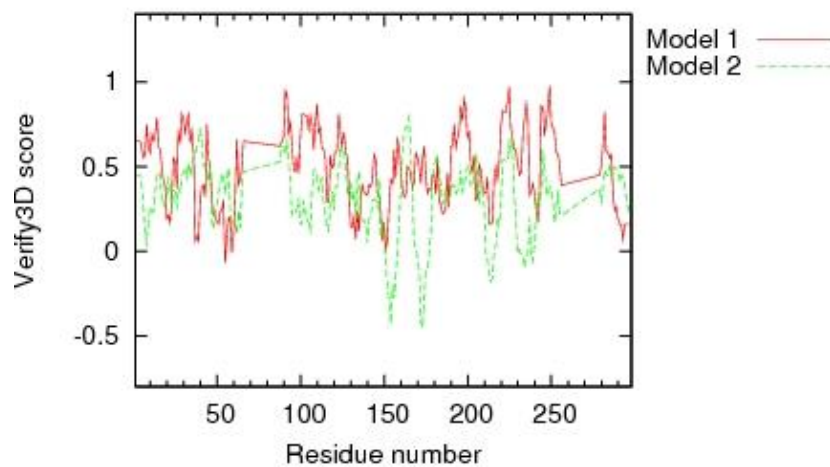


Procheck G-factor for all dihedral angles

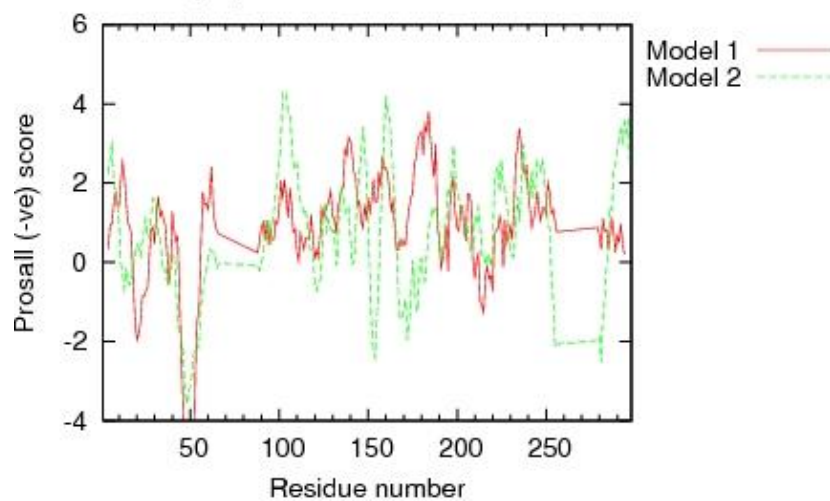


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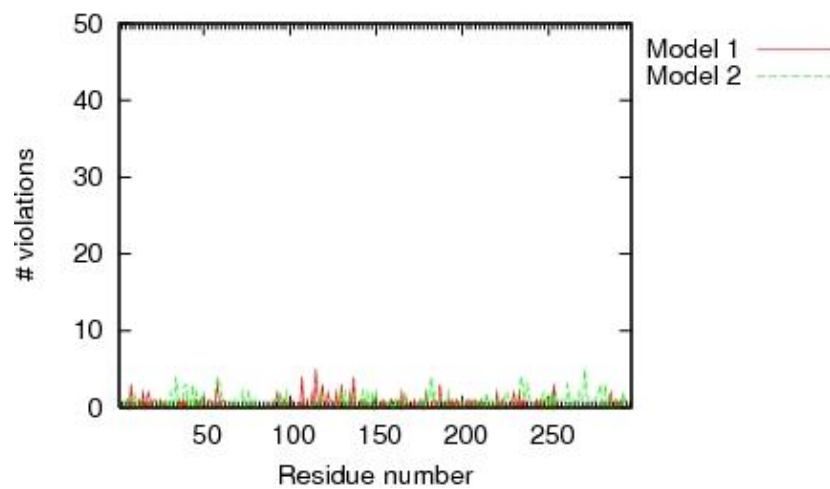
Verify3D score over window of 7 residues

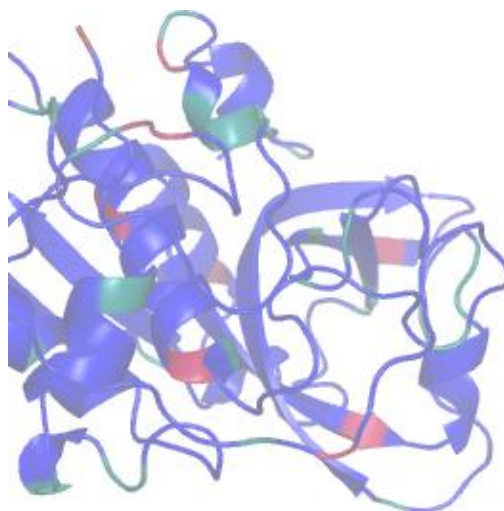


ProsaII (-ve) score over window of 7 residues



Residual VdW violations from MolProbity





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

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generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

Summary of structure quality factors

Analyses performed for all residues.

Total structures computed	currently unknown		
Number of structures used	2		
RMSD Values			
	all	ordered ^e	Selected ^f
All backbone atoms	6.9 Å	5.8 Å	6.9 Å
All heavy atoms	7.2 Å	6.6 Å	7.2 Å
Structure Quality Factors - overall statistics			
	Mean score	SD	Z-score ^g
Procheck G-factor ^e (phi / psi only)	-0.62	N/A	-2.12
Procheck G-factor ^e (all dihedral angles)	-0.50	N/A	-2.96
Verify3D	0.40	0.1273	-0.96
ProsaII (-ve)	0.43	0.0424	-0.91
MolProbity clashscore	19.95	5.3669	-1.90
Ramachandran Plot Summary from Procheck ^f			
Most favoured regions	79.0%		
Additionally allowed regions	19.6%		
Generously allowed regions	0.8%		
Disallowed regions	0.6%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	90%		
Allowed regions	7.6%		
Disallowed regions	2.4%		

^e Residues with sum of phi and psi order parameters > 1.8

Ordered residue ranges:

^f Residues selected based on: all residues

Selected residue ranges: all

^g With respect to mean and standard deviation for 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 DocfISIRT1CathB by PSVS

Output from PDBStat

S(phi)|S(psi) V/S Residue number

Text output from PDBStat of phi psi order

#	CHAIN										.GT.	SUM.GT.
#	RES	ID	DIH	S(phi)	S(psi)	S(chi1)	S(chi2)	S(chi3)	S(chi4)	S(chi5)	0.90	1.6
#	-----											
	LEU	M	1		0.274	0.999	0.464	706.223				
	PRO	M	2	1.000	0.999						2	2
	ALA	M	3	0.845	0.936	706.283	705.986					3
	SER	M	4	0.719	0.188	0.908	706.046	706.047				
	PHE	M	5	0.812	0.018							
	ASP	M	6	0.710	0.173							
	ALA	M	7	0.986	1.000	706.378	706.058				7	7
	ARG	M	8	0.993	0.997						8	8
	GLU	M	9	0.997	0.108	0.836	0.618					
	GLN	M	10	0.927	0.268	0.604	0.574	0.384				
	TRP	M	11	0.774	0.700	0.760	0.949					
	PRO	M	12	0.272	0.501							
	GLN	M	13	0.924	0.951						13	13
	CYS	M	14	0.565	0.955	0.602						
	PRO	M	15	0.984	0.179	0.882	0.812					
	THR	M	16	0.966	0.587	0.683						
	ILE	M	17	0.933	0.965						17	17
	LYS	M	18	0.867	0.925							18
	GLU	M	19	0.978	0.017							
	ILE	M	20	0.944	0.066							
	ARG	M	21	0.929	0.263	0.989	0.296					
	ASP	M	22	0.918	0.912	1.000	0.568	706.007	706.753	706.821	22	22
	GLN	M	23	0.971	0.378	0.494	0.454	0.351				
	GLY	M	24	0.426	0.950							
	SER	M	25	0.988	0.686							
	CYS	M	26	0.662	0.993	0.369						
	GLY	M	27	0.992	0.523	706.876						
	SER	M	28	0.966	0.997	0.992	706.491				28	28
	CYS	M	29	0.875	0.987							29
	TRP	M	30	0.426	1.000							
	ALA	M	31	0.954	0.120	706.372	706.838	706.855				
	PHE	M	32	0.998	0.023	0.852	0.431					
	GLY	M	33	0.984	0.478	706.183	706.130					
	ALA	M	34	0.999	0.239	705.979	706.897	706.010	706.835	706.589		
	VAL	M	35	0.922	0.249	1.000	706.071	706.170	706.049			
	GLU	M	36	0.970	0.043	0.999	0.993	0.944	705.977	706.676		
	ALA	M	37	0.998	0.126	706.888	706.456					
	ILE	M	38	0.908	0.999	0.881	0.971	706.867	706.502	706.816	38	38
	SER	M	39	0.821	0.111	0.926	706.222	706.118	705.922	706.730		
	ASP	M	40	0.996	0.984	0.988	0.778				40	40
	ARG	M	41	0.219	0.661							
	ILE	M	42	0.992	0.198	0.936	0.275					
	CYS	M	43	0.190	0.868							
	ILE	M	44	0.990	0.155	0.479	0.546					
	HIS	M	45	0.980	0.825	1.000	0.482	706.228				45
	THR	M	46	0.996	0.925	0.974	706.172	706.118	705.996	706.721	46	46

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[illegible]

PSVS Software Environment

HIS	M	131	0.878	0.988								131
HIS	M	132	0.426	0.219	0.633	0.984						
VAL	M	133	0.900	0.900	0.752							133
ASN	M	134	0.977	0.999	0.418	0.360	706.823	706.125	706.767		134	134
GLY	M	135	0.428	0.948	705.995	706.128	706.847					
SER	M	136	0.978	0.005	0.983	706.893						
ARG	M	137	0.997	0.985	0.704	0.177					137	137
PRO	M	138	0.965	0.914	0.772	0.231					138	138
PRO	M	139	0.820	0.990								139
CYS	M	140	0.962	0.806	0.994	705.900						140
THR	M	141	0.618	0.453	0.719	705.996						
GLY	M	142	0.726	0.320	705.917	706.888						
GLU	M	143	0.701	0.913	0.591	0.990						
GLY	M	144	0.779	0.936	705.986	705.909						
ASP	M	145	1.000	0.252	0.490	0.664	706.021					
THR	M	146	0.942	0.067	0.489	705.949						
PRO	M	147	0.978	0.994	0.311	0.466					147	147
LYS	M	148	0.920	0.158	0.306	0.984						
CYS	M	149	0.973	0.979	0.998	706.898					149	149
SER	M	150	0.982	0.988	0.461	706.021	706.277				150	150
LYS	M	151	0.994	0.763								
ILE	M	152	0.794	0.120	0.672	0.524	706.151					
CYS	M	153	0.990	0.989	0.930	706.132	706.780				153	153
GLU	M	154	1.000	0.338	0.305	0.999	0.396					
PRO	M	155	0.999	0.056	0.189	0.848	706.611					
GLY	M	156	0.186	0.998	706.366	706.260	706.688					
TYR	M	157	0.999	0.015								
SER	M	158	0.772	0.147								
PRO	M	159	0.933	0.596								
THR	M	160	0.987	0.135								
TYR	M	161	0.974	0.985							161	161
LYS	M	162	1.000	1.000	0.118	0.998					162	162
GLN	M	163	0.133	0.953								
ASP	M	164	0.968	0.335	0.950	0.958						
LYS	M	165	0.963	0.999	0.990	0.449	0.966	0.928	706.729		165	165
HIS	M	166	0.954	0.837	0.284	1.000						166
TYR	M	167	0.984	0.811	0.696	0.758						167
GLY	M	168	0.934	0.998	706.160	705.975					168	168
TYR	M	169	1.000	0.241	0.488	0.532						
ASN	M	170	0.662	0.947	0.574	0.402						
SER	M	171	0.951	0.969							171	171
TYR	M	172	0.568	0.157	0.594	0.005						
SER	M	173	0.996	0.048	0.965	706.072	706.145					
VAL	M	174	0.920	0.999	1.000	706.091					174	174
SER	M	175	0.951	0.999	0.841	706.053					175	175

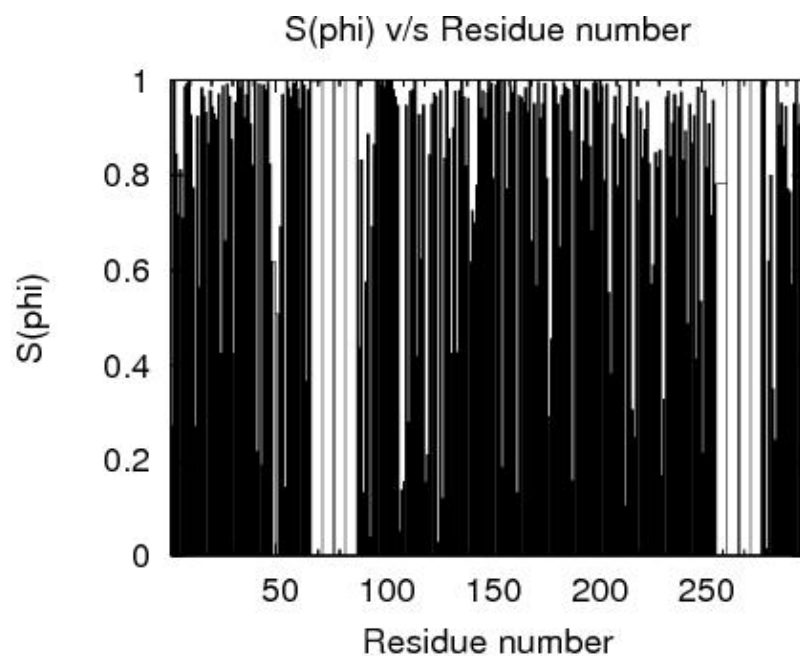
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GLY	M	193	0.790	0.863						
ALA	M	194	0.871	0.689	706.868					
PHE	M	195	0.983	0.963	1.000			195		195
SER	M	196	0.979	0.486	0.907					
VAL	M	197	0.862	0.169	0.451	706.806				
TYR	M	198	0.684	0.939	0.358	0.982				
SER	M	199	0.994	0.320	0.966					
ASP	M	200	0.994	0.170	0.974	0.984				
PHE	M	201	0.955	0.186	0.997	0.994	706.823	706.292	706.734	
LEU	M	202	1.000	0.410	0.789	0.210				
LEU	M	203	0.987	0.377	0.994	1.000	706.151	705.936	706.749	
TYR	M	204	0.790	0.965	0.607	0.548				
LYS	M	205	0.992	0.110						
SER	M	206	0.553	0.932	0.988	706.889				
GLY	M	207	0.383	0.479	706.803	706.624				
VAL	M	208	0.908	0.083	0.237					
TYR	M	209	0.966	0.132	0.533	0.115				
GLN	M	210	0.778	0.102	0.410					
HIS	M	211	0.989	0.174	0.364	0.541	706.436			
VAL	M	212	0.888	0.996	0.565	706.098	706.478			212
THR	M	213	0.878	0.356	0.641	706.600				
GLY	M	214	0.106	0.294	706.284	706.145				
GLU	M	215	0.945	0.010	0.393	0.554	0.970			
MET	M	216	0.998	0.121	0.737	0.508				
MET	M	217	0.307	0.993						
GLY	M	218	0.249	0.972	706.402					
GLY	M	219	0.965	0.950	706.013	706.216		219		219
HIS	M	220	0.747	0.110	0.393	0.906				
ALA	M	221	0.939	0.001	706.151	706.243	706.129	706.759	706.835	
ILE	M	222	0.837	0.353	0.707					
ARG	M	223	0.897	0.089	0.323	0.999				
ILE	M	224	0.955	0.198	0.986	0.999				
LEU	M	225	0.825	0.874	0.770	0.925	706.176	706.269		225
GLY	M	226	0.572	0.353	706.201	706.293				
TRP	M	227	0.612	0.429	0.281	0.771				
GLY	M	228	0.848	0.705	706.004	706.897				
VAL	M	229	0.816	0.357	0.271	706.482				
GLU	M	230	0.854	0.128	0.416	0.996	0.986			
ASN	M	231	0.169	0.993	0.638					
GLY	M	232	0.329	0.441	706.287	706.092				
THR	M	233	0.964	0.998	0.916	706.475		233		233
PRO	M	234	0.977	0.998	0.871	0.801		234		234
TYR	M	235	0.839	0.087	0.947	0.603				
TRP	M	236	0.911	0.115	0.969	0.966	705.956			
LEU	M	237	0.970	0.990	0.480	0.554		237		237
VAL	M	238	0.712	0.992	0.987	706.899				
ALA	M	239	0.944	0.123	706.126	706.253				
ASN	M	240	0.975	0.323	0.711	0.869	706.275			
SER	M	241	0.832	0.693	0.616					
TRP	M	242	0.894	0.840	0.990	0.101				242
ASN	M	243	0.488	0.460	0.978	0.982				
THR	M	244	0.950	0.912	0.887	706.029	706.009	244		244
ASP	M	245	0.868	0.848	0.852	0.581				245
TRP	M	246	0.926	0.217	0.986					
GLY	M	247	0.414	0.580	706.317	705.963				
ASP	M	248	0.985	0.467	0.985	0.978				
ASN	M	249	0.535	0.772	0.580	0.928				
GLY	M	250	0.215	0.984	706.038	706.260				
PHE	M	251	0.978	0.235	0.996					
PHE	M	252	0.817	0.900	0.485	0.804	706.562			252
LYS	M	253	0.909	0.976	0.632	0.198		253		253
ILE	M	254	0.717	0.160	0.283	0.347				

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LEU	M	255	0.958	0.946	0.602	0.537	706.030	706.133		255	255
ARG	M	256	0.782	706.533	1.000	0.987	0.584	0.995	1.000		
ARG	M	267	706.295	706.369	706.060	706.233	706.256	706.018		267	267
ARG	M	278	706.077	706.755	706.195	706.792	706.012	706.860		278	278
GLY	M	279	706.421	0.970	706.891	706.734	706.209	706.081	706.727	279	279
GLN	M	280	0.015	0.924	0.717	0.858	0.763	705.981			
ASP	M	281	0.620	0.561	0.935	0.874					
HIS	M	282	0.800	0.763	0.455	0.647					
CYS	M	283	0.351	0.994	0.265	706.332					
GLY	M	284	0.244	0.243	706.883						
ILE	M	285	0.998	0.985	0.566	0.491				285	285
GLU	M	286	0.906	0.936	0.995	0.419	1.000			286	286
SER	M	287	0.952	0.976	0.722	706.314				287	287
GLU	M	288	0.861	0.705							
VAL	M	289	0.945	0.136	0.999						
VAL	M	290	0.772	0.089	0.358	706.870	705.903	706.842			
ALA	M	291	0.766	0.339	706.193	706.013					
GLY	M	292	0.571	0.121	706.154	706.128					
ILE	M	293	0.951	0.154	1.000	0.997	706.583				
PRO	M	294	1.000	0.326	0.996	0.624	705.901				
ARG	M	295	0.907	0.987	0.464					295	295
THR	M	296	0.950	0.228	0.662	706.456	705.919	706.865			
ASP	M	297	1.000	706.898	0.351	0.820	706.240	706.322		297	297

JPEG image of S(phi)~Residue_number Plot



JPEG image of S(psi)~Residue_number Plot

S(phi)|S(psi) V/S Residue number

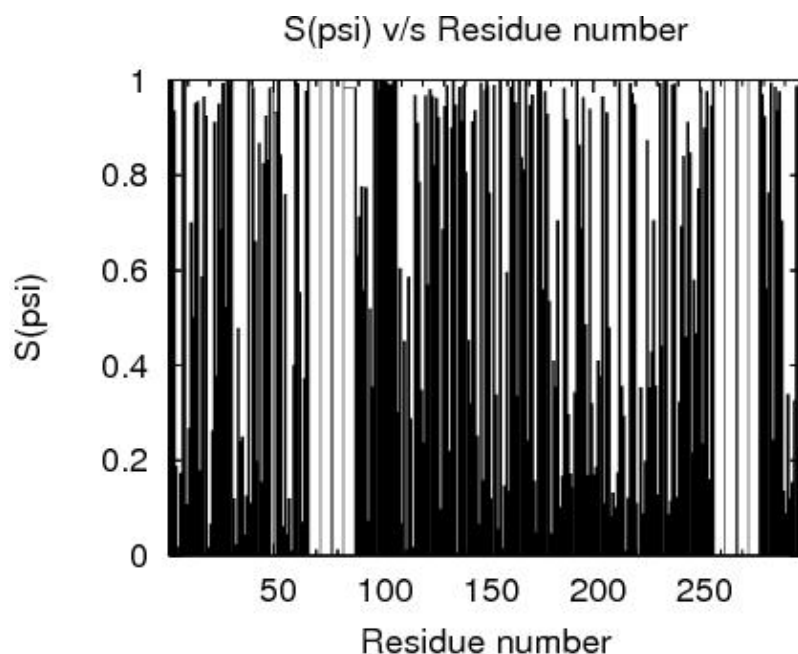


Table of Backbone and Heavy Atom RMSD

Text report of backbone and heavy atom RMSD for ordered regions

```
>
> Kabsch RMSD data for family `DocflSIRT1CathB.pdb'
>
> Kabsch RMSD of backbone atoms in res. M[7..8],M[60..61],M[65..88],M[97..107],M[123..124],M[137..138]
> Kabsch RMSD of backbone atoms in res. M[7..8],M[60..61],M[65..88],M[97..107],M[123..124],M[137..138]
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[7..8],[60..61],[65..88],[97..107],[123..124]
> Range of RMSD values to reference struct. is 3.585 to 9.261

> Kabsch RMSD of heavy atoms in res. M[7..8],M[60..61],M[65..88],M[97..107],M[123..124],M[137..138]
> Kabsch RMSD of heavy atoms in res. M[7..8],M[60..61],M[65..88],M[97..107],M[123..124],M[137..138]
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[7..8],[60..61],[65..88],[97..107],[123..124]
> Range of RMSD values to reference struct. is 3.811 to 10.281
```

Text report of backbone RMSD for entire protein

```
> Kabsch RMSD of backb atoms in res. *[1..297],for model 1 is: 2.768 (*)
> Kabsch RMSD of backb atoms in res. *[1..297],for model 2 is: 11.122
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[1..297], is: 6.945
> Range of RMSD values to reference struct. is 2.768 to 11.122
```

Text report of heavy atom RMSD for entire protein

```
> Kabsch RMSD of heavy atoms in res. *[1..297],for model 1 is: 2.846 (*)
> Kabsch RMSD of heavy atoms in res. *[1..297],for model 2 is: 11.486
>
```

PSVS Software Environment

```
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[1..297], is: 7.166
> Range of RMSD values to reference struct. is 2.846 to 11.486
```

Summary of heavy atom and backbone RMSDs over the whole protein and ordered residues

RMSD Values

	all residues	ordered residues	selected residues
All backbone atoms	6.9	5.8	6.9
All heavy atoms	7.2	6.6	7.2

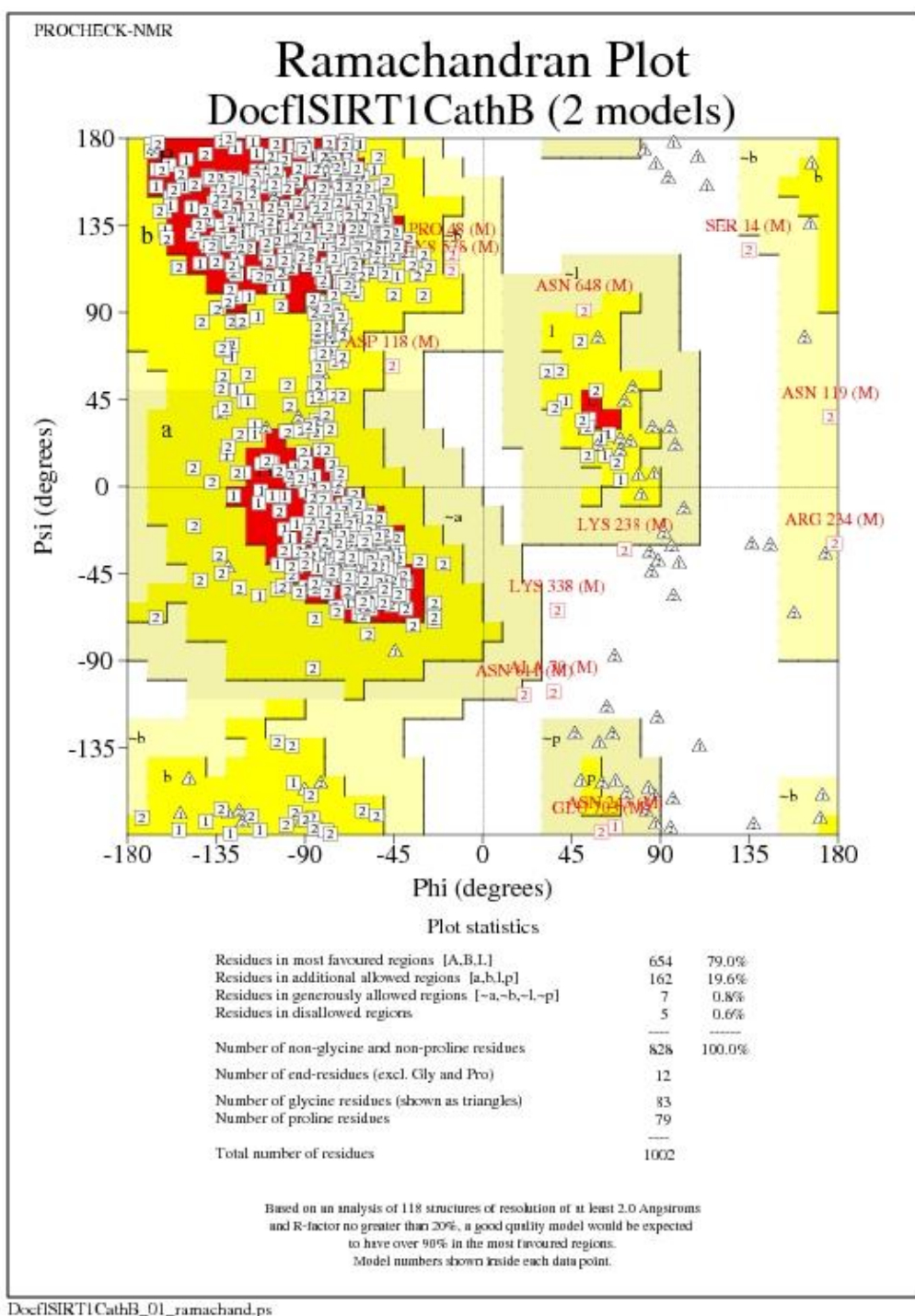
Output from PROCHECK

Ramachandran Plot for all models

Text summary of Ramachandran Plot

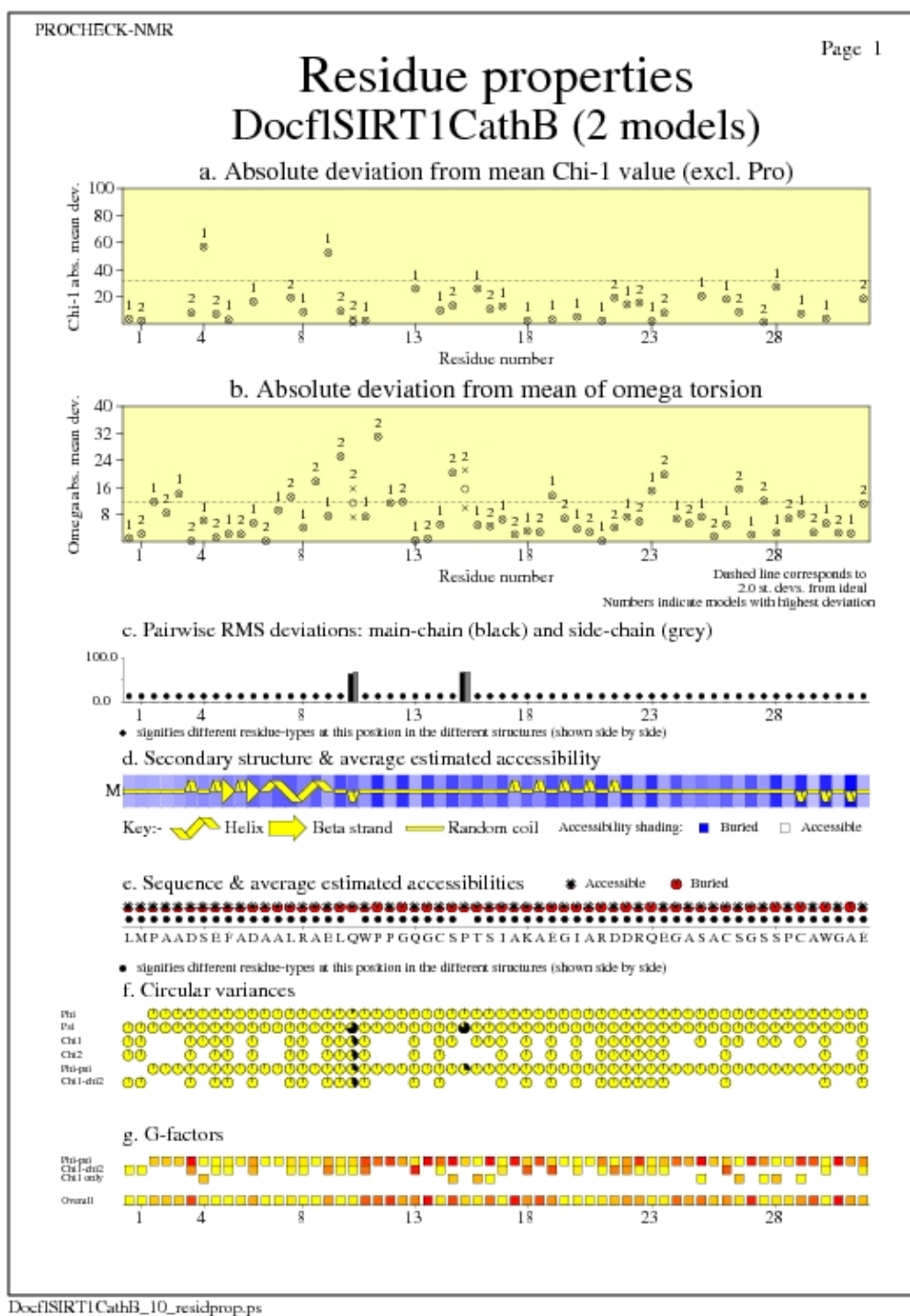
```
+-----<<< P R O C H E C K       S U M M A R Y >>>-----+
|
| DocflSIRT1CathB_002.rin    0.0                                1002 residues |
|
*| Ramachandran plot:    79.0% core    19.6% allow    0.8% gener    0.6% disall |
|
*| All Ramachandrans:    62 labelled residues (out of 989)
+| Chi1-chi2 plots:      10 labelled residues (out of 569)
```

JPEG image for all model Ramachandran Plot

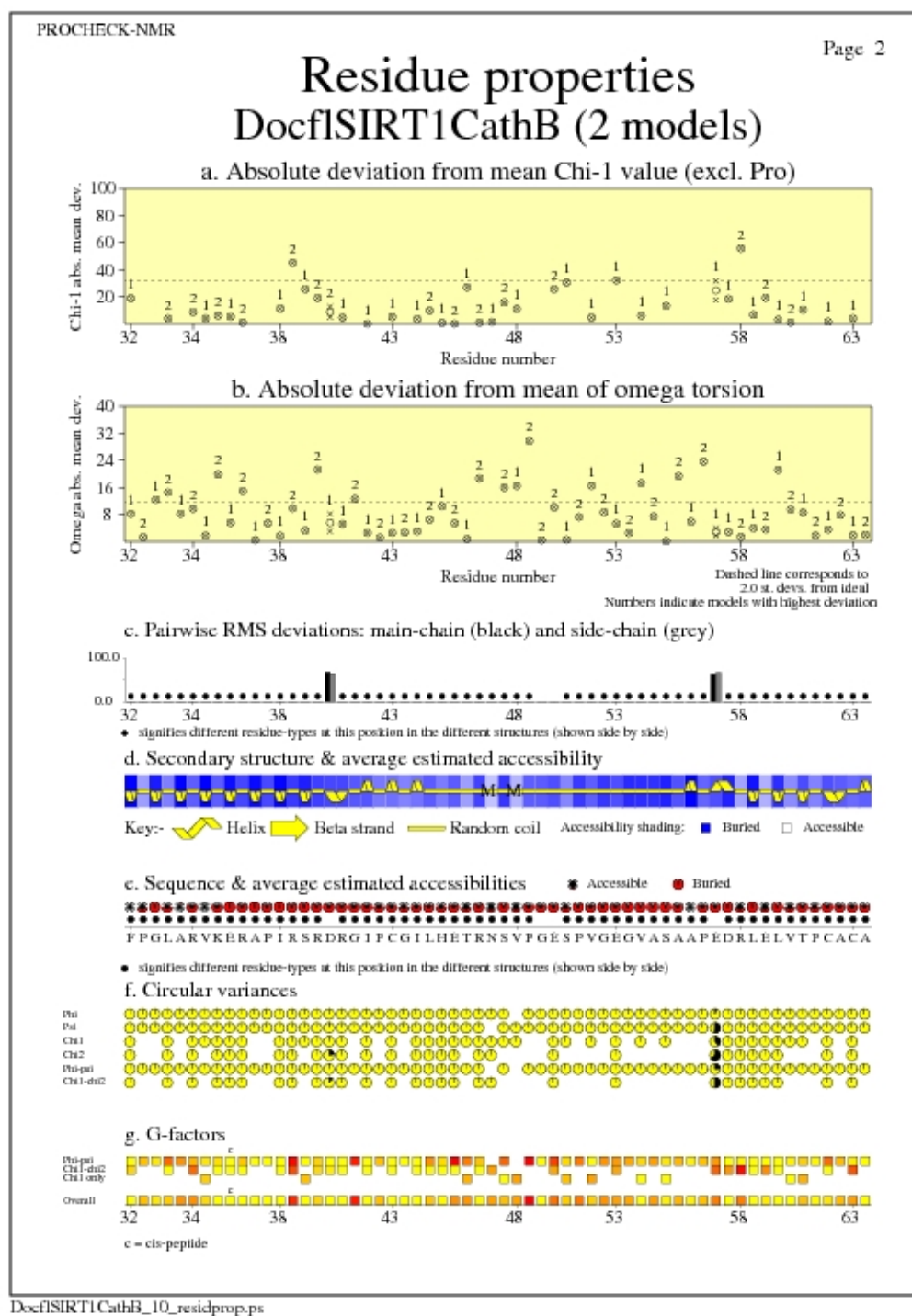


Residue Properties for all models

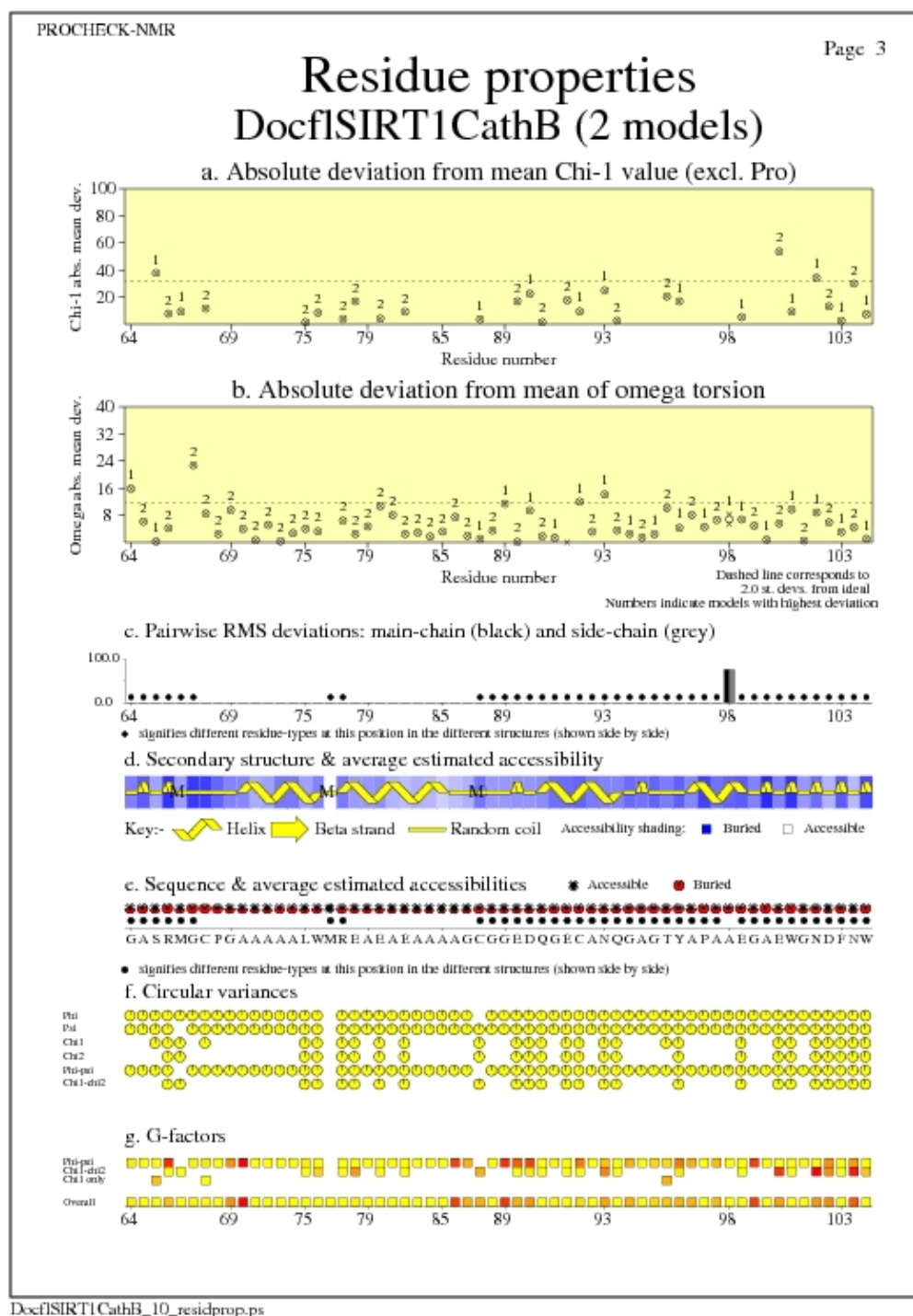
JPEG for all model Residue Properties - page \$num_n



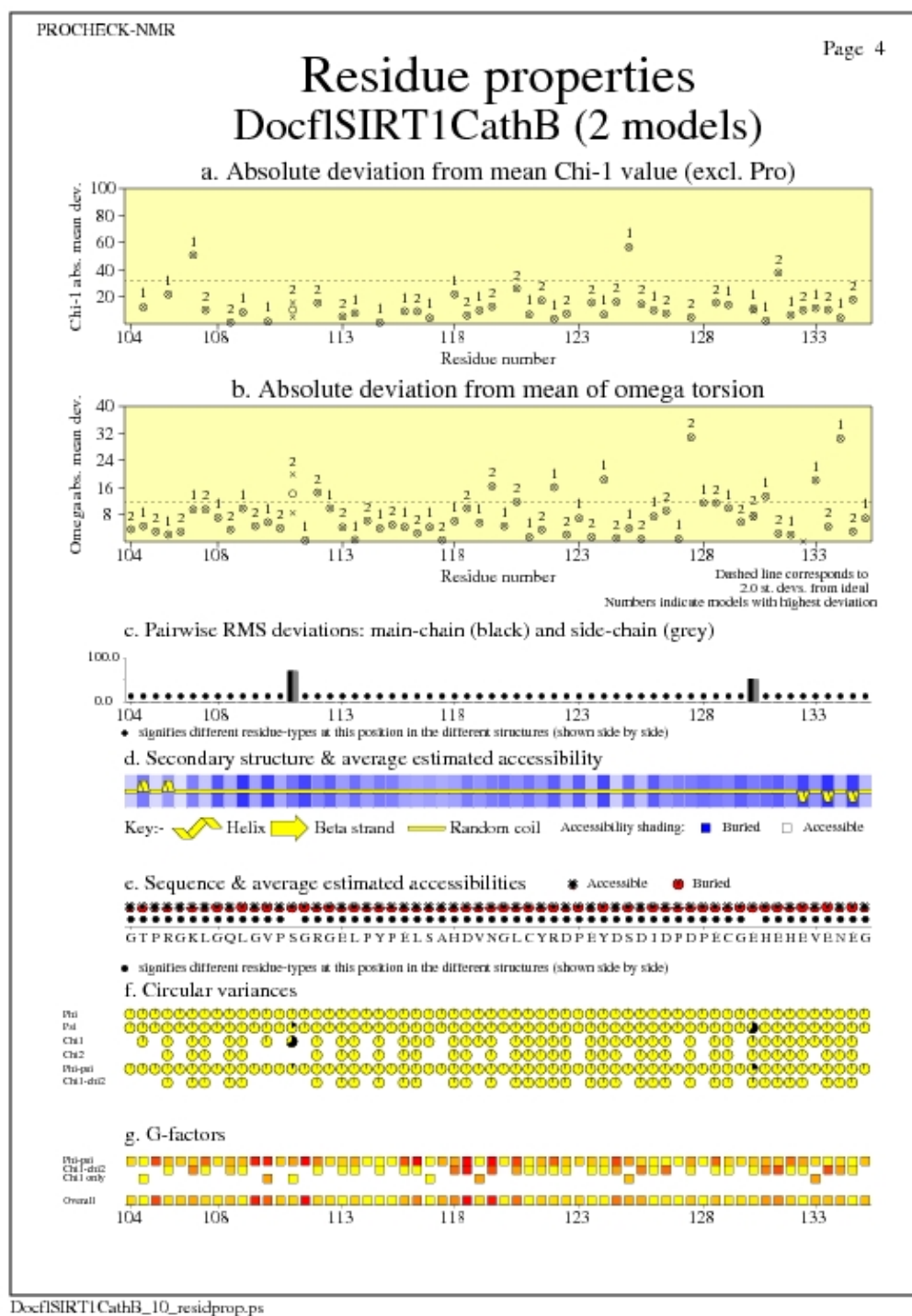
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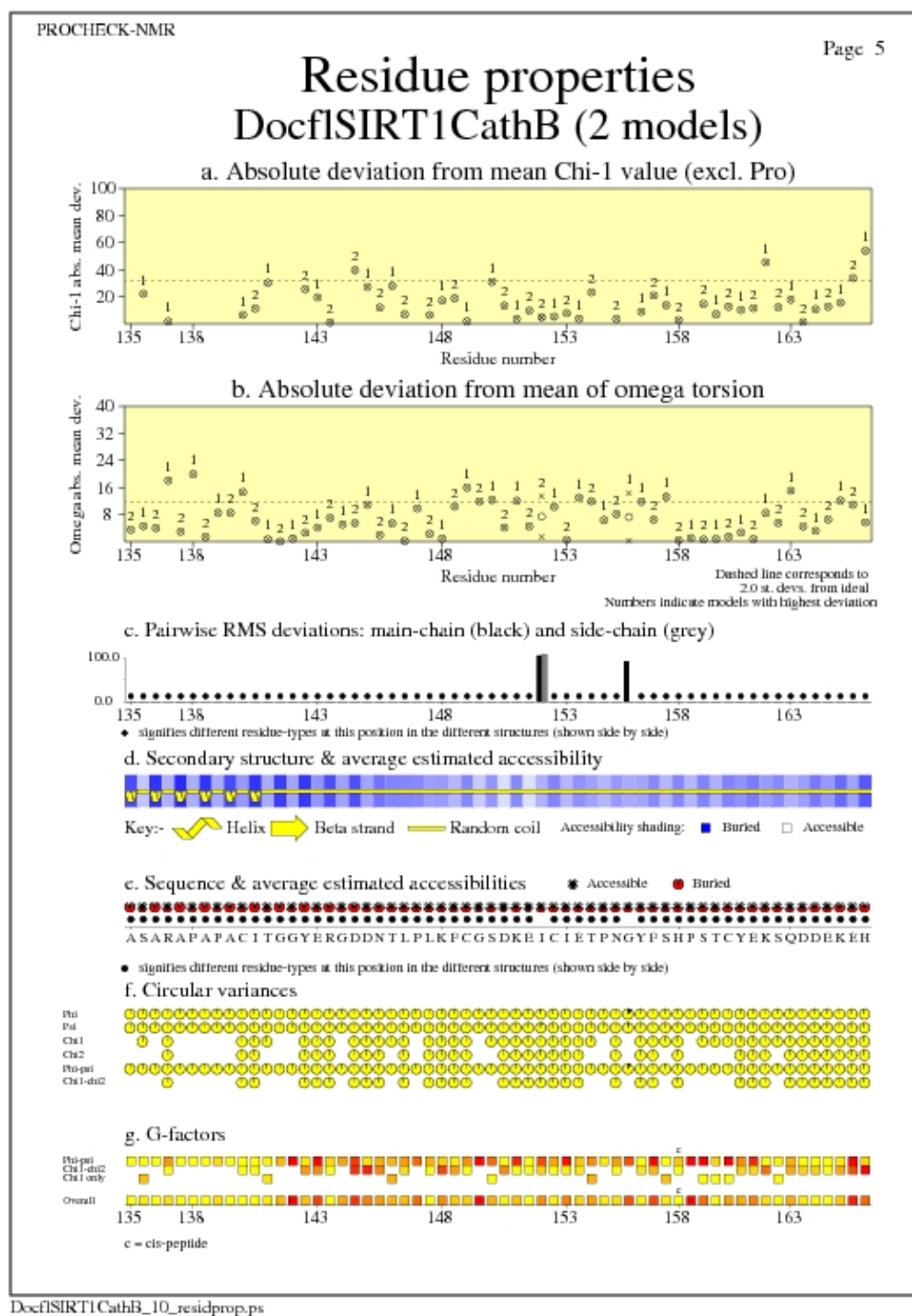
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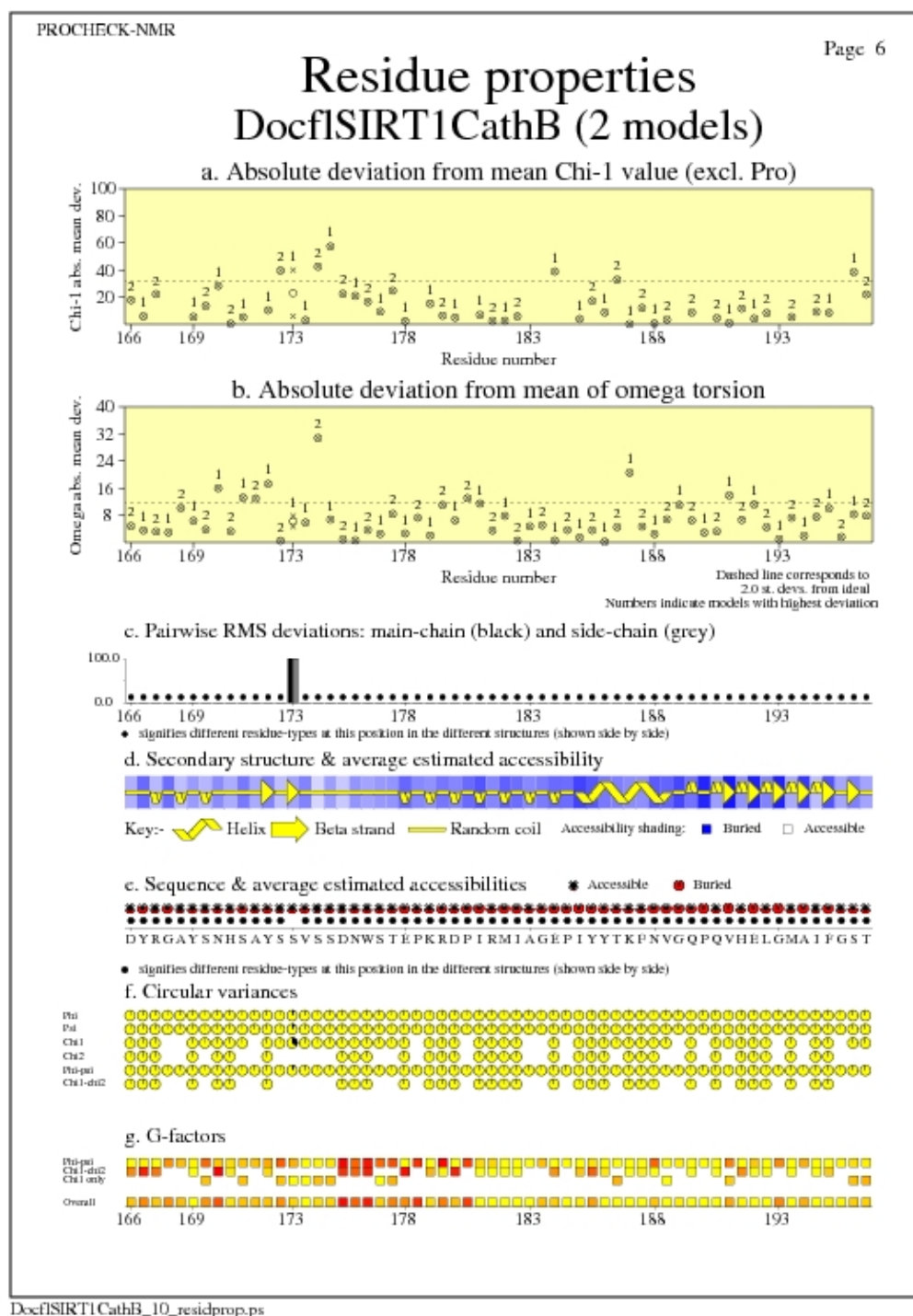
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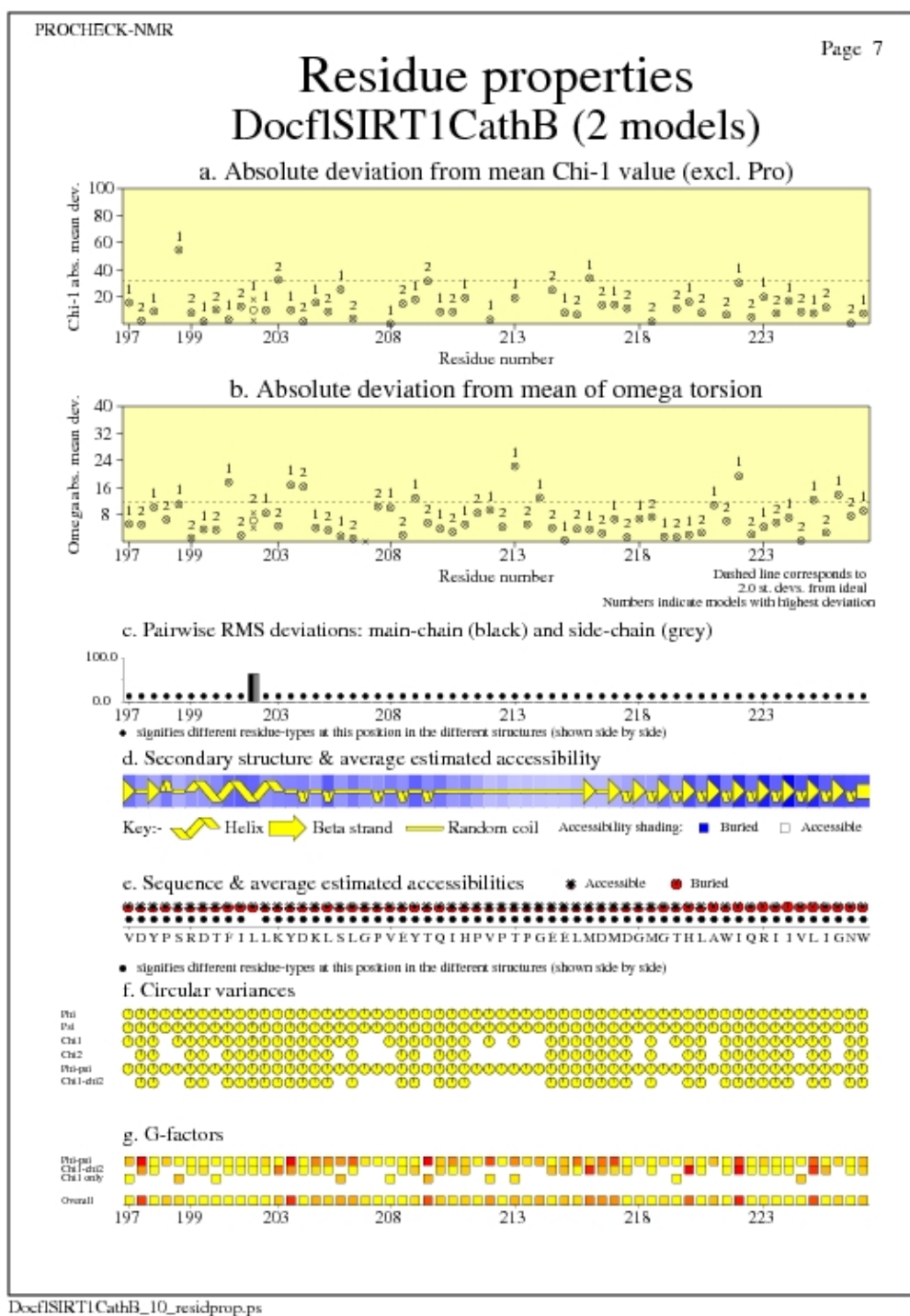
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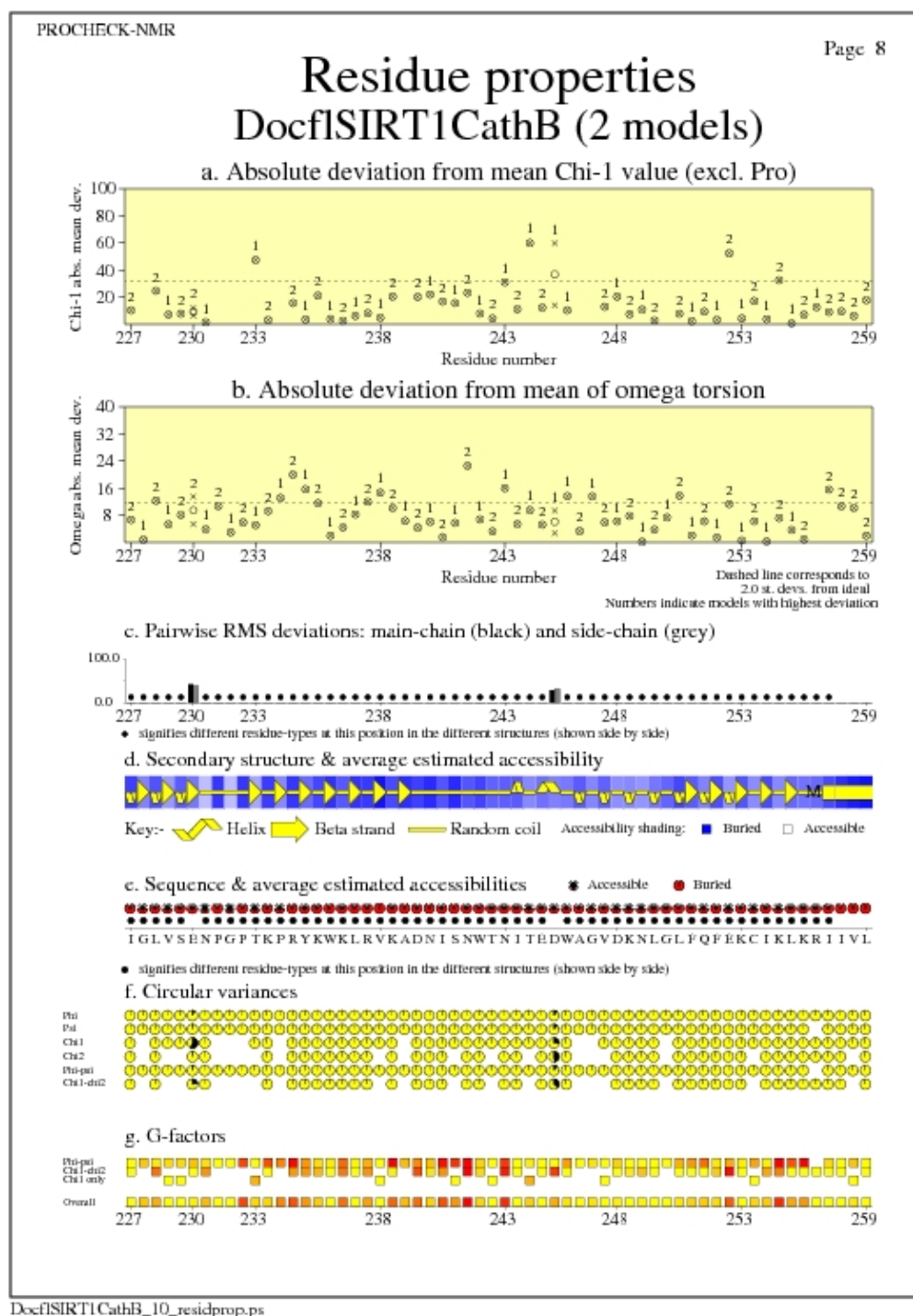
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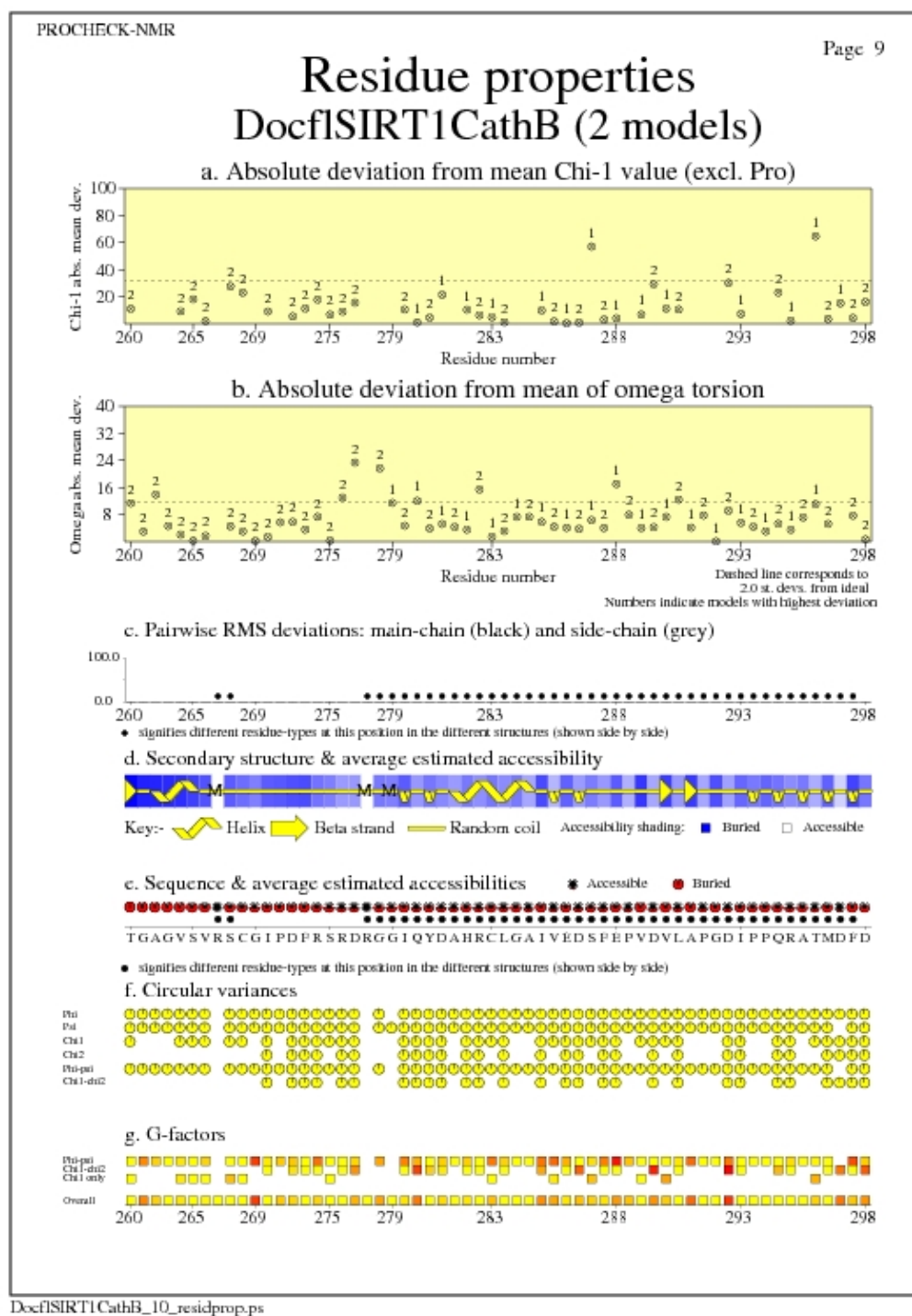
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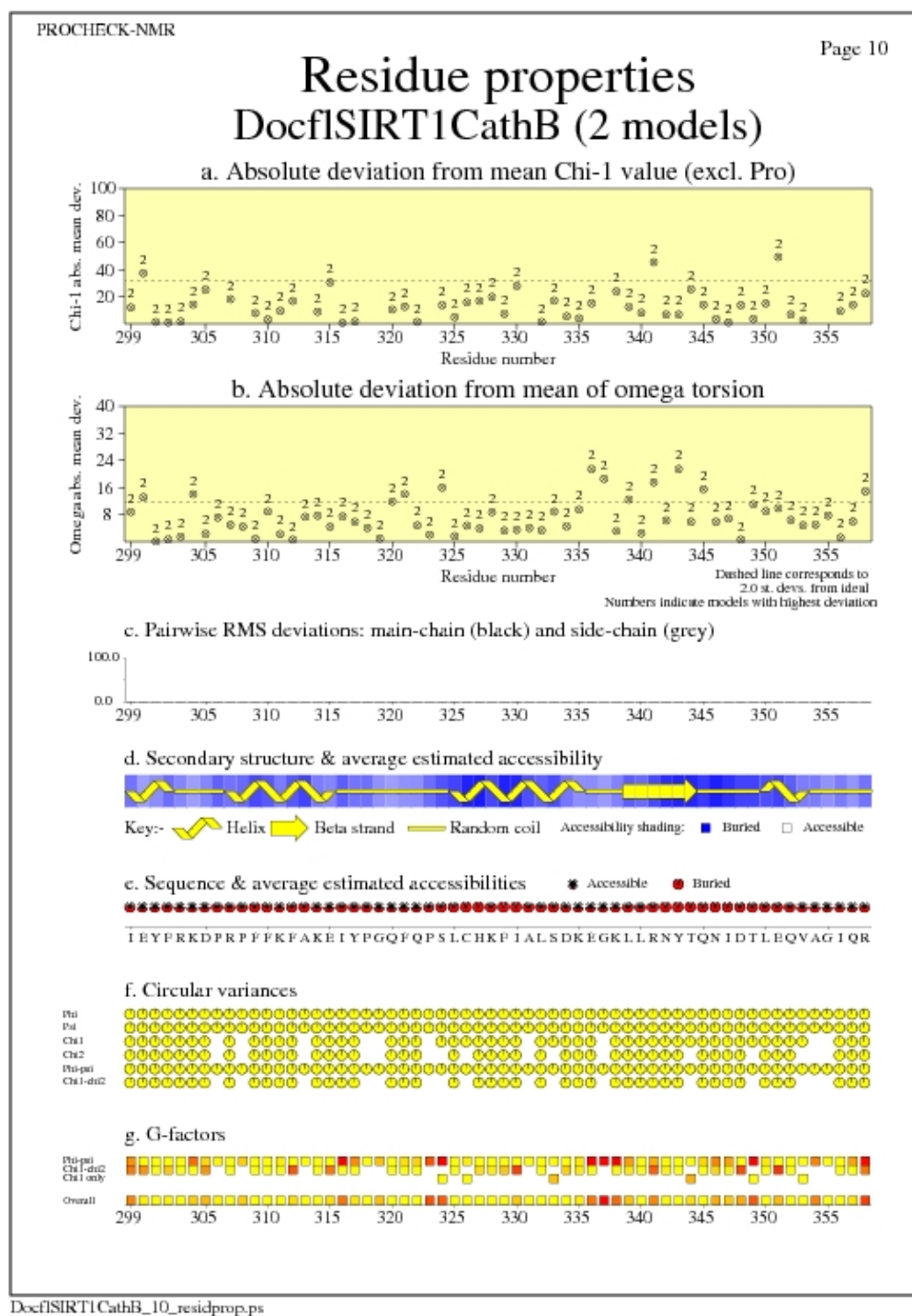
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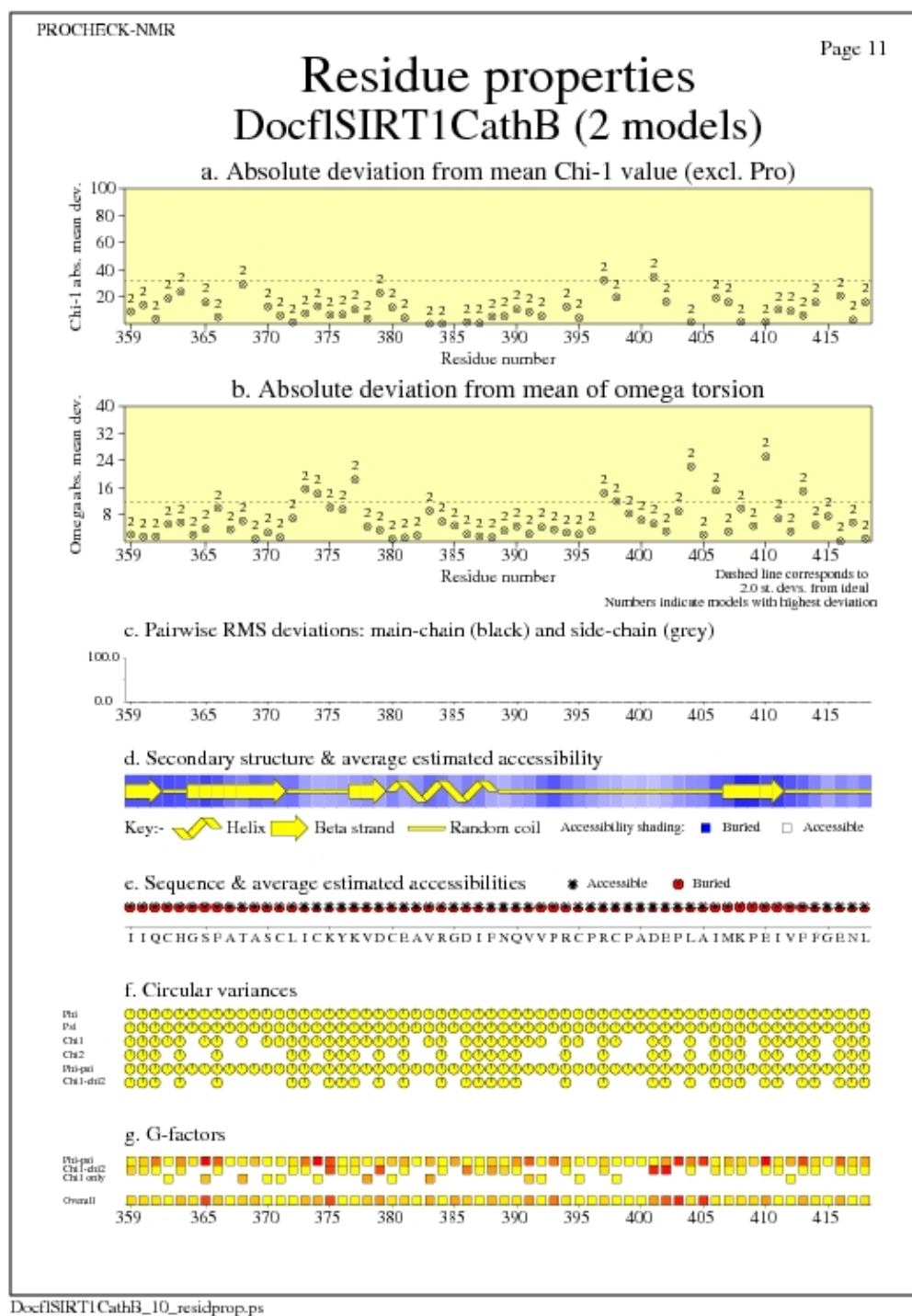
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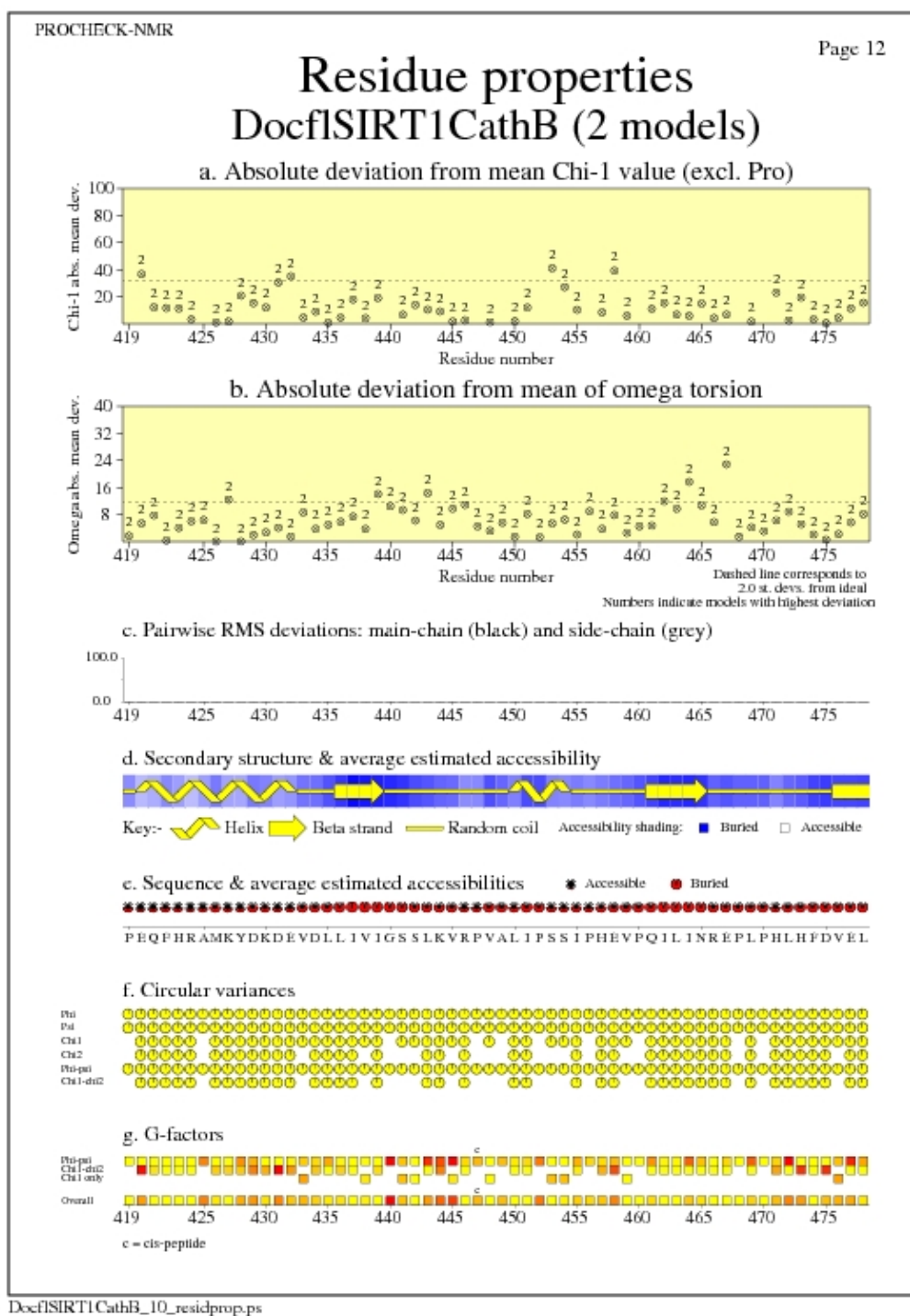
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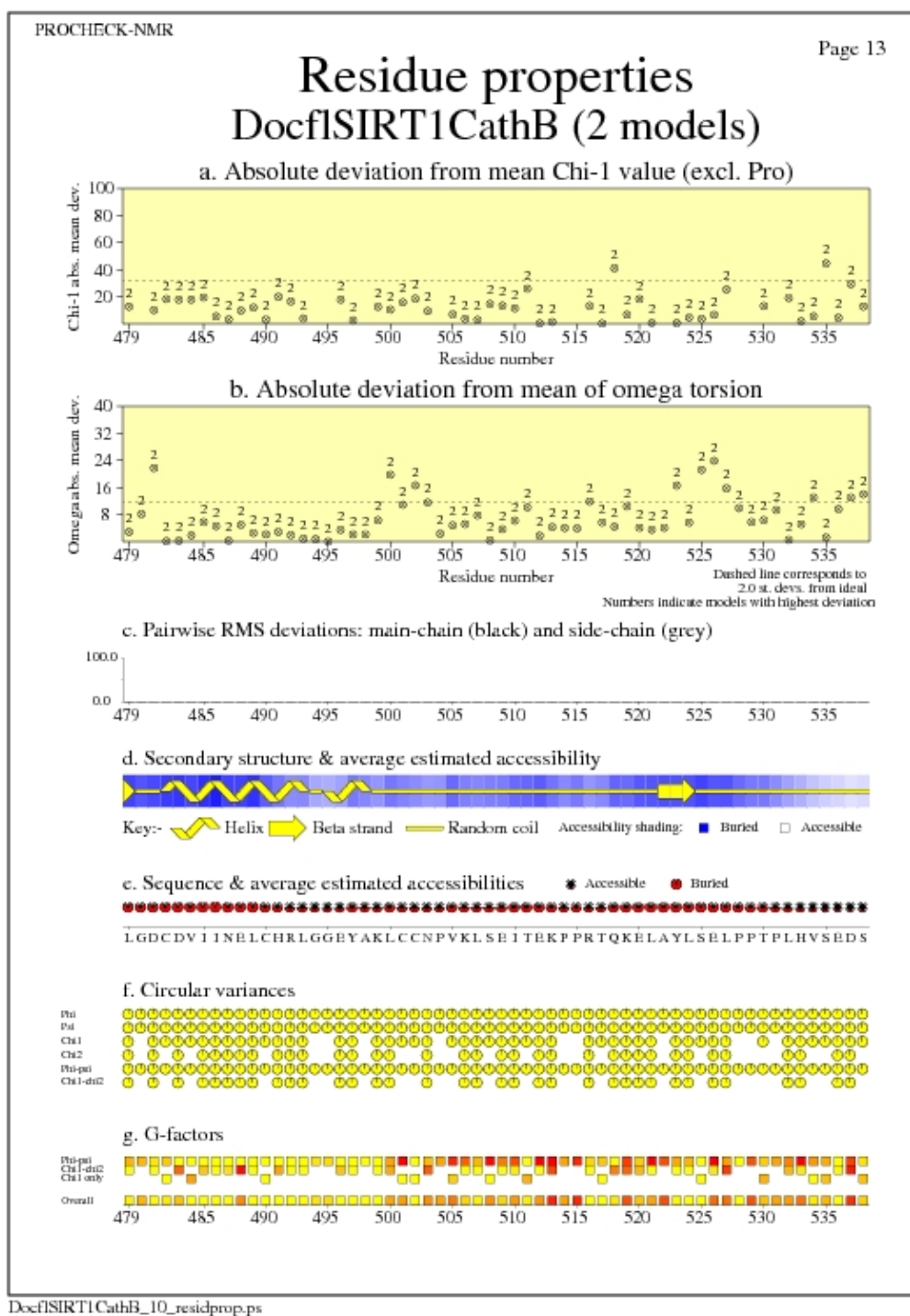
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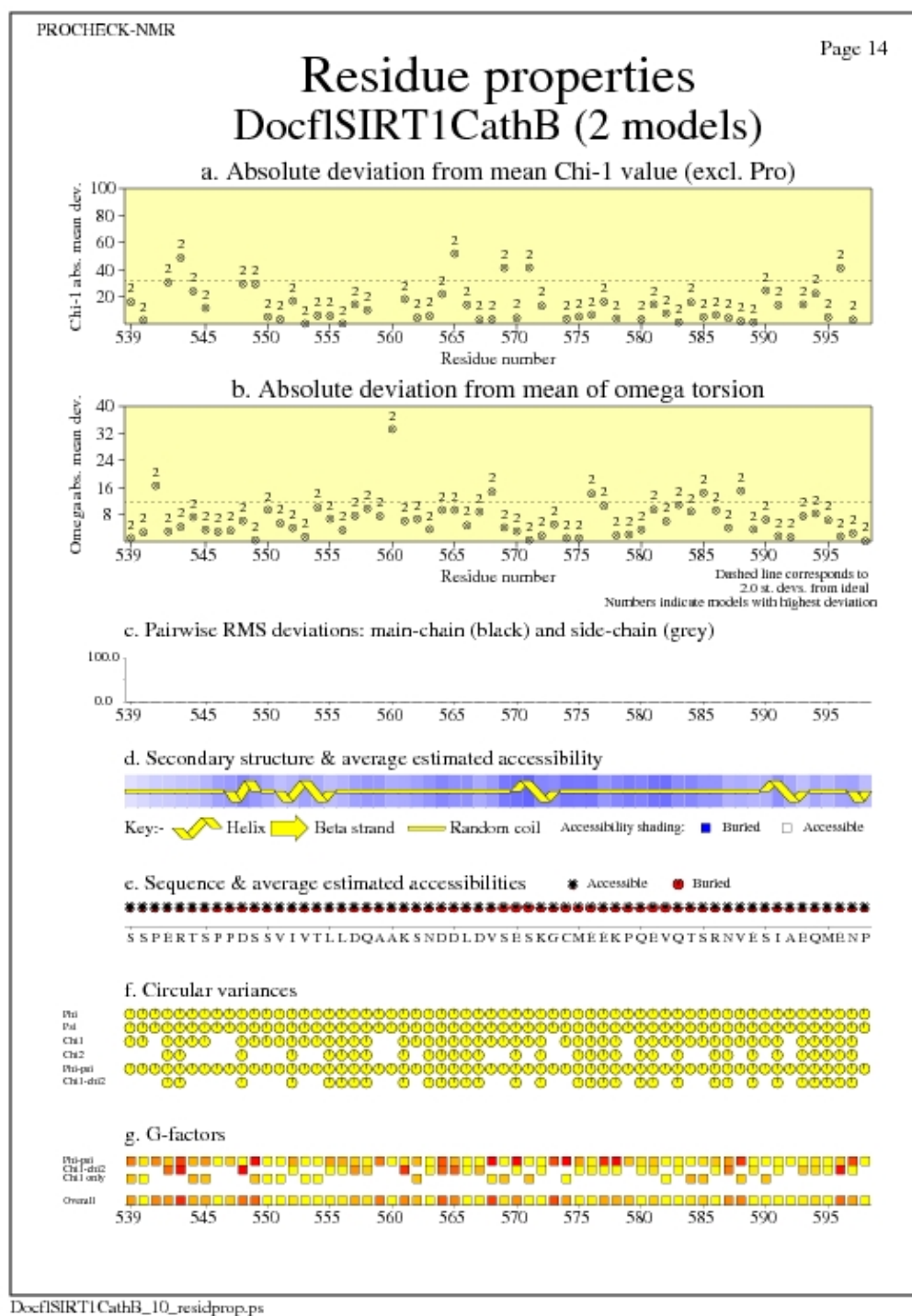
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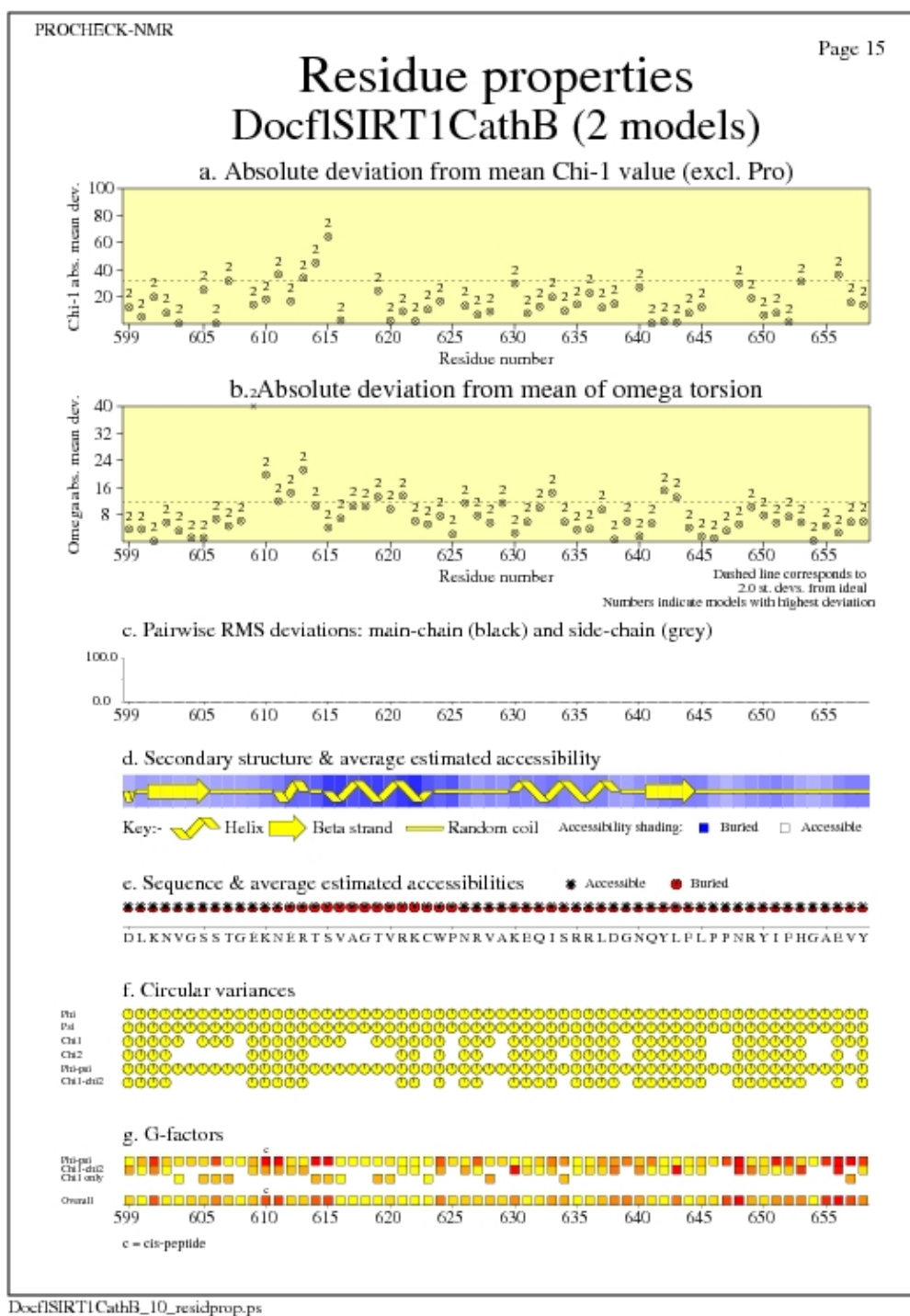
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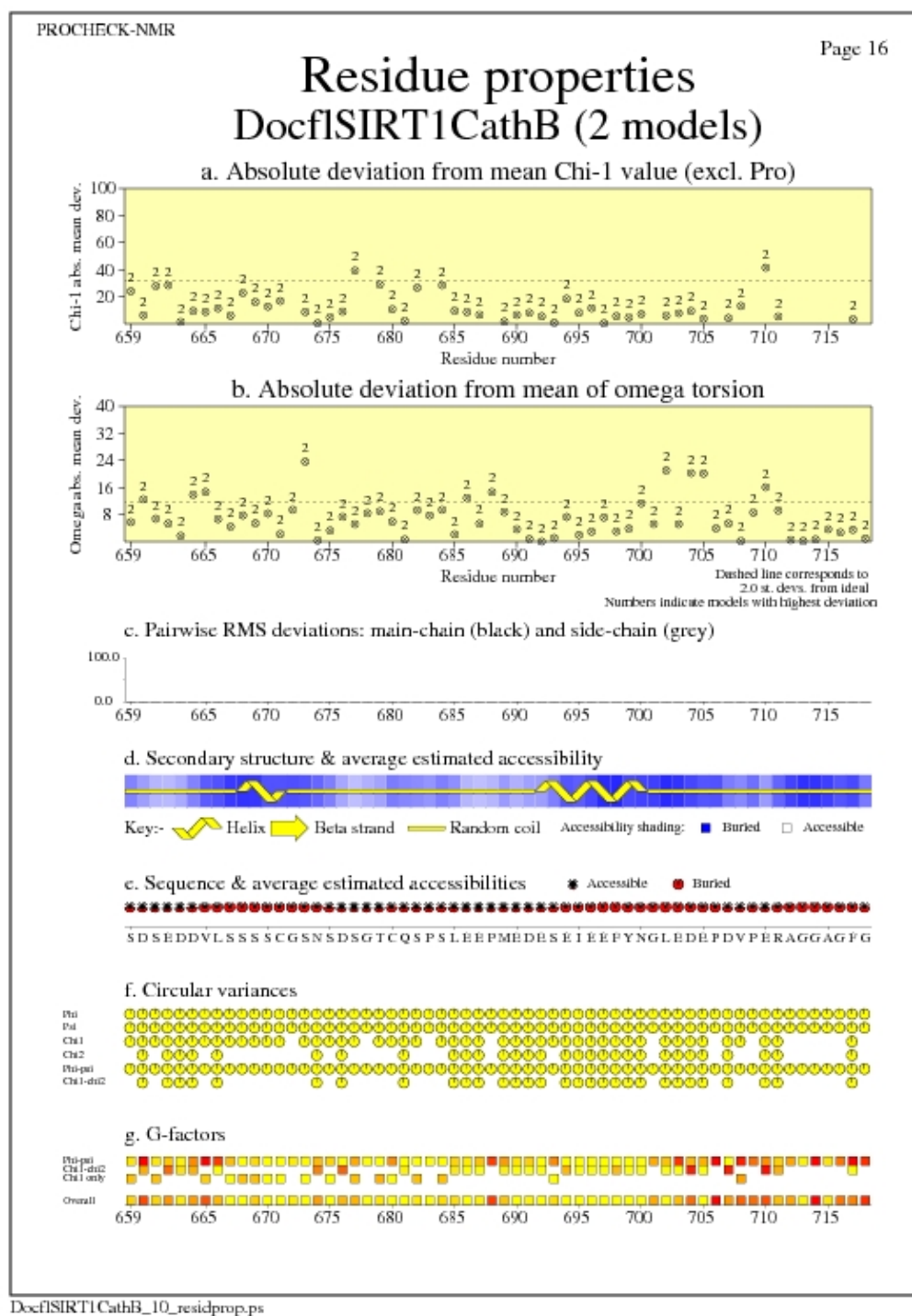
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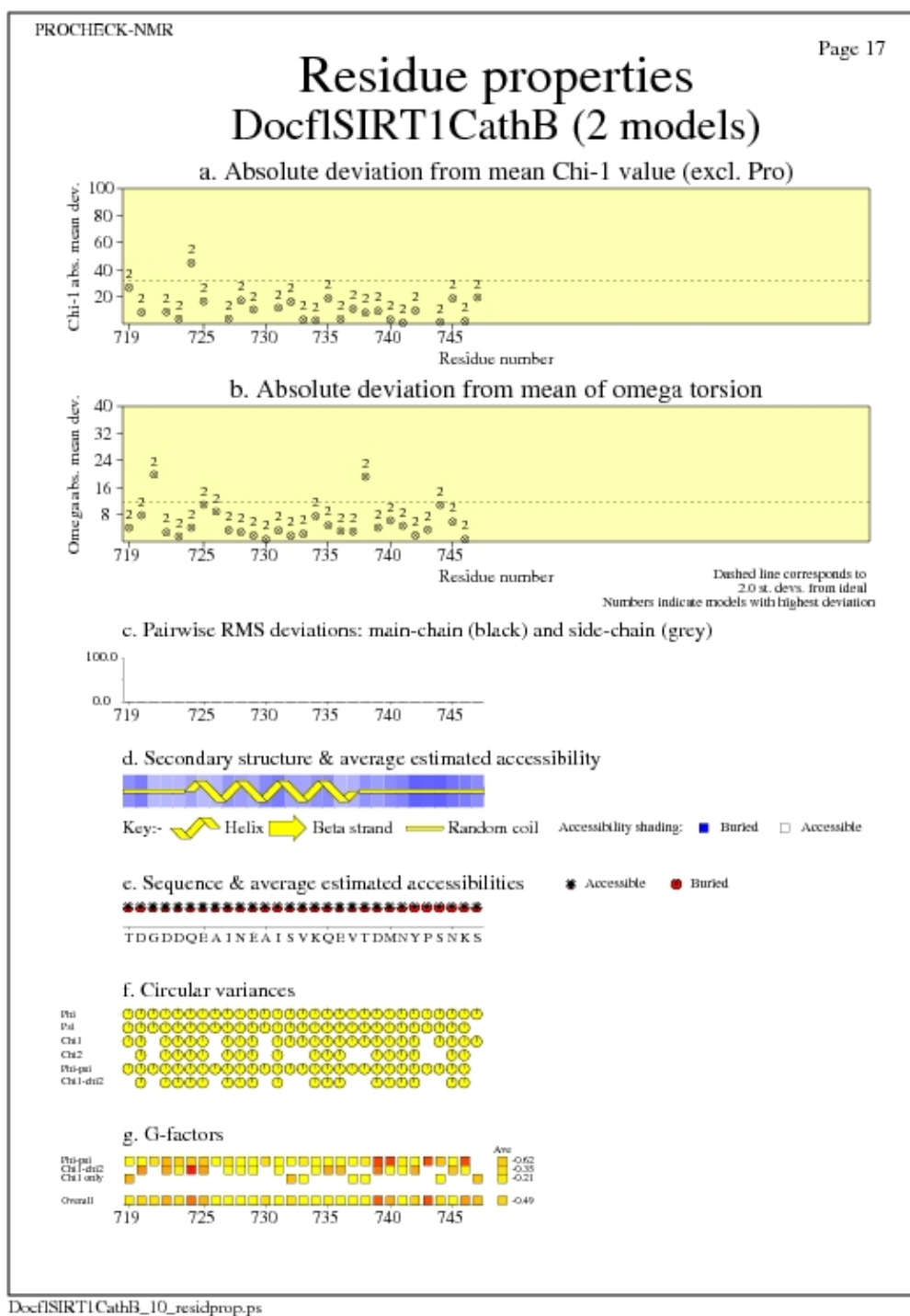
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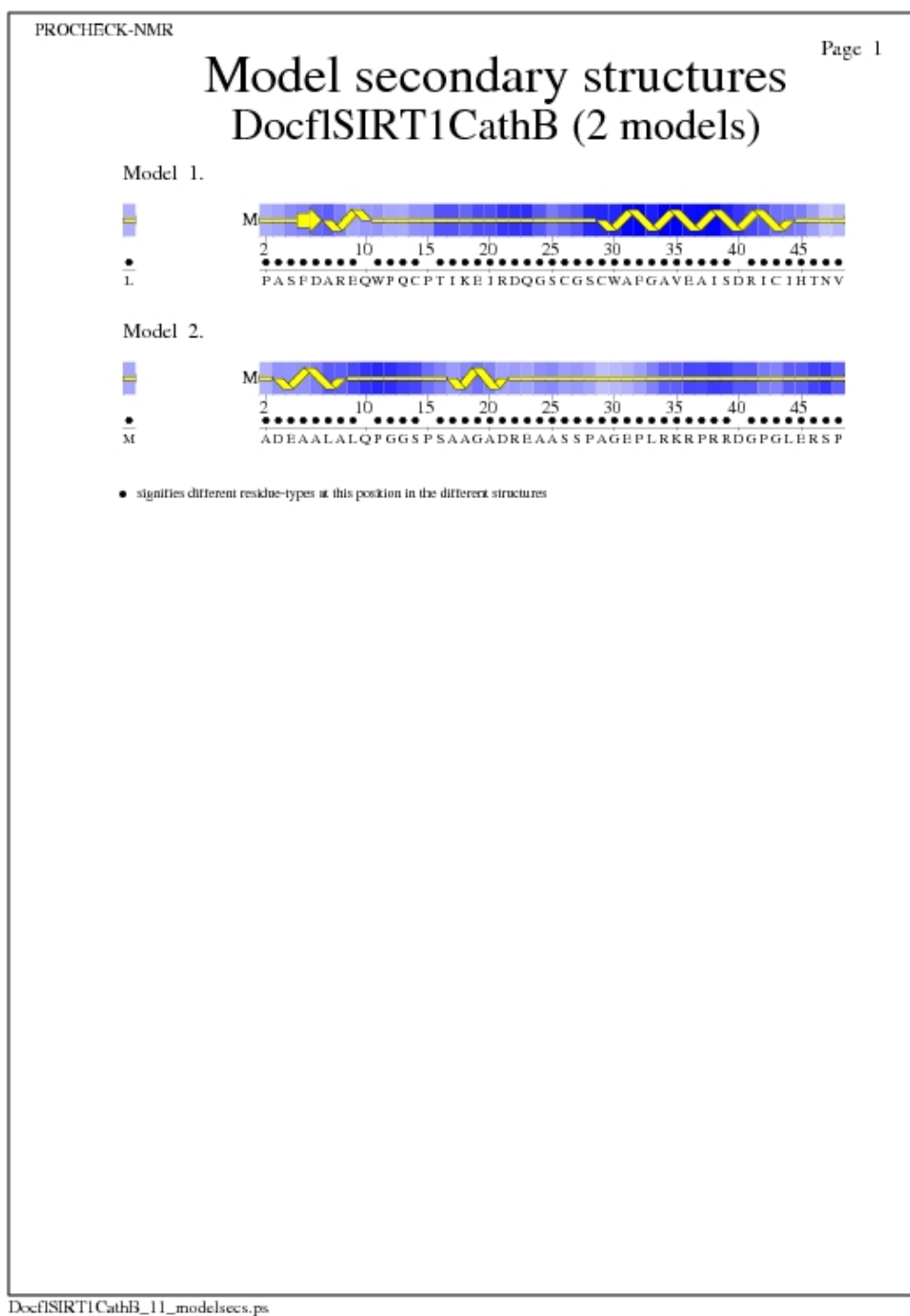


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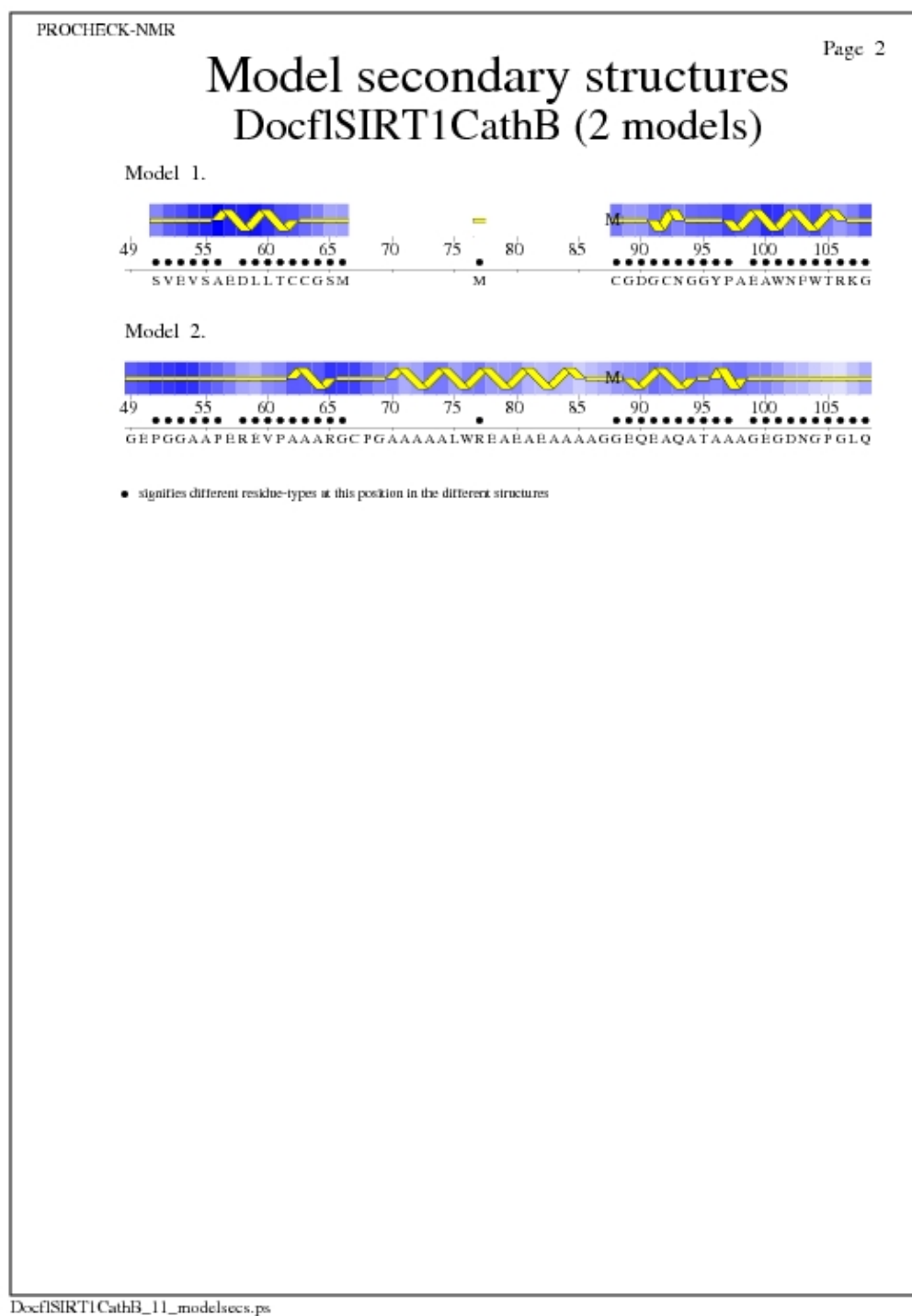


Model Secondary Structures from Proccheck

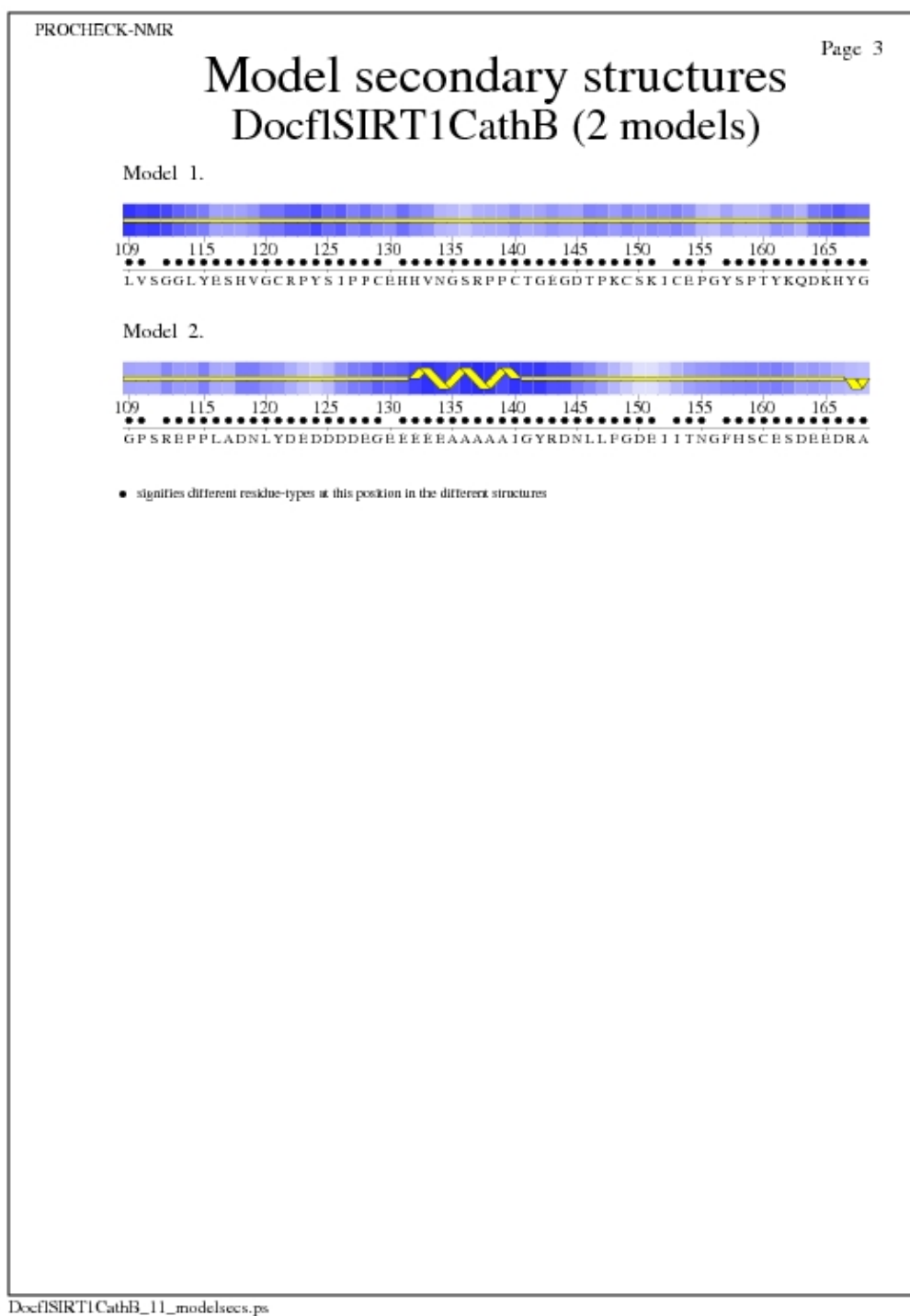
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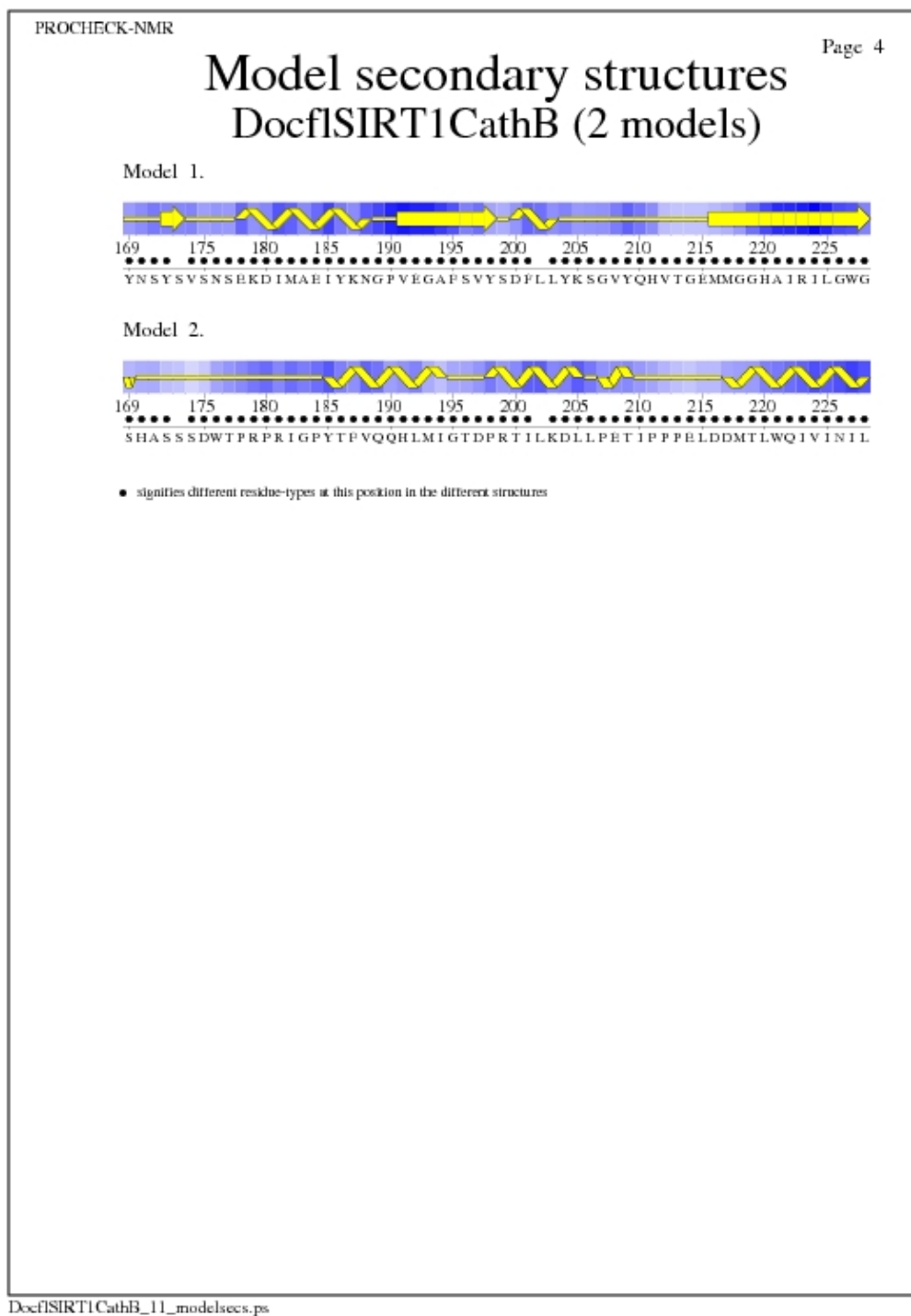
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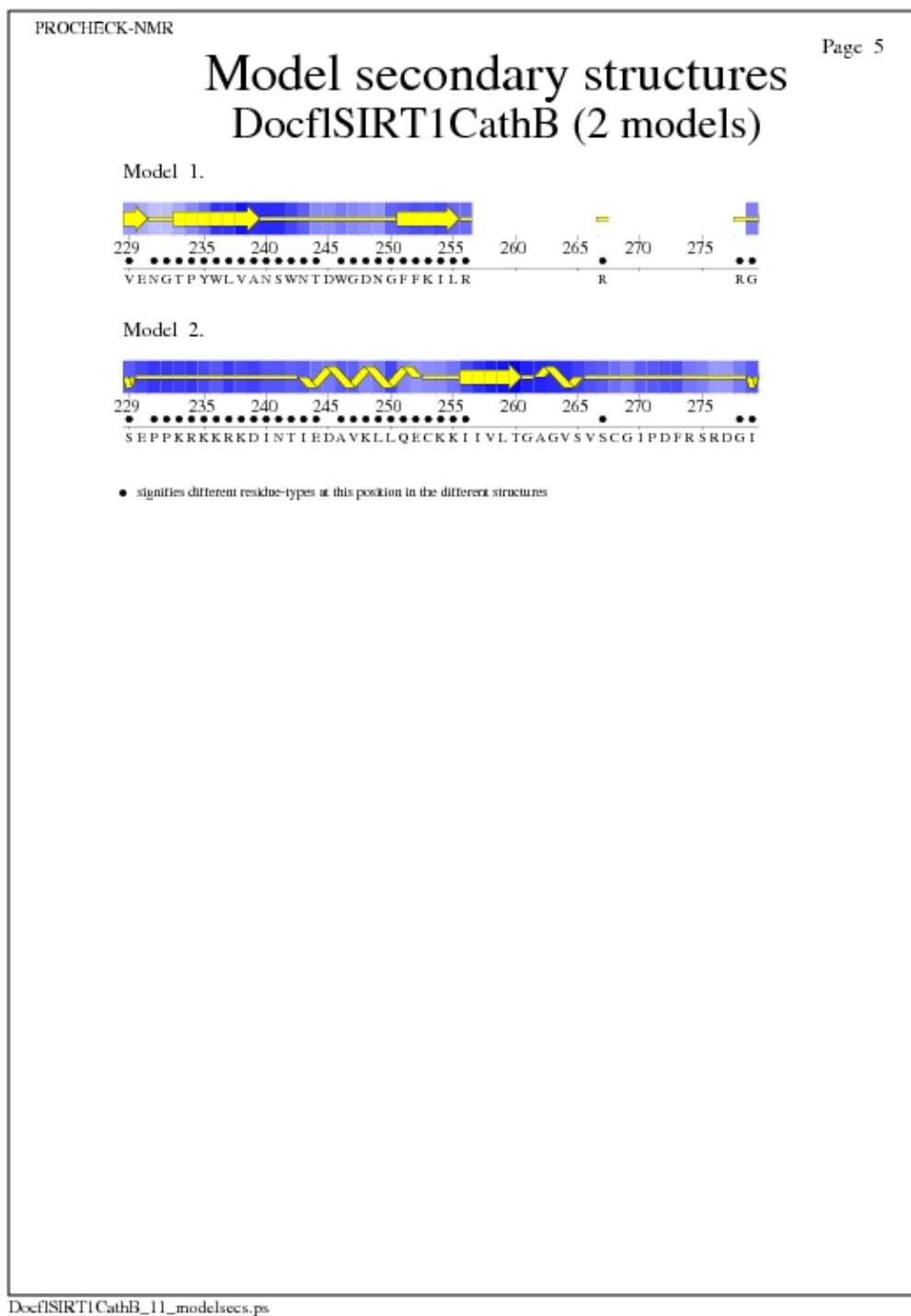
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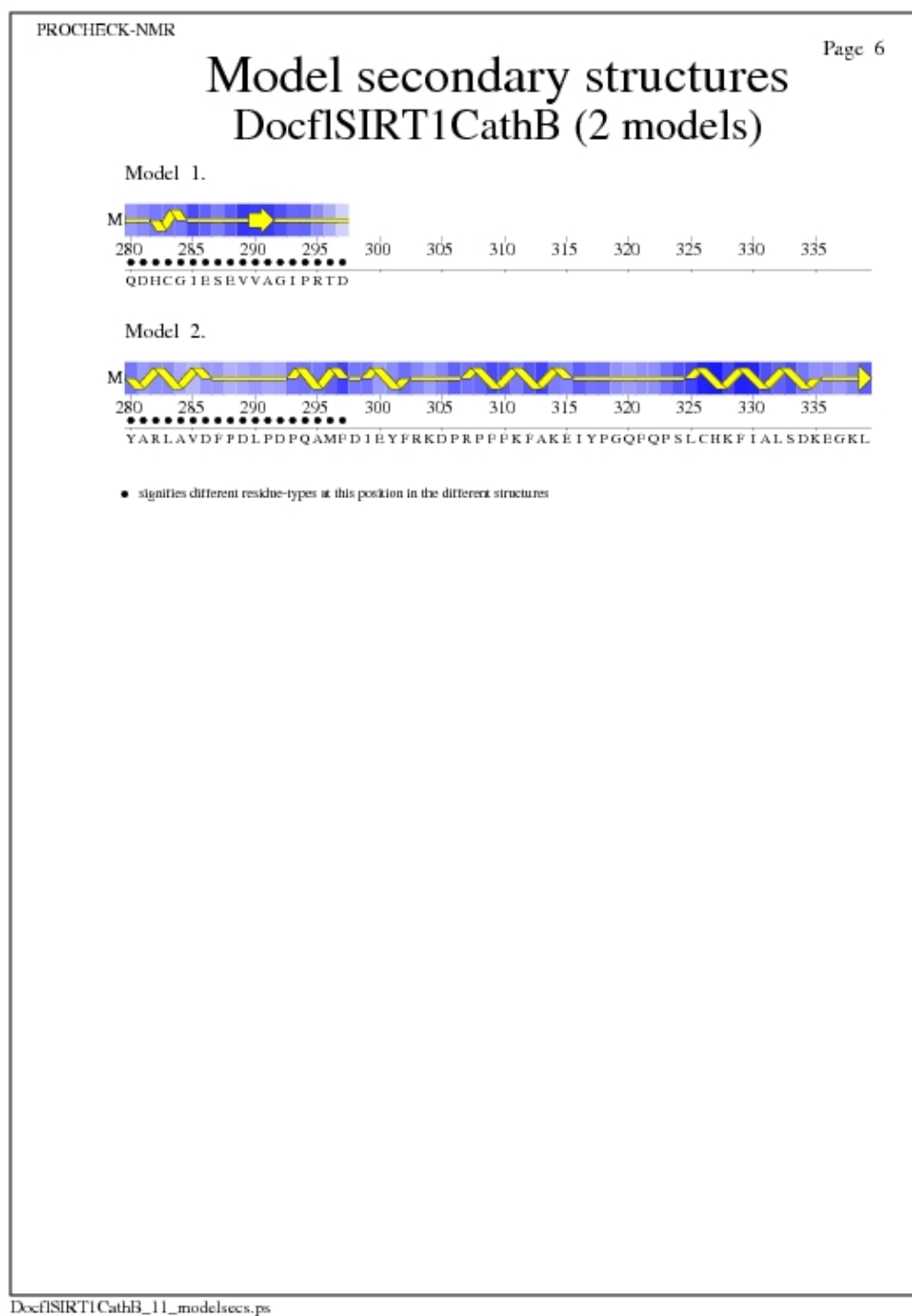
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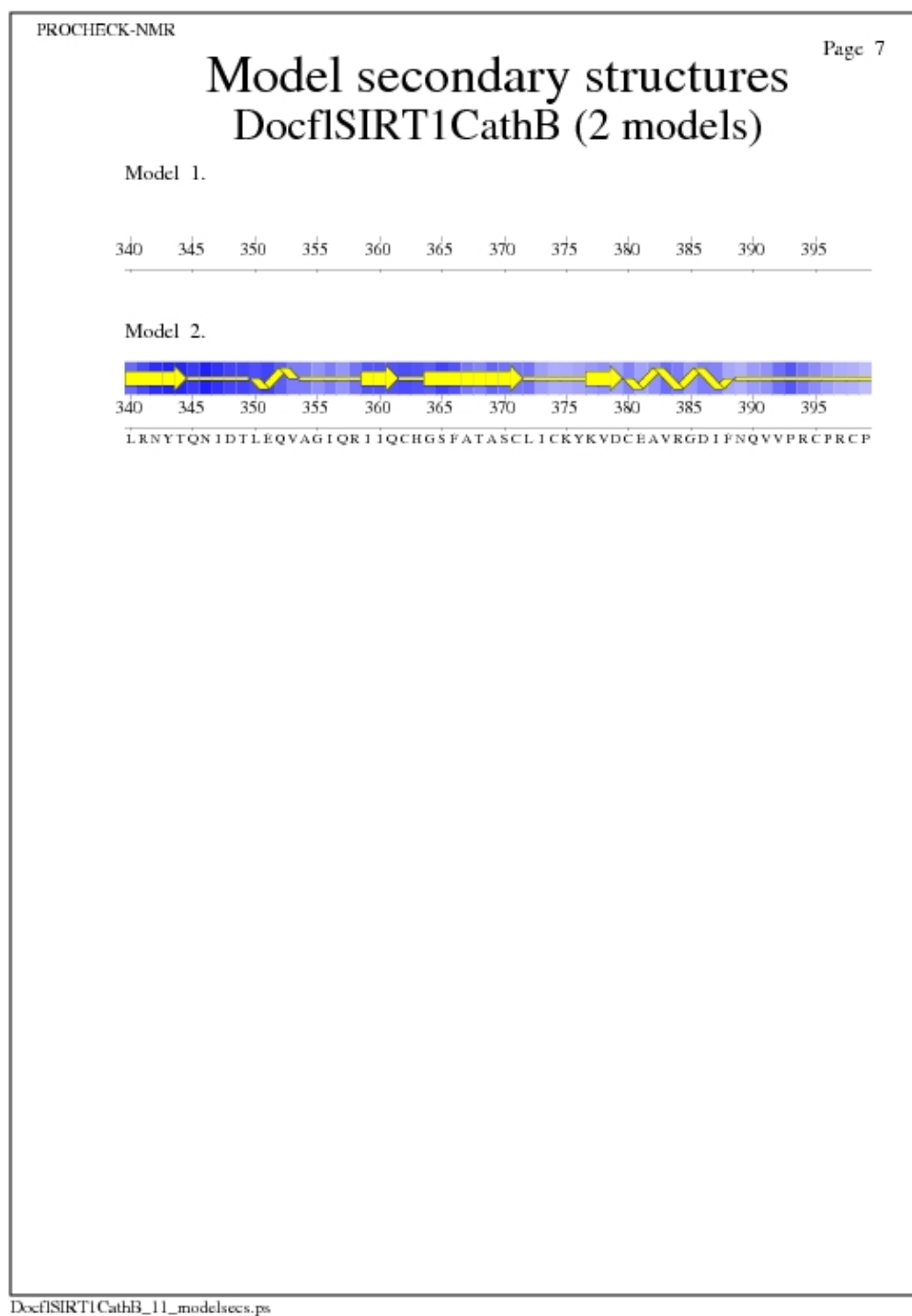
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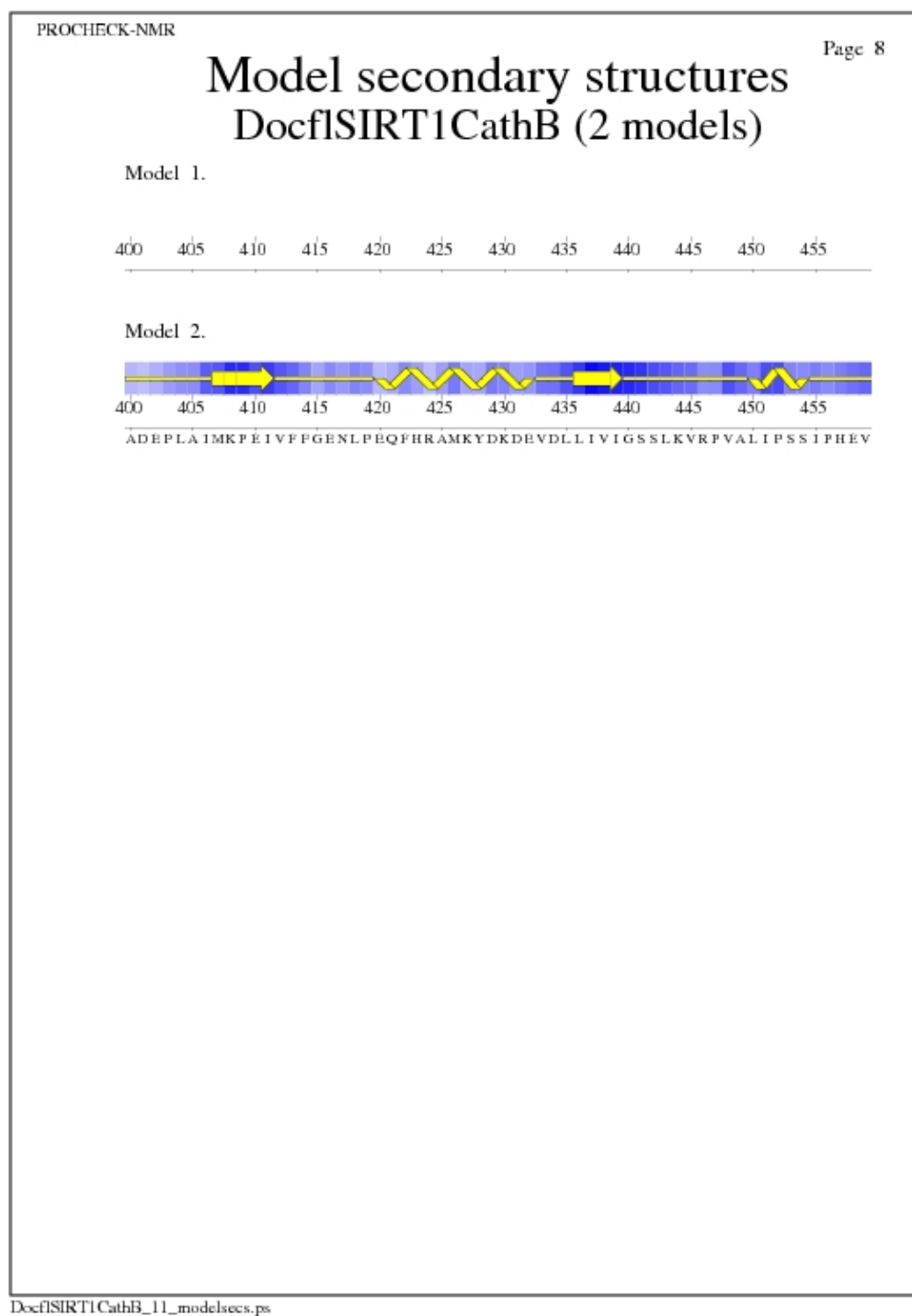
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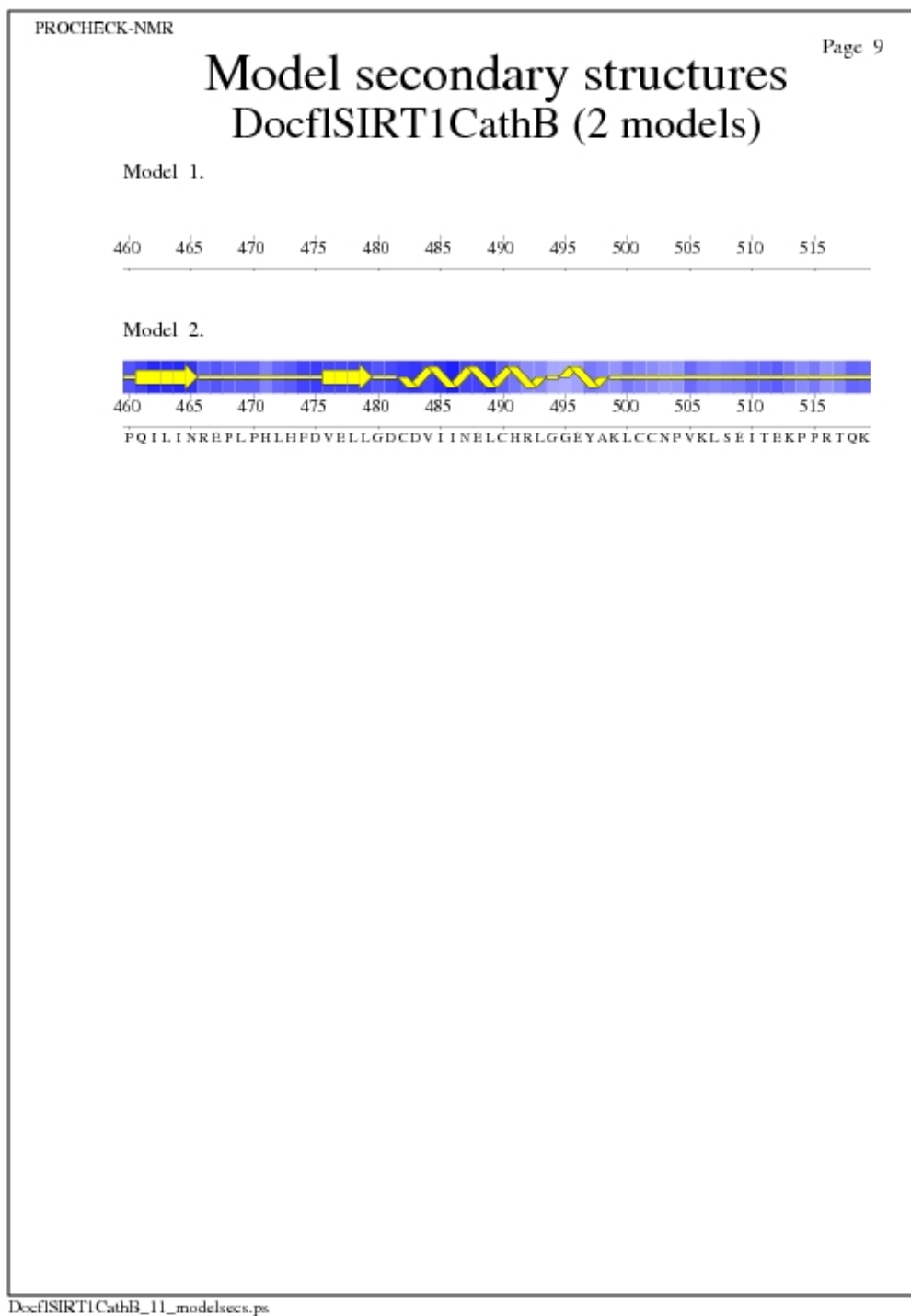
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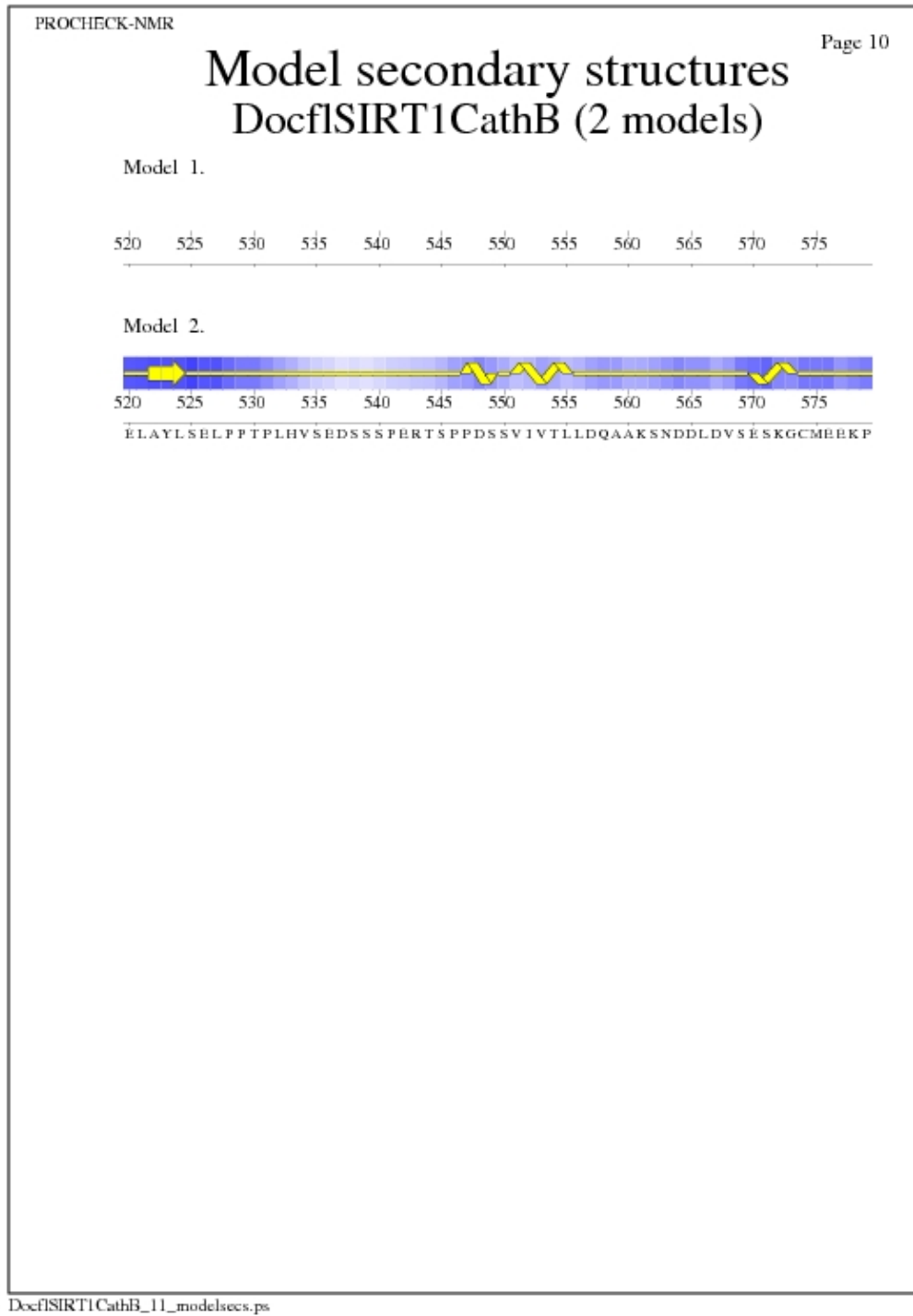
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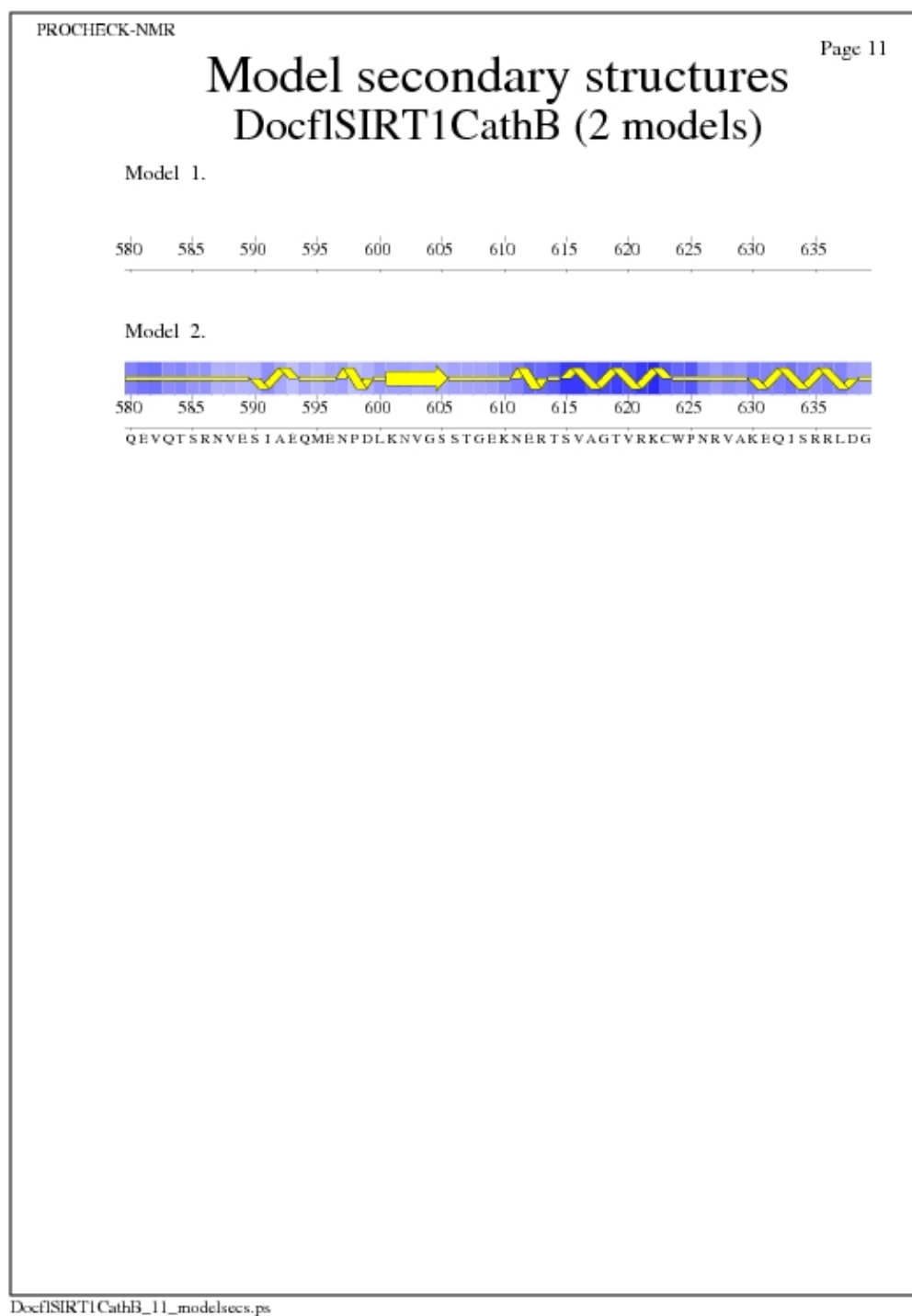
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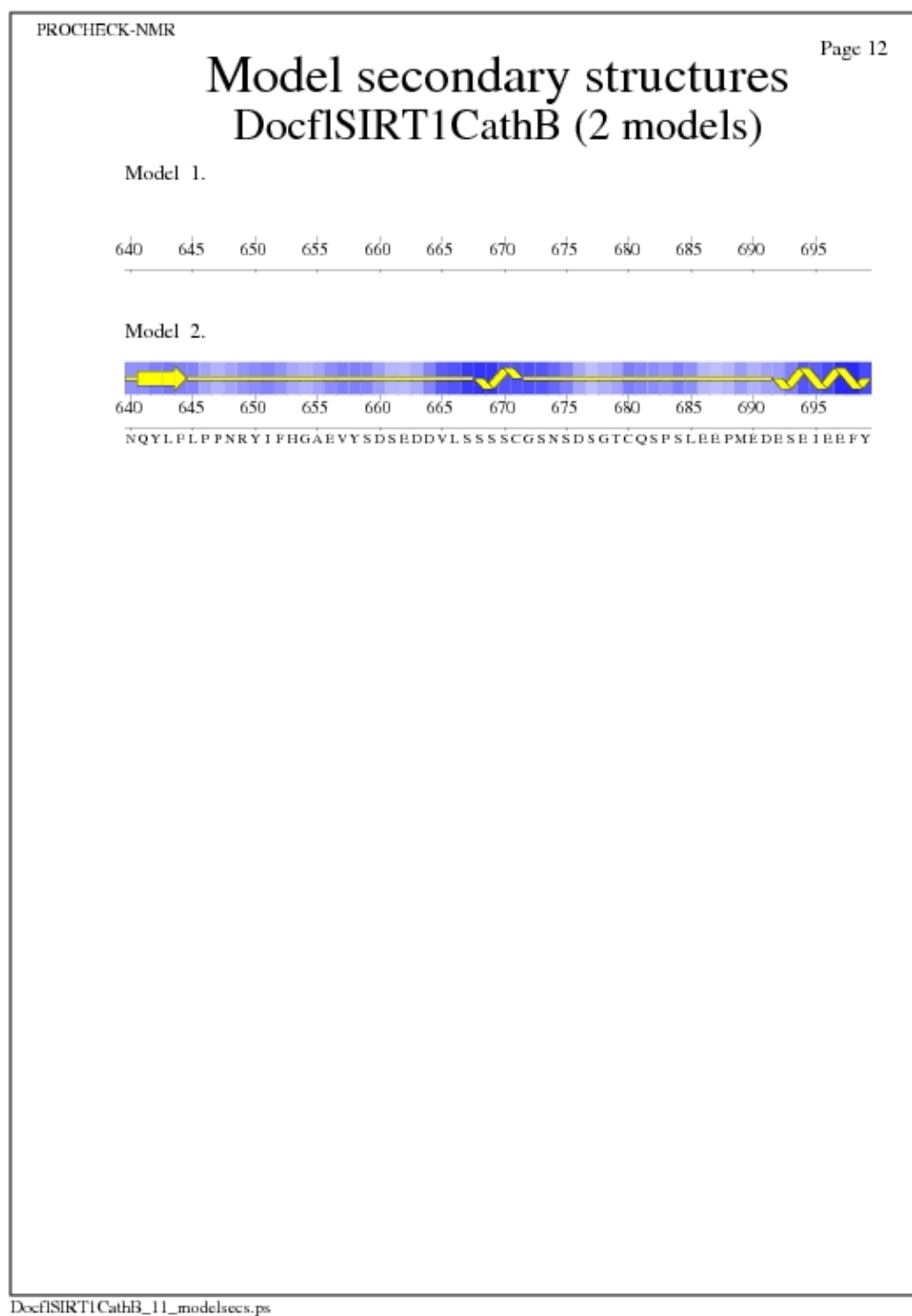
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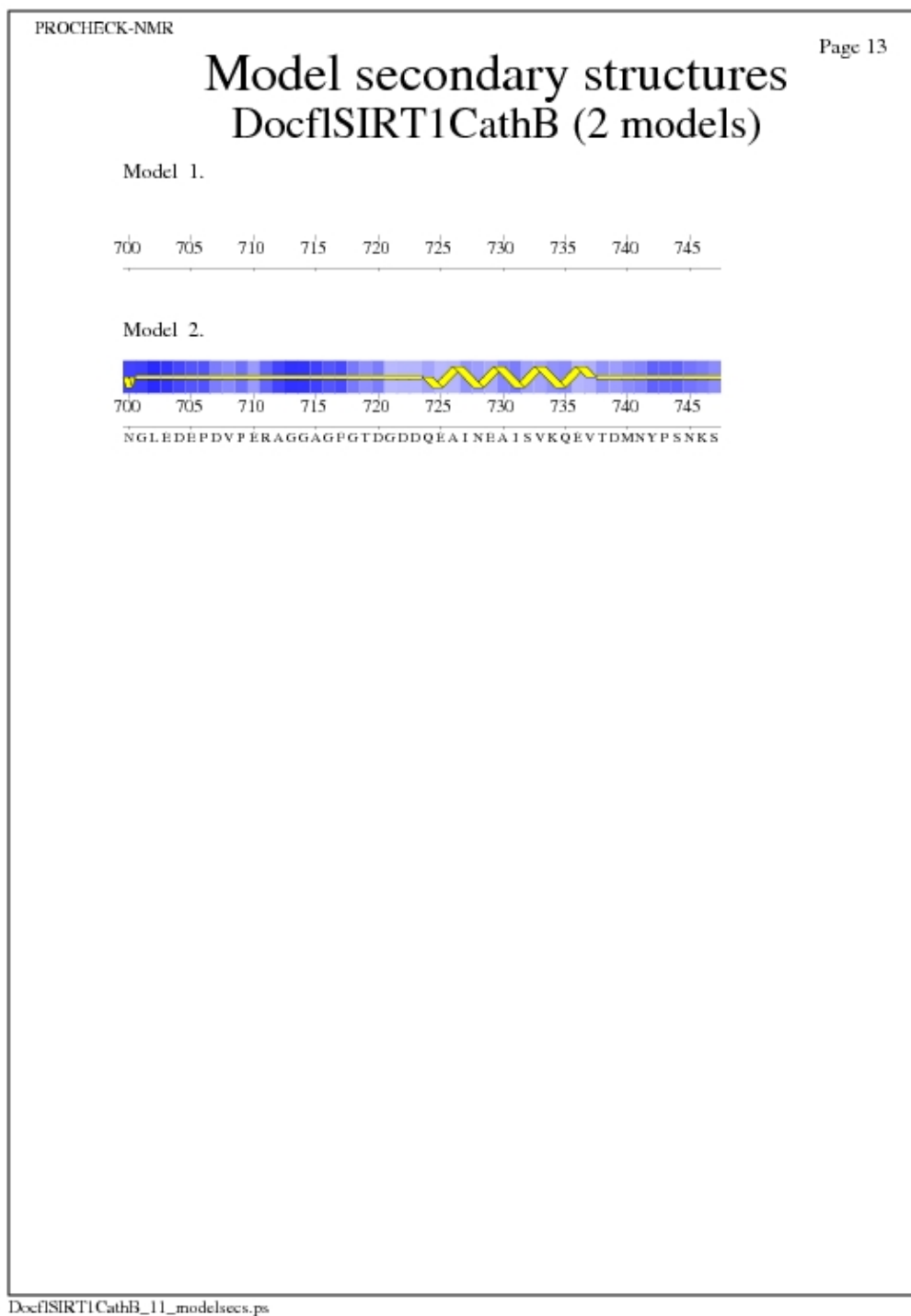
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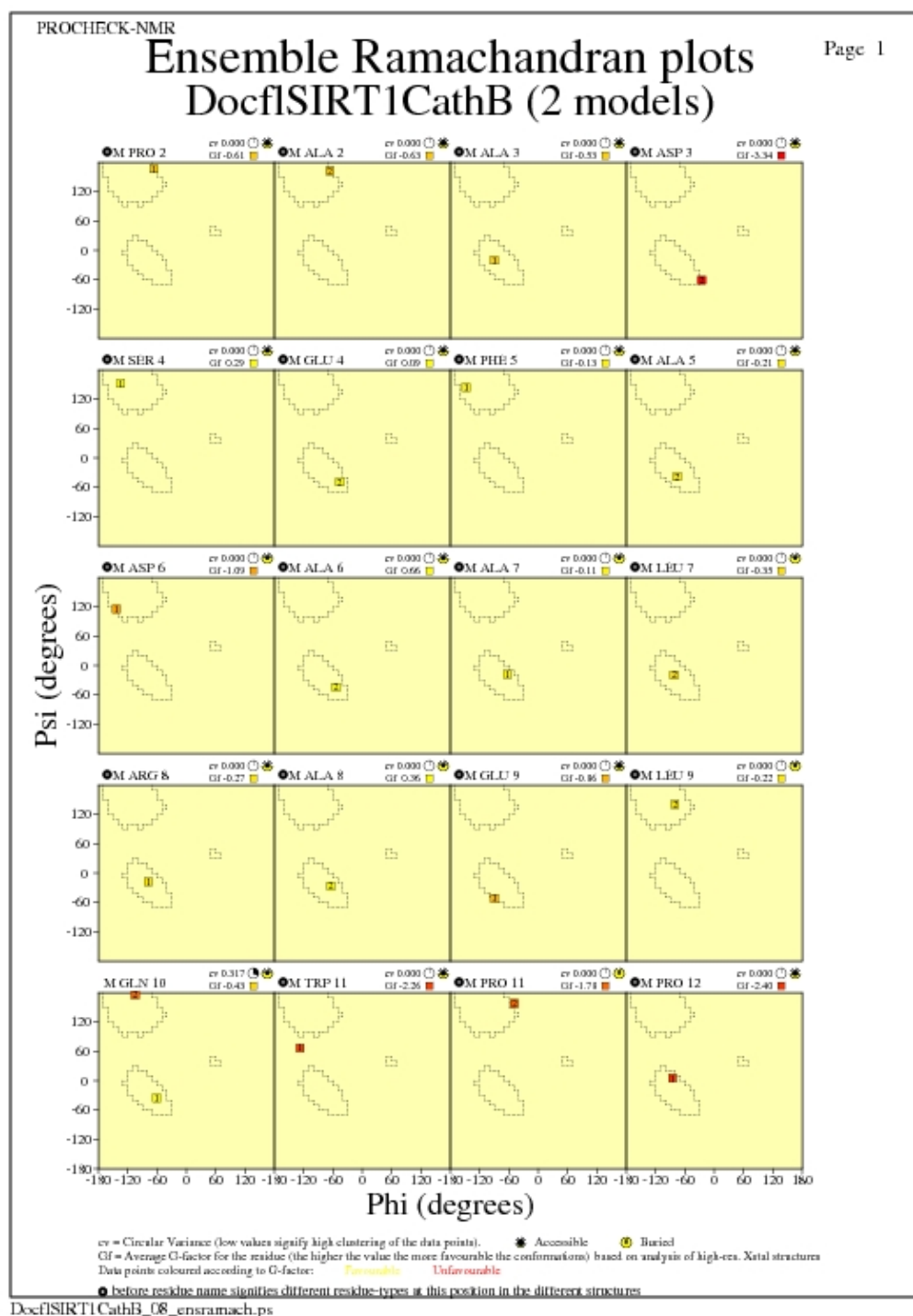


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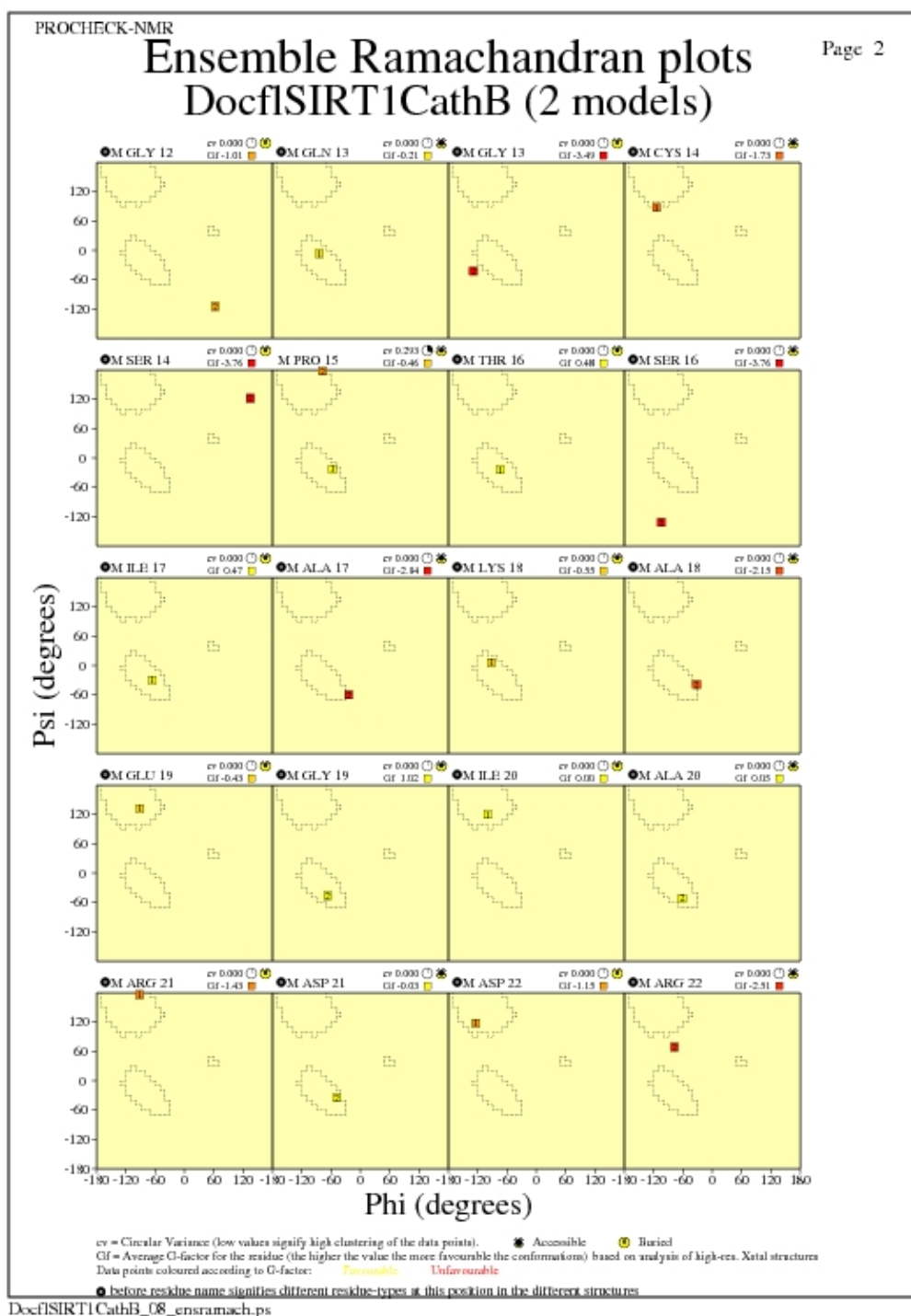


Ramachandran Plots for each residue

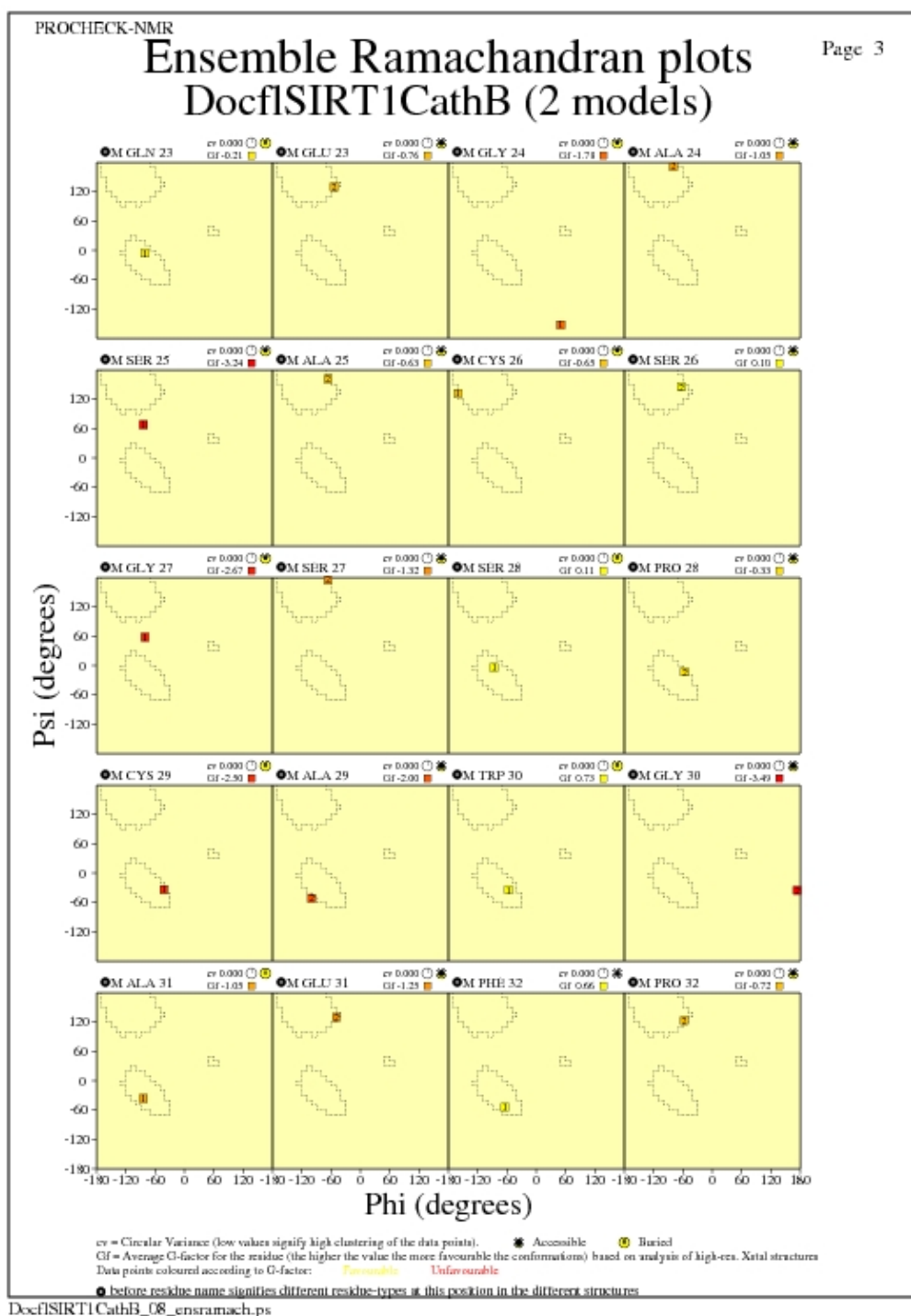
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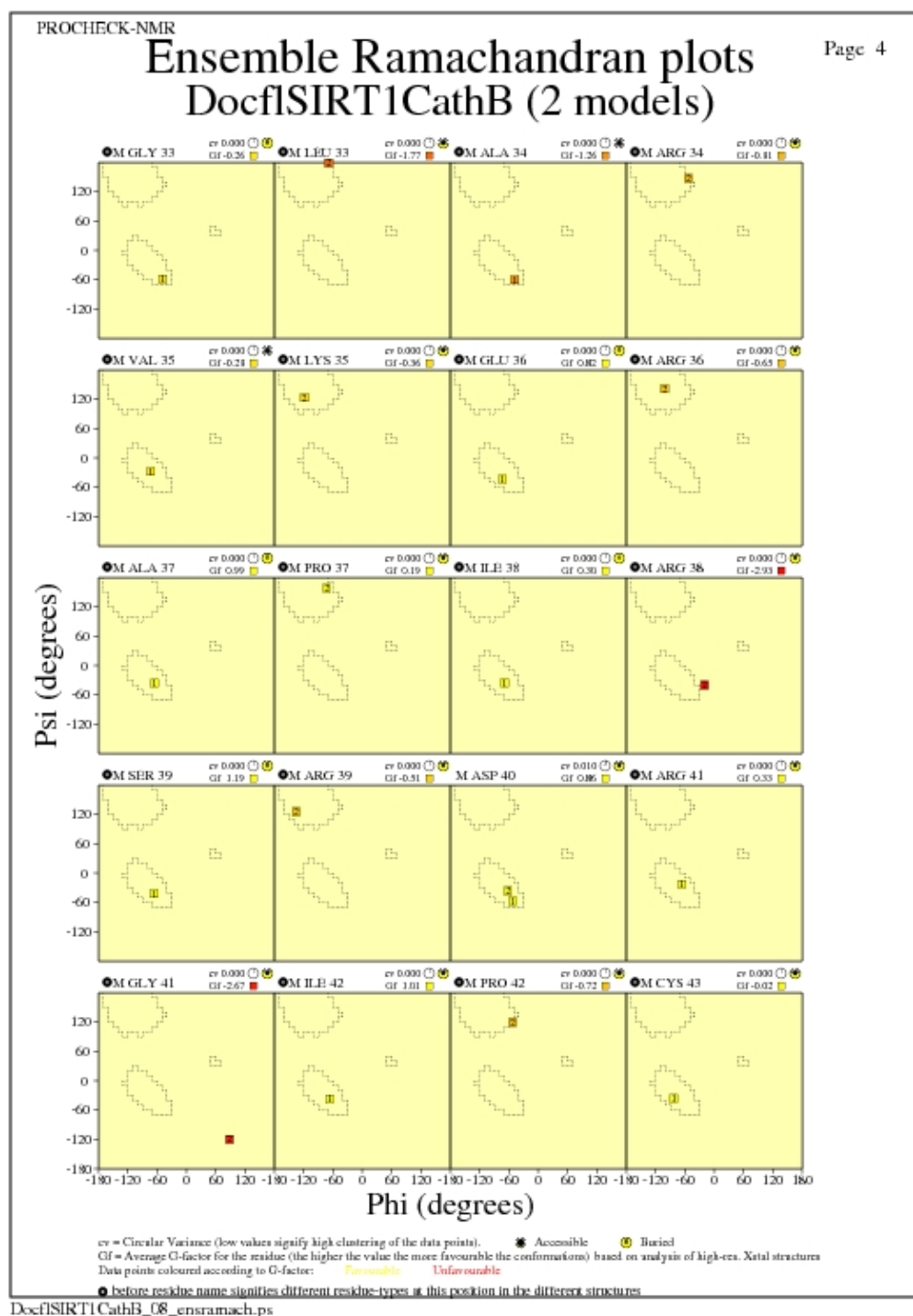
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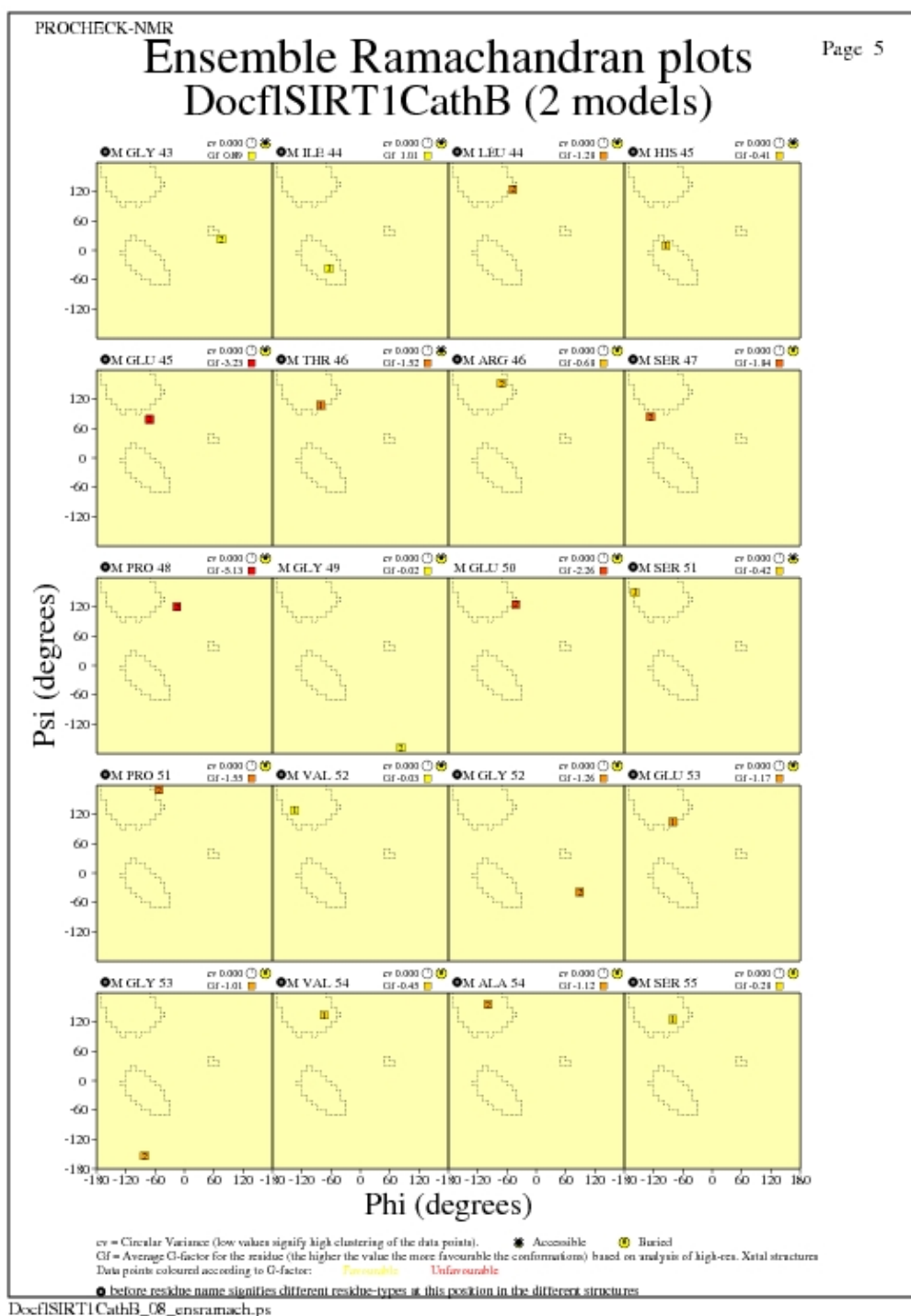
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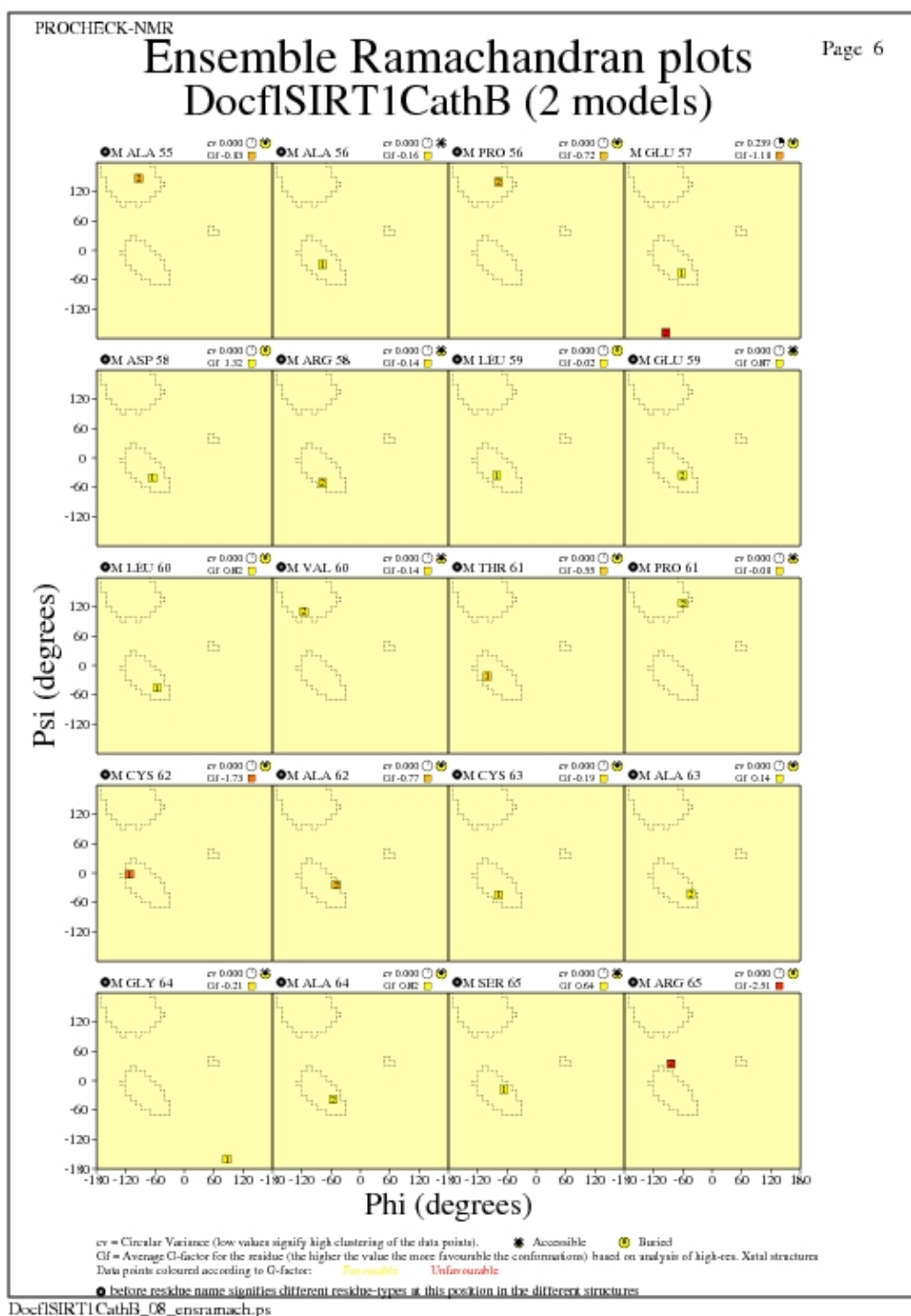
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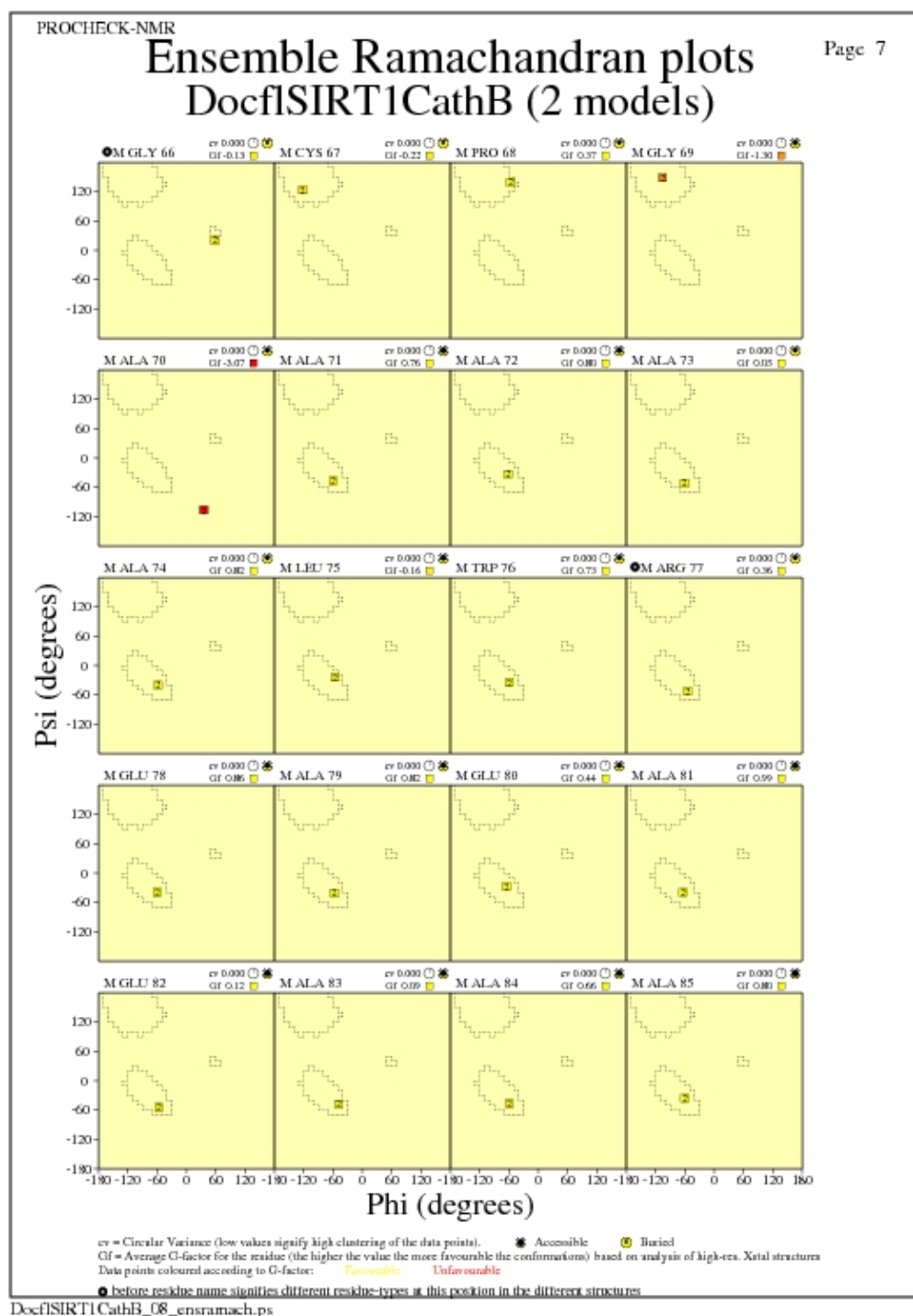
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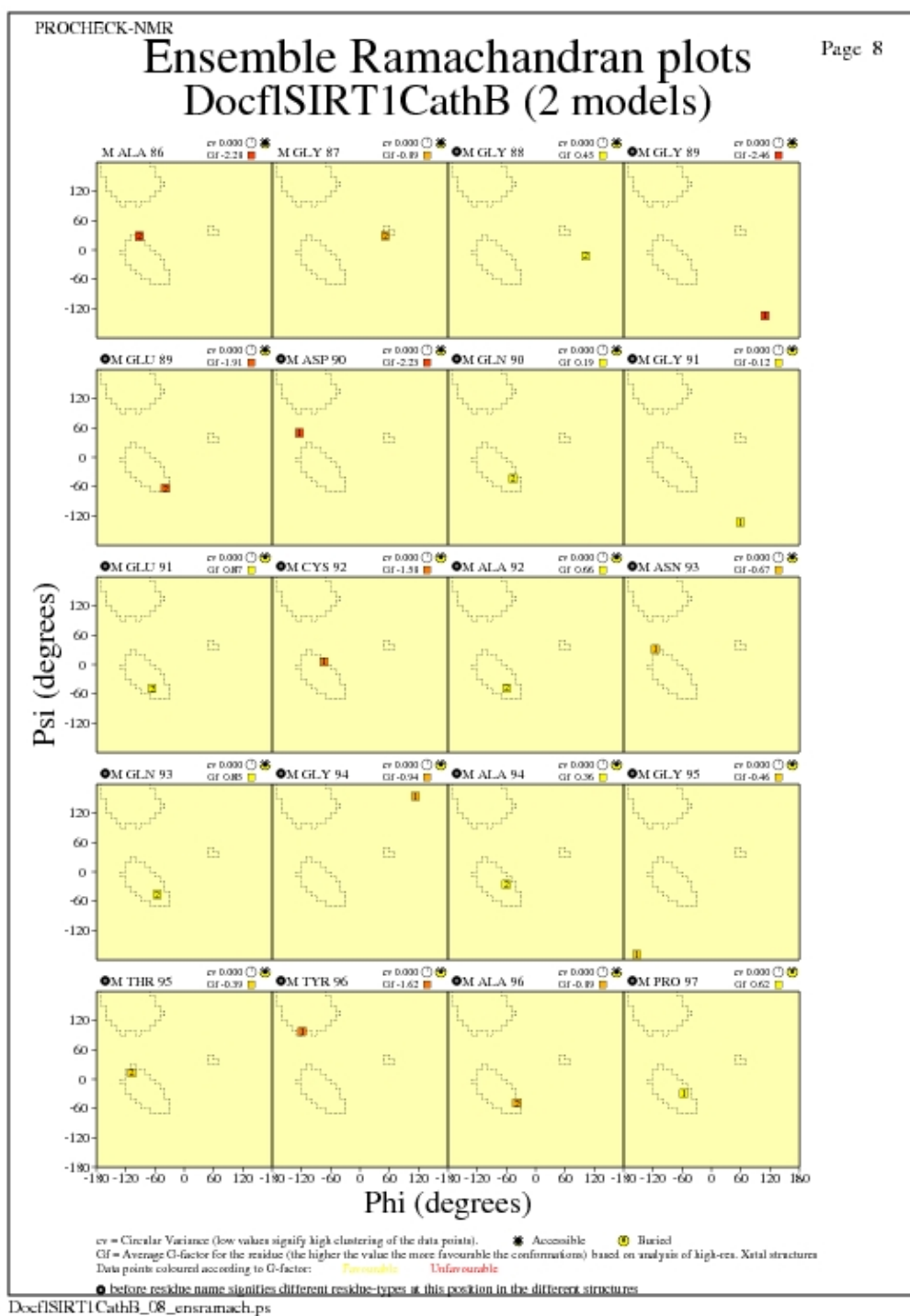
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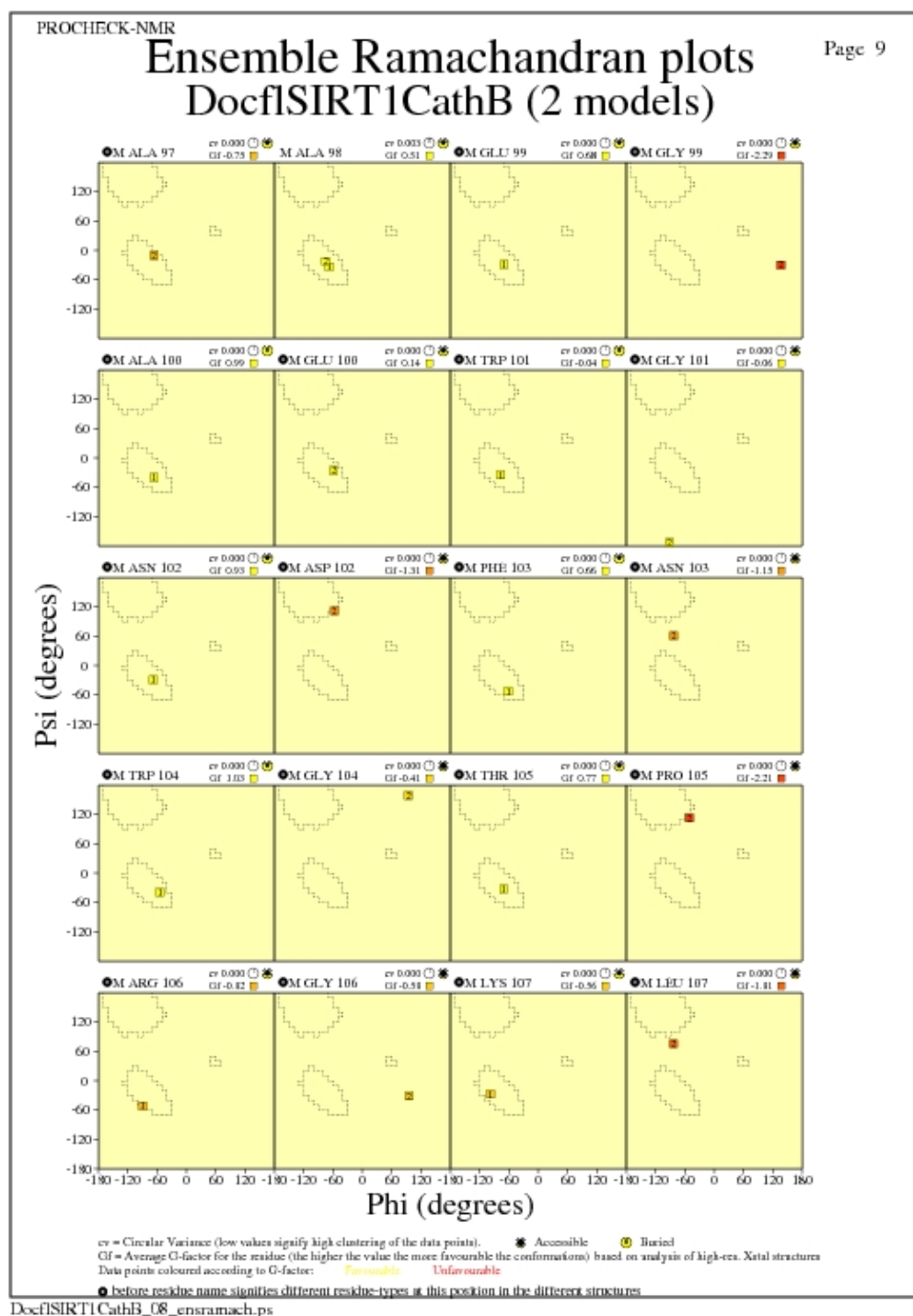
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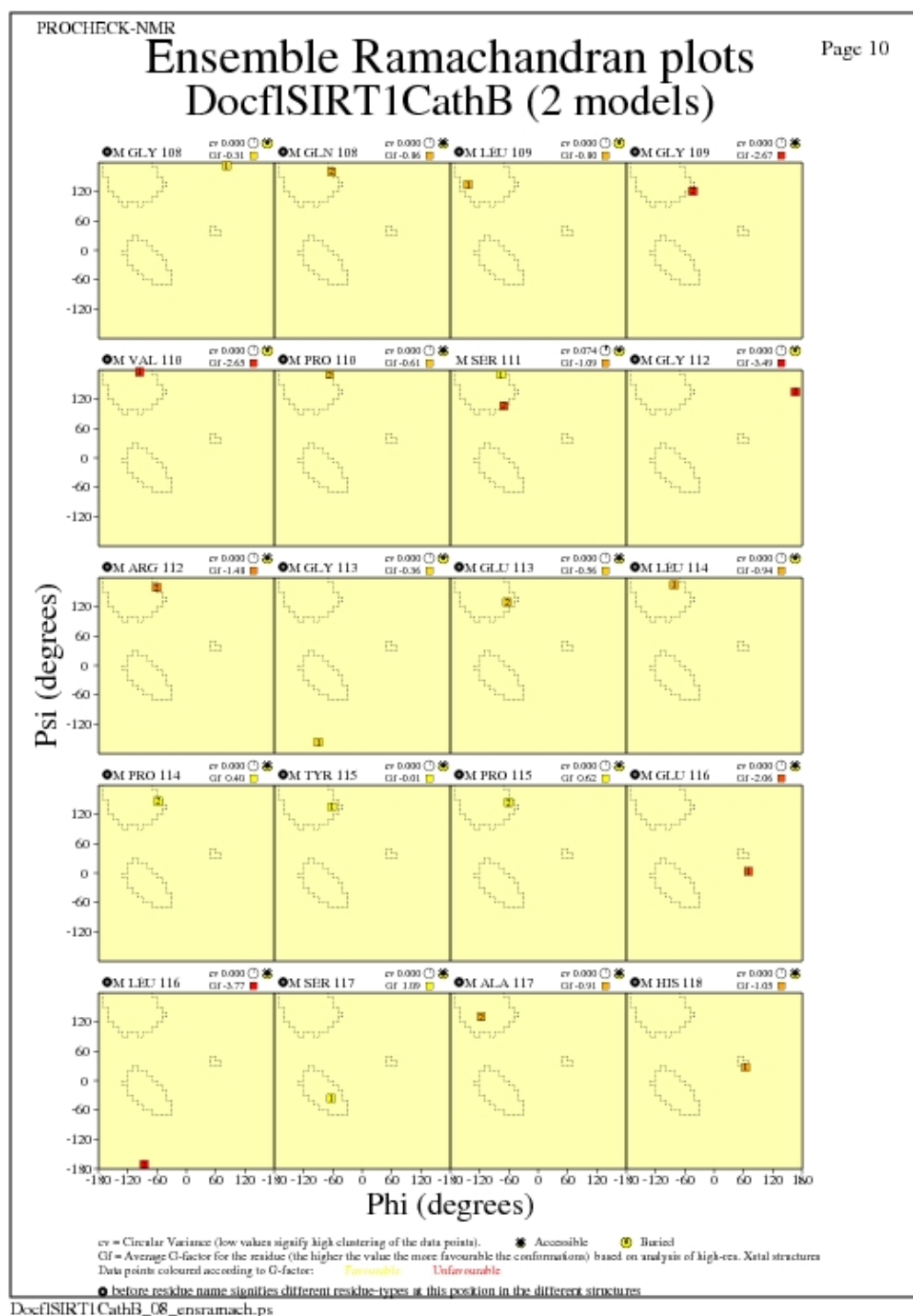
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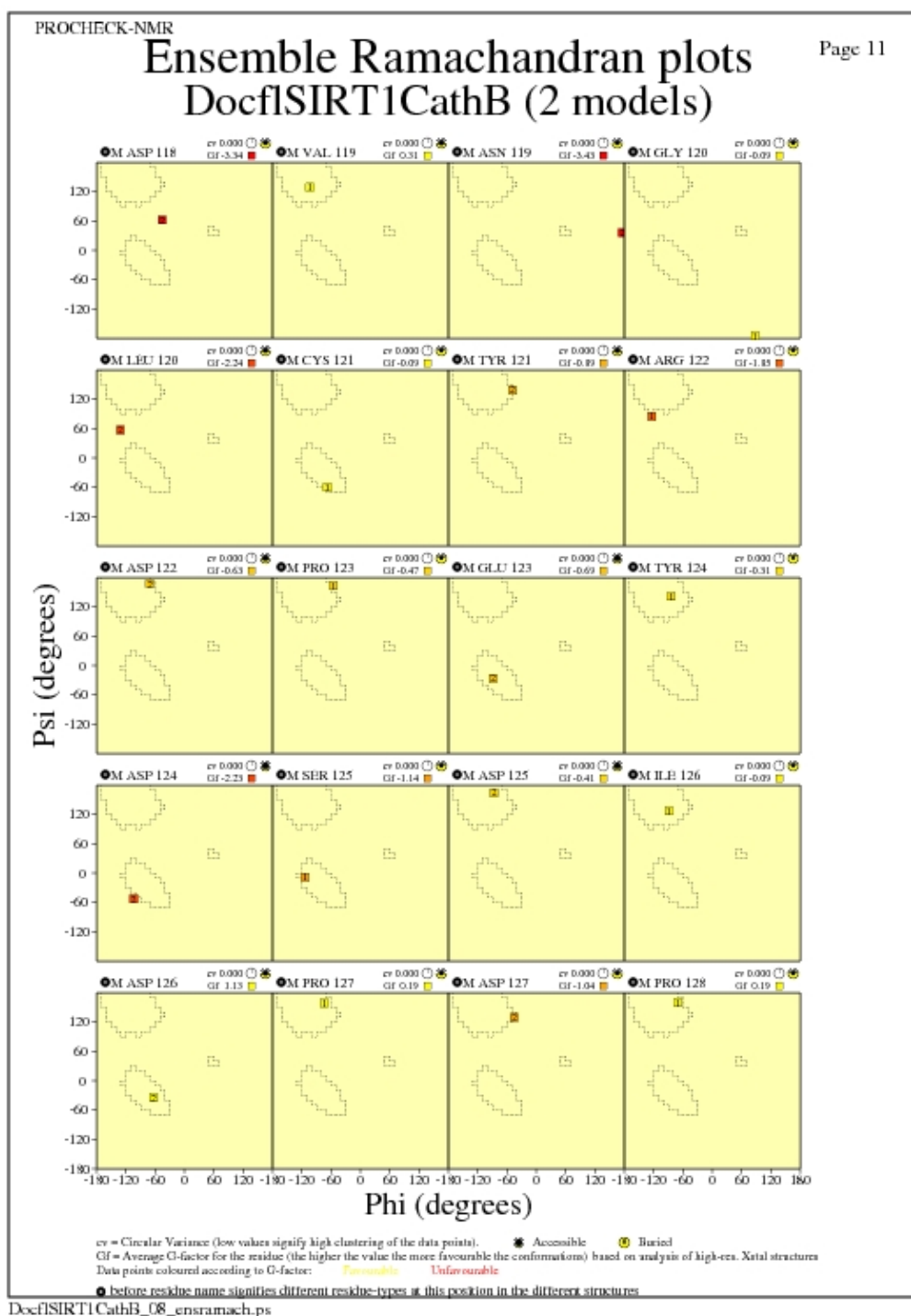
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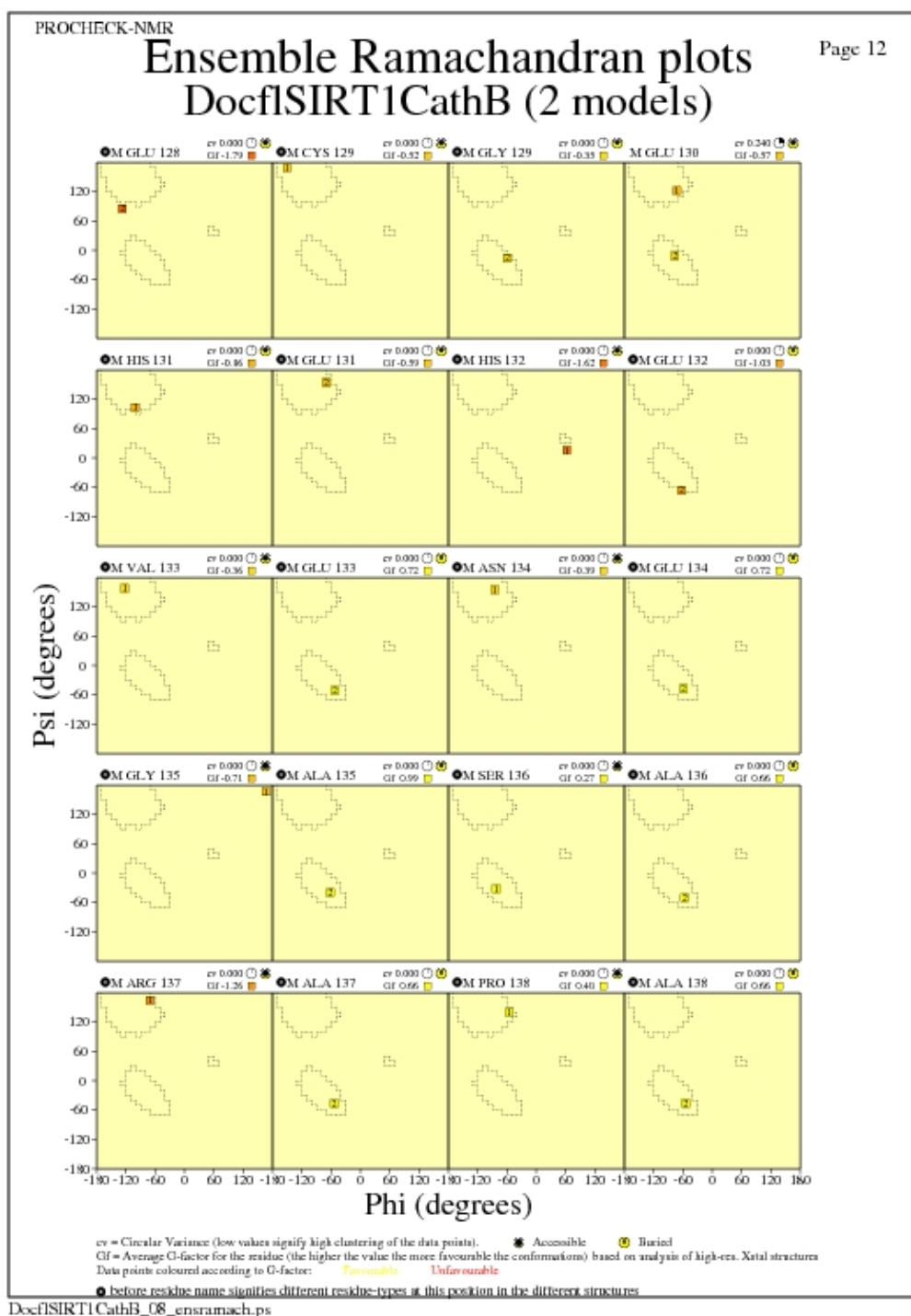
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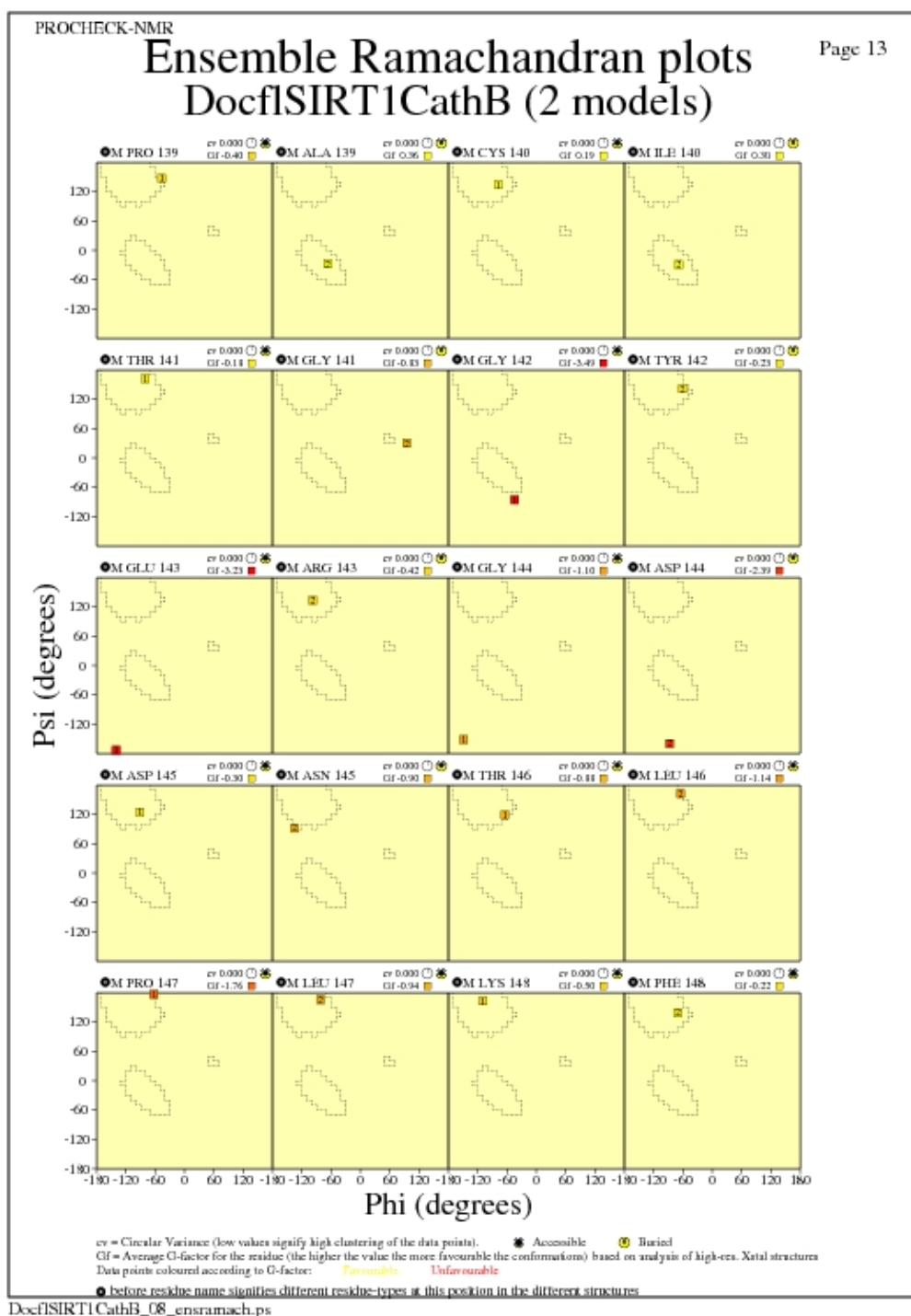
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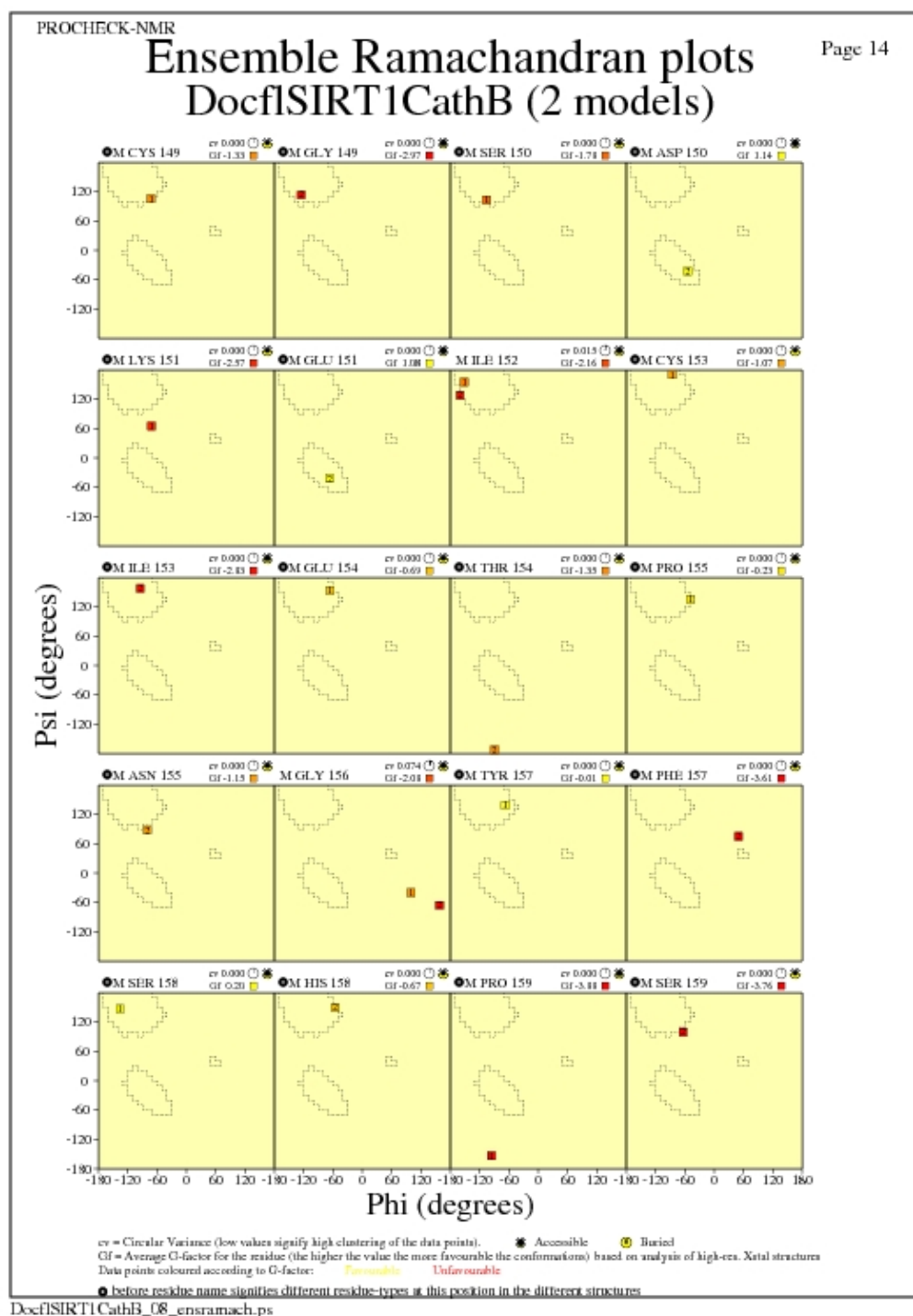
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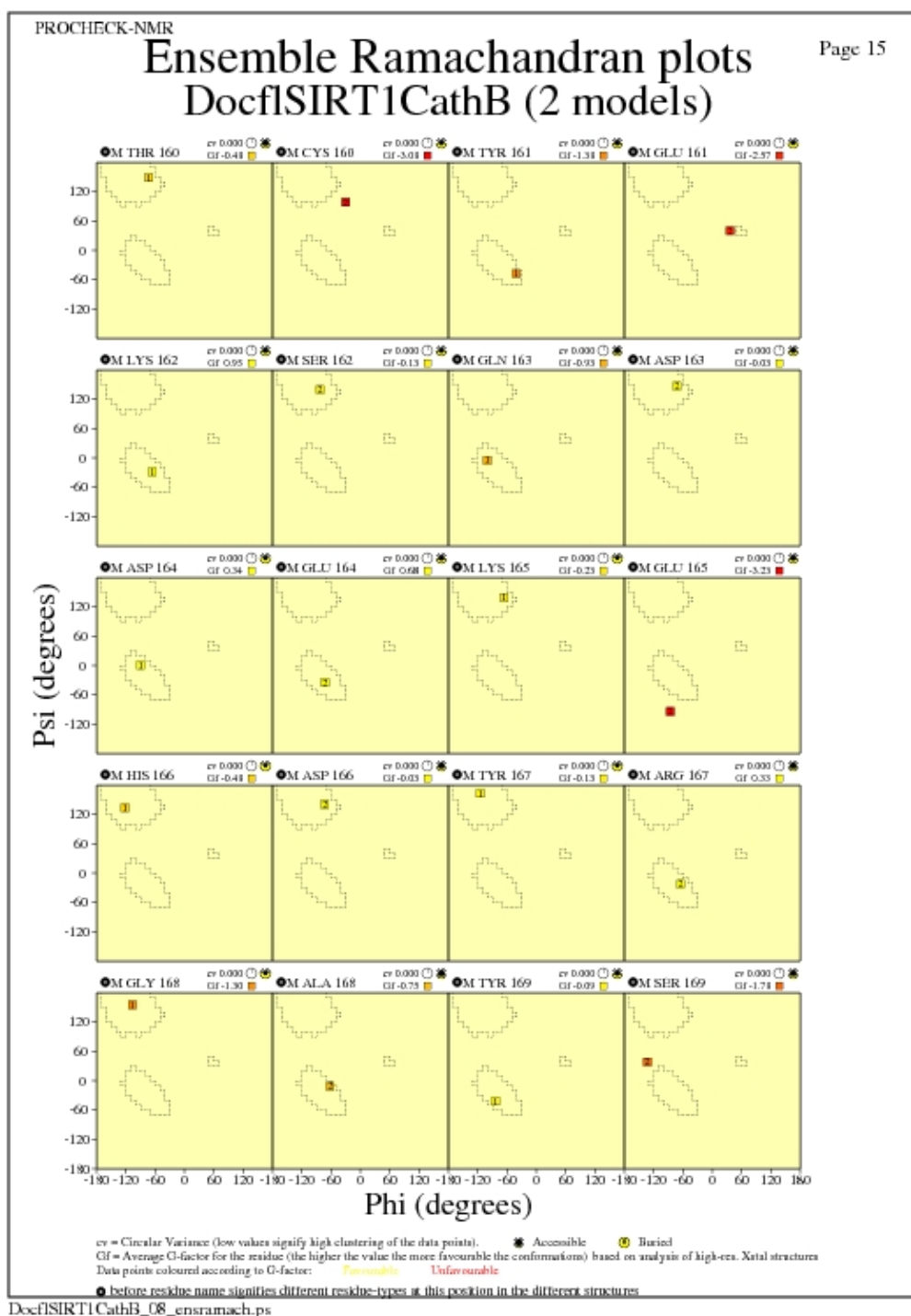
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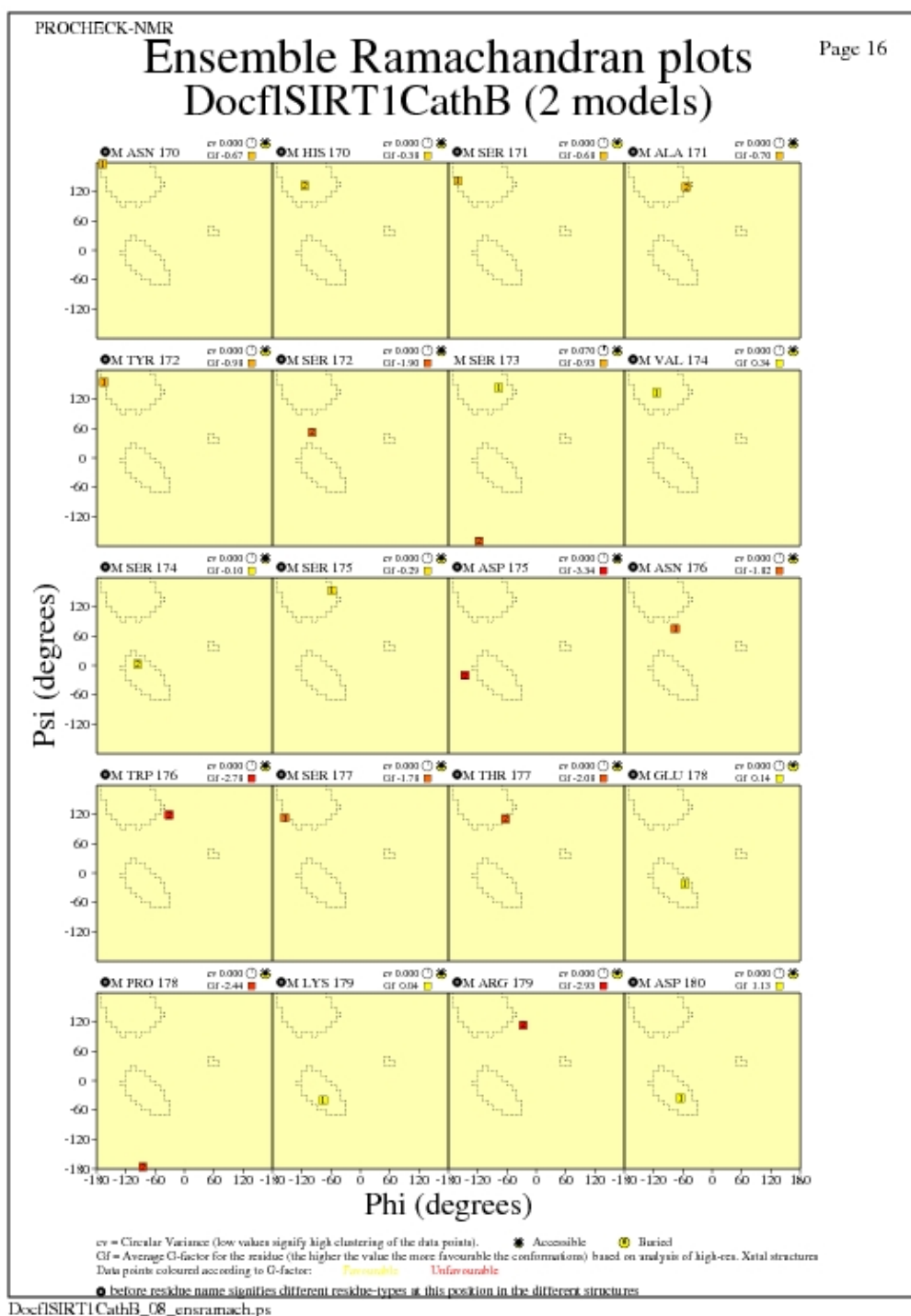
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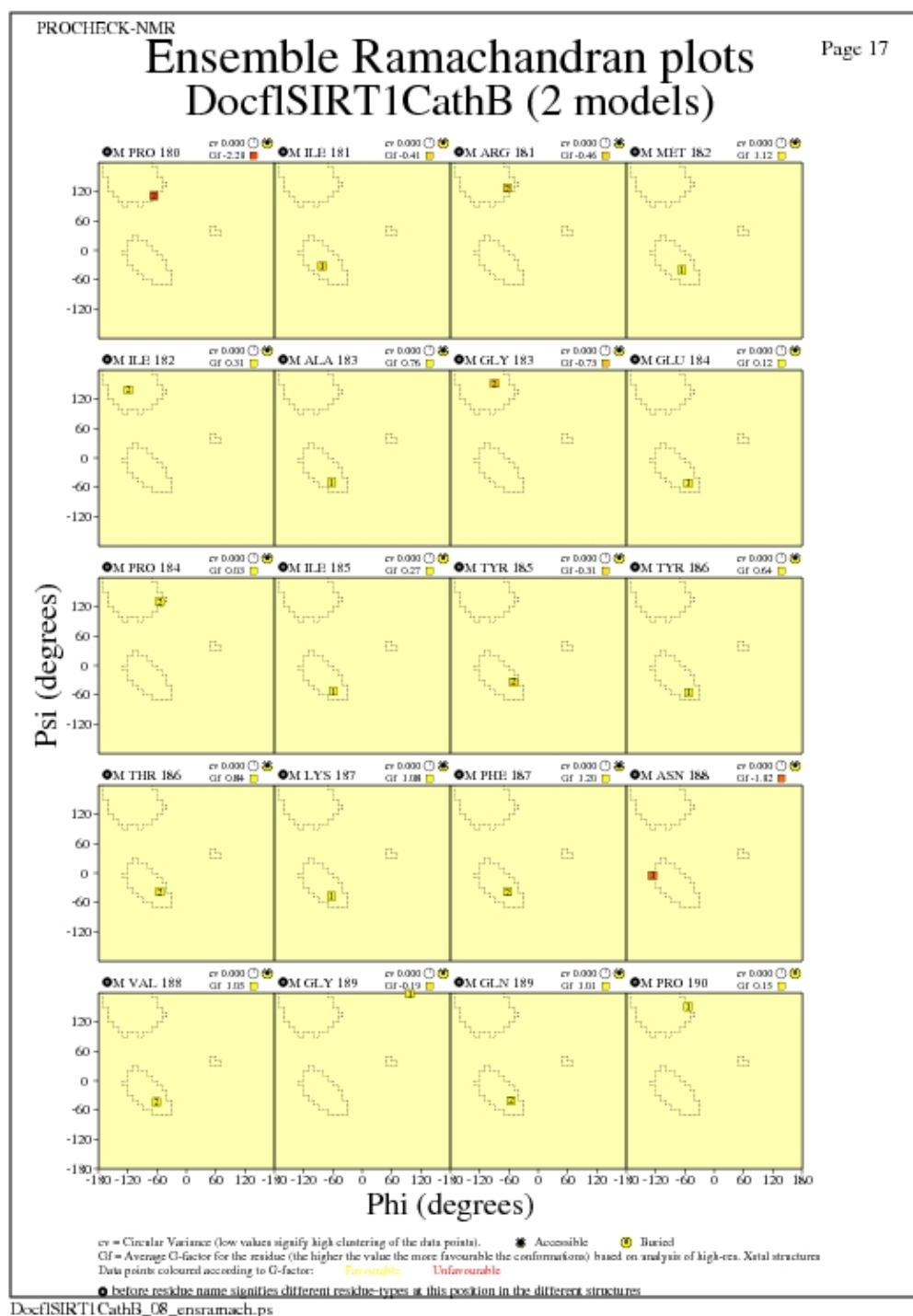
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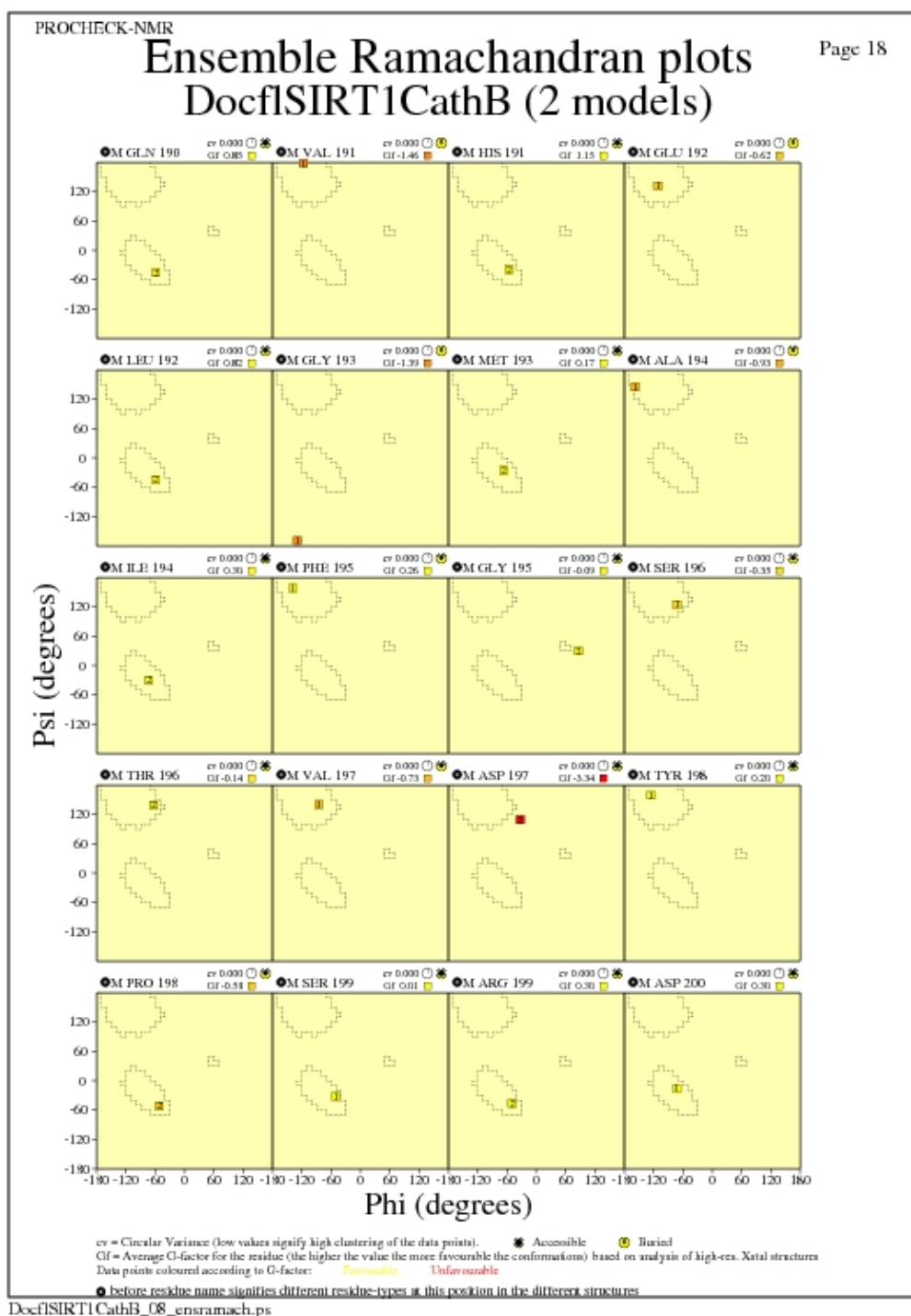
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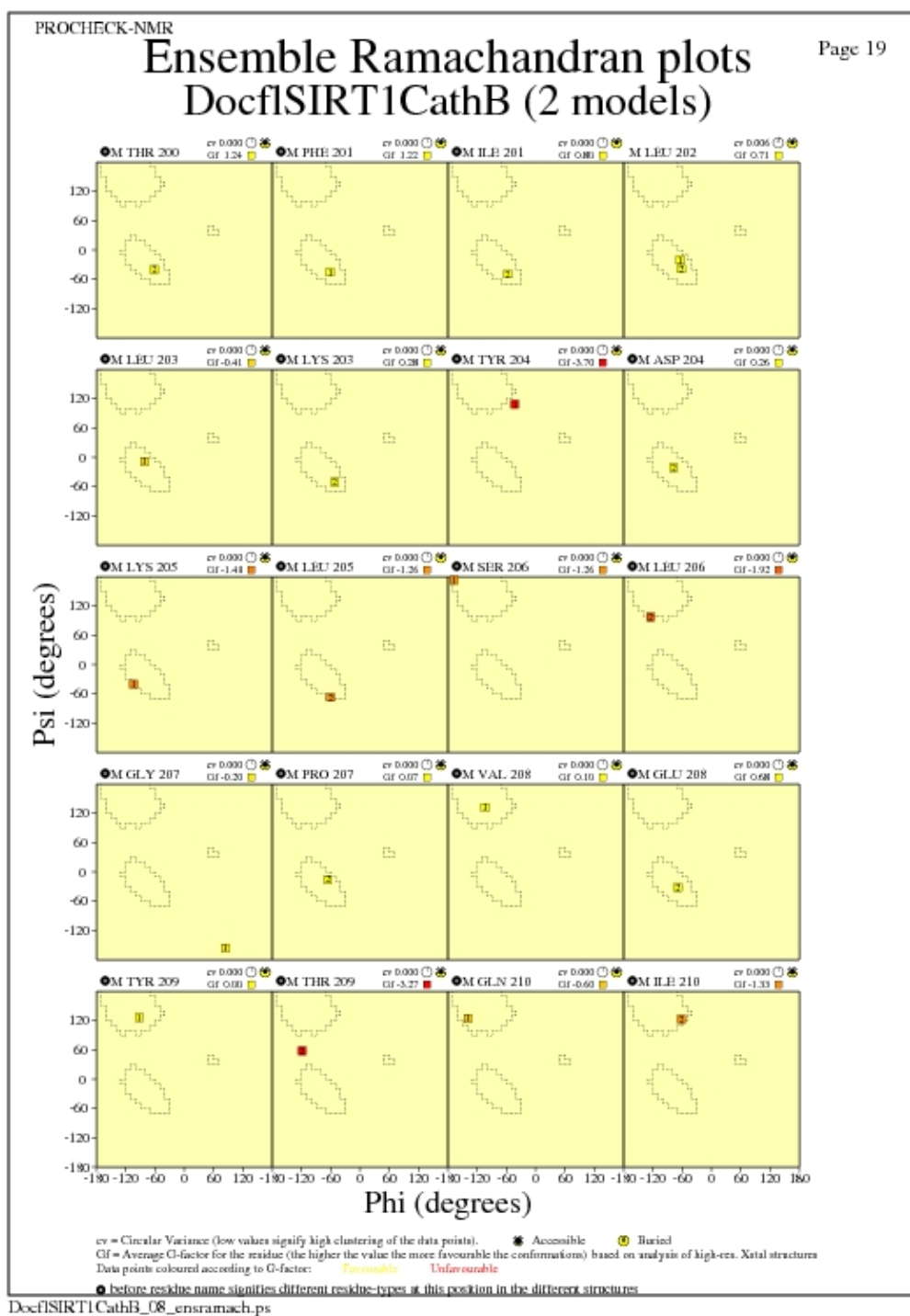
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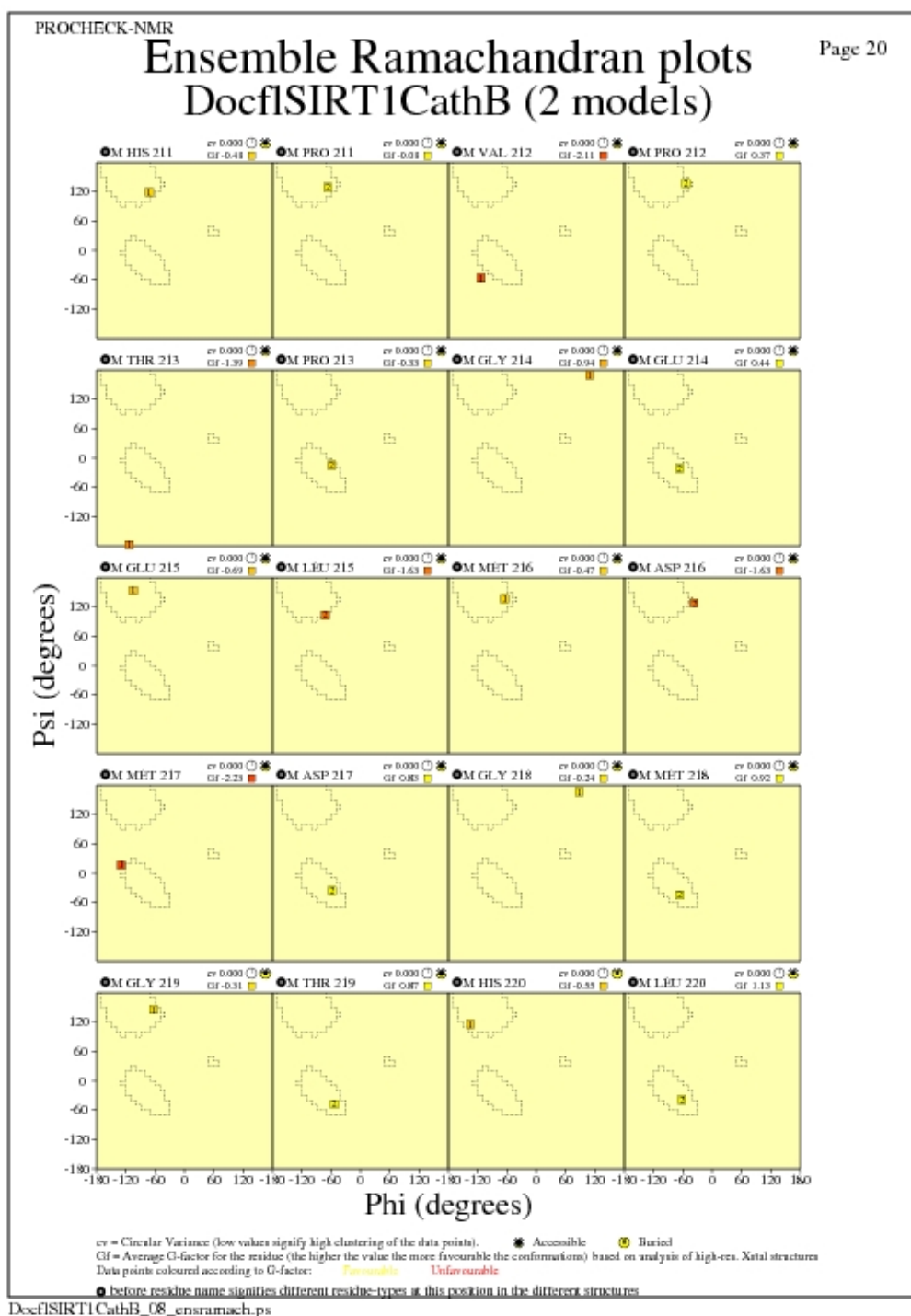
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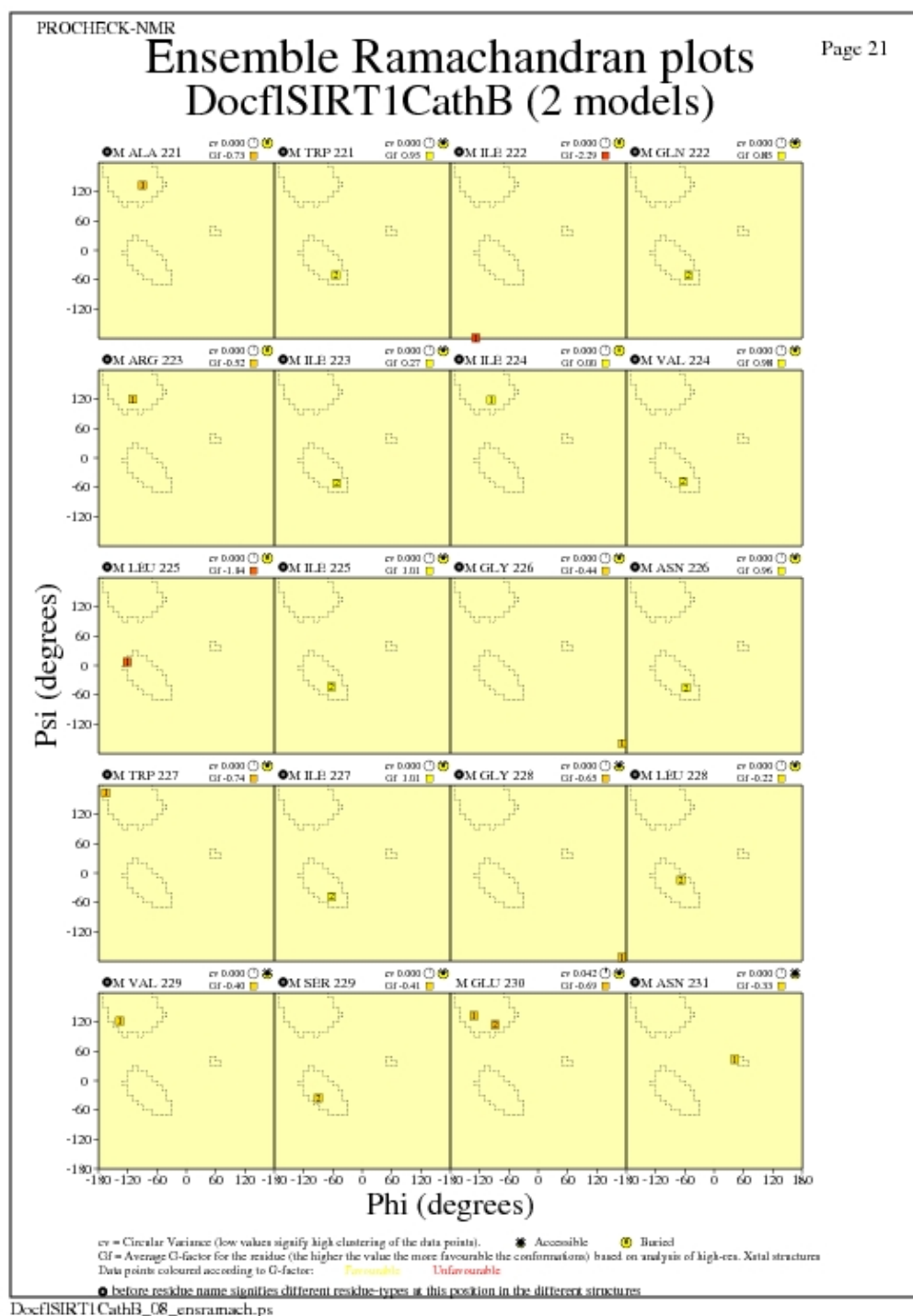
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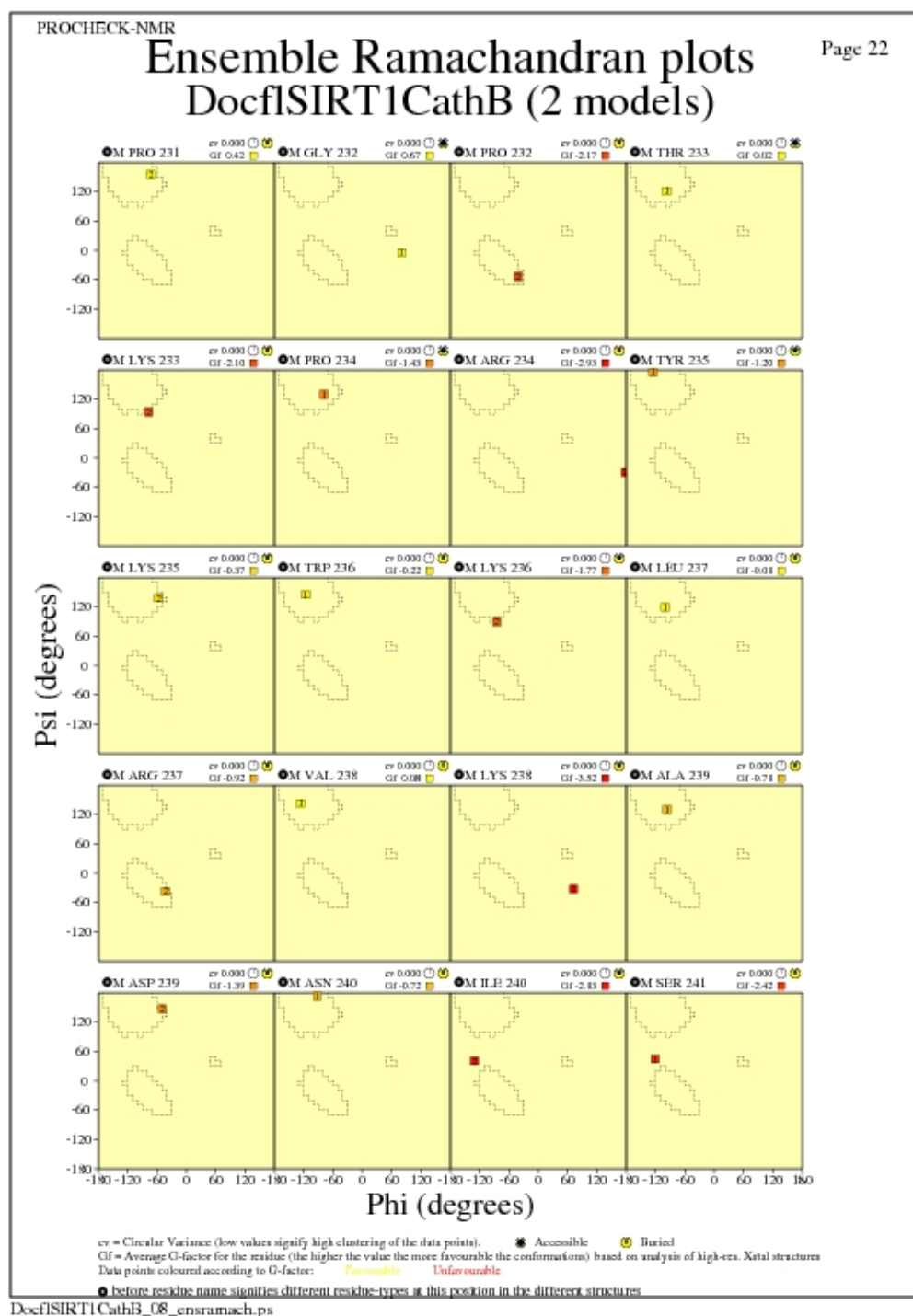
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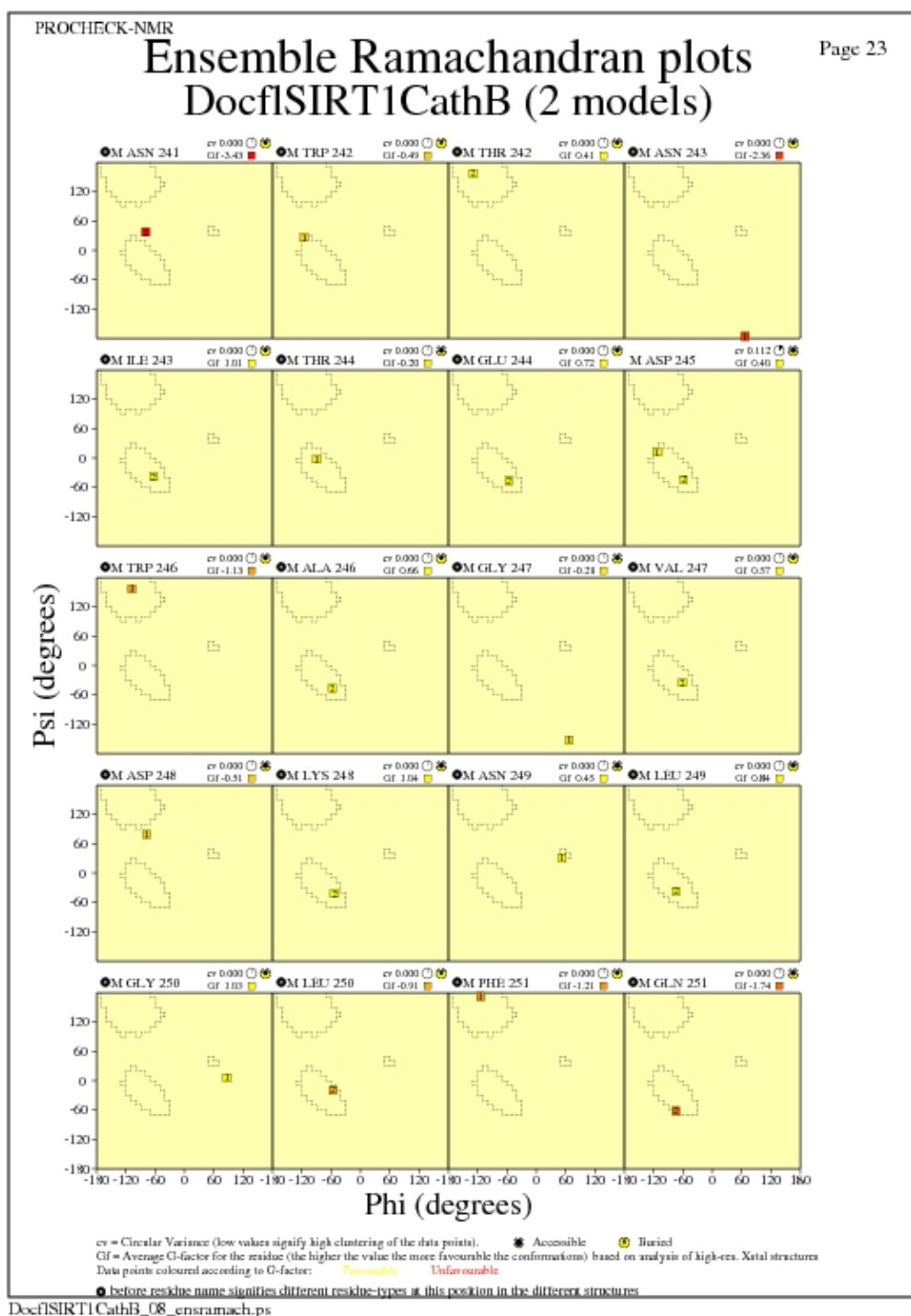
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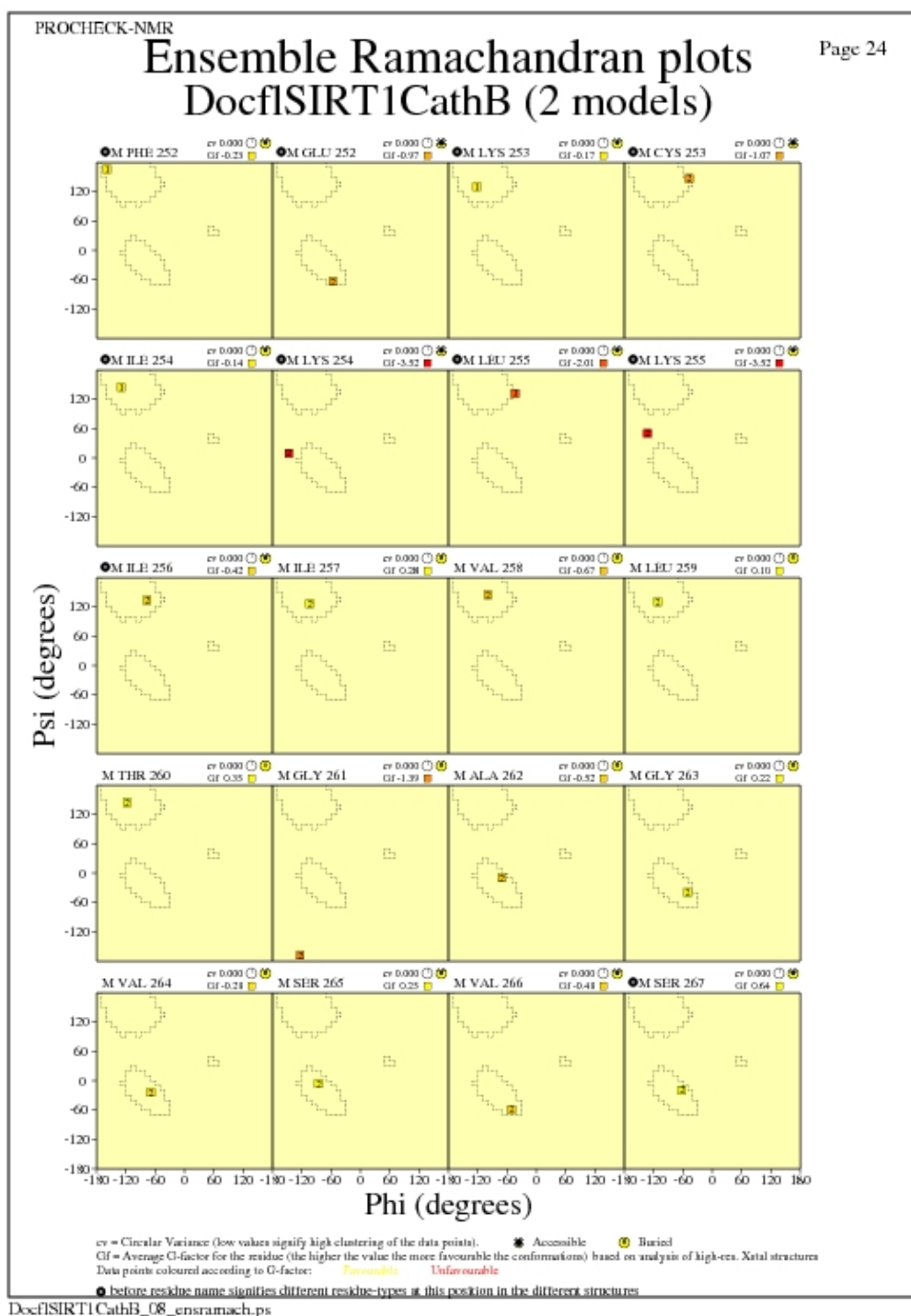
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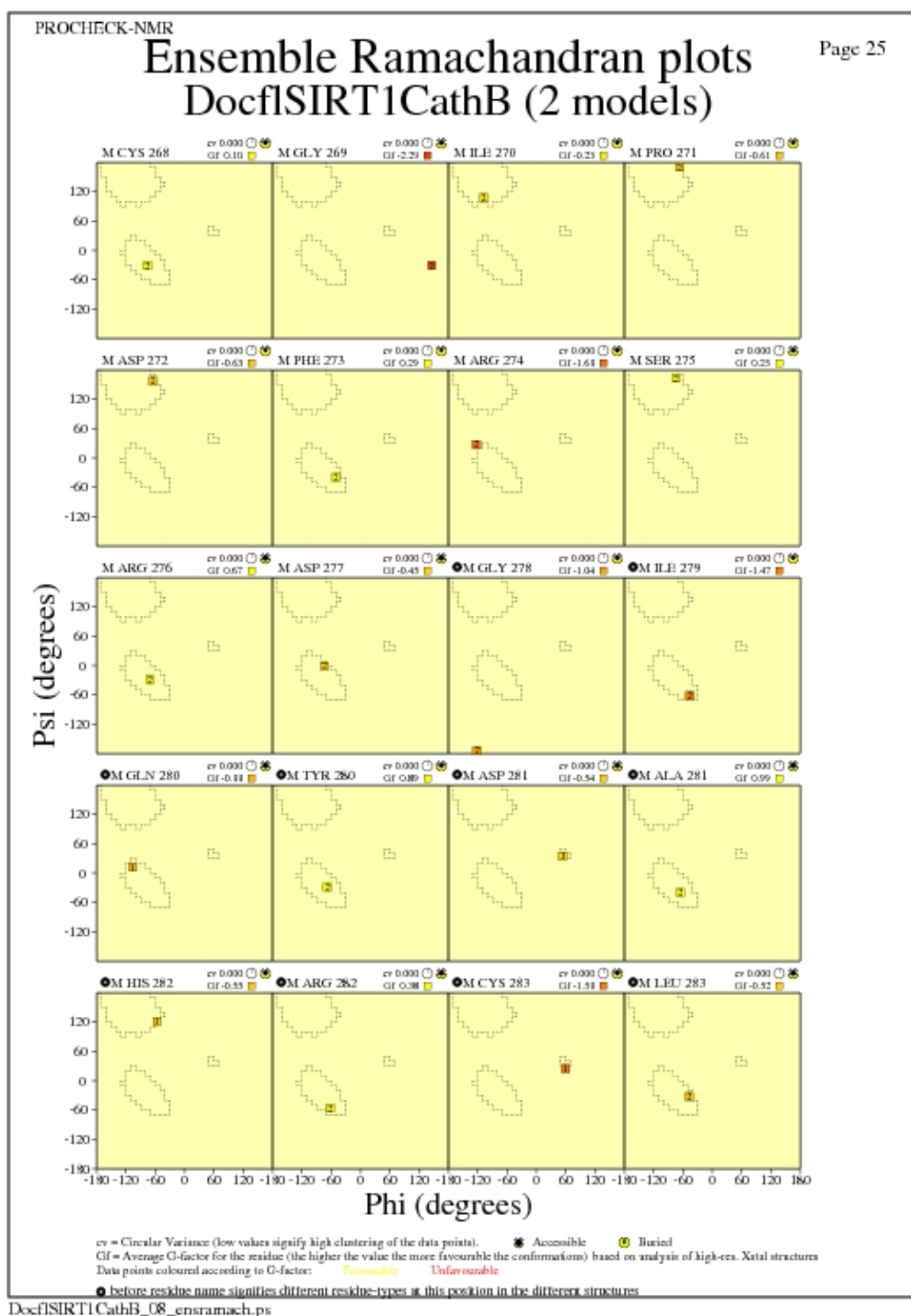
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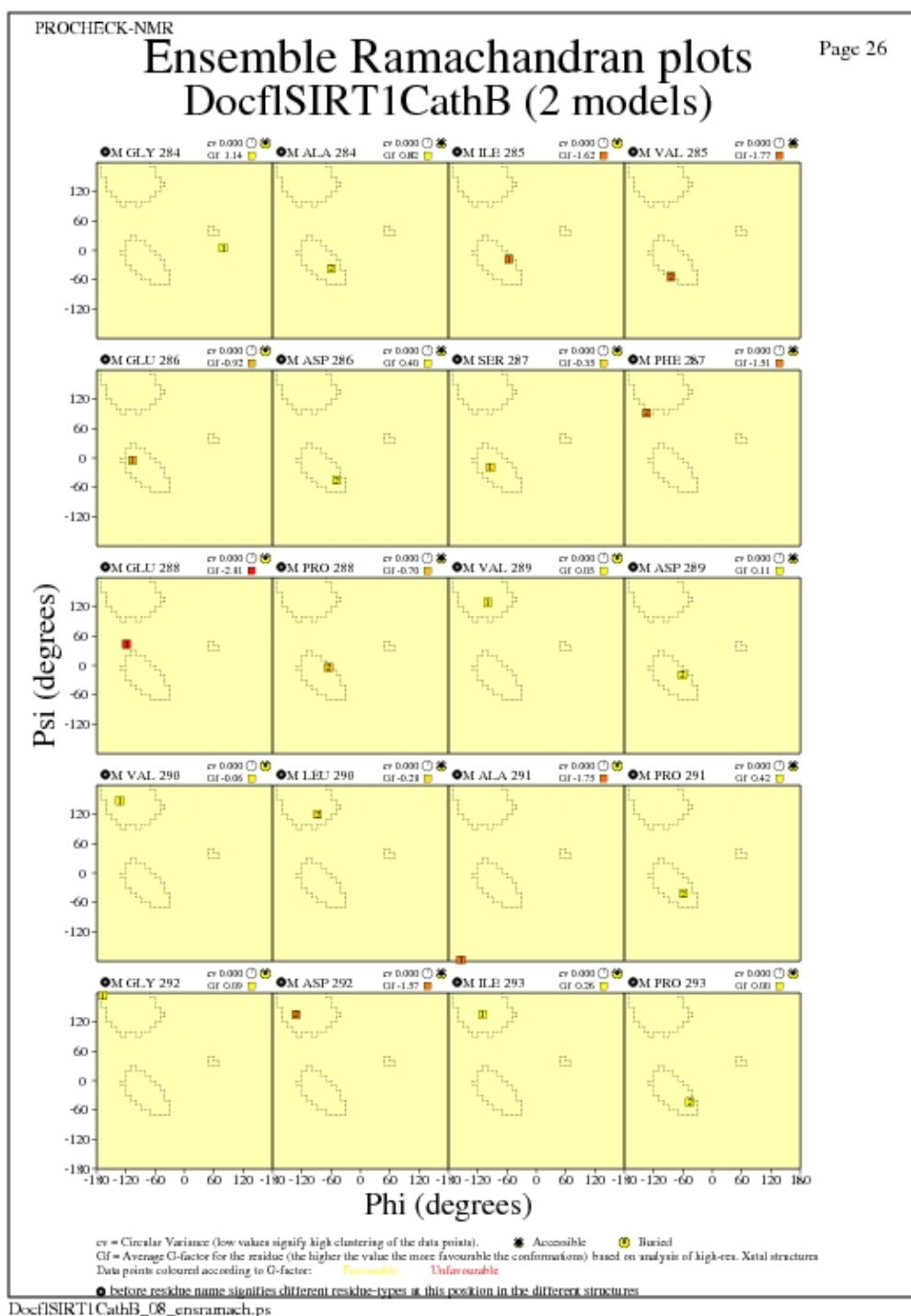
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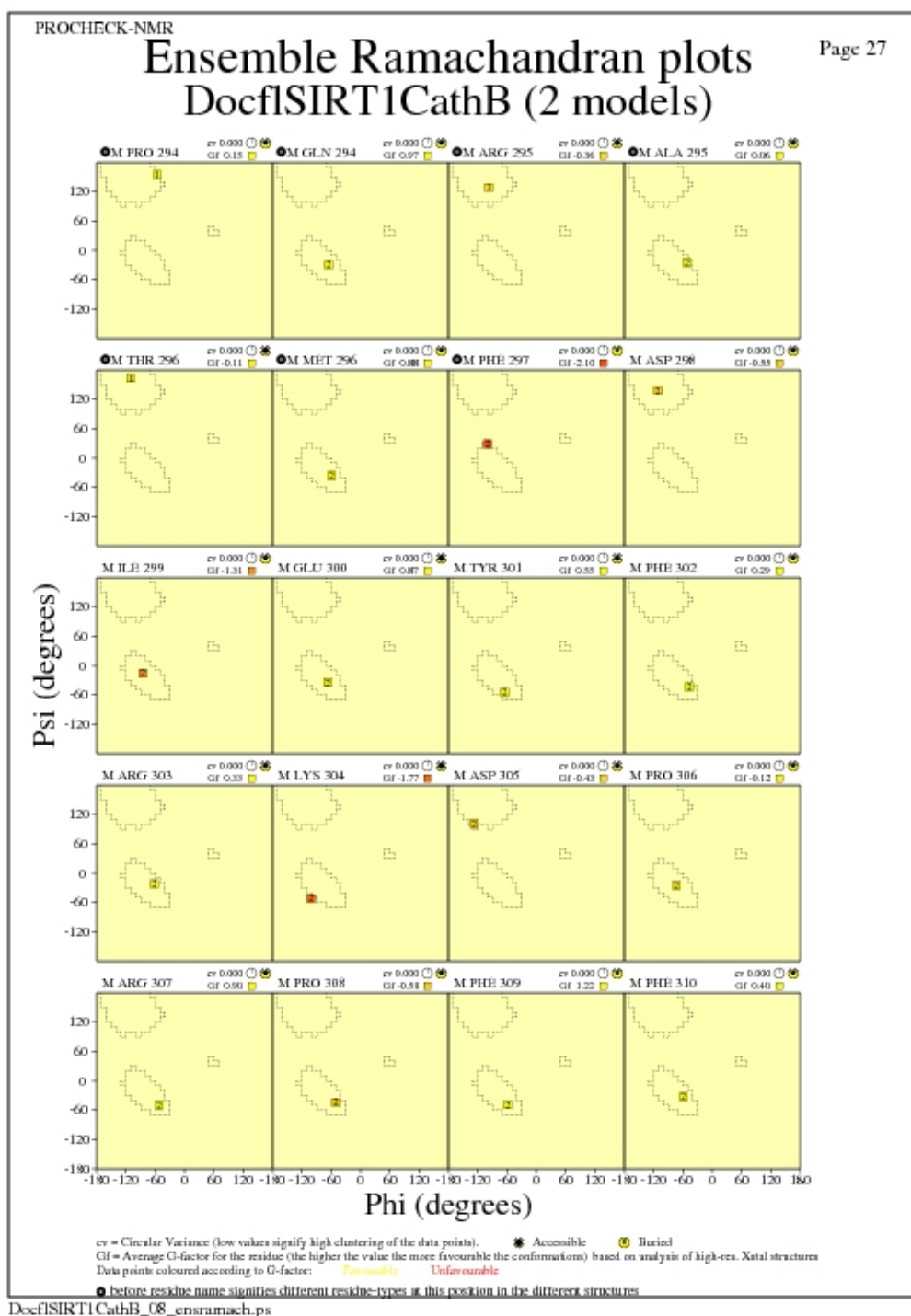
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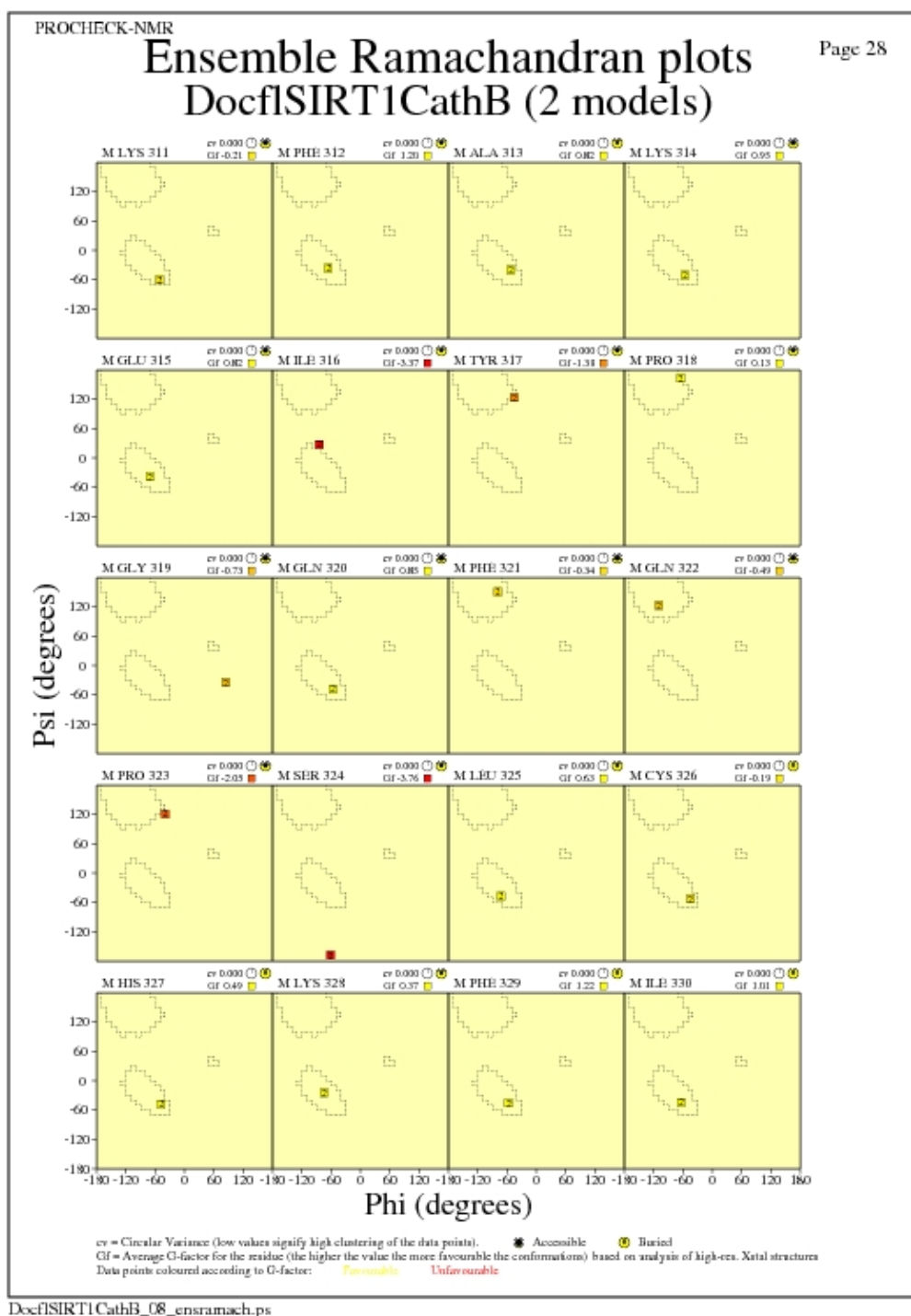
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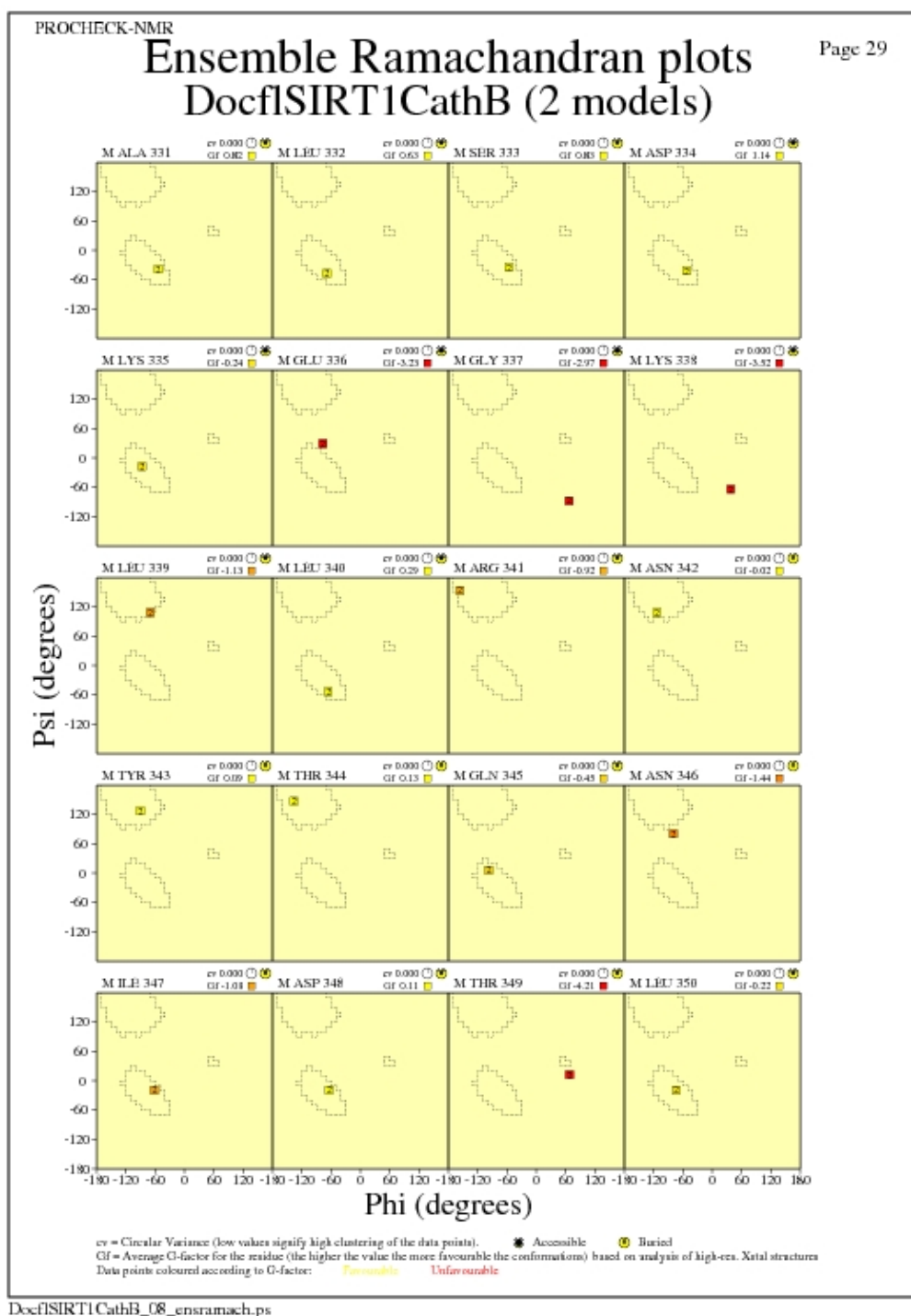
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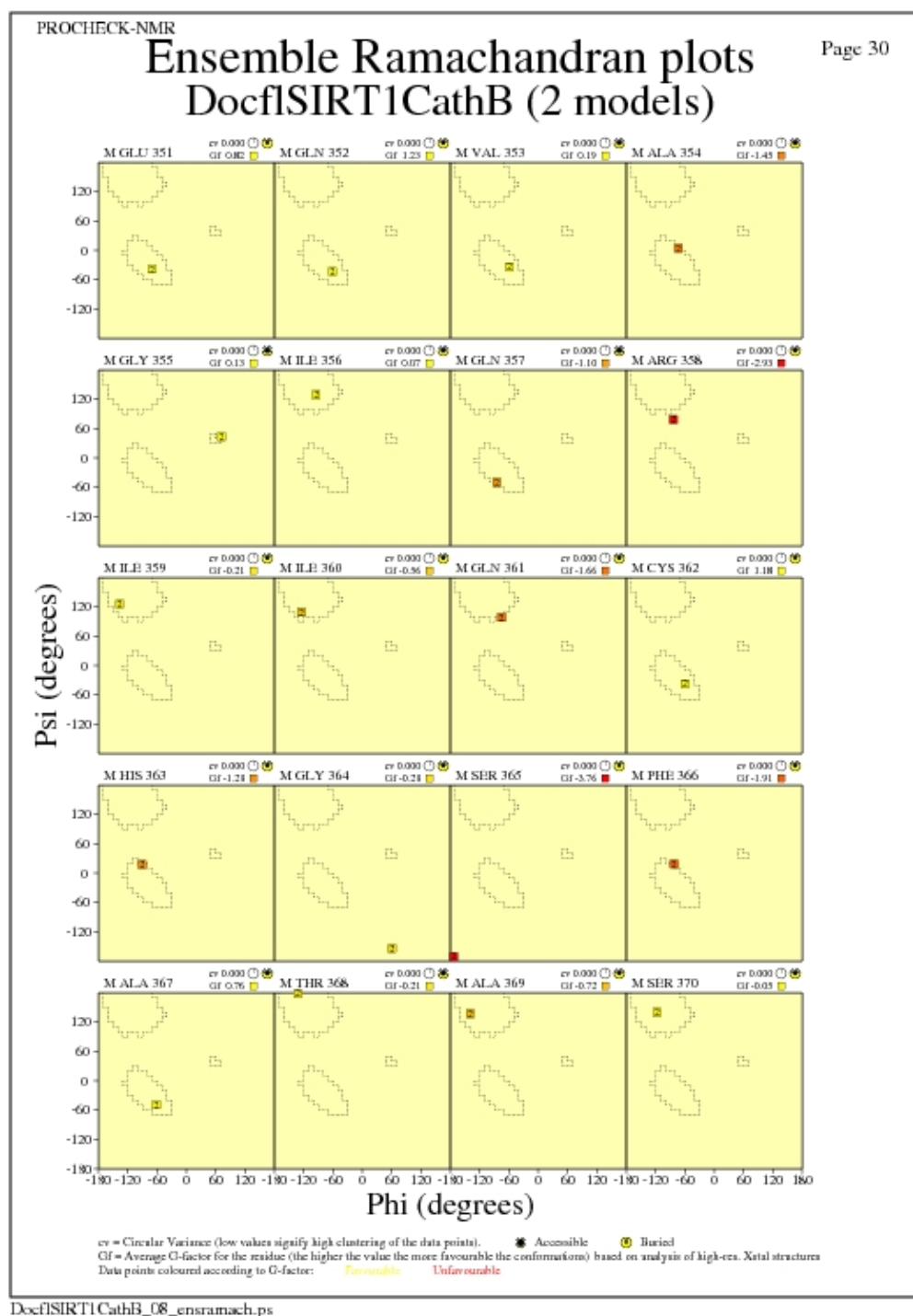
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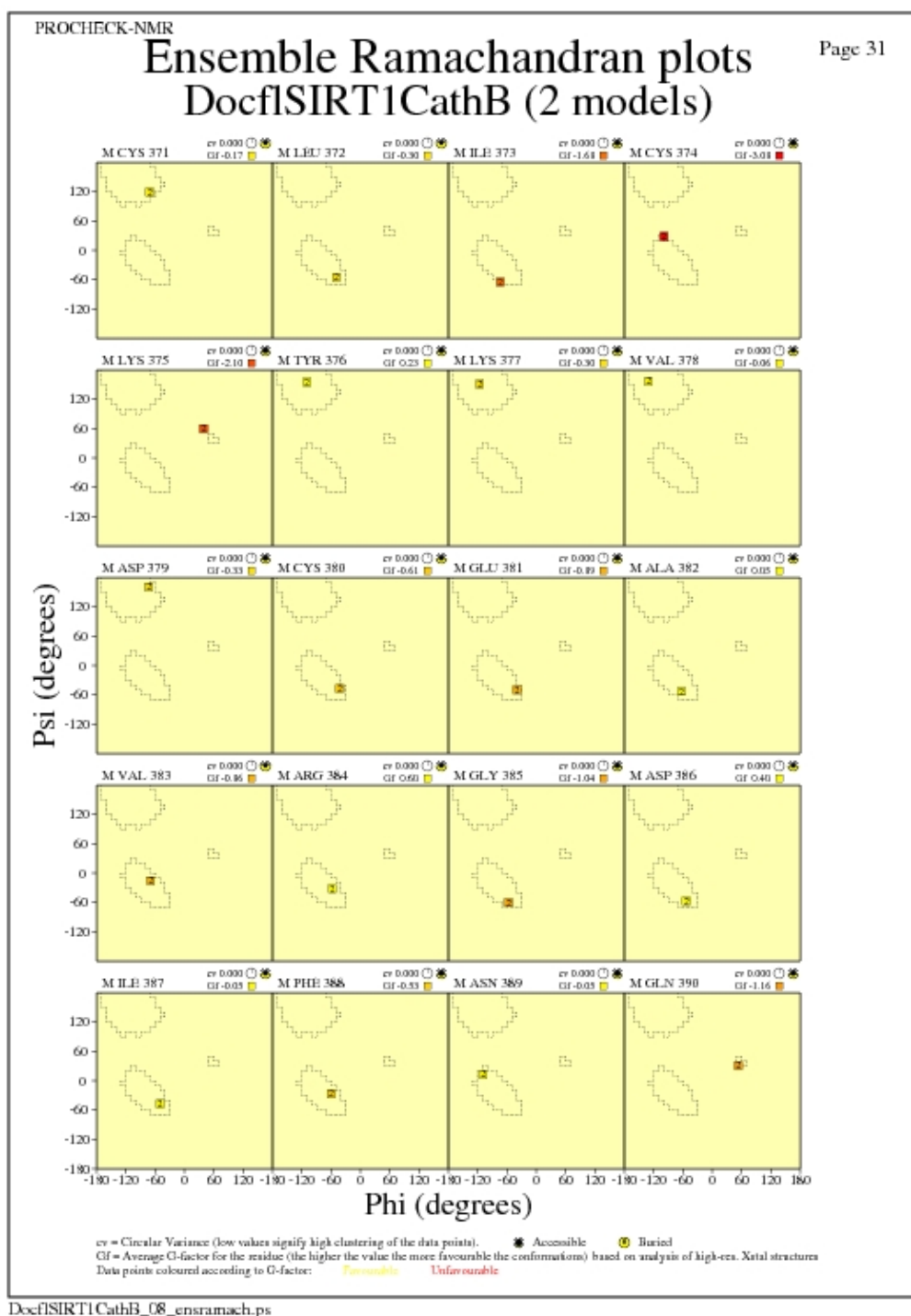
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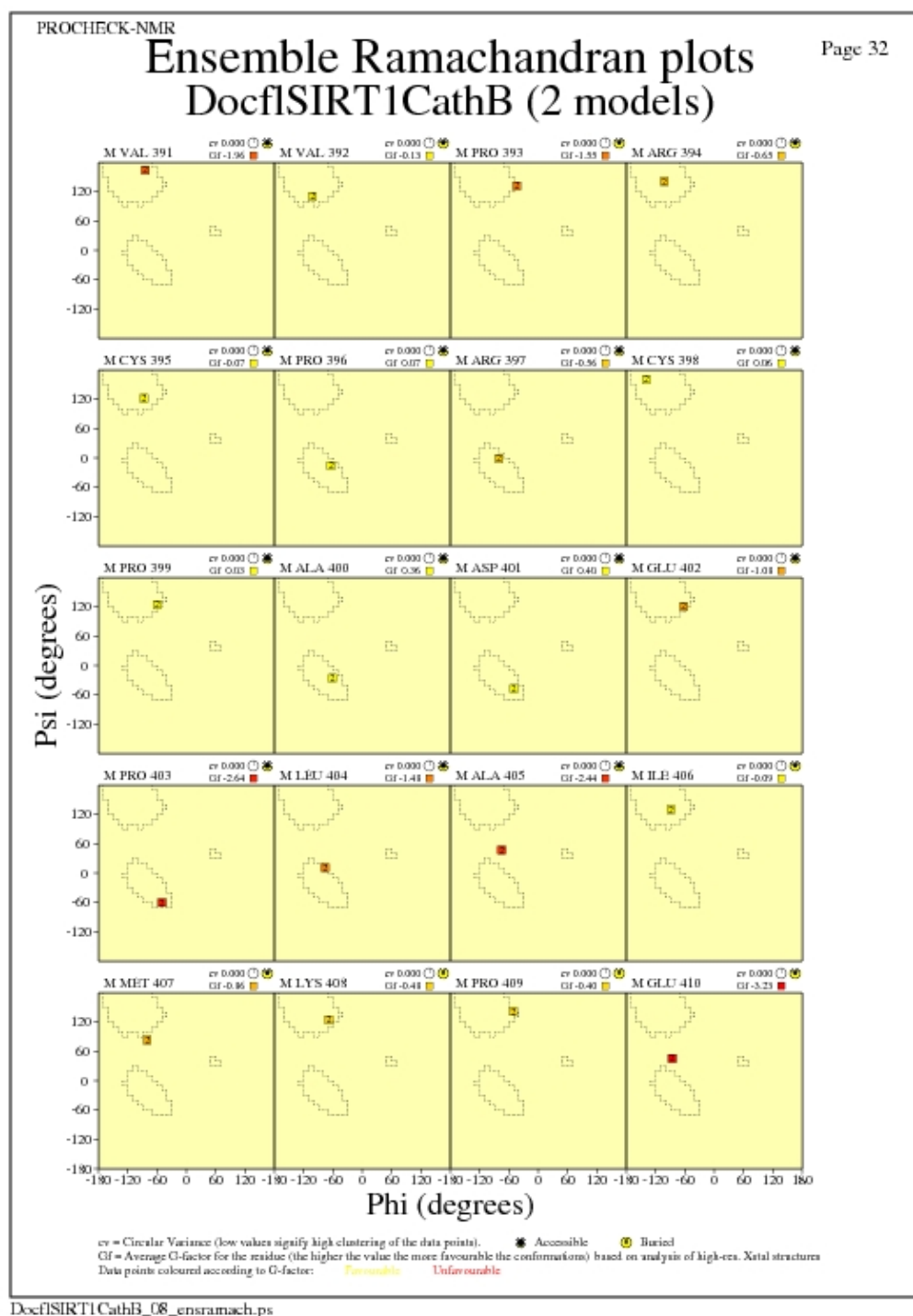
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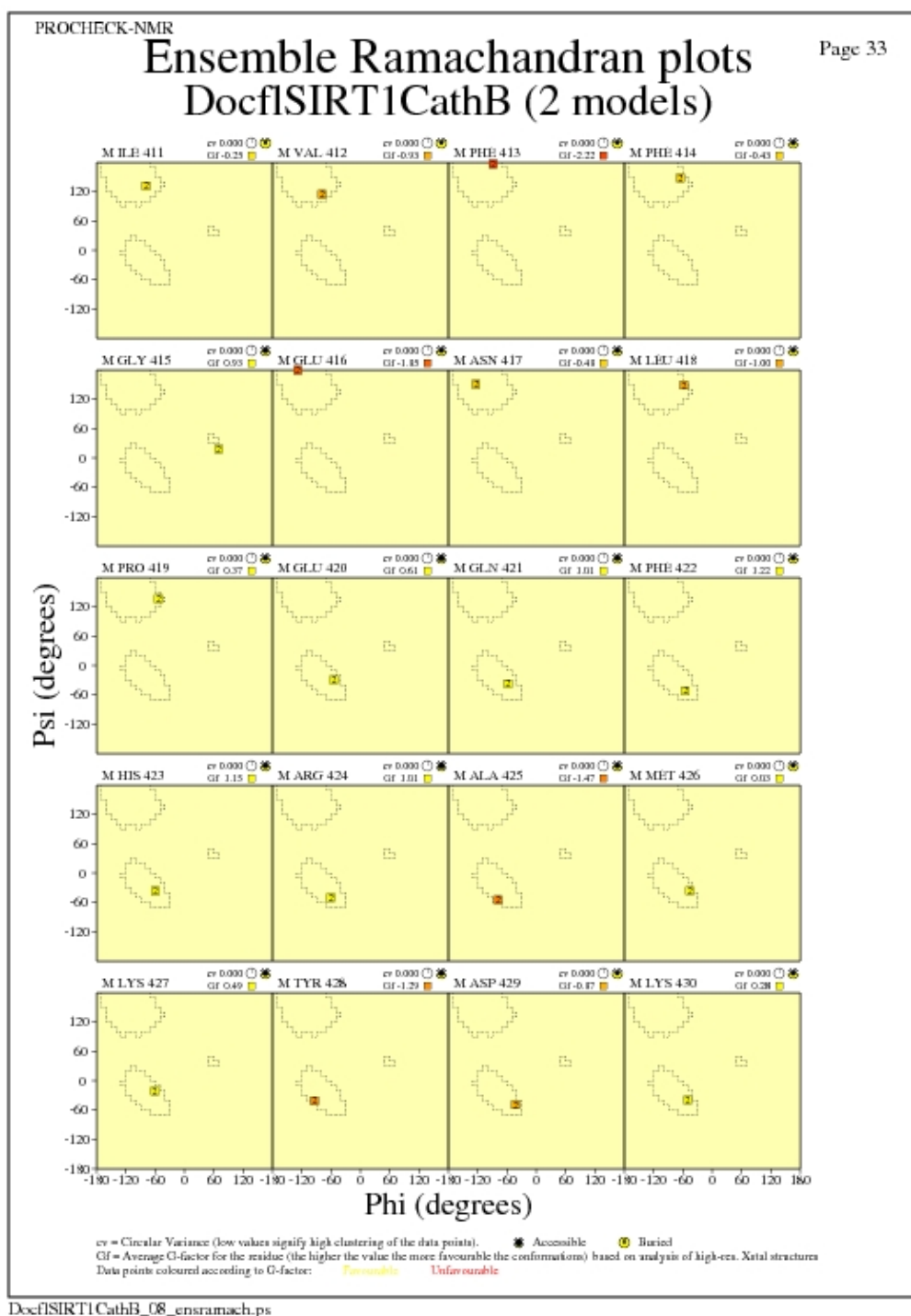
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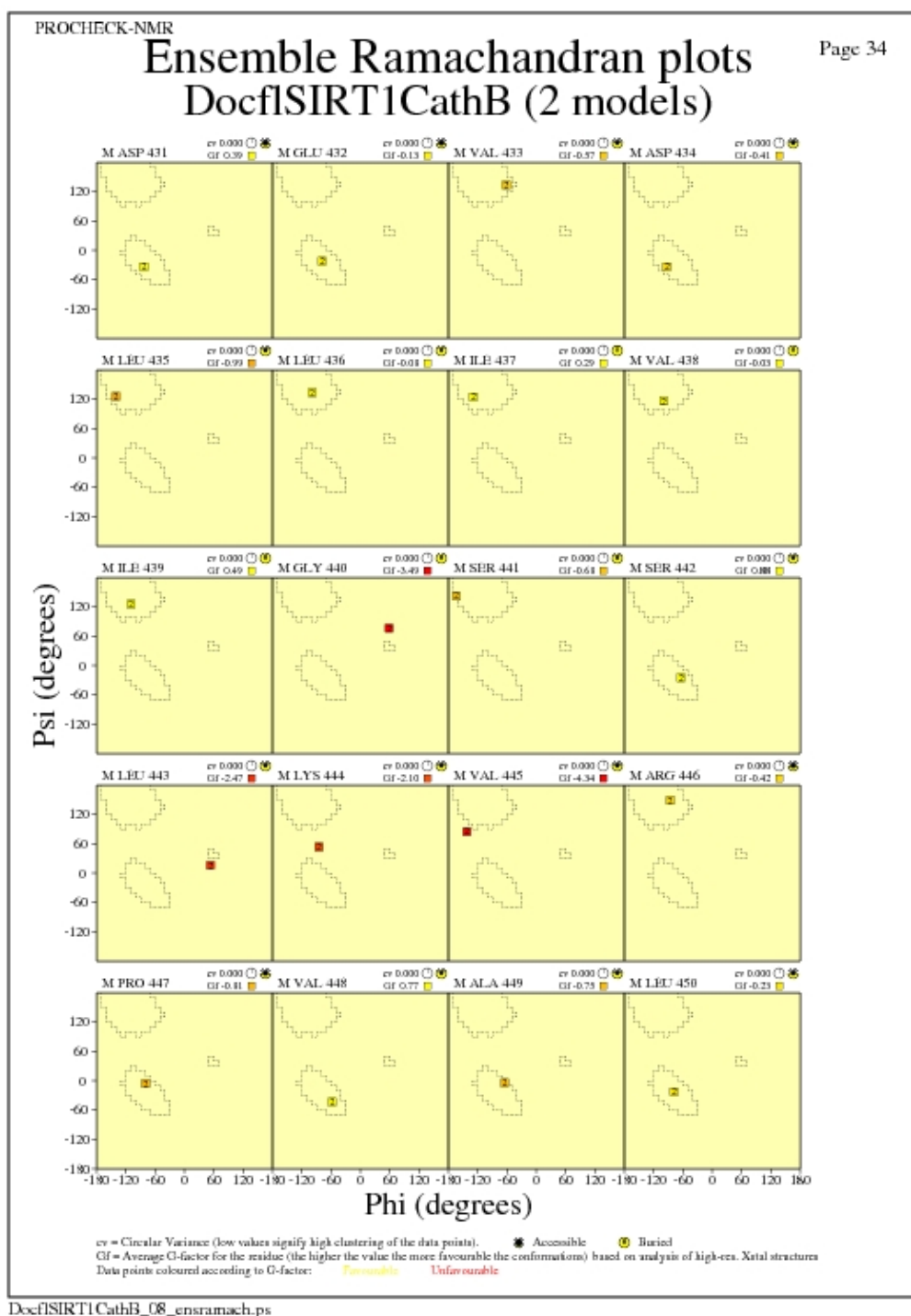
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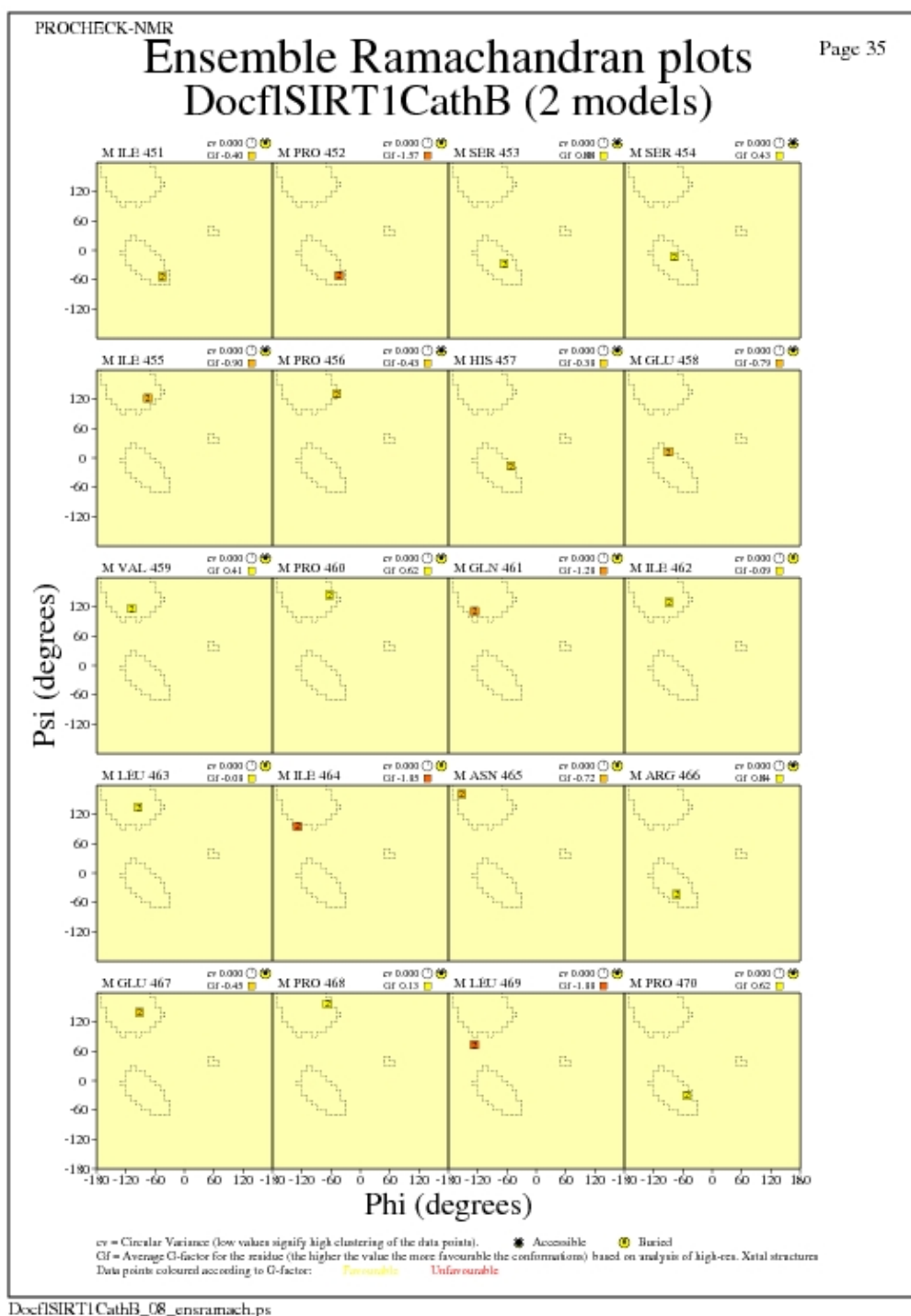
JPEG for residue Ramachandran Plots - page \$num_n



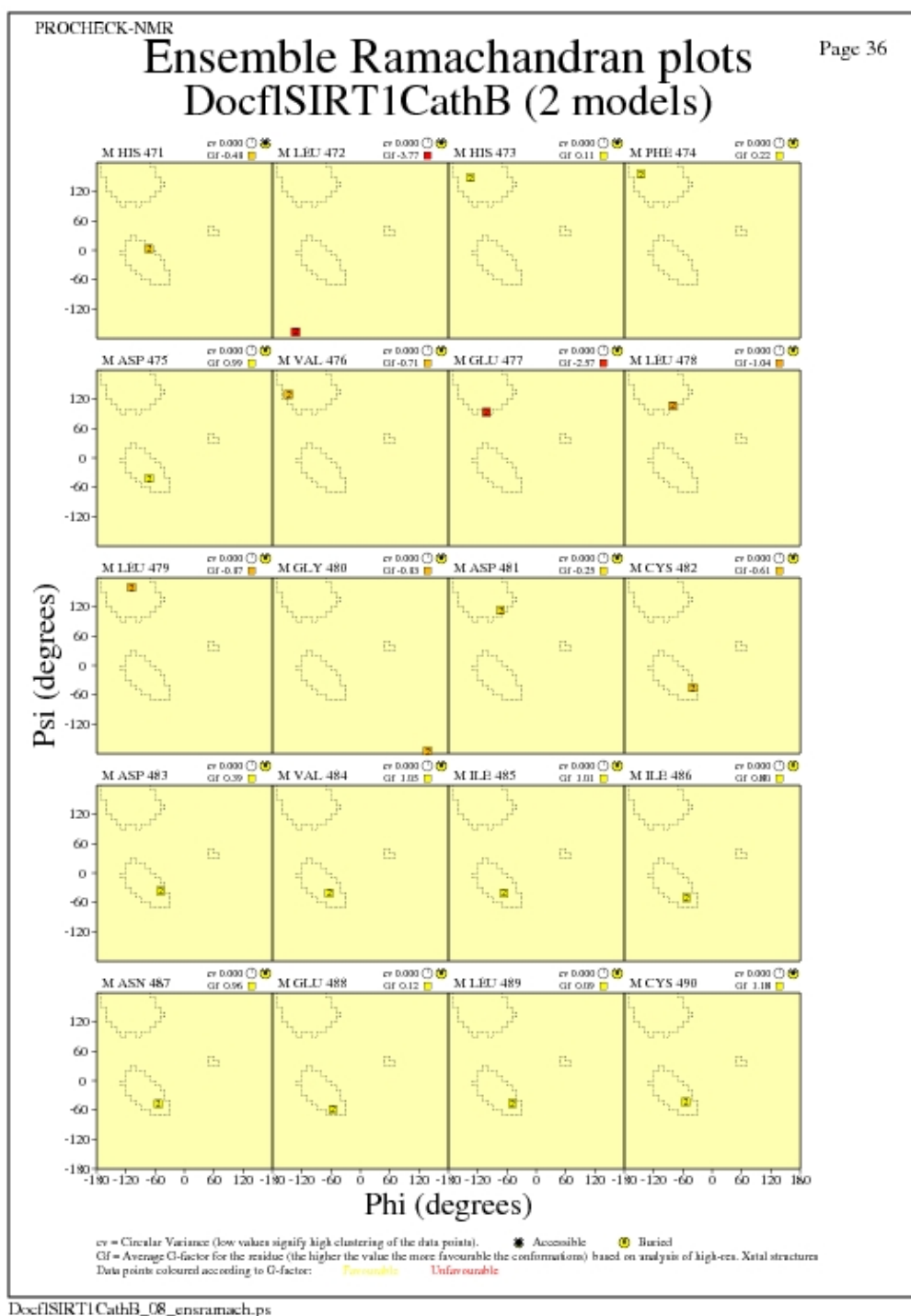
JPEG for residue Ramachandran Plots - page \$num_n



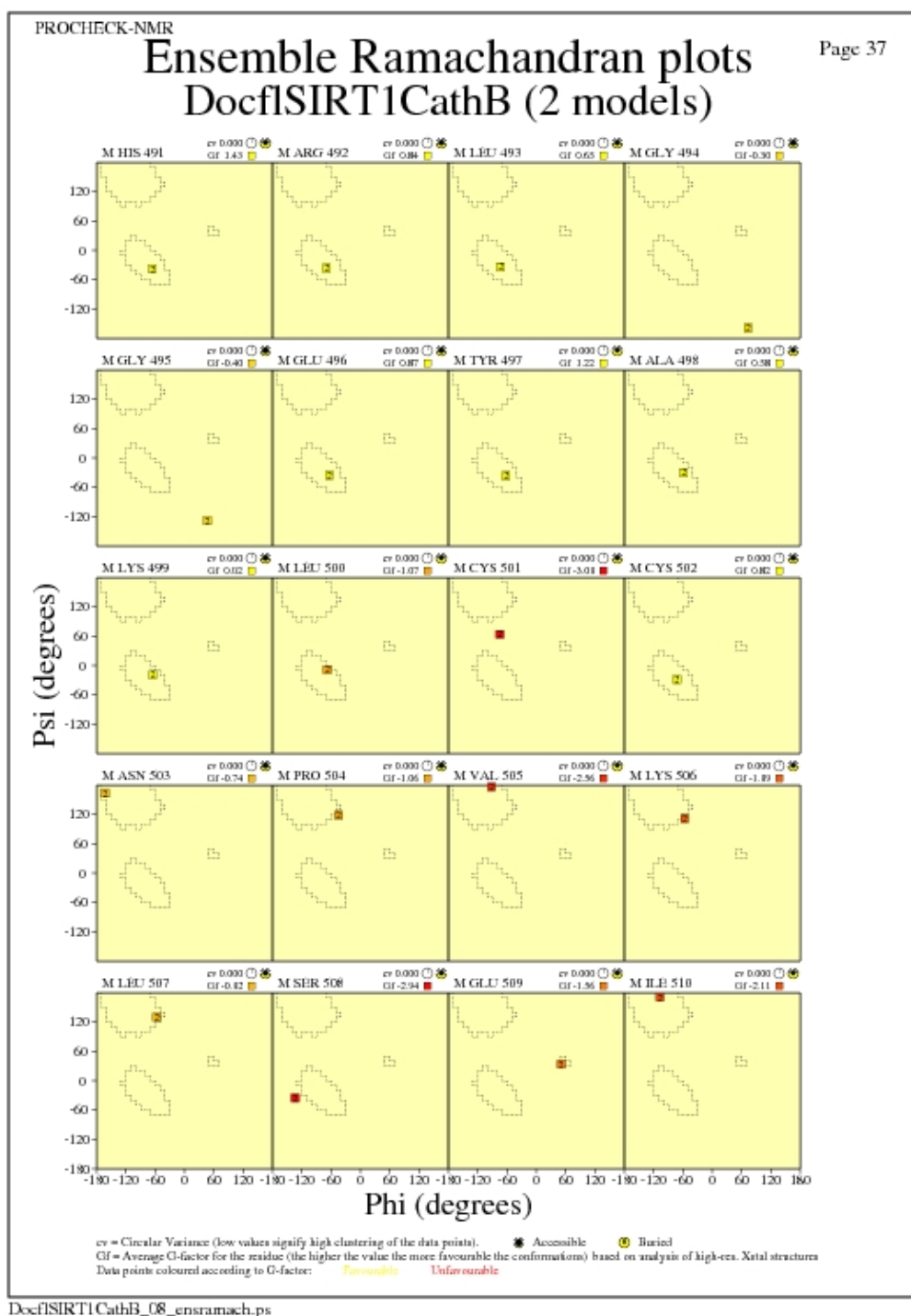
JPEG for residue Ramachandran Plots - page \$num_n



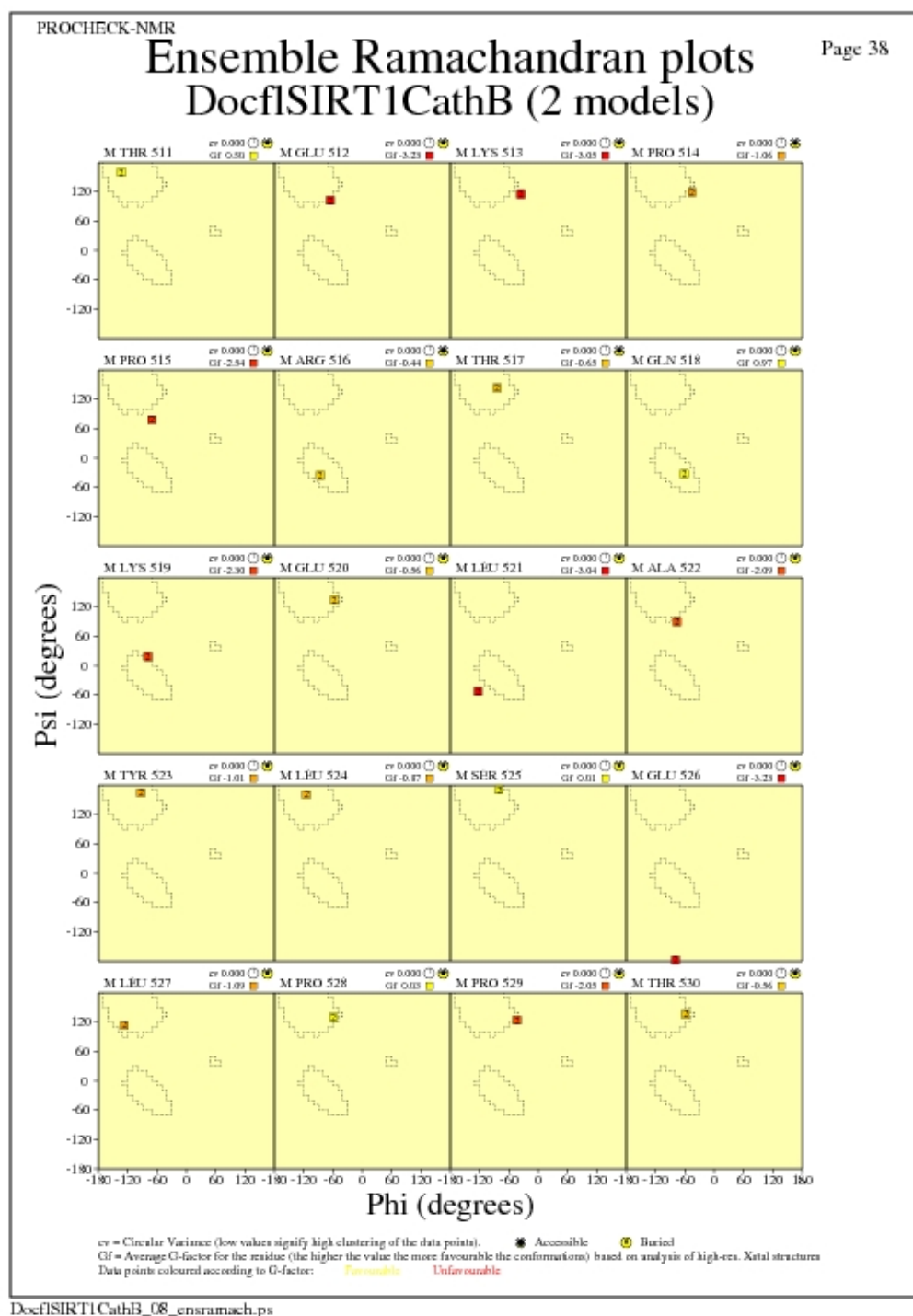
JPEG for residue Ramachandran Plots - page \$num_n



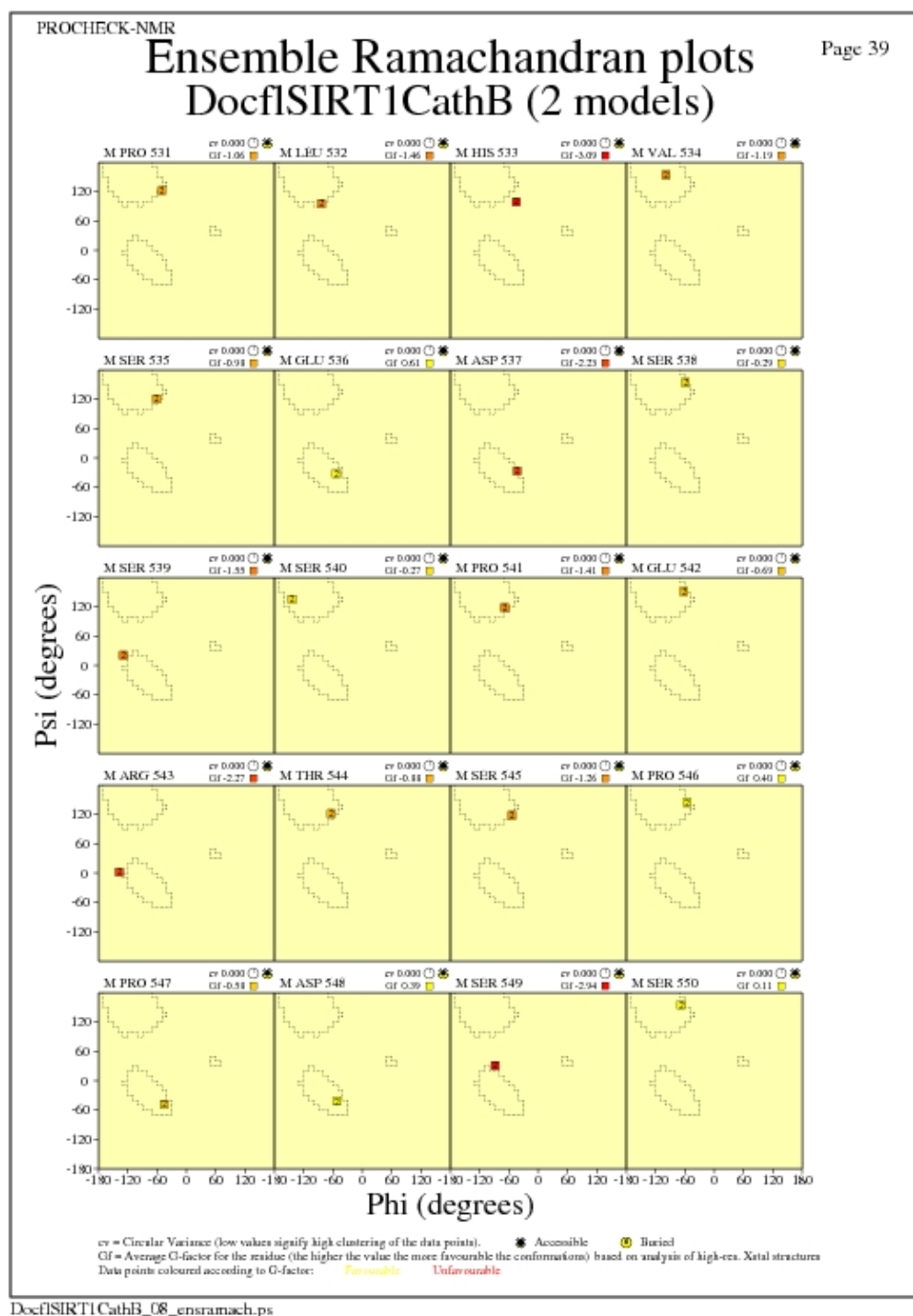
JPEG for residue Ramachandran Plots - page \$num_n



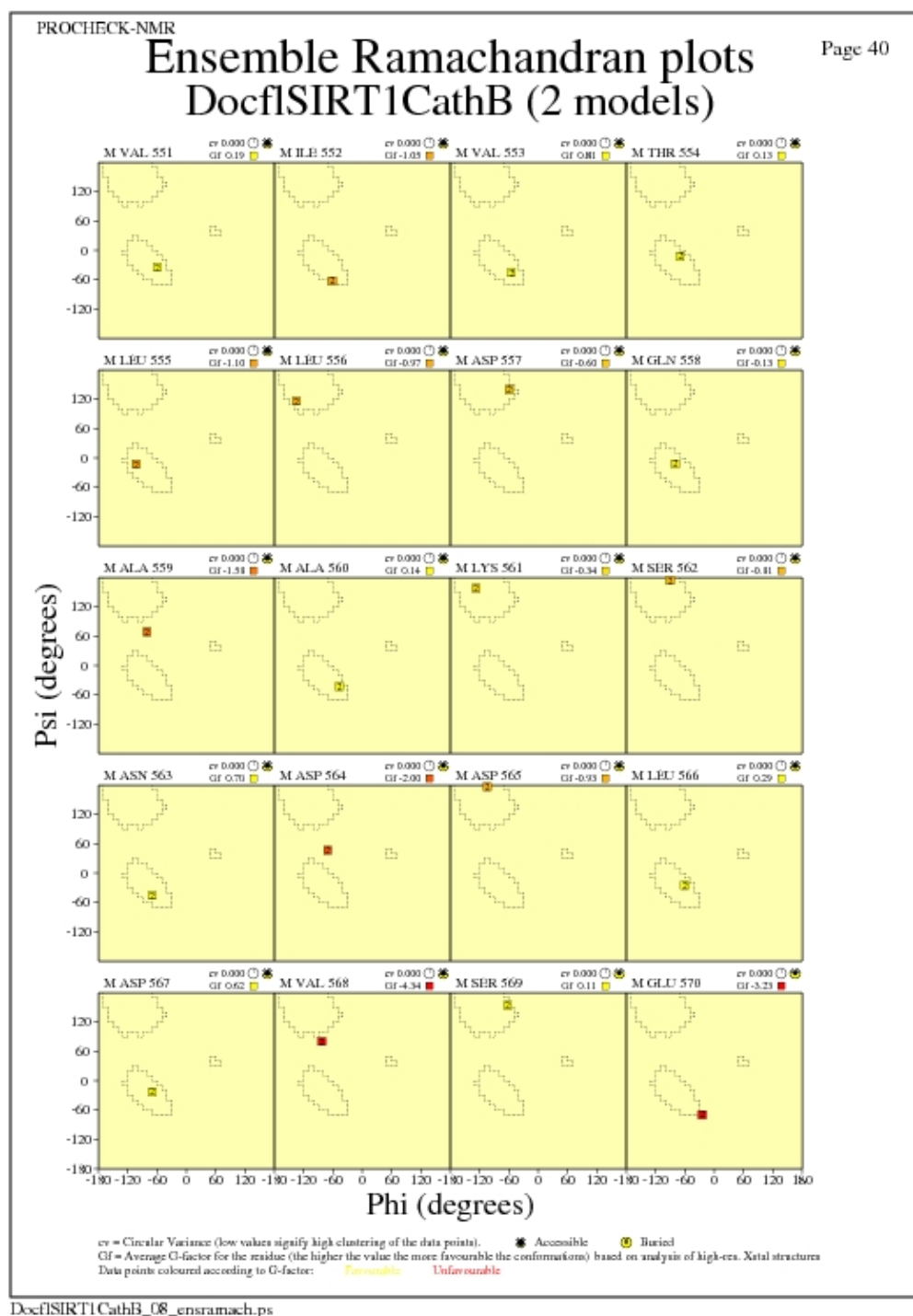
JPEG for residue Ramachandran Plots - page \$num_n



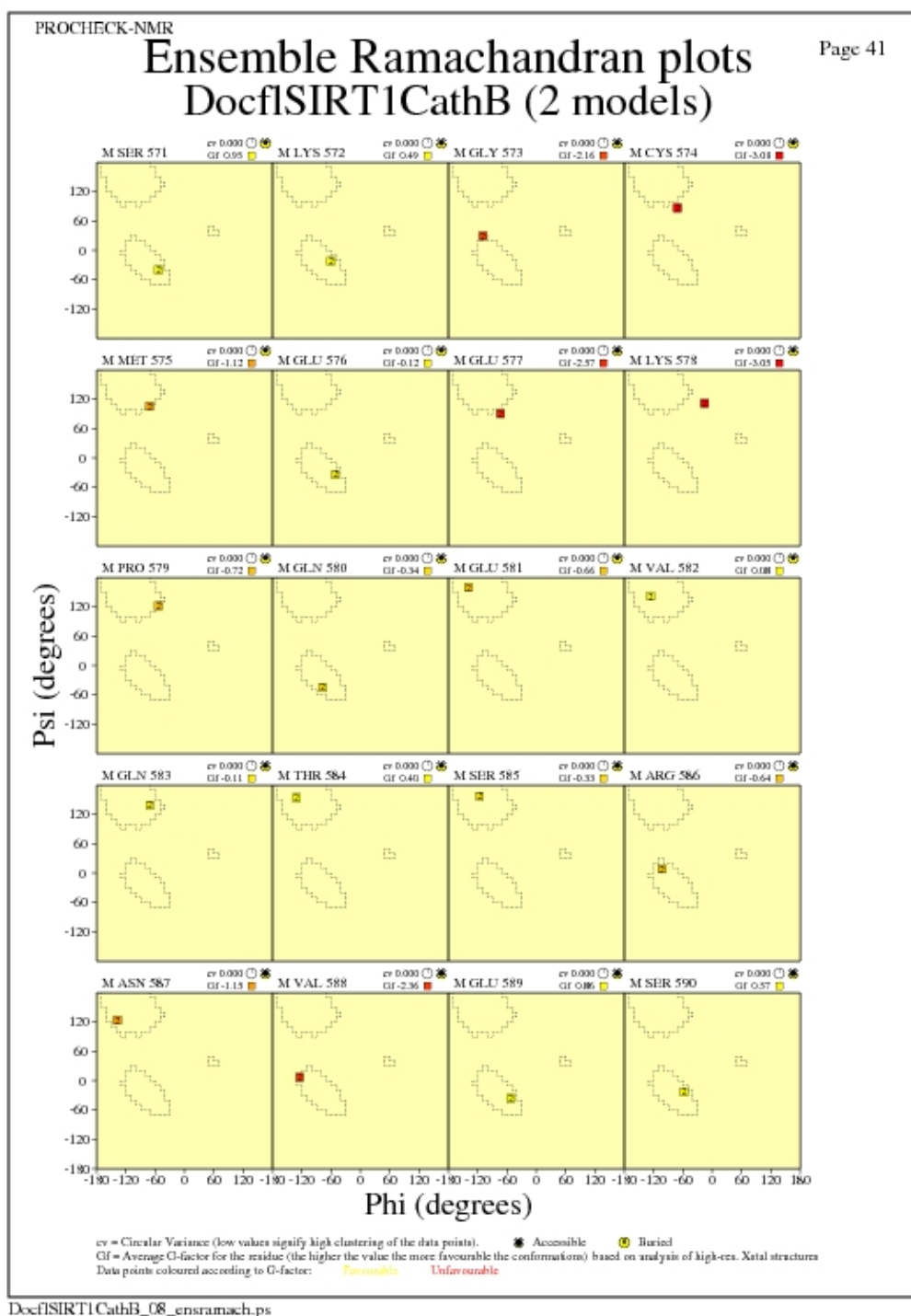
JPEG for residue Ramachandran Plots - page \$num_n



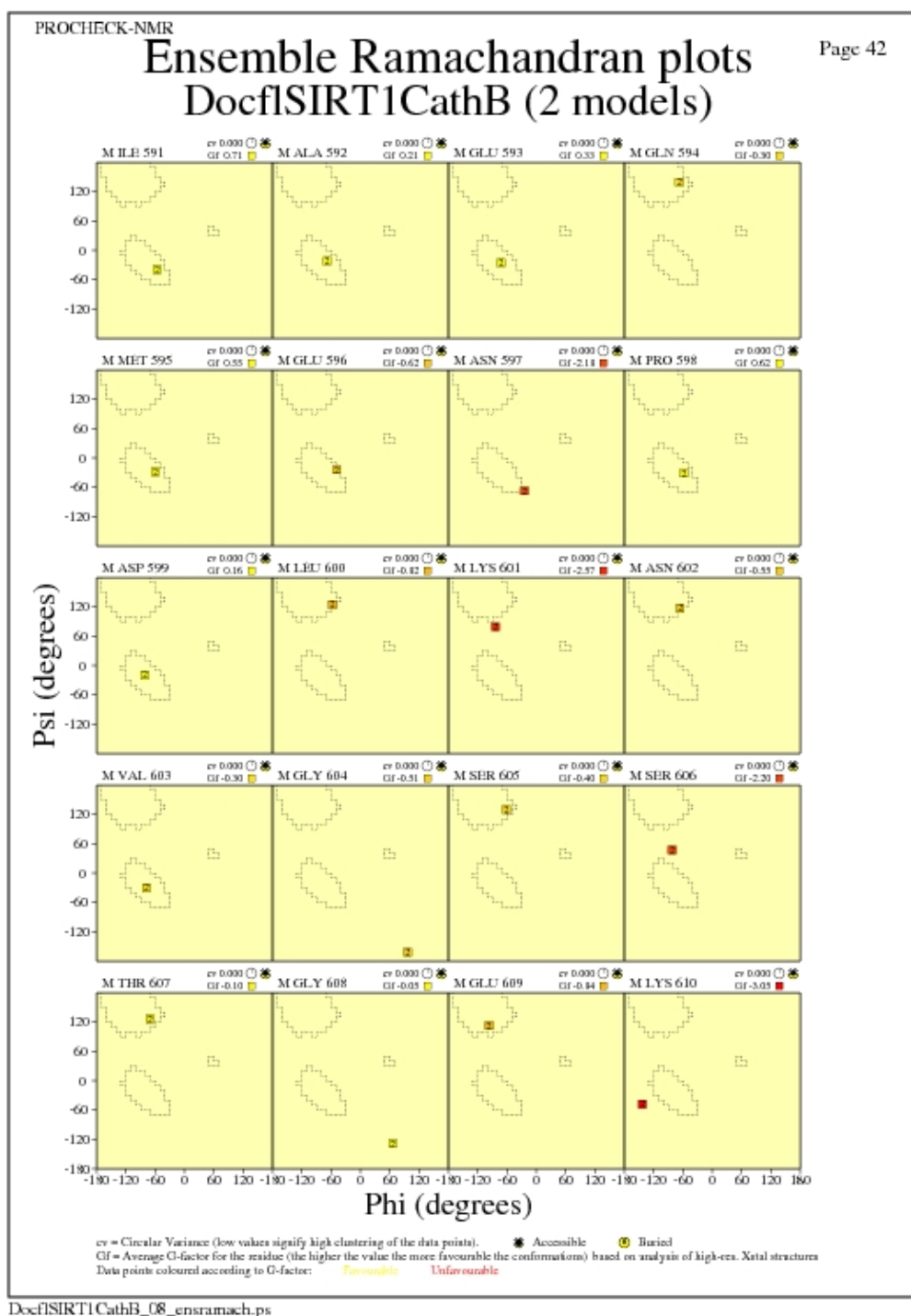
JPEG for residue Ramachandran Plots - page \$num_n



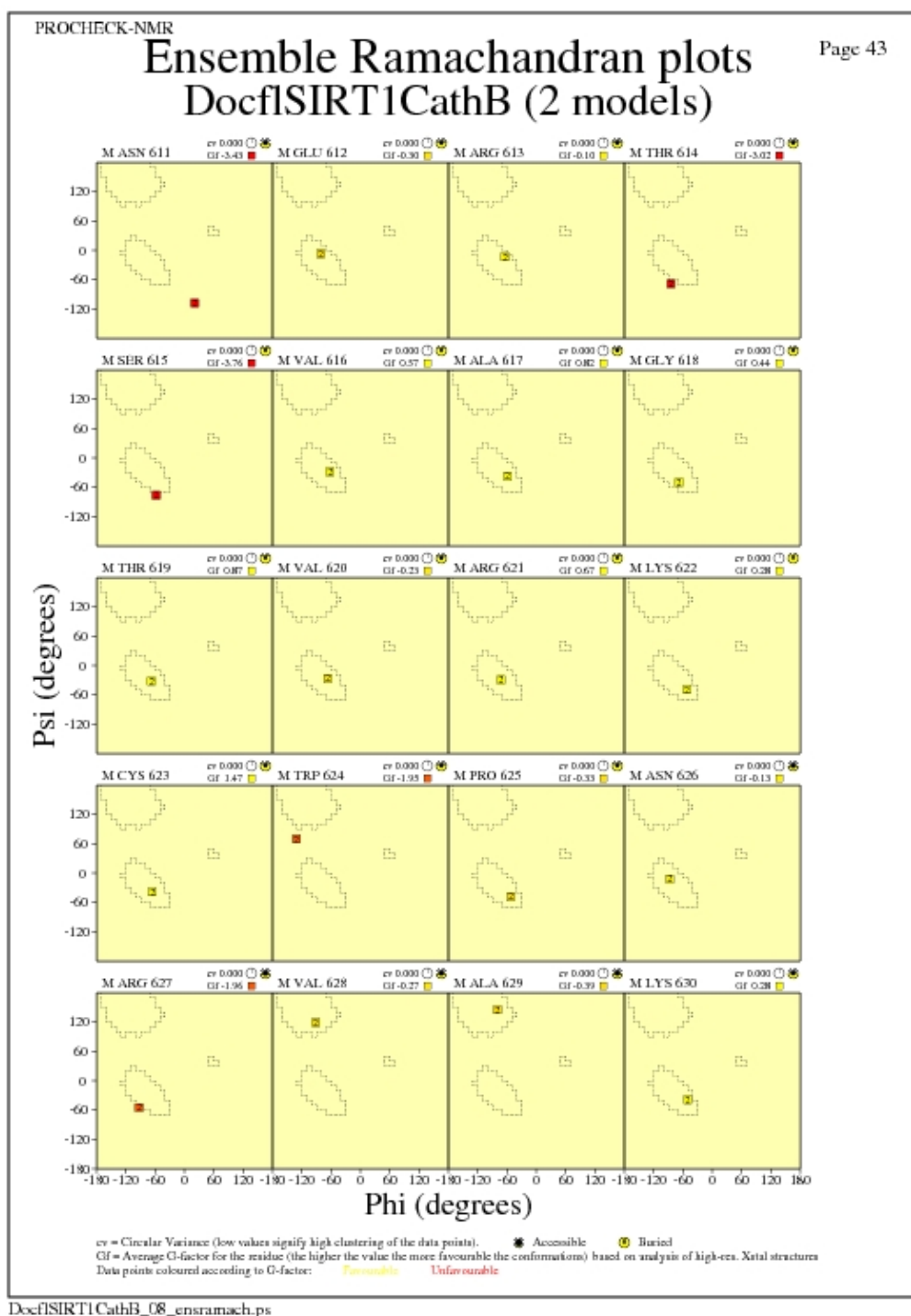
JPEG for residue Ramachandran Plots - page \$num_n



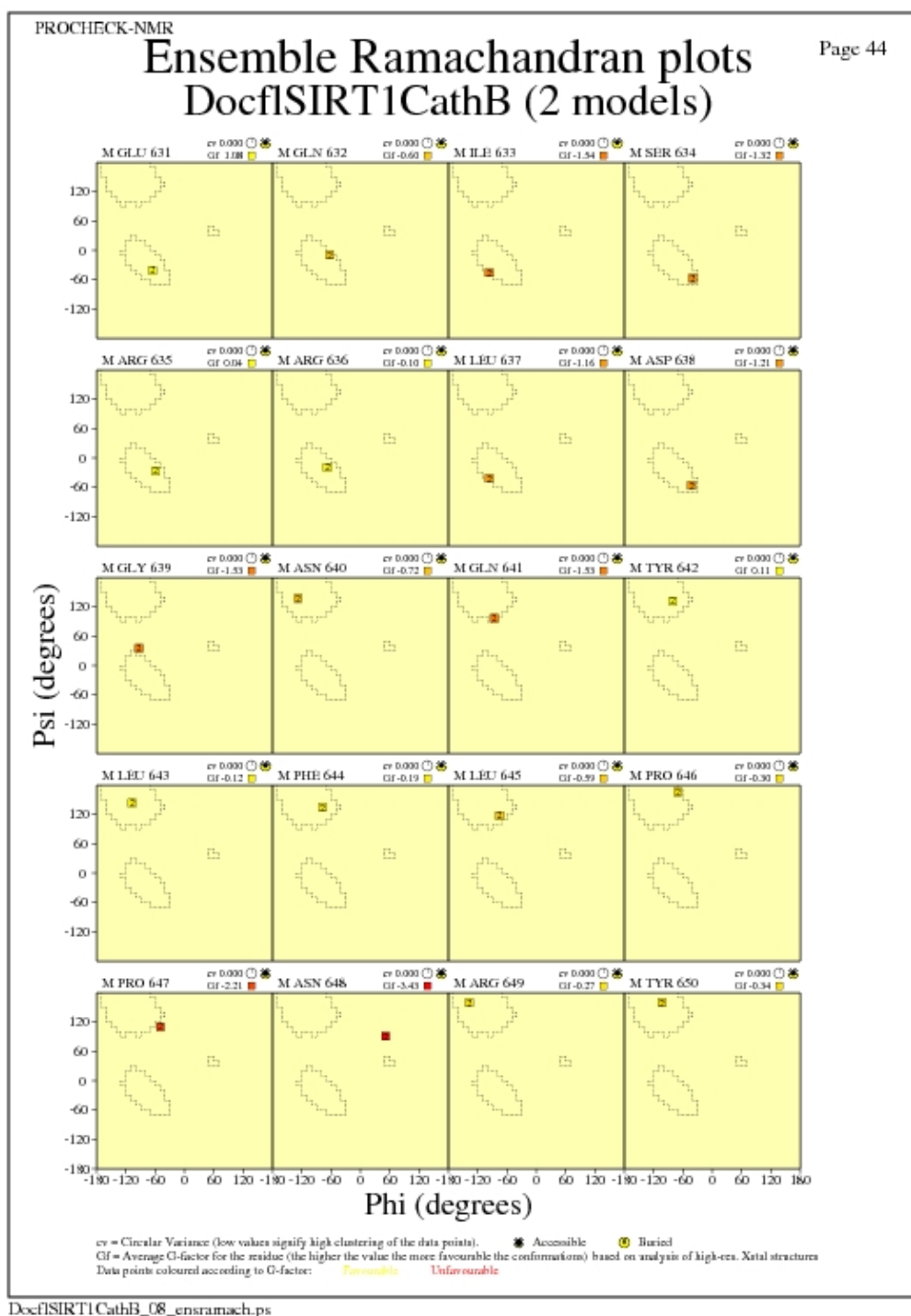
JPEG for residue Ramachandran Plots - page \$num_n



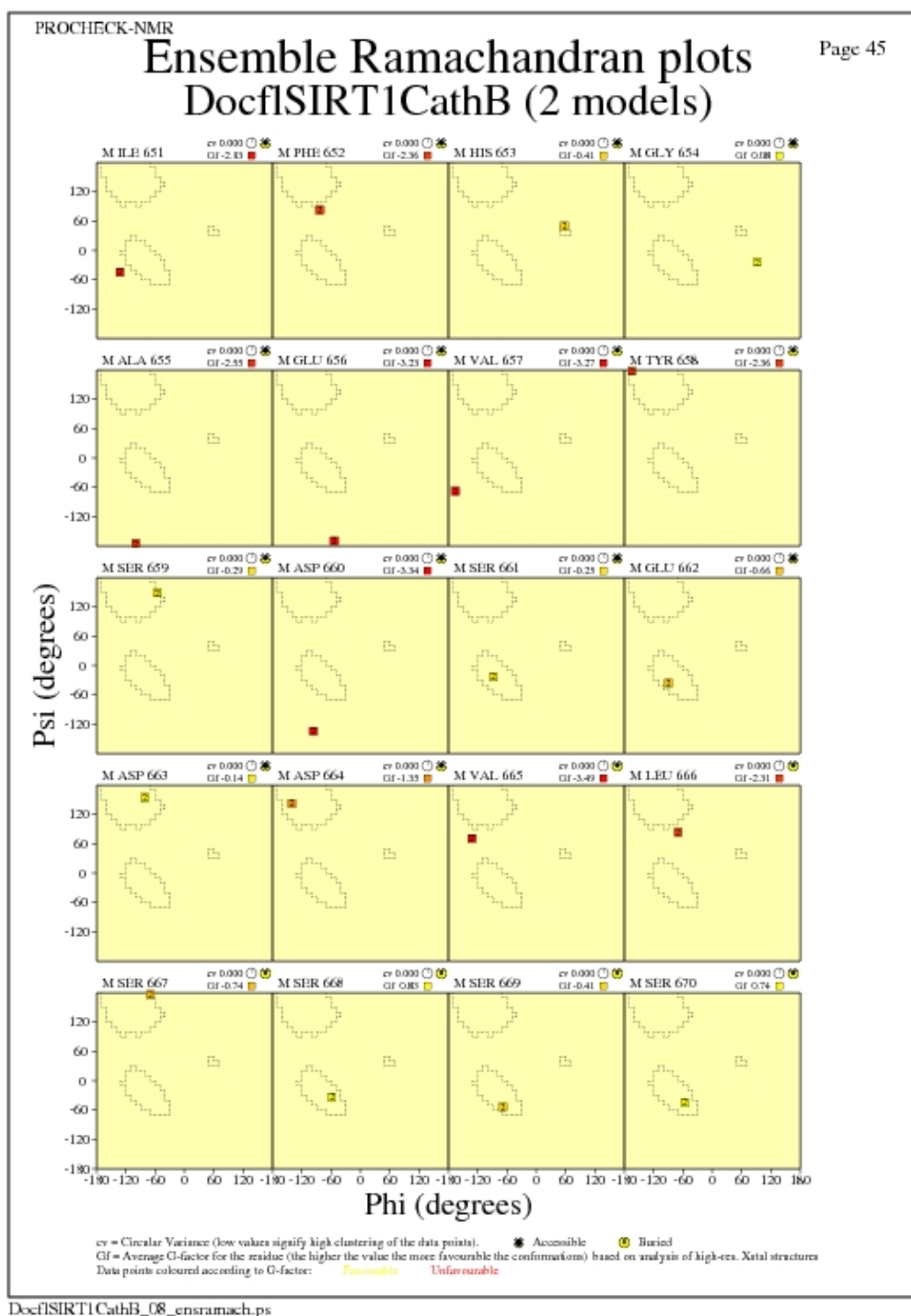
JPEG for residue Ramachandran Plots - page \$num_n



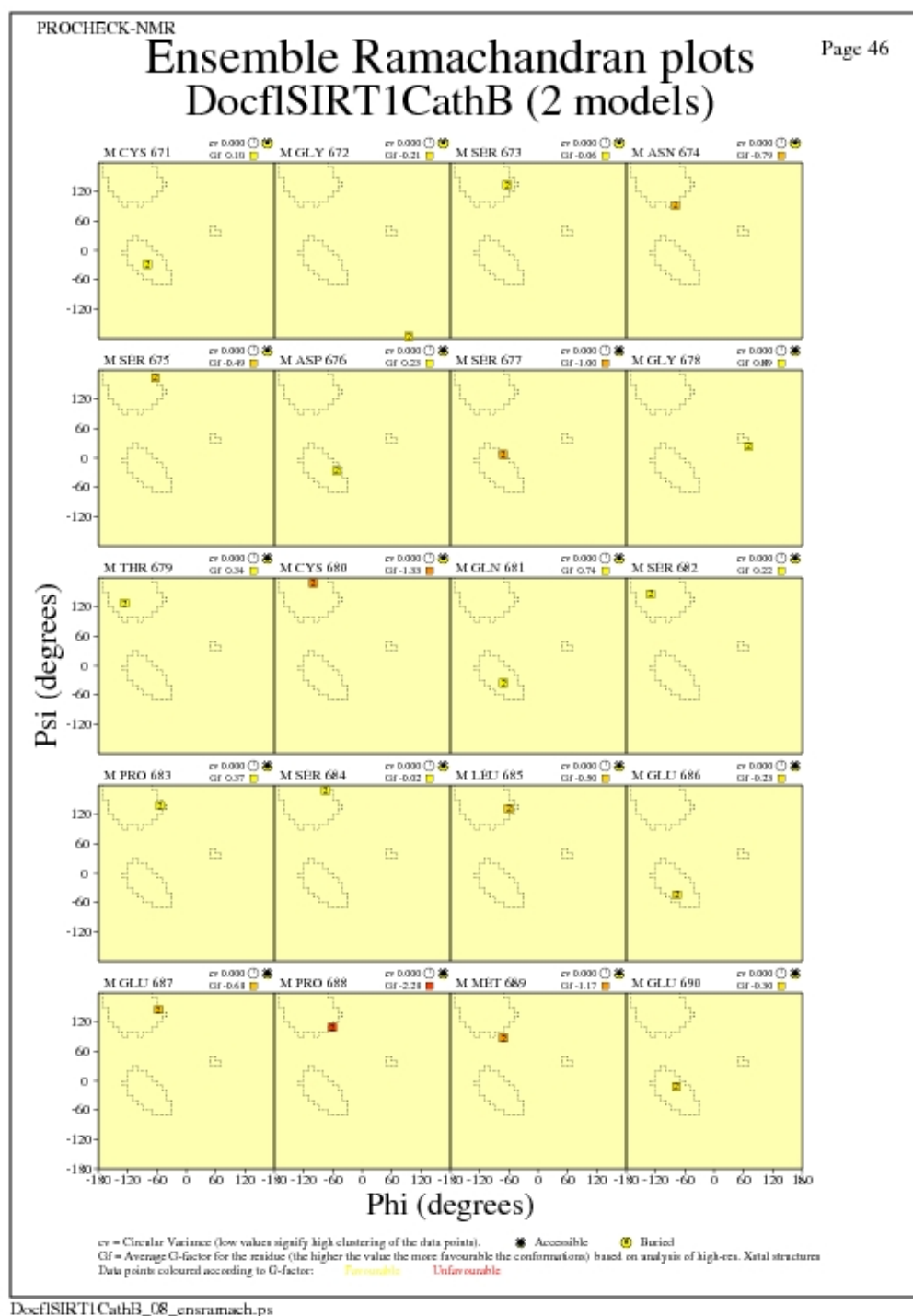
JPEG for residue Ramachandran Plots - page \$num_n



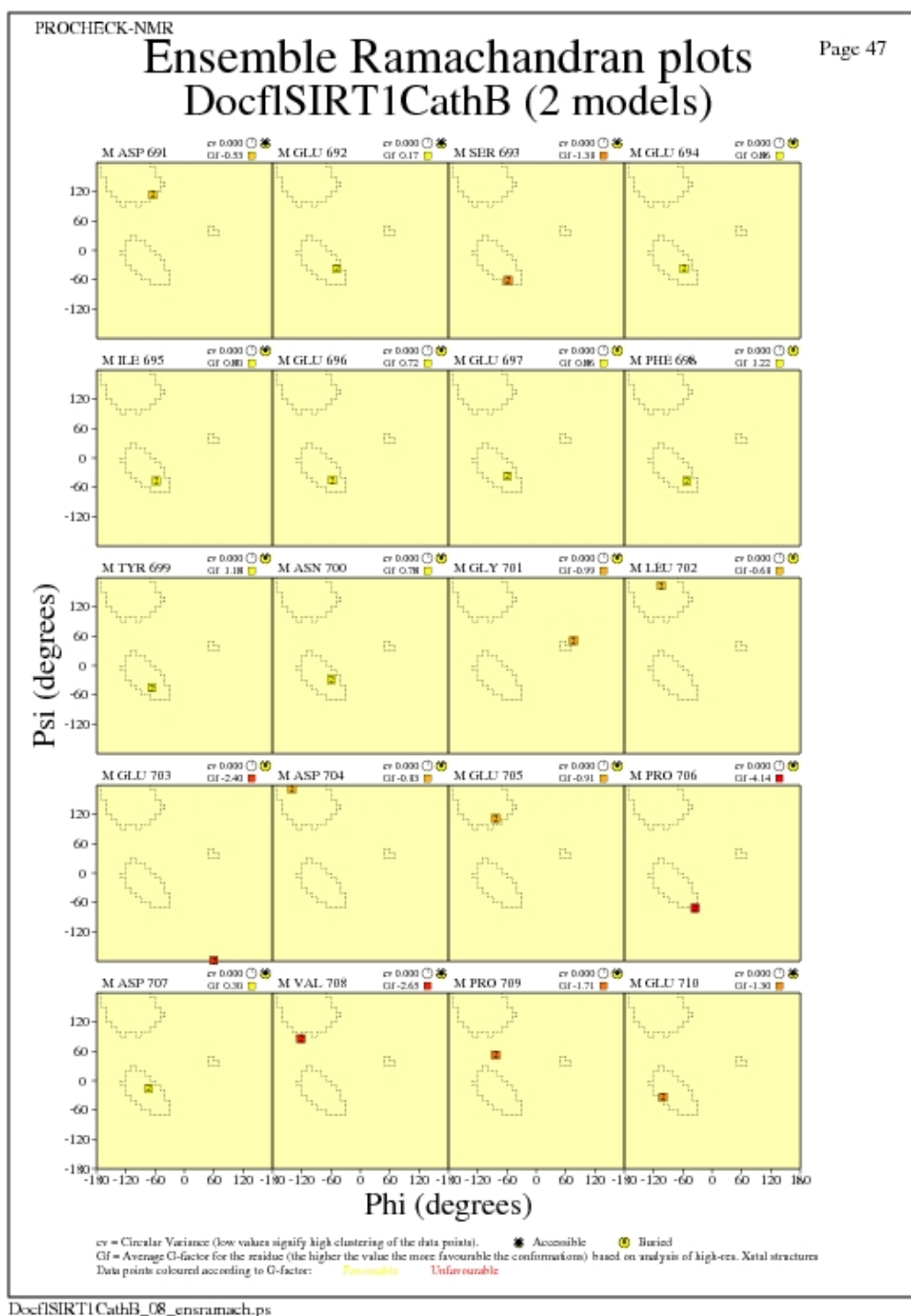
JPEG for residue Ramachandran Plots - page \$num_n



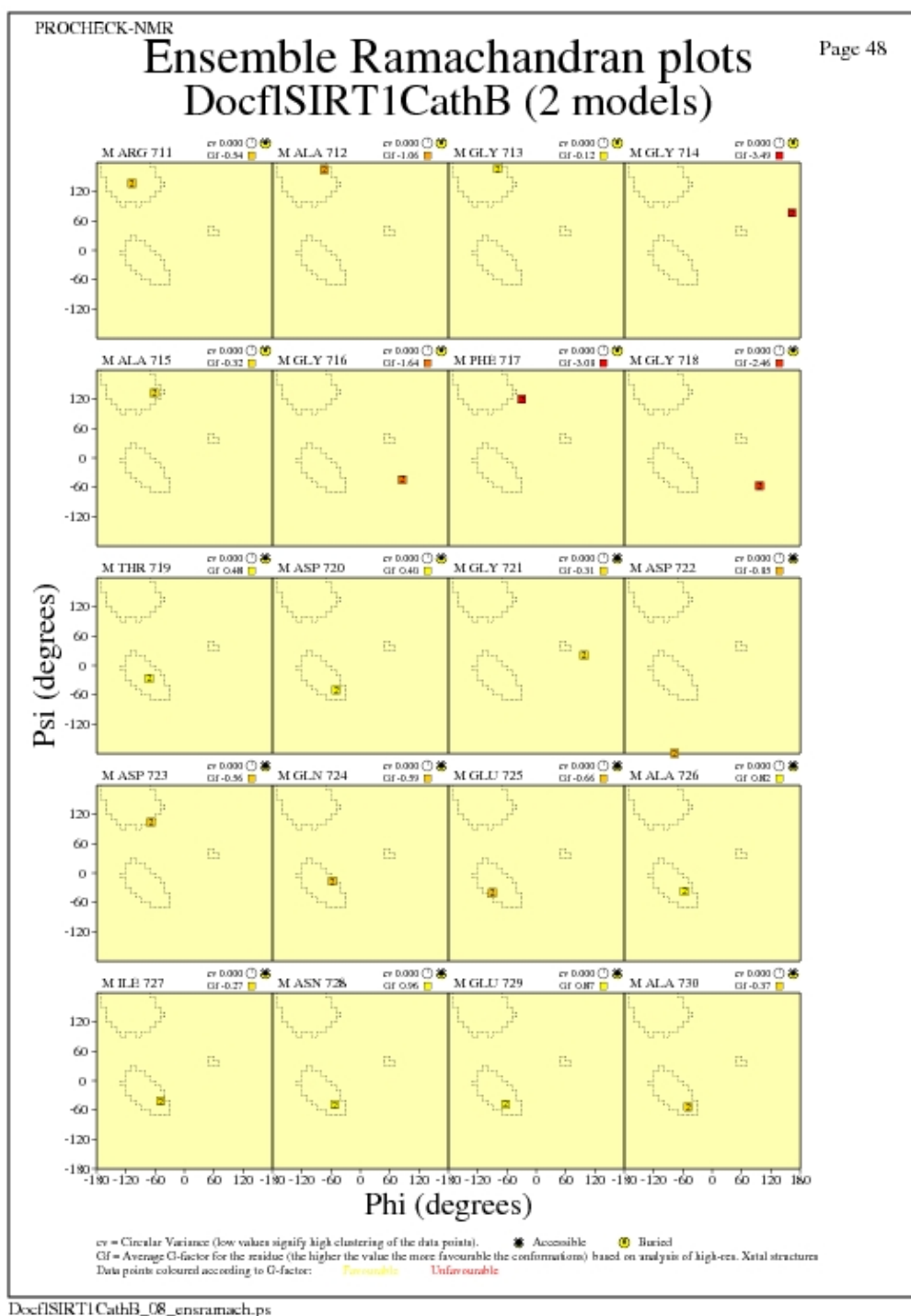
JPEG for residue Ramachandran Plots - page \$num_n



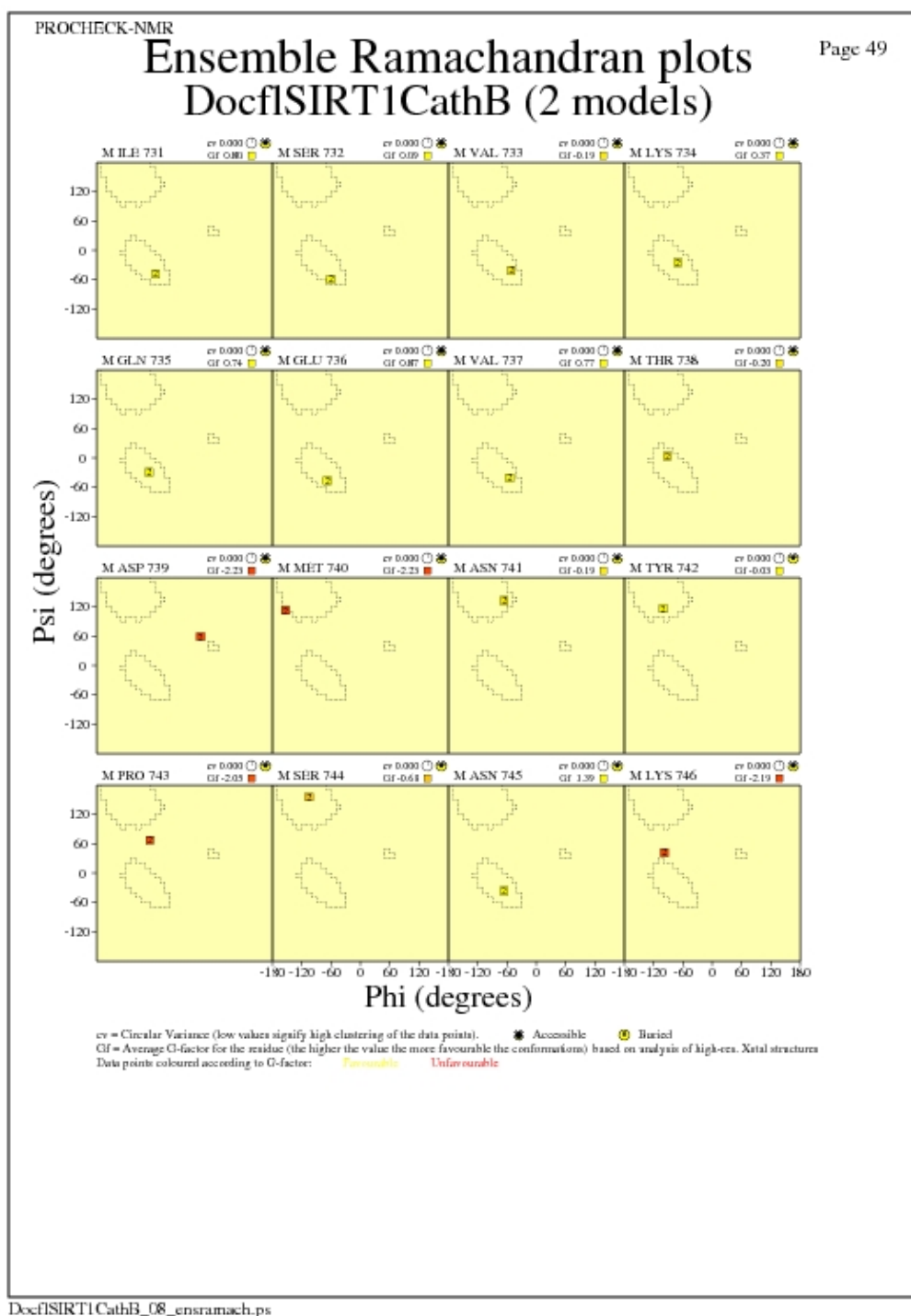
JPEG for residue Ramachandran Plots - page \$num_n



JPEG for residue Ramachandran Plots - page \$num_n



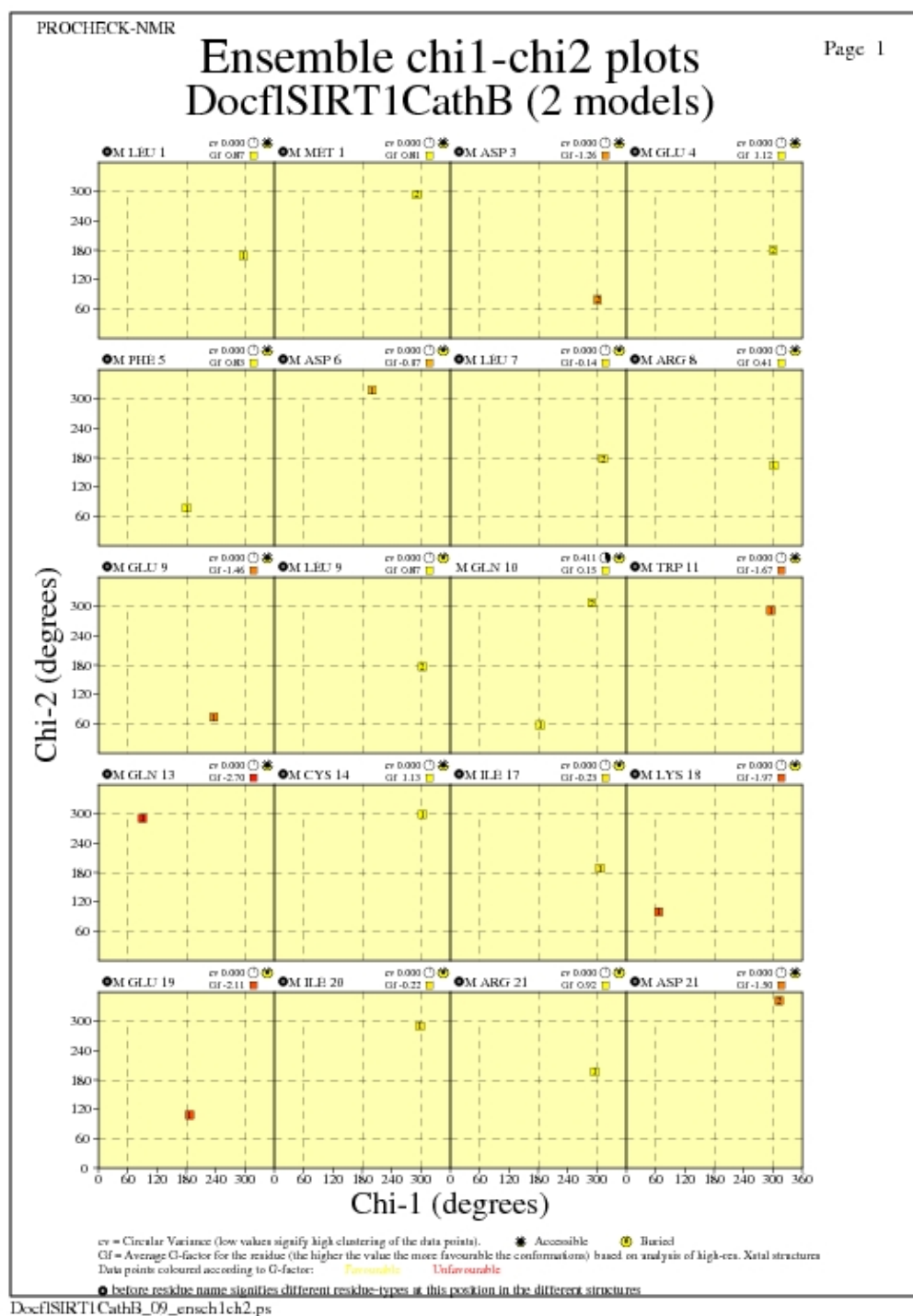
JPEG for residue Ramachandran Plots - page \$num_n



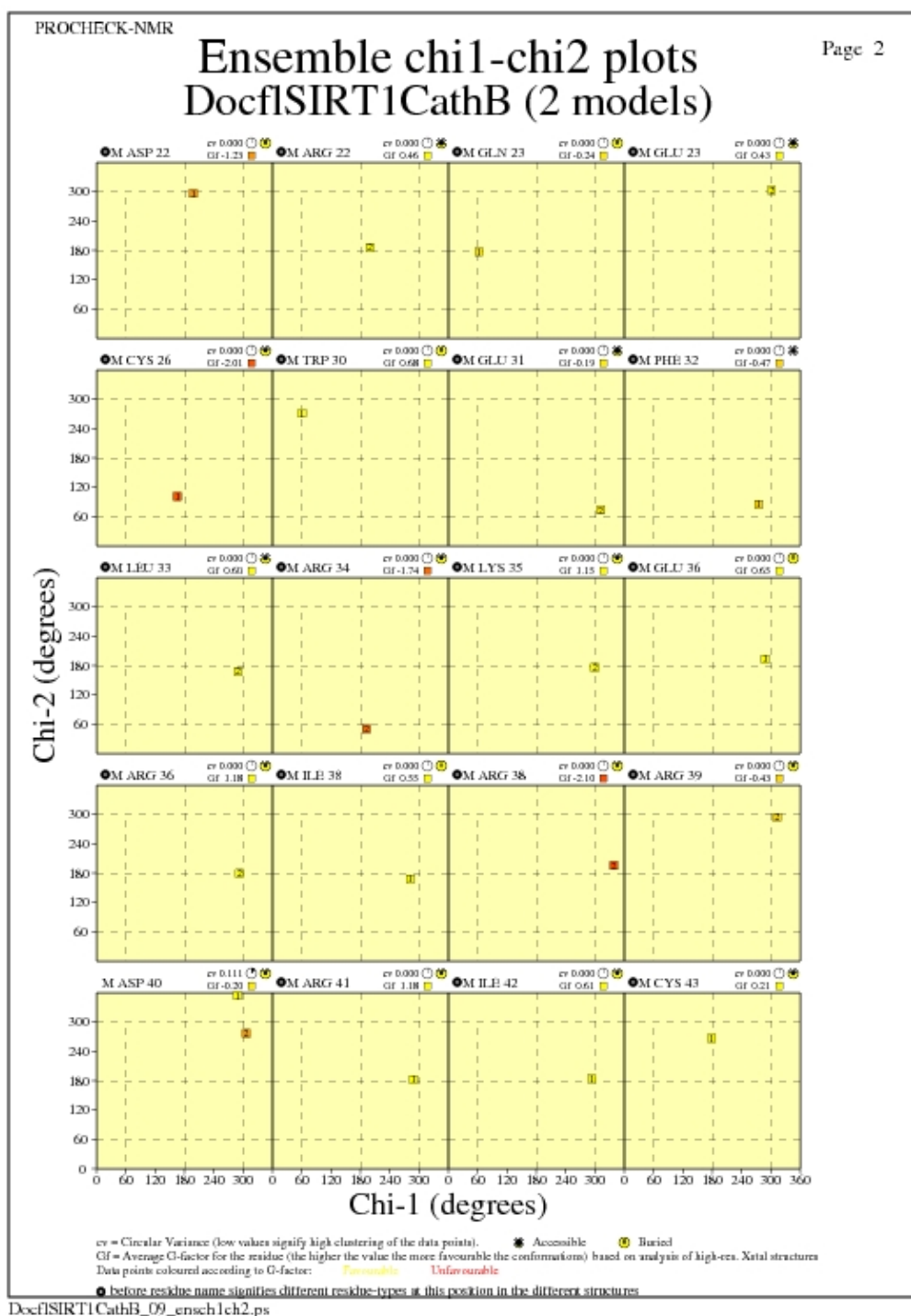
Ramachandran analysis for each residue from Molprobit

Chi1-Chi2 Plots for each residue

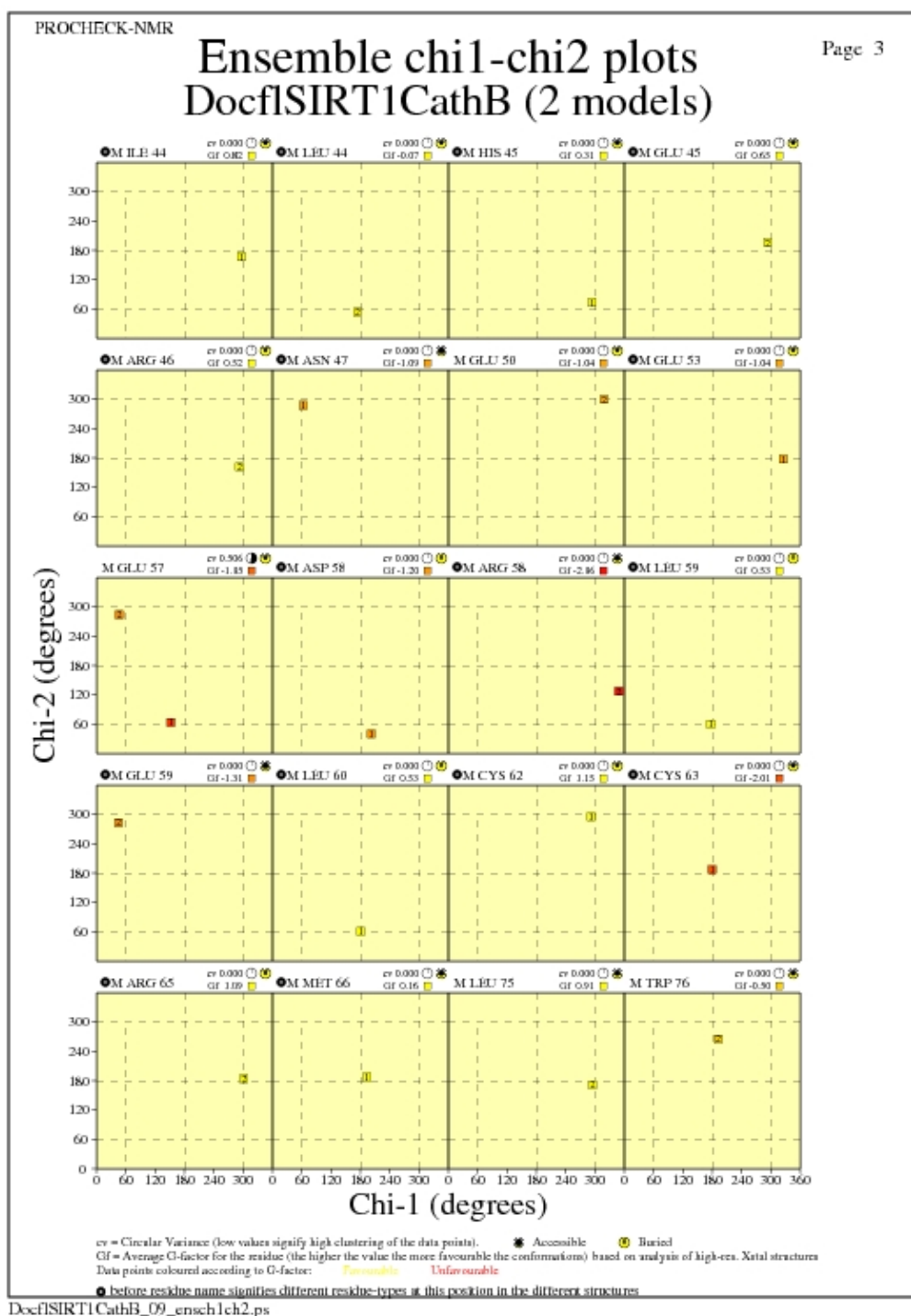
JPEG for residue Chi1-Chi2 Plots - page \$num_n



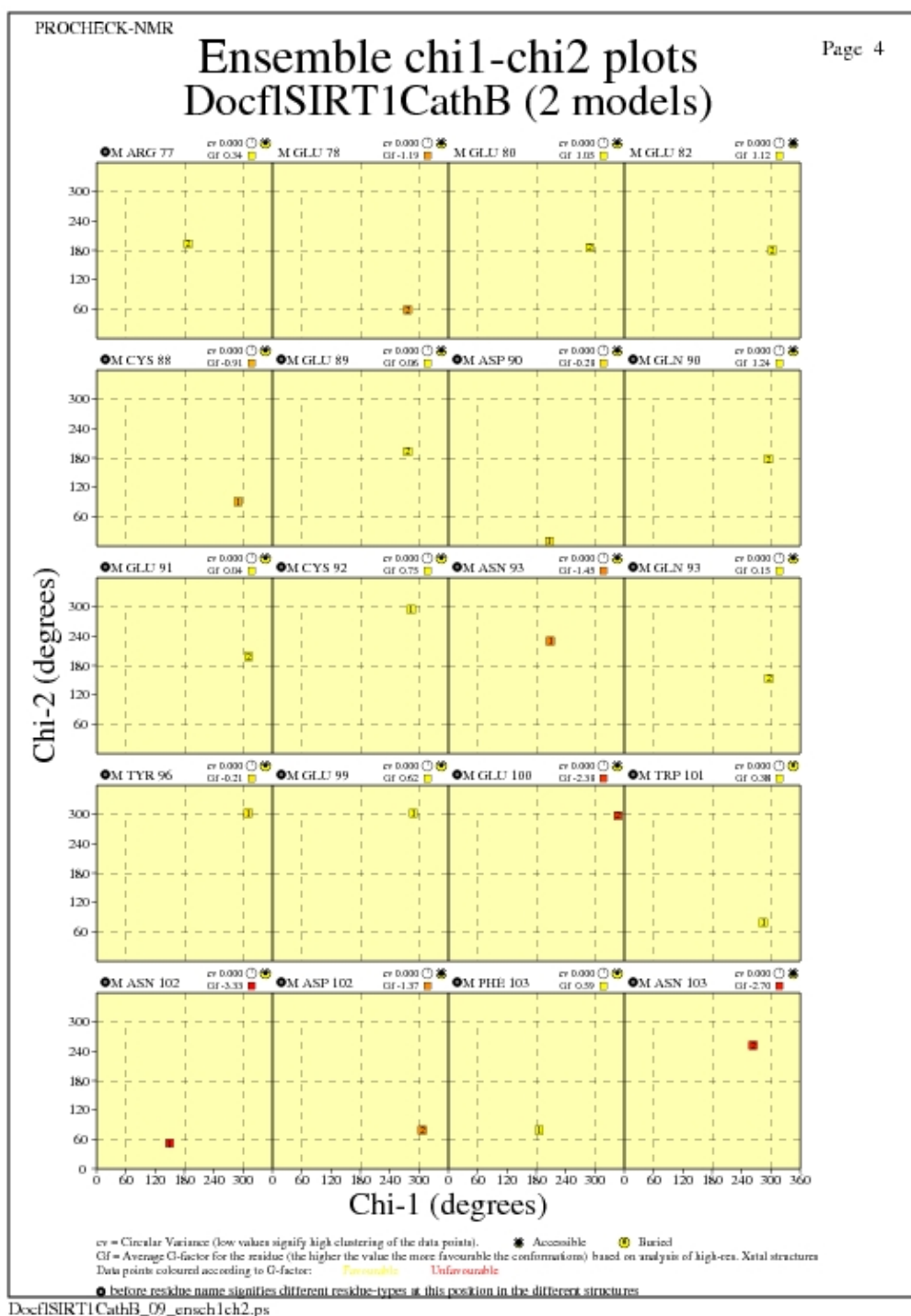
JPEG for residue Chi1-Chi2 Plots - page \$num_n



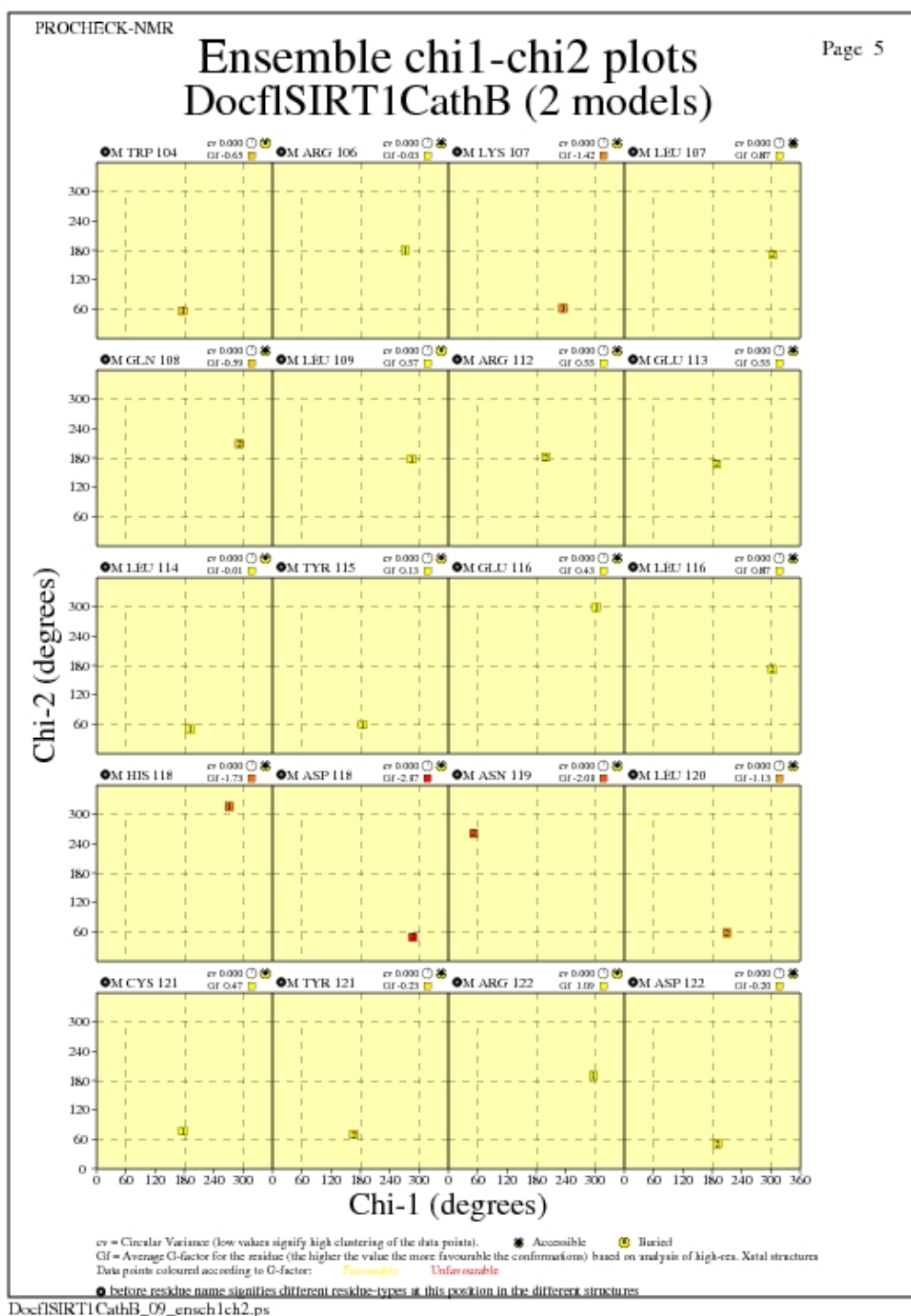
JPEG for residue Chi1-Chi2 Plots - page \$num_n



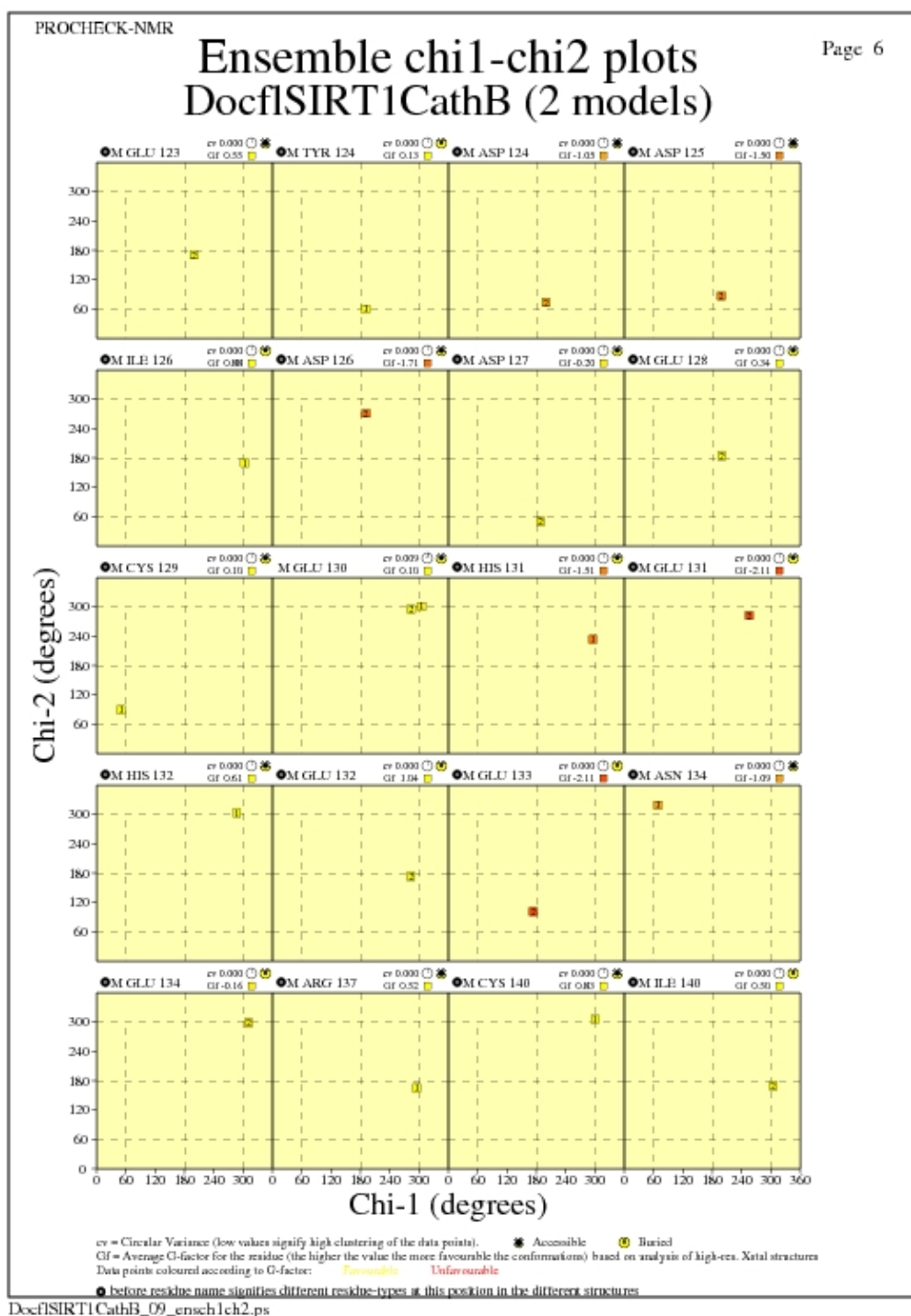
JPEG for residue Chi1-Chi2 Plots - page \$num_n



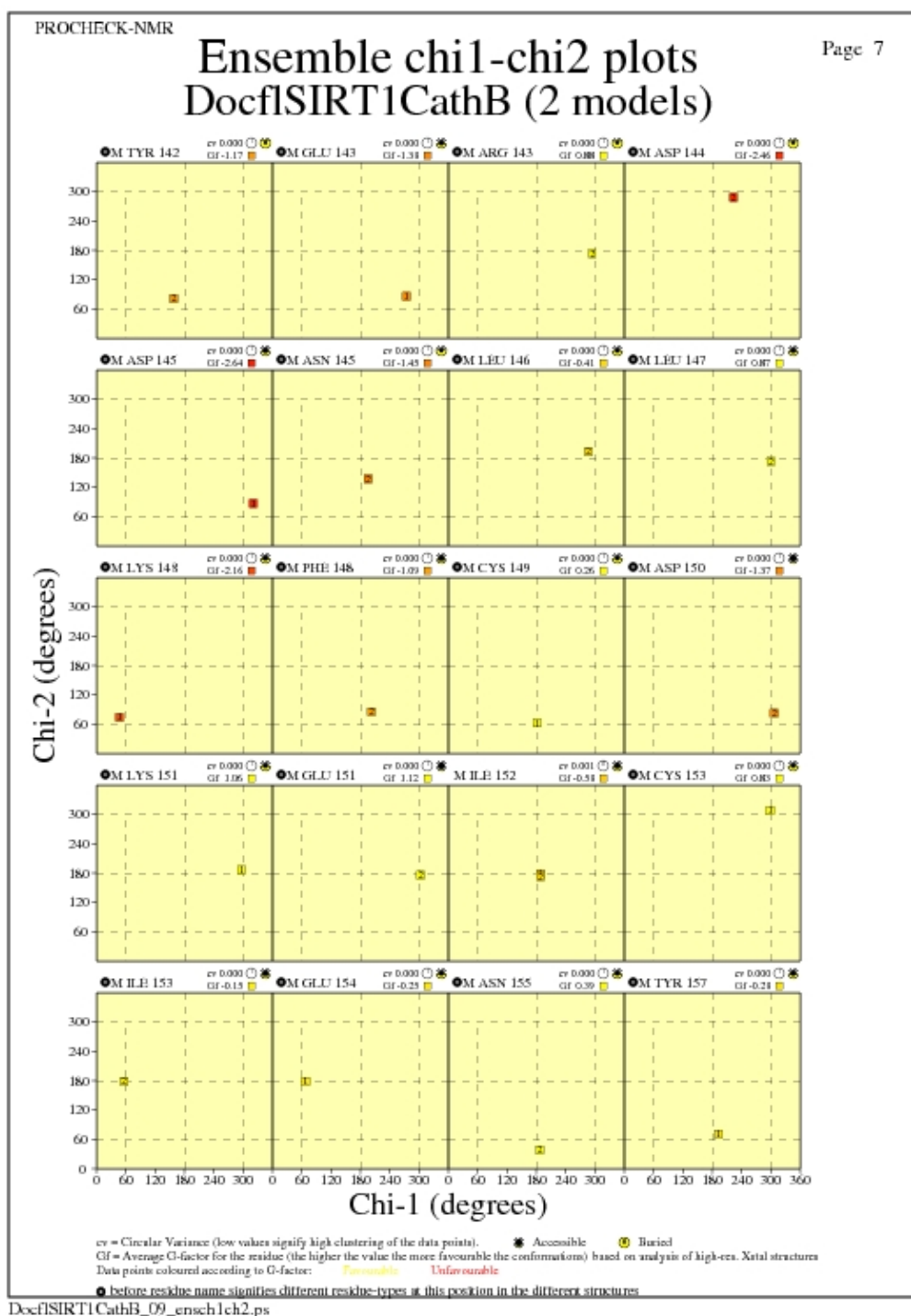
JPEG for residue Chi1-Chi2 Plots - page \$num_n



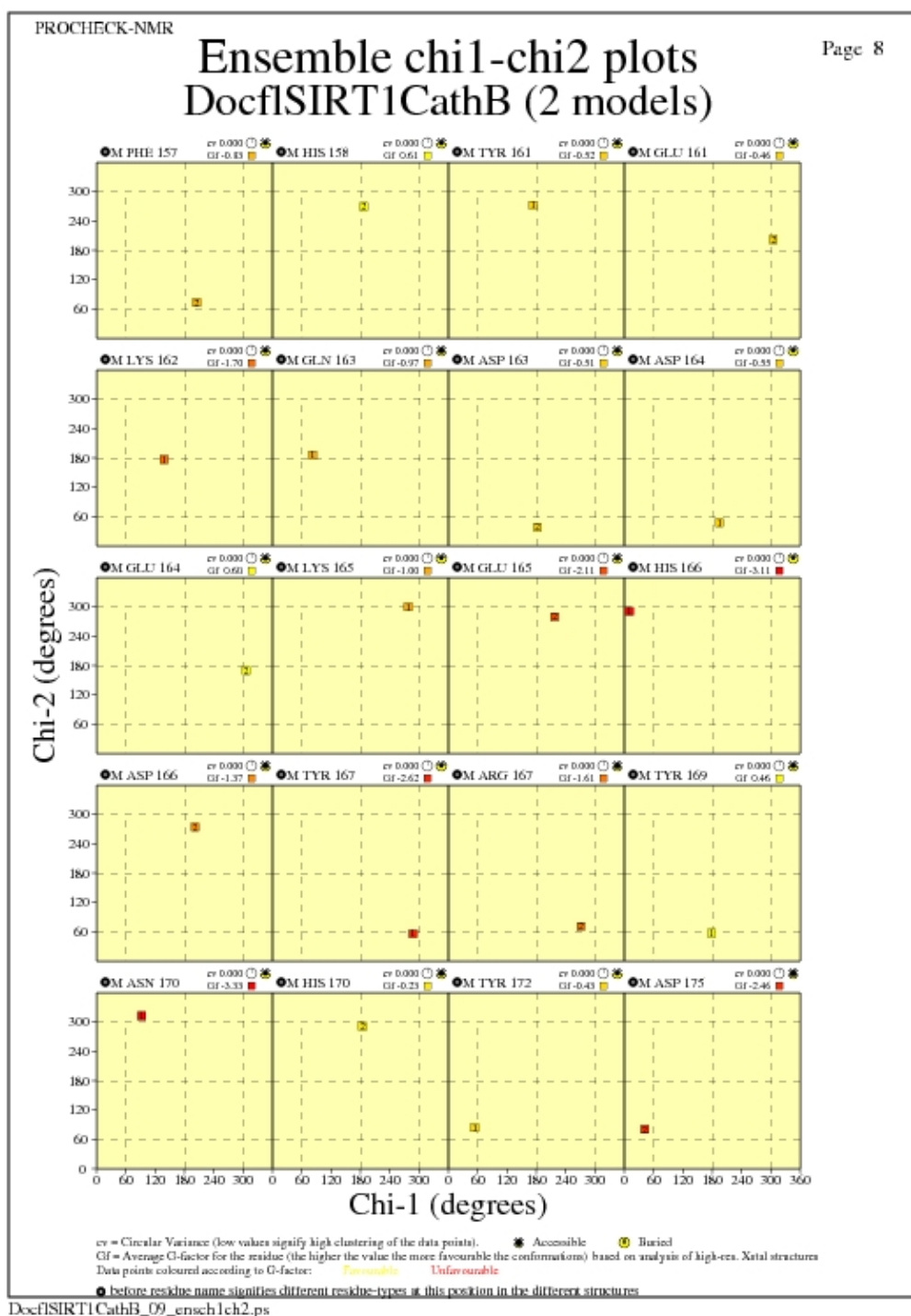
JPEG for residue Chi1-Chi2 Plots - page \$num_n



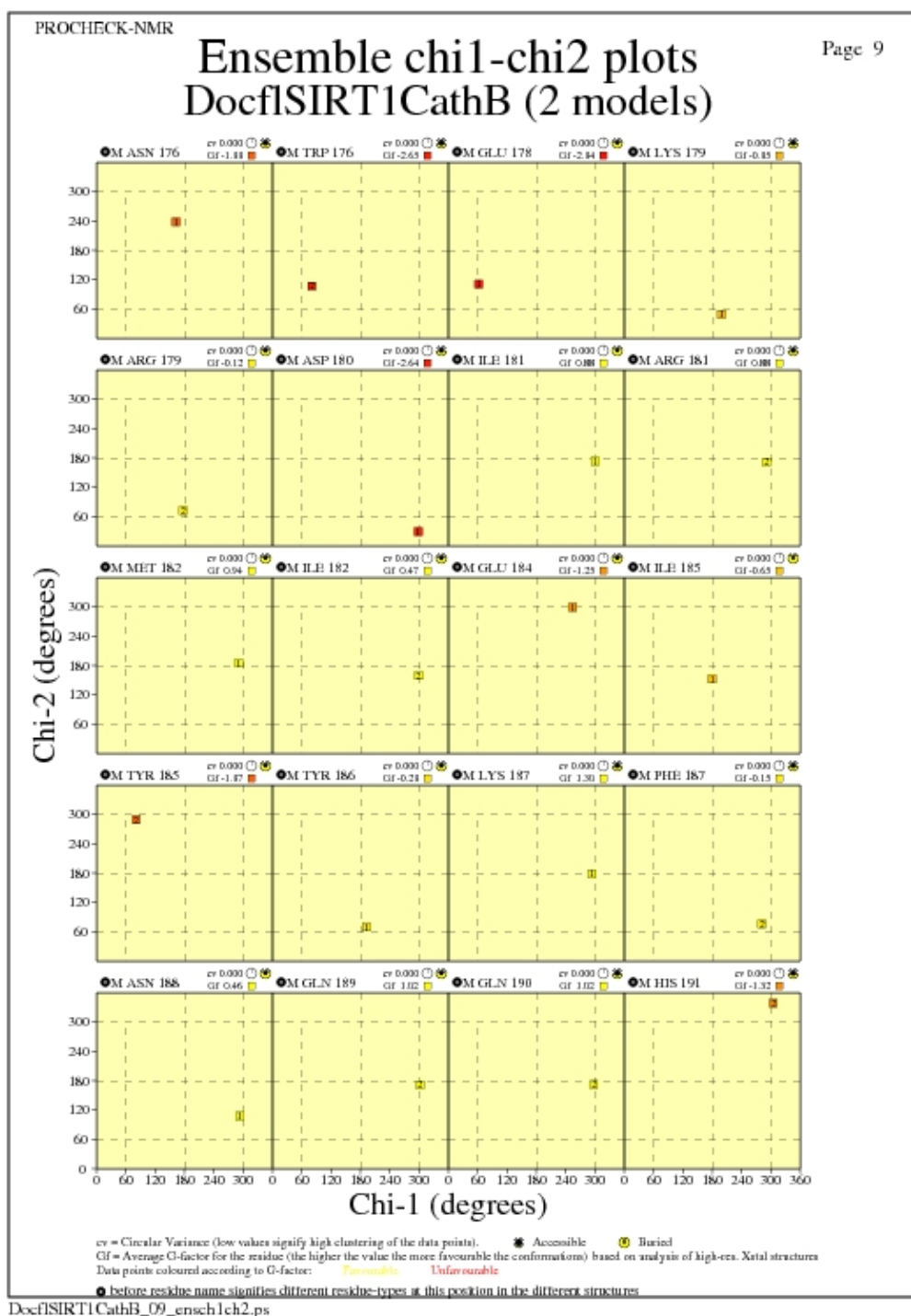
JPEG for residue Chi1-Chi2 Plots - page \$num_n



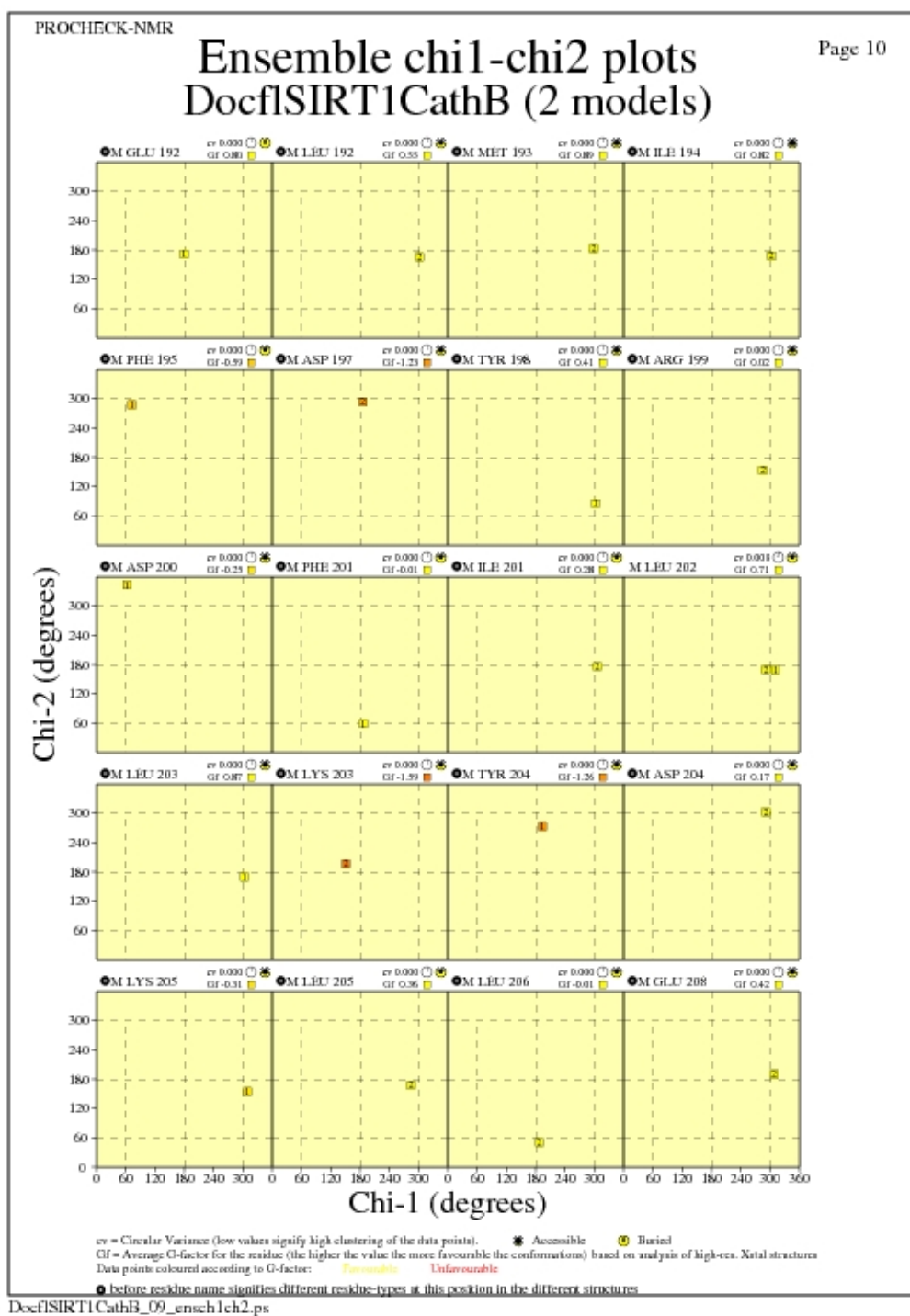
JPEG for residue Chi1-Chi2 Plots - page \$num_n



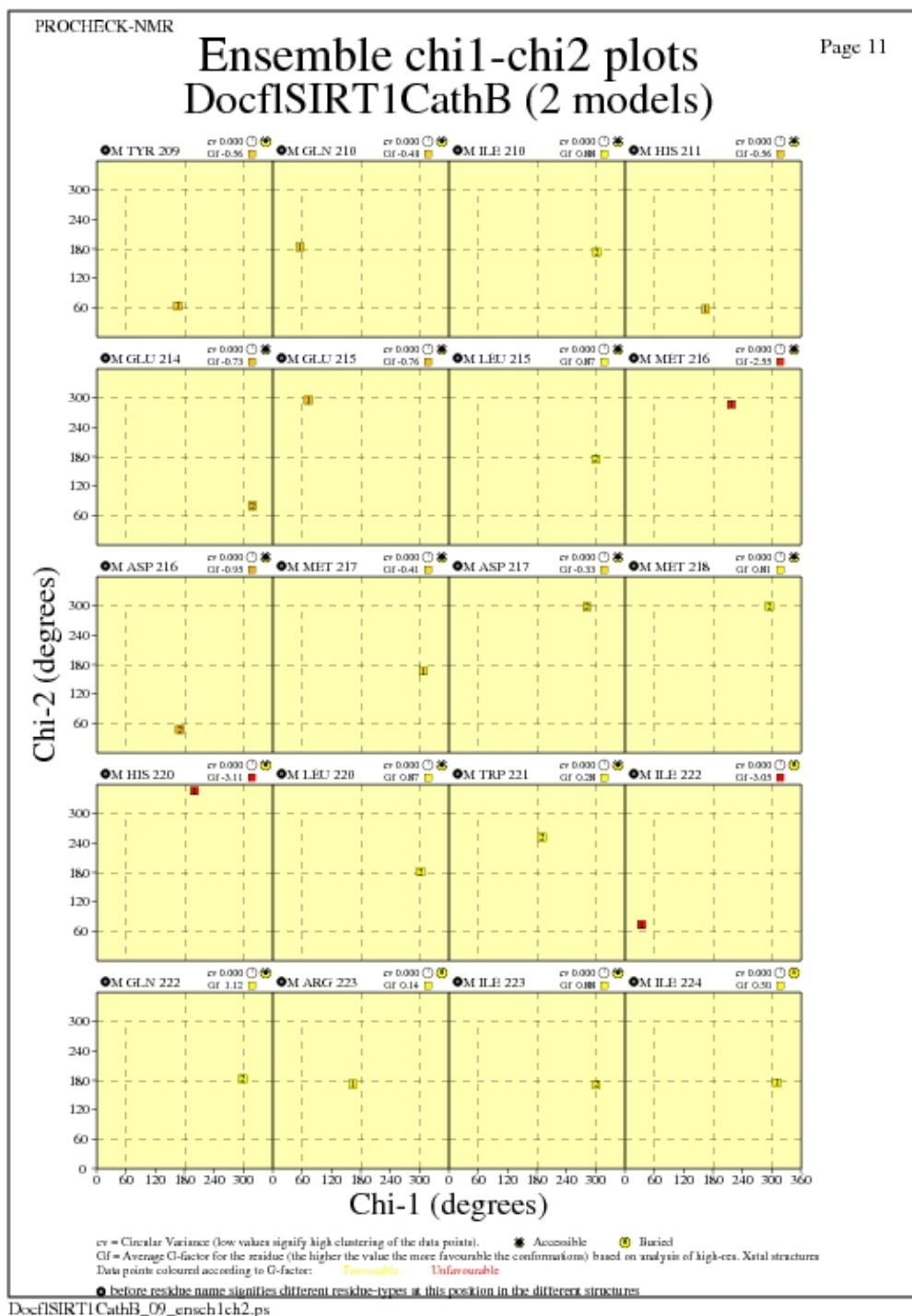
JPEG for residue Chi1-Chi2 Plots - page \$num_n



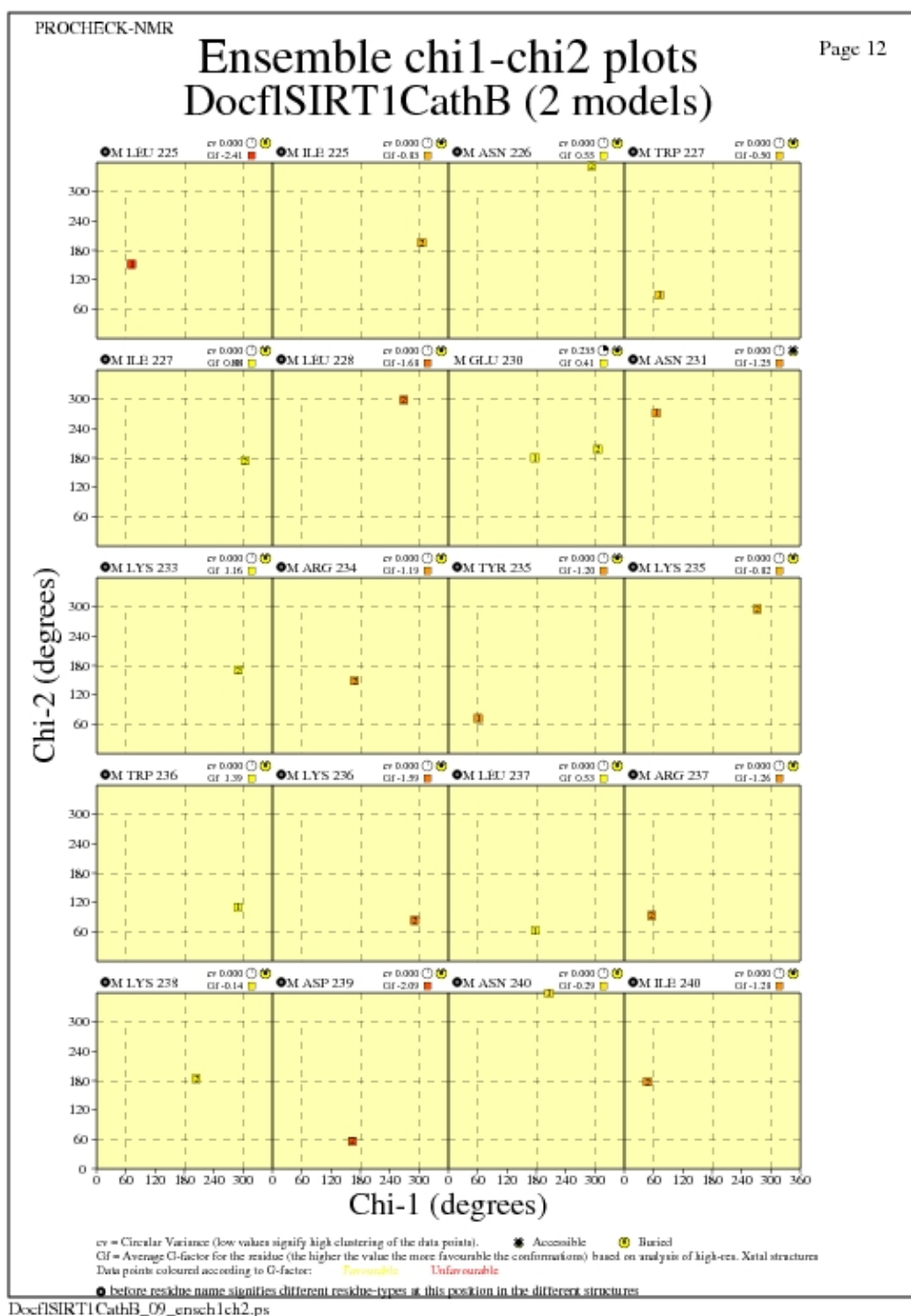
JPEG for residue Chi1-Chi2 Plots - page \$num_n



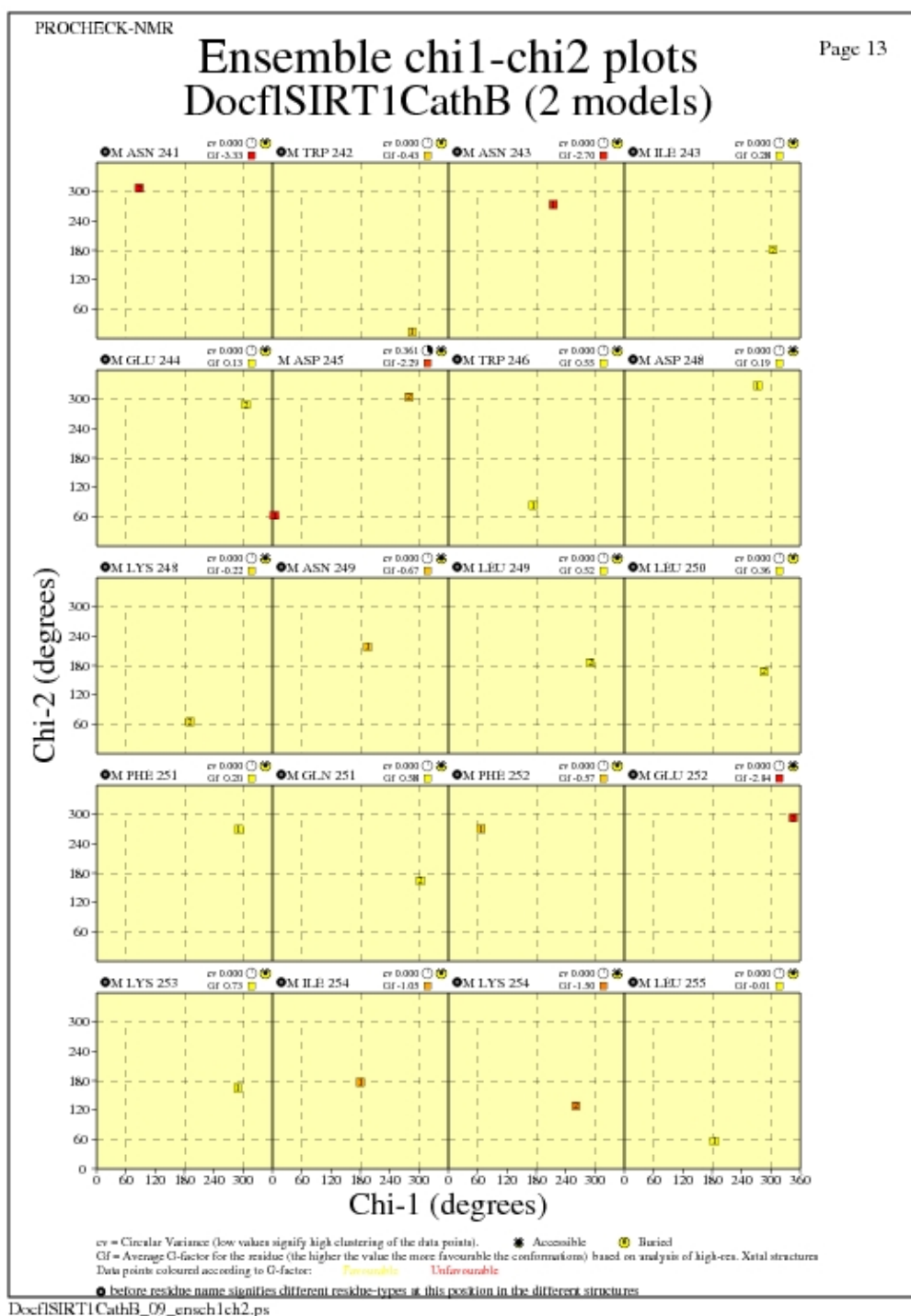
JPEG for residue Chi1-Chi2 Plots - page \$num_n



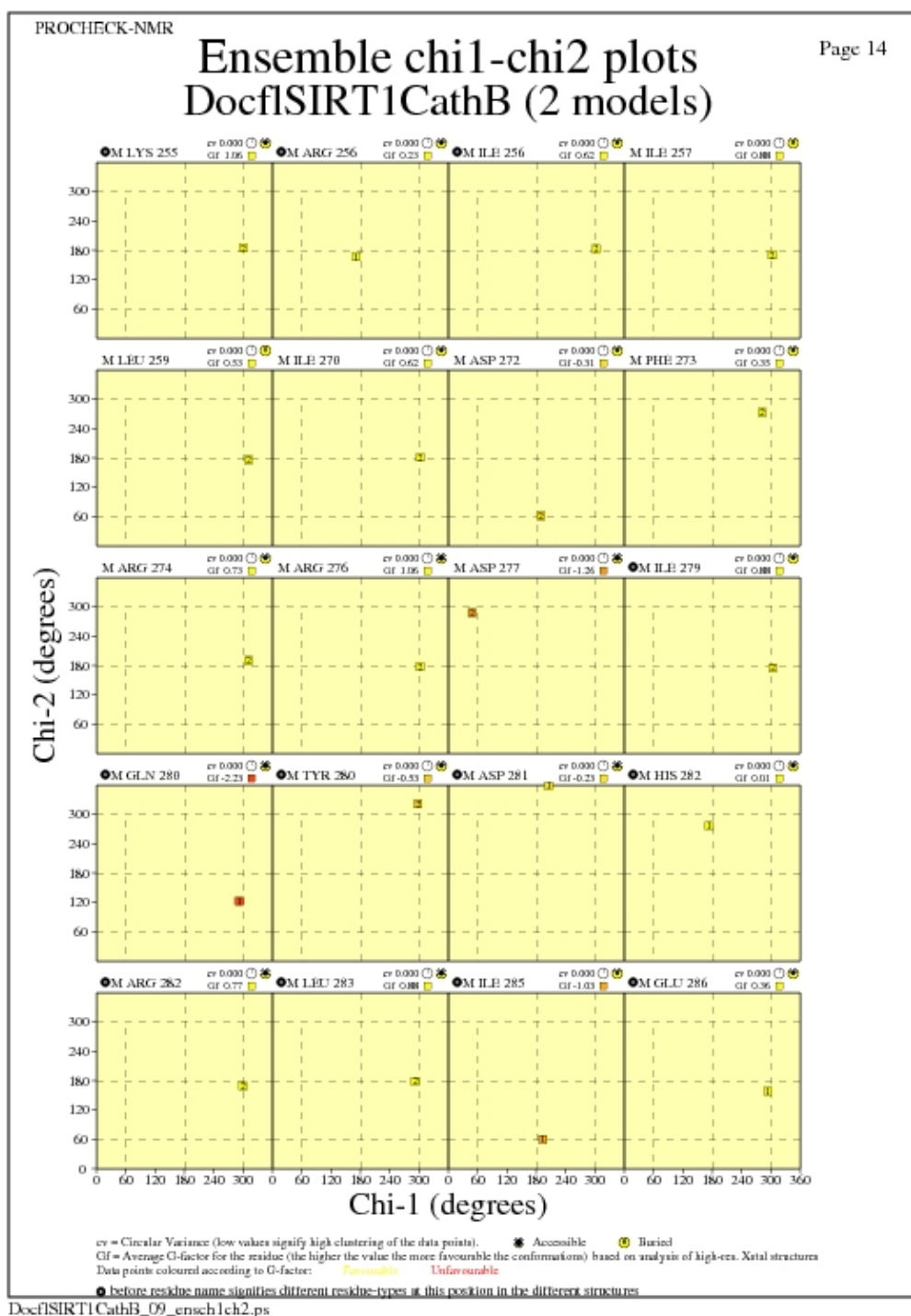
JPEG for residue Chi1-Chi2 Plots - page \$num_n



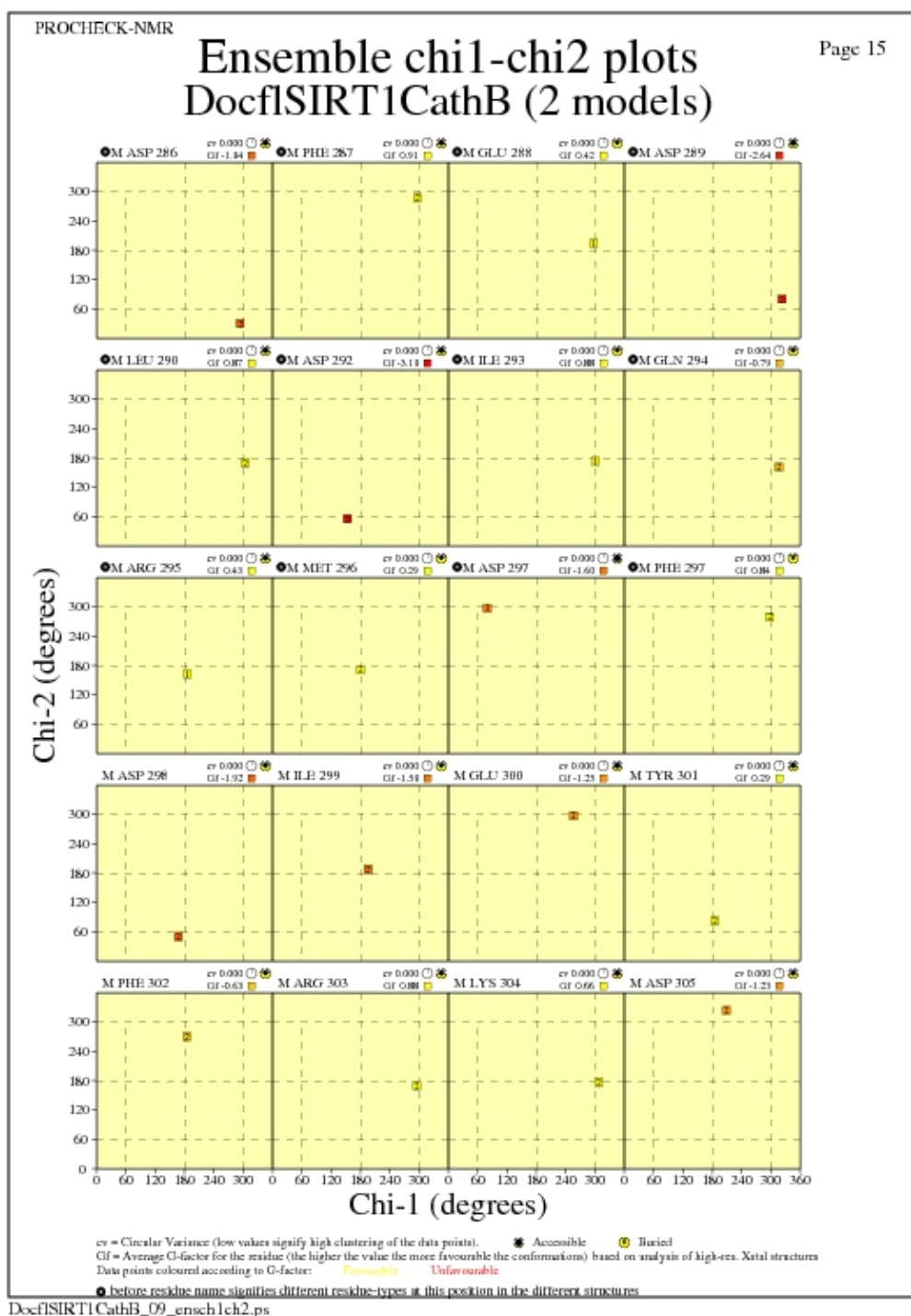
JPEG for residue Chi1-Chi2 Plots - page \$num_n



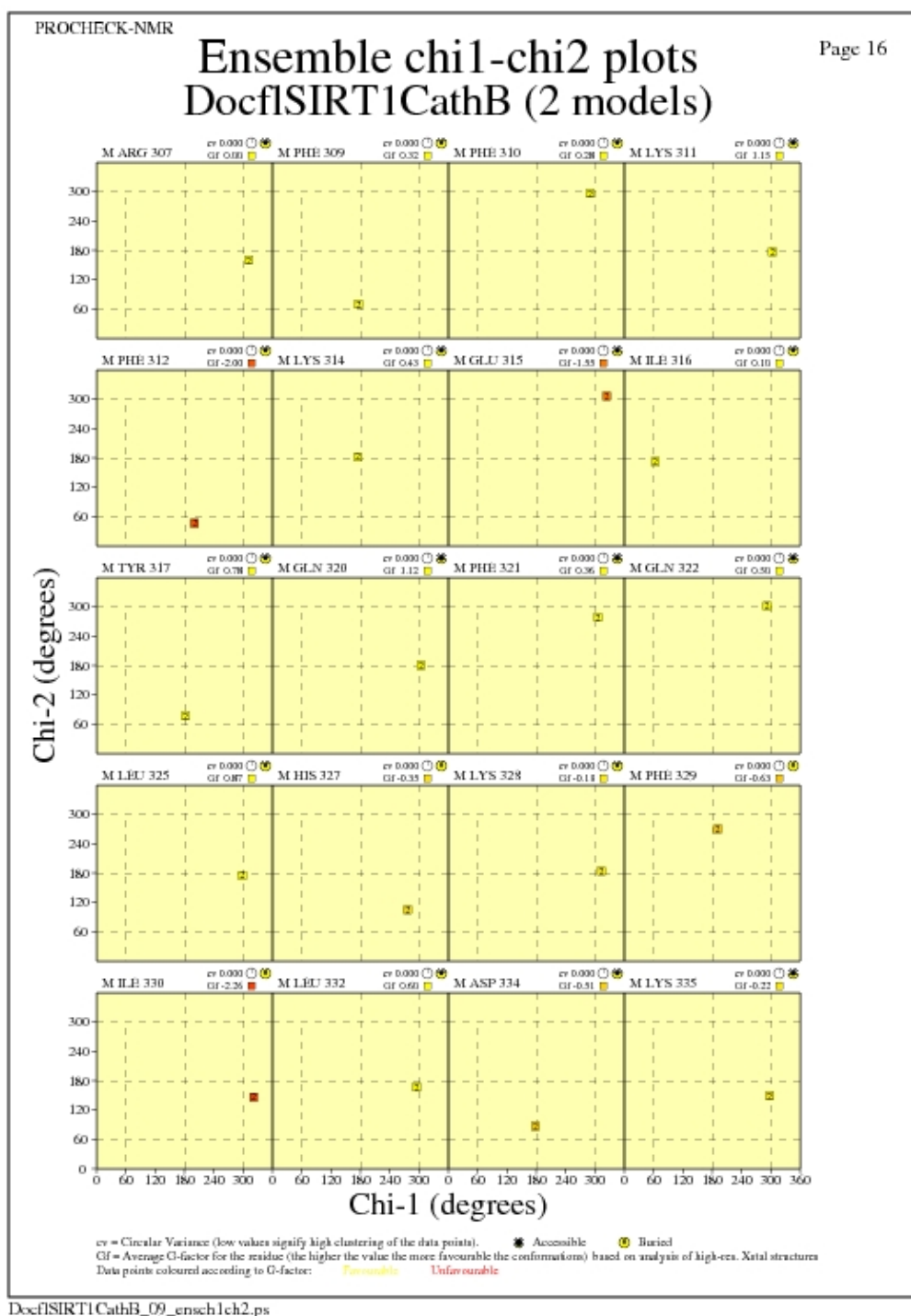
JPEG for residue Chi1-Chi2 Plots - page \$num_n



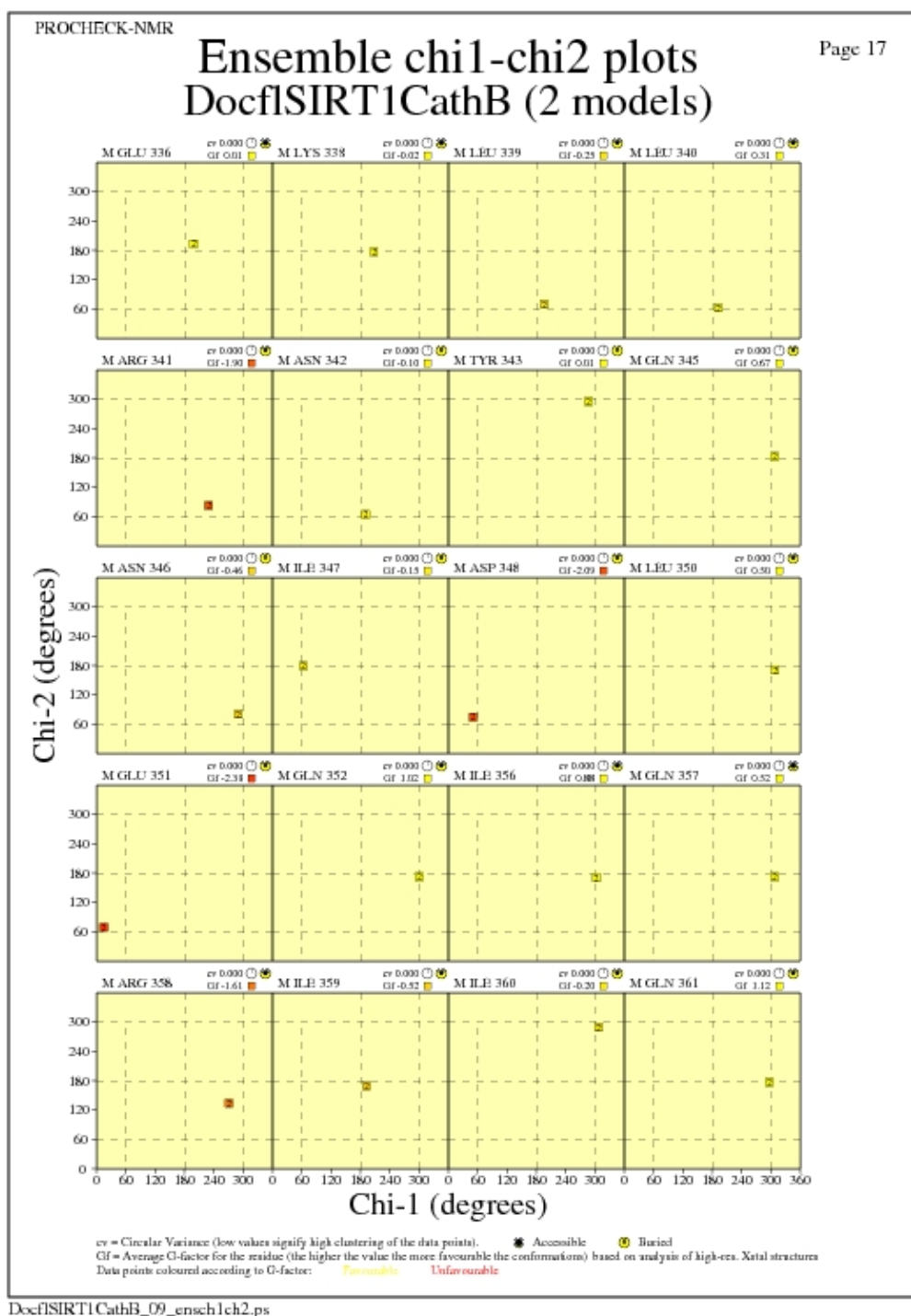
JPEG for residue Chi1-Chi2 Plots - page \$num_n



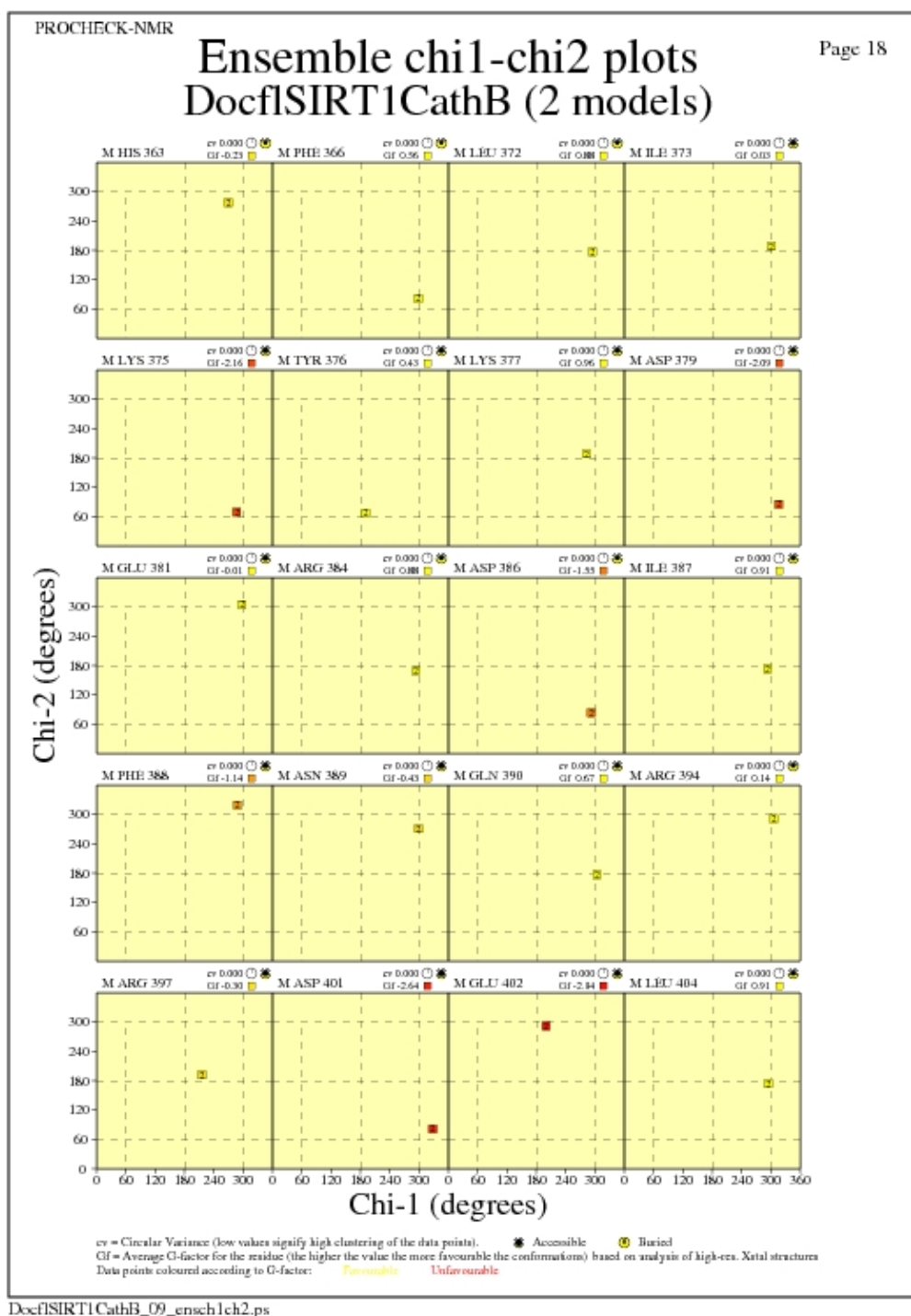
JPEG for residue Chi1-Chi2 Plots - page \$num_n



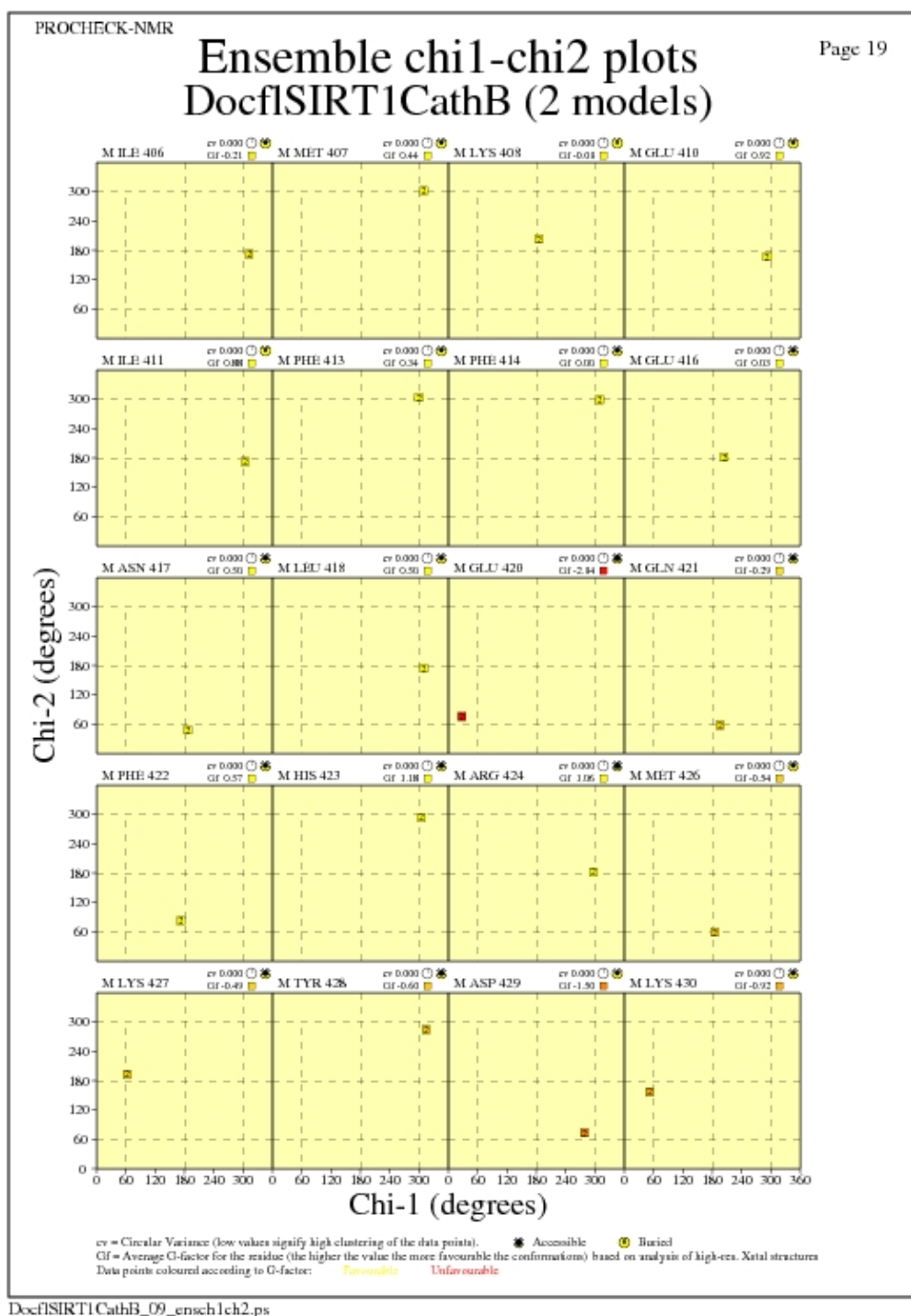
JPEG for residue Chi1-Chi2 Plots - page \$num_n



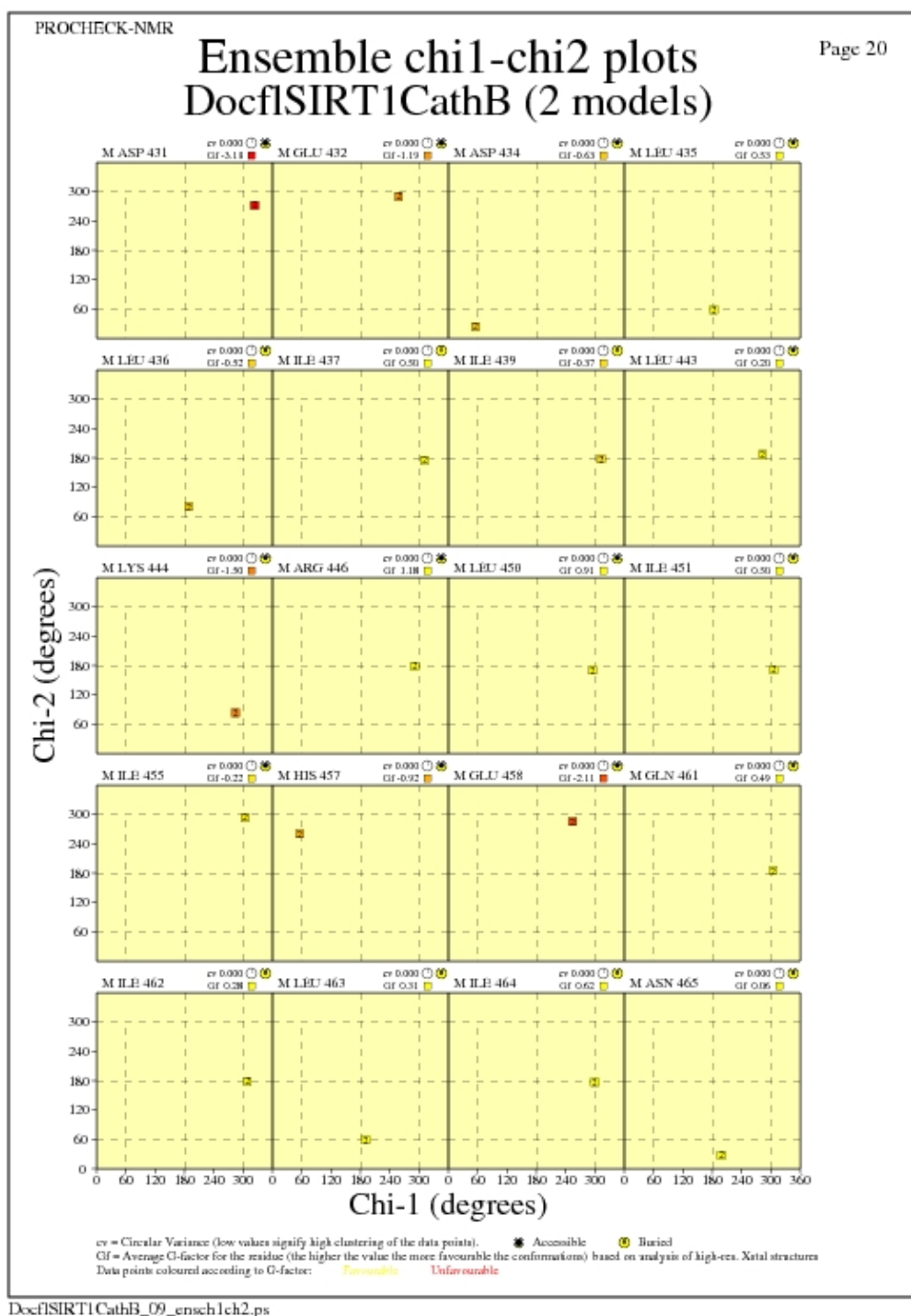
JPEG for residue Chi1-Chi2 Plots - page \$num_n



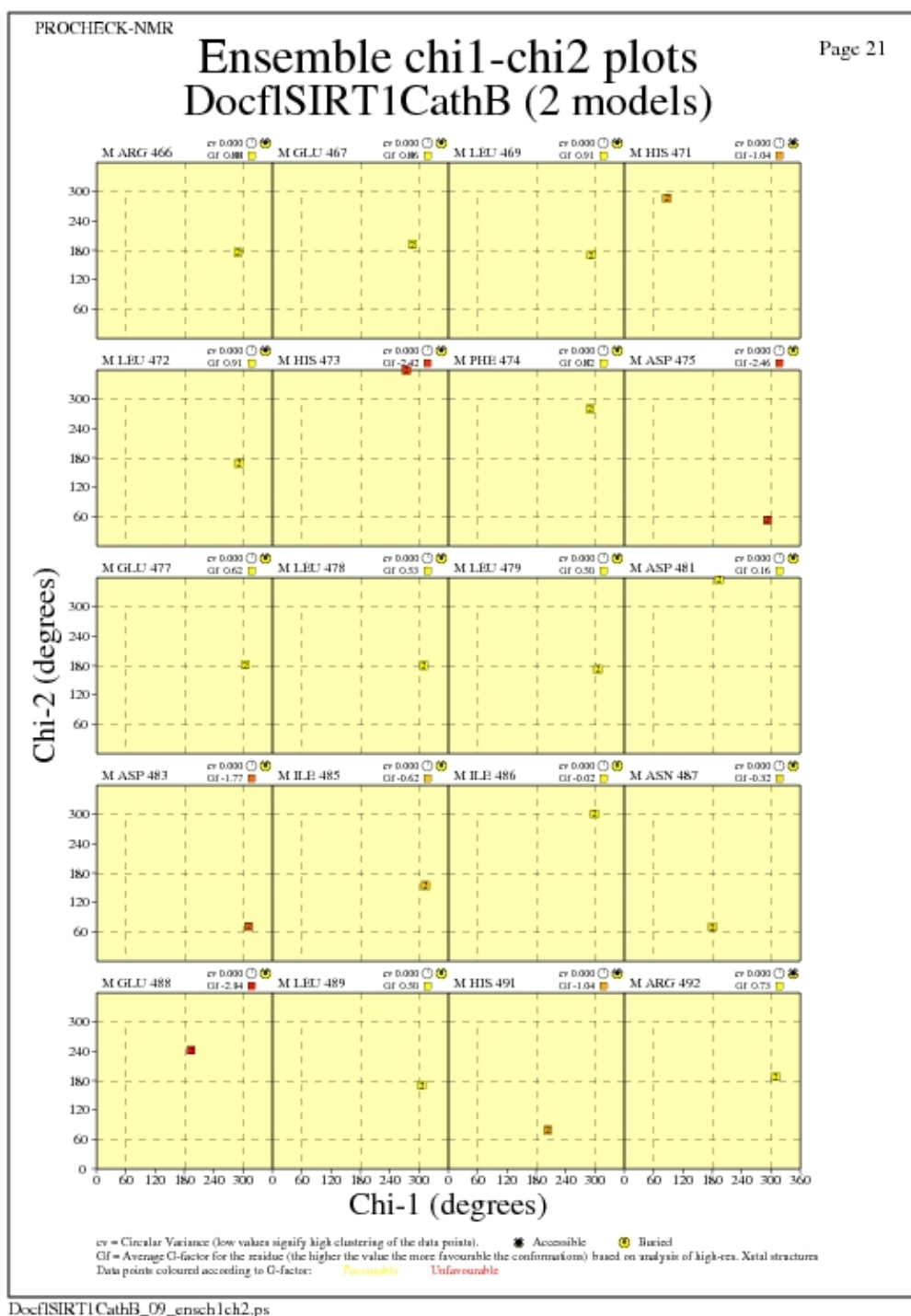
JPEG for residue Chi1-Chi2 Plots - page \$num_n



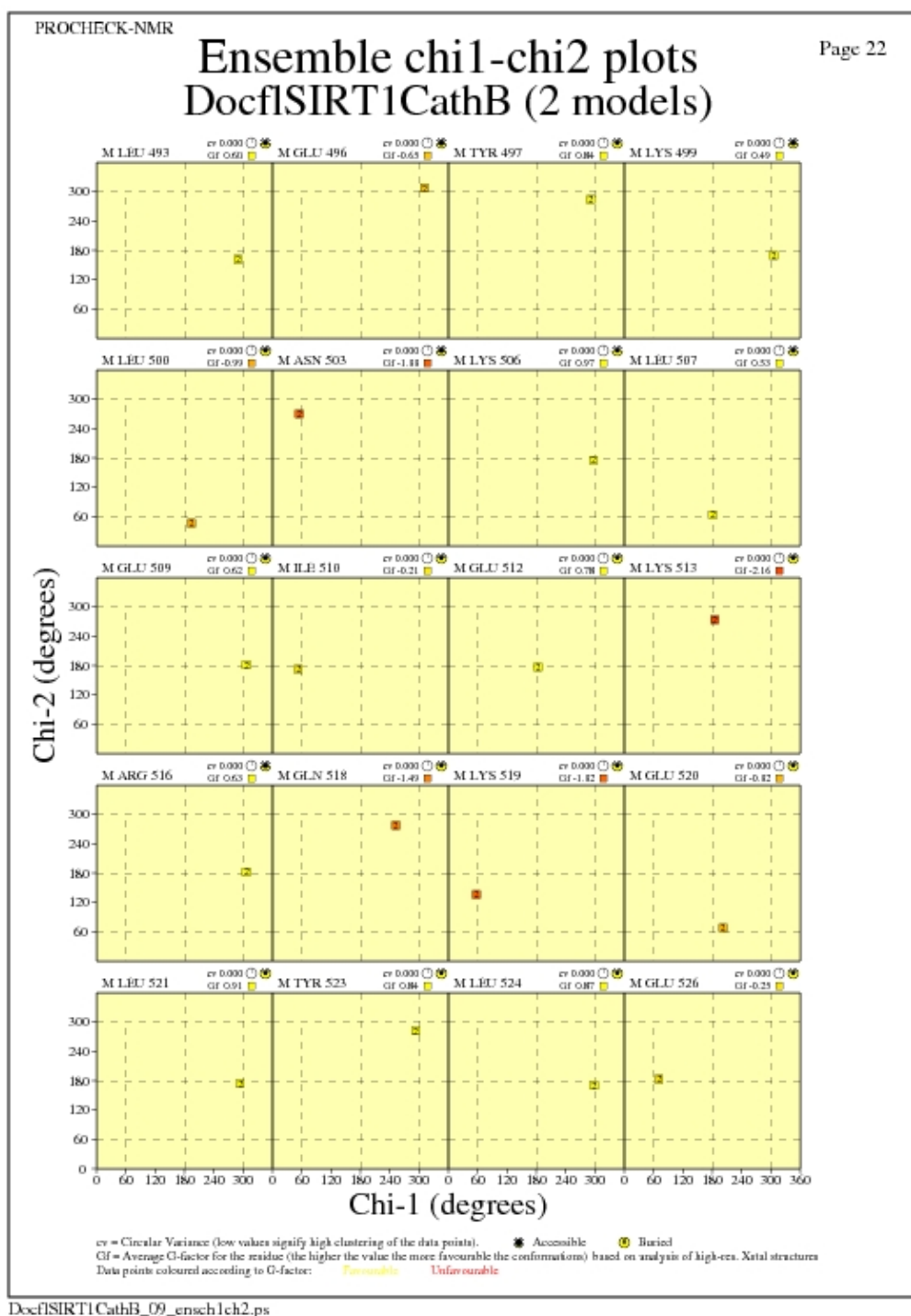
JPEG for residue Chi1-Chi2 Plots - page \$num_n



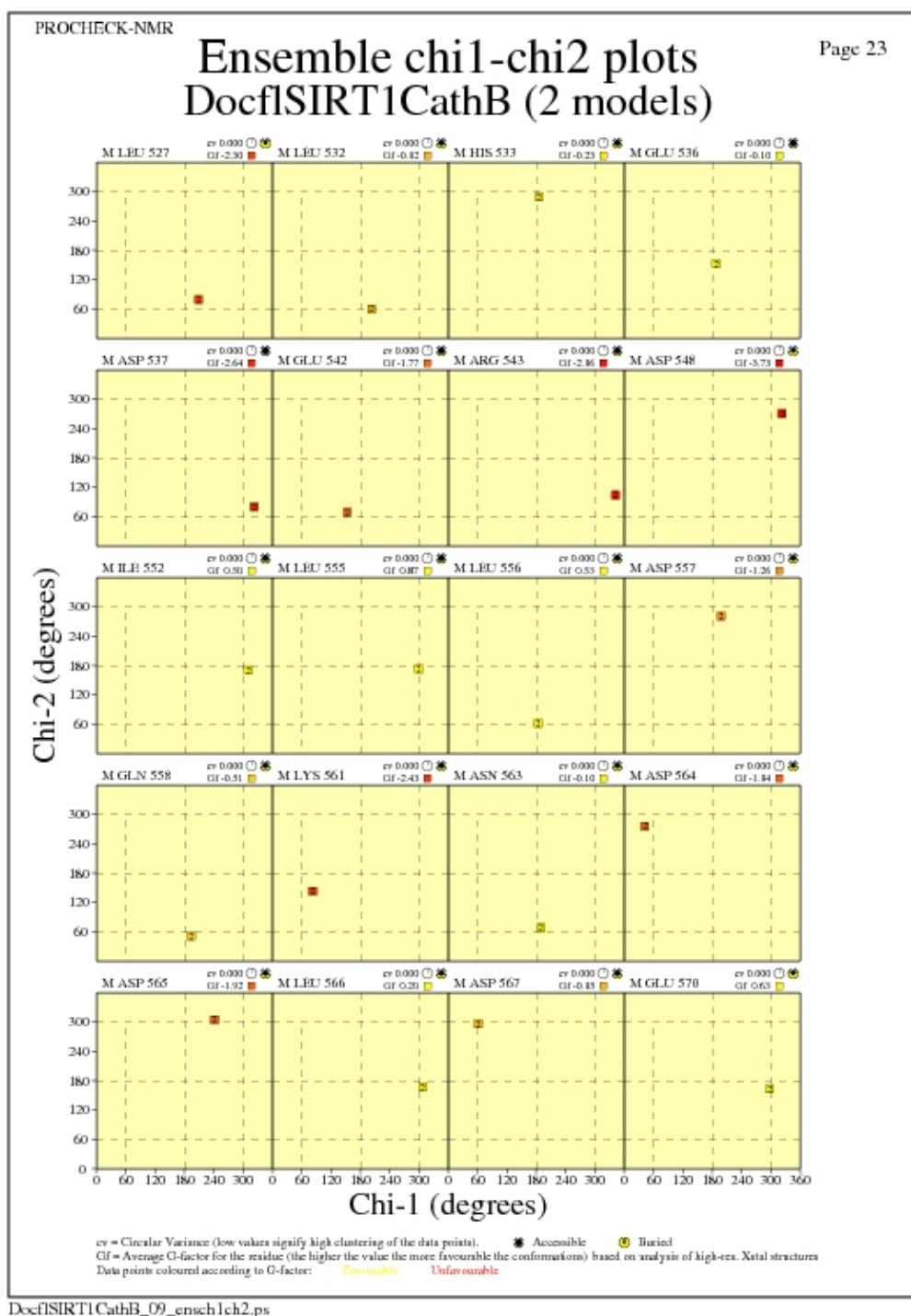
JPEG for residue Chi1-Chi2 Plots - page \$num_n



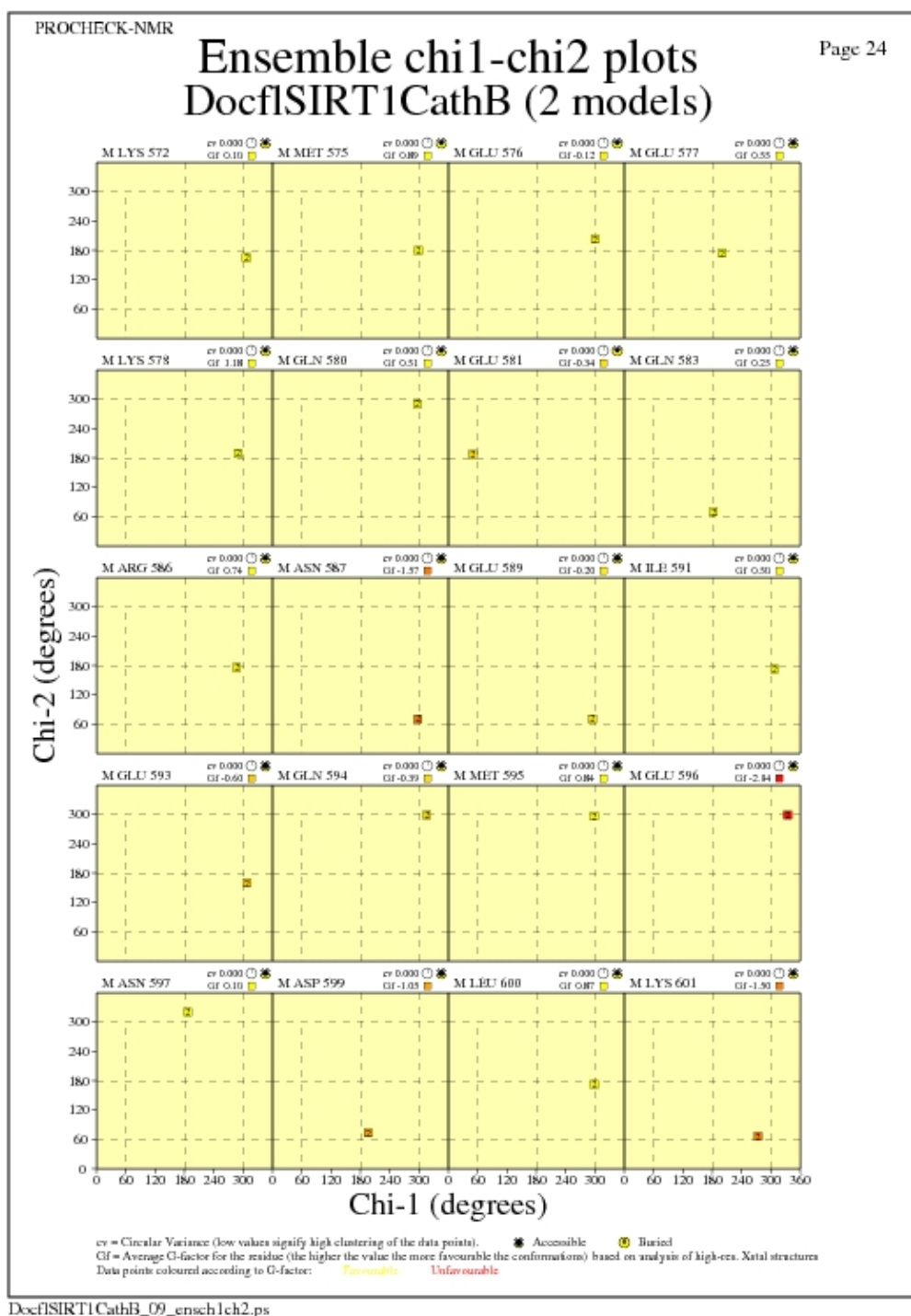
JPEG for residue Chi1-Chi2 Plots - page \$num_n



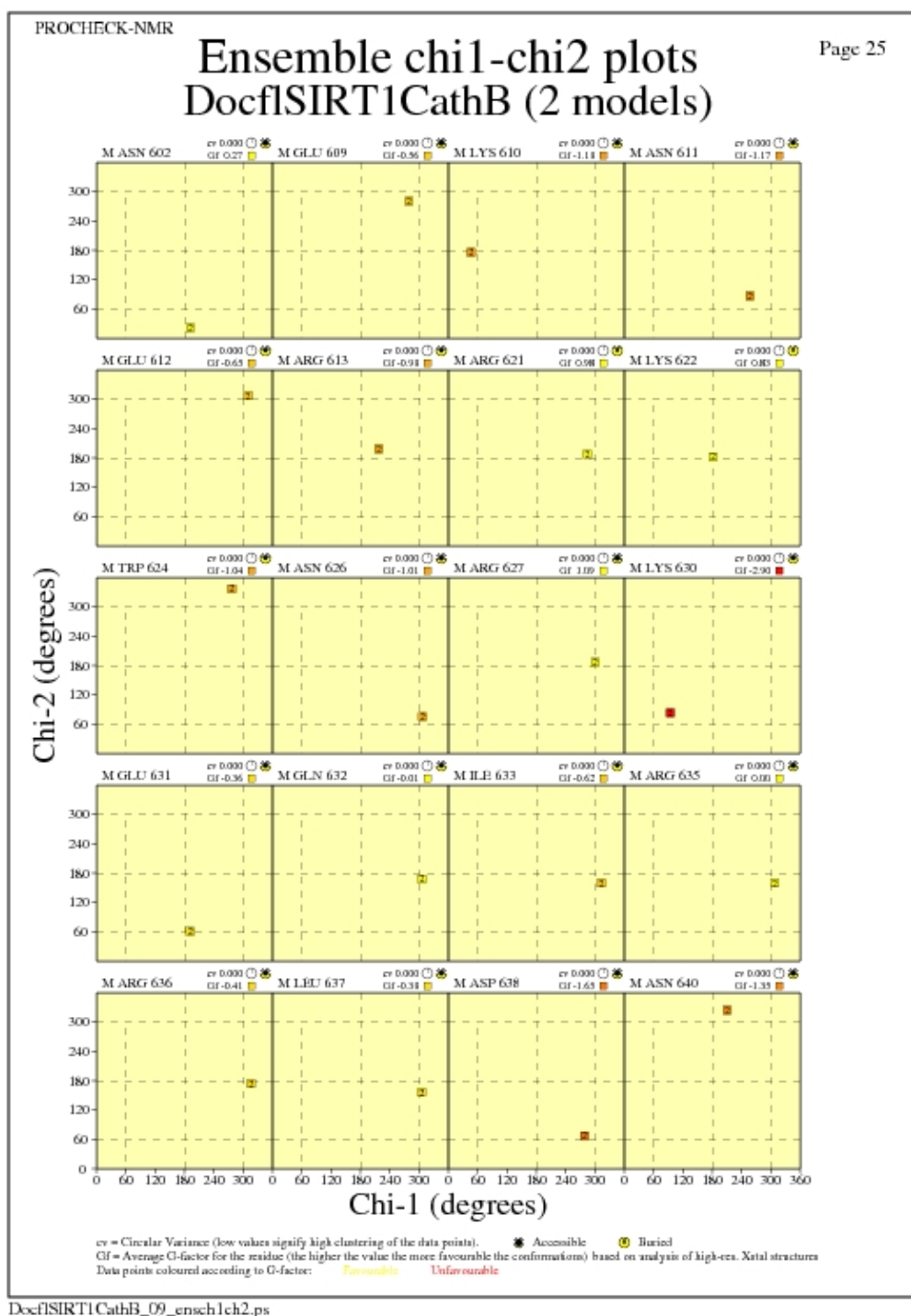
JPEG for residue Chi1-Chi2 Plots - page \$num_n



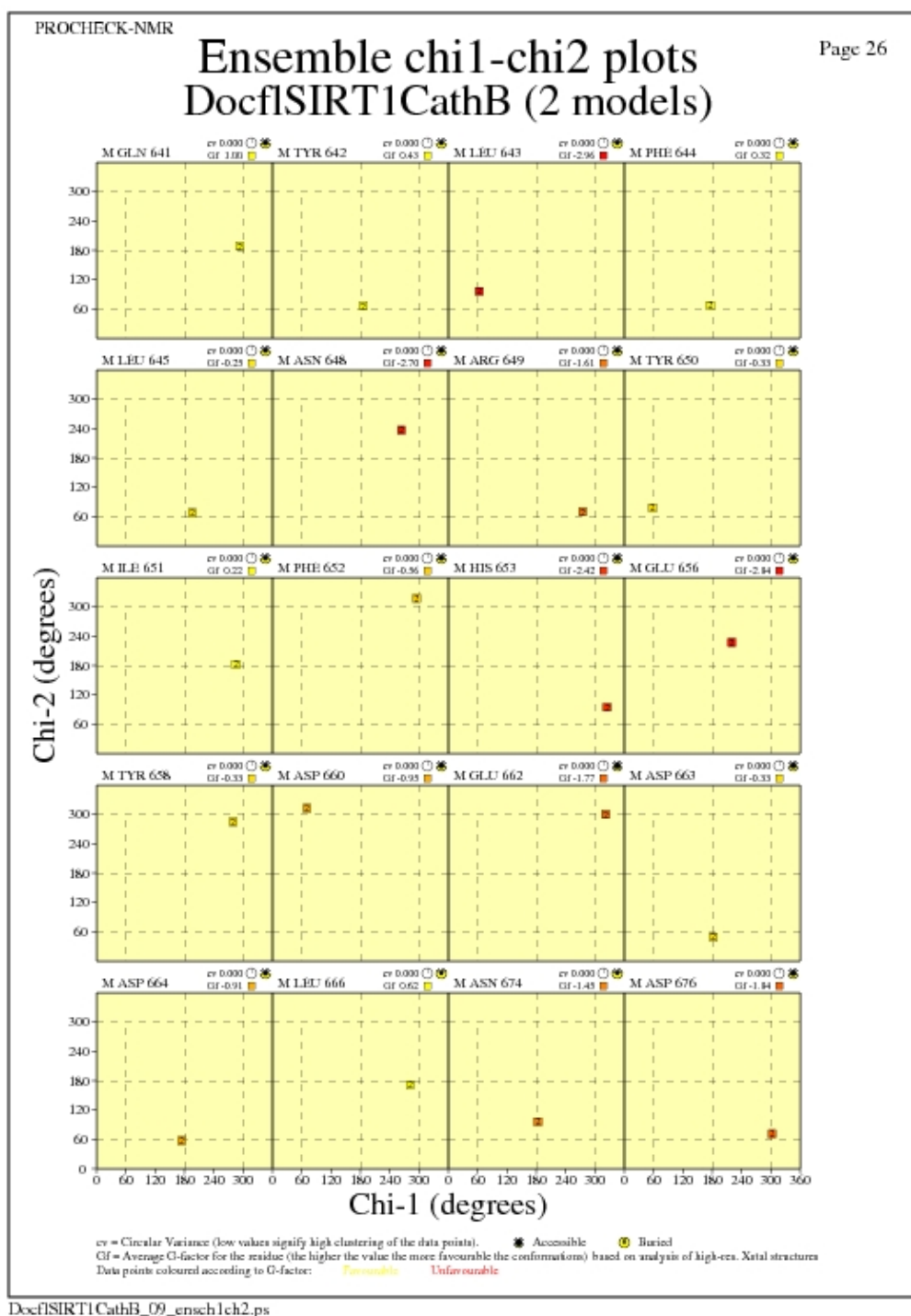
JPEG for residue Chi1-Chi2 Plots - page \$num_n



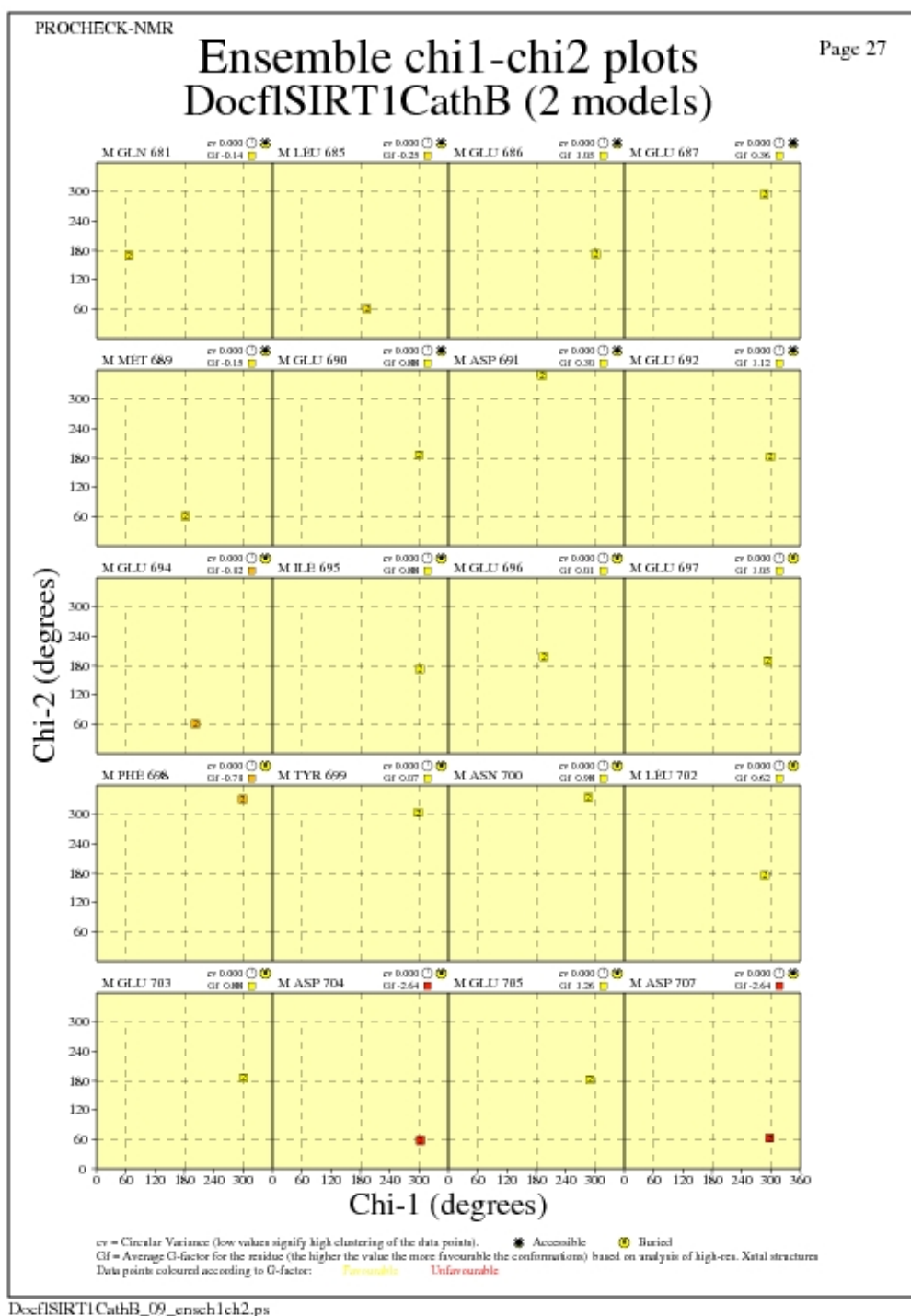
JPEG for residue Chi1-Chi2 Plots - page \$num_n



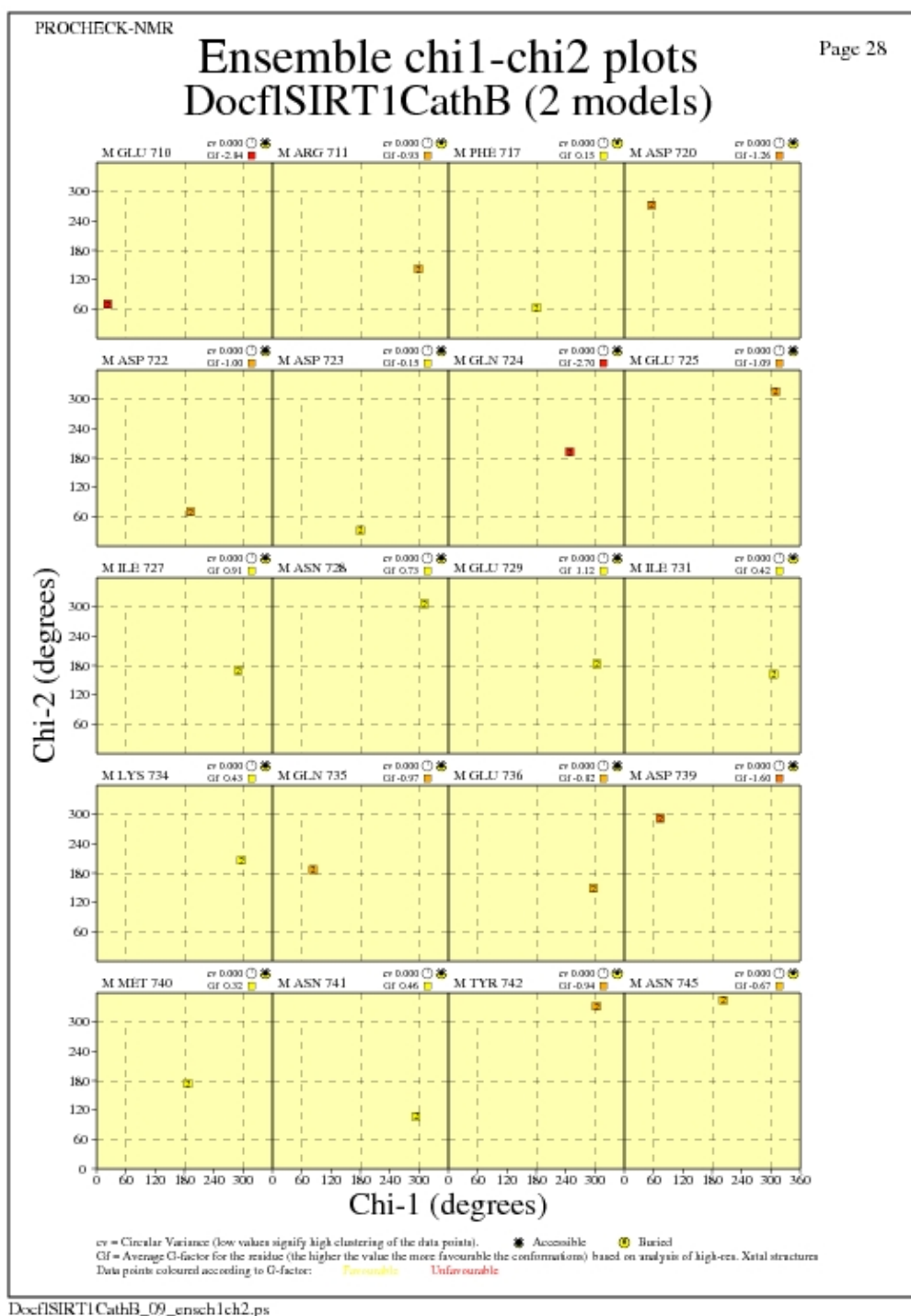
JPEG for residue Chi1-Chi2 Plots - page \$num_n



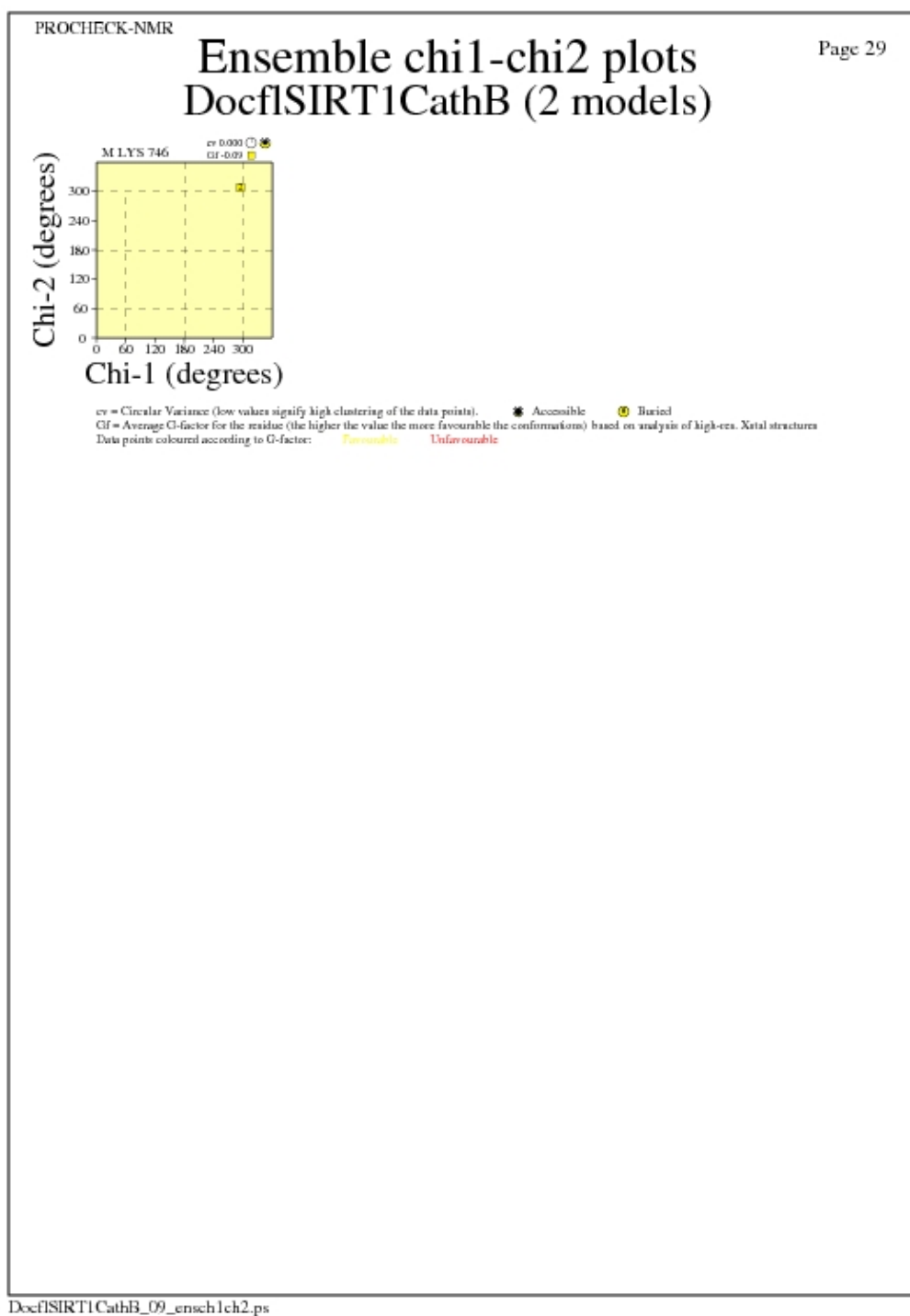
JPEG for residue Chi1-Chi2 Plots - page \$num_n



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

Procheck G-factor for phi-psi

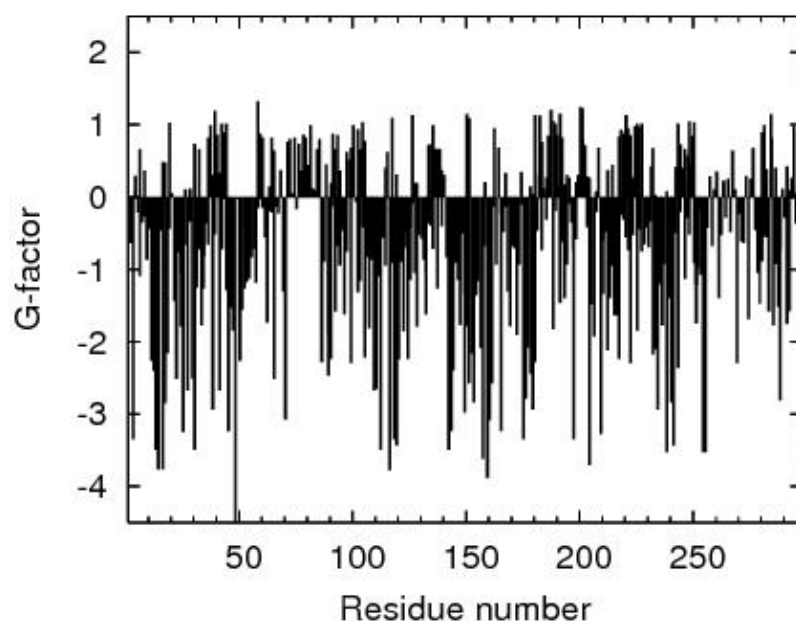


Table of Procheck G-factors for phi-psi for ordered residues

No ordered residues found for phipsi_gfactor.

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

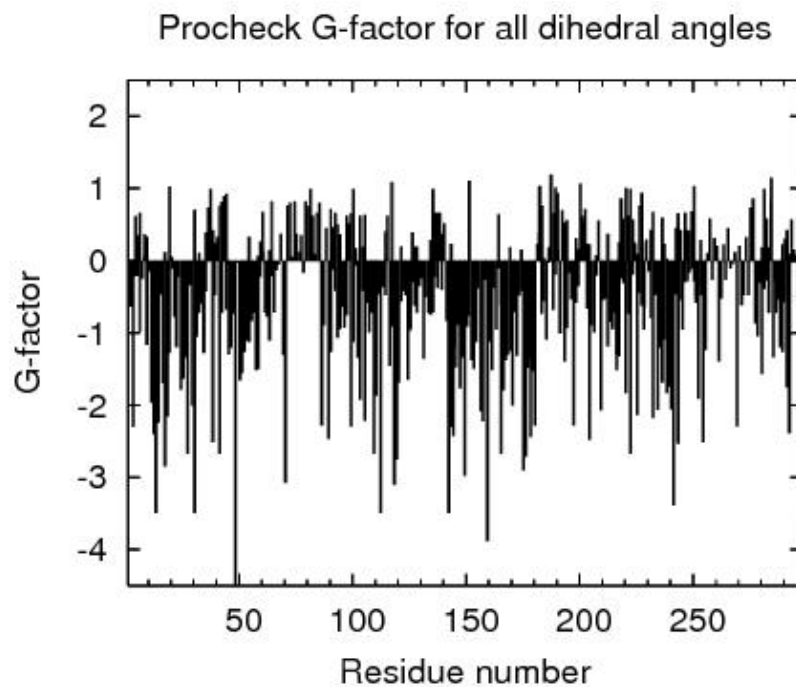


Table of Procheck G-factors for all dihedrals for ordered residues

No ordered residues found for alldih_gfactor.

Output from Verify3D

Verify3D Score over a window of \$wsize_s residues

JPEG image for Verify3D Score

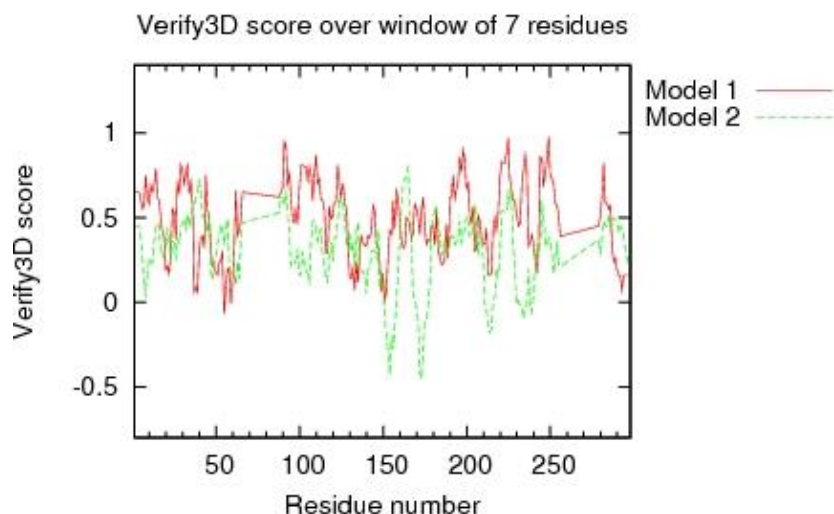


Table of Verify3D scores for ordered residues across all models

No ordered residues found for verify3d.

Output from Prosall

Prosall Score over a window of \$wsize_s residues

JPEG image for Prosall Score

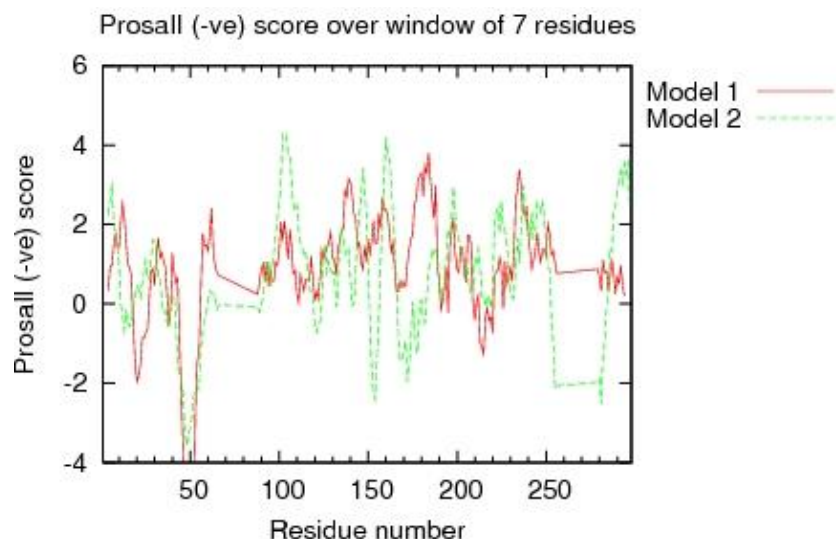


Table of Verify3D scores for ordered residues across all models

No ordered residues found for verify3d.

Output from MolProbity

VdW violations from MAGE

JPEG image for MAGE VdW violation

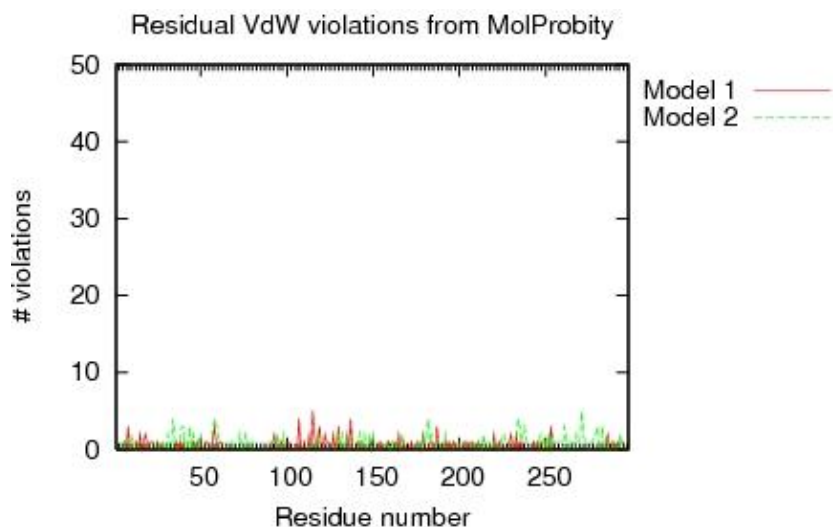


Table of MAGE VdW violations for ordered residues across all models

No ordered residues found for mage_clash.

List of bad contacts calculated by MAGE for model \$num_n

/farm/software/bin/probe

: 3712:M 285 ILE 3HG2 :M 286 GLU 2HG : -0.748: 0

Prosall Score over a window of \$winsize_s residues

PSVS Software Environment

: 3712:M 286 GLU O :M 176 ASN HA : -0.484: 0
: 3712:M 100 ALA 1HB :M 59 LEU 1HD2 : -0.682: 0
: 3712:M 187 LYS 2HZ :M 184 GLU HA : -0.662: 0
: 3712:M 188 ASN OD1 :M 187 LYS NZ : -0.470: 0
: 3712:M 183 ALA O :M 187 LYS 2HG : -0.424: 0
: 3712:M 53 GLU CD :M 21 ARG 2HH2 : -0.599: 0
: 3712:M 107 LYS HA :M 107 LYS NZ : -0.597: 0
: 3712:M 107 LYS 3HZ :M 107 LYS HA : -0.466: 0
: 3712:M 208 VAL 1HG2 :M 233 THR HB : -0.593: 0
: 3712:M 229 VAL HA :M 233 THR O : -0.431: 0
: 3712:M 137 ARG 2HH2 :M 245 ASP CG : -0.581: 0
: 3712:M 115 TYR HD2 :M 124 TYR O : -0.581: 0
: 3712:M 130 GLU CD :M 135 GLY 2HA : -0.570: 0
: 3712:M 137 ARG 1HH2 :M 130 GLU CD : -0.540: 0
: 3712:M 115 TYR CD1 :M 116 GLU 1HG : -0.512: 0
: 3712:M 115 TYR CE1 :M 116 GLU 1HG : -0.445: 0
: 3712:M 115 TYR CD1 :M 127 PRO HA : -0.441: 0
: 3712:M 137 ARG HE :M 137 ARG 1HB : -0.409: 0
: 3712:M 135 GLY 2HA :M 130 GLU OE1 : -0.403: 0
: 3712:M 115 TYR CE1 :M 127 PRO 2HB : -0.400: 0
: 3712:M 200 ASP OD2 :M 211 HIS HA : -0.579: 0
: 3712:M 8 ARG CZ :M 8 ARG 1HB : -0.572: 0
: 3712:M 8 ARG 1HH2 :M 6 ASP CG : -0.430: 0
: 3712:M 62 CYS 1HB :M 58 ASP O : -0.543: 0
: 3712:M 58 ASP HA :M 122 ARG NH1 : -0.542: 0
: 3712:M 165 LYS NZ :M 58 ASP OD2 : -0.447: 0
: 3712:M 110 VAL 3HG1 :M 165 LYS 2HD : -0.424: 0
: 3712:M 57 GLU CD :M 122 ARG NH2 : -0.404: 0
: 3712:M 36 GLU 2HB :M 223 ARG CZ : -0.540: 0
: 3712:M 292 GLY 1HA :M 172 TYR CE2 : -0.526: 0
: 3712:M 19 GLU OE1 :M 18 LYS NZ : -0.525: 0
: 3712:M 15 PRO O :M 18 LYS 2HG : -0.512: 0
: 3712:M 13 GLN O :M 15 PRO 2HD : -0.405: 0
: 3712:M 203 LEU O :M 205 LYS 2HG : -0.523: 0
: 3712:M 22 ASP 1HB :M 243 ASN 2HD2 : -0.514: 0
: 3712:M 38 ILE 2HG2 :M 54 VAL 1HG2 : -0.502: 0
: 3712:M 143 GLU 1HG :M 92 CYS O : -0.502: 0
: 3712:M 123 PRO 2HG :M 119 VAL O : -0.499: 0
: 3712:M 113 GLY 2HA :M 119 VAL CG2 : -0.465: 0
: 3712:M 113 GLY 2HA :M 119 VAL 3HG2 : -0.405: 0

PSVS Software Environment

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: 3712:M 192 GLU O :M 289 VAL HA : -0.493: 0
: 3712:M 235 TYR HE2 :M 230 GLU 1HB : -0.488: 0
: 3712:M 236 TRP O :M 253 LYS HA : -0.455: 0
: 3712:M 207 GLY O :M 253 LYS 1HB : -0.450: 0
: 3712:M 230 GLU CD :M 253 LYS 3HZ : -0.429: 0

: 3712:M 17 ILE 1HG1 :M 40 ASP CG : -0.467: 0
: 3712:M 97 PRO O :M 101 TRP HD1 : -0.466: 0
: 3712:M 294 PRO 2HD :M 293 ILE HA : -0.466: 0
: 3712:M 48 VAL 3HG1 :M 46 THR 1HG2 : -0.460: 0
: 3712:M 247 GLY 1HA :M 204 TYR O : -0.444: 0
: 3712:M 61 THR O :M 149 CYS 1HB : -0.442: 0
: 3712:M 25 SER 1HB :M 141 THR O : -0.433: 0
: 3712:M 197 VAL 3HG2 :M 220 HIS 1HB : -0.428: 0
: 3712:M 220 HIS O :M 194 ALA HA : -0.404: 0
: 3712:M 295 ARG CZ :M 168 GLY O : -0.424: 0
: 3712:M 179 LYS 2HE :M 179 LYS HA : -0.422: 0
: 3712:M 154 GLU OE2 :M 118 HIS HA : -0.420: 0
: 3712:M 93 ASN 2HD2 :M 93 ASN HA : -0.417: 0
: 3712:M 159 PRO 1HB :M 163 GLN CD : -0.415: 0
#sum2 ::16.16 clashscore : 16.16 clashscore B

```

List of bad contacts calculated by MAGE for model \$num_n

/farm/software/bin/probe

```

: 11242:M 492 ARG 1HD :M 247 VAL 1HG2 : -0.861: 0
: 11242:M 250 LEU 1HB :M 247 VAL HA : -0.559: 0

: 11242:M 44 LEU HA :M 40 ASP 1HB : -0.849: 0
: 11242:M 46 ARG 2HG :M 44 LEU HG : -0.536: 0
: 11242:M 22 ARG CZ :M 40 ASP HA : -0.530: 0
: 11242:M 40 ASP H :M 44 LEU 3HD1 : -0.479: 0
: 11242:M 46 ARG 2HH2 :M 239 ASP CG : -0.419: 0

: 11242:M 222 GLN HA :M 98 ALA 1HB : -0.822: 0
: 11242:M 225 ILE HB :M 98 ALA 2HB : -0.662: 0
: 11242:M 225 ILE 1HG1 :M 192 LEU 3HD1 : -0.509: 0
: 11242:M 192 LEU 2HD1 :M 189 GLN HA : -0.489: 0

: 11242:M 271 PRO HA :M 266 VAL 2HG2 : -0.794: 0
: 11242:M 271 PRO 1HB :M 278 GLY 1HA : -0.666: 0
: 11242:M 271 PRO 1HB :M 278 GLY CA : -0.461: 0
: 11242:M 269 GLY O :M 271 PRO 2HD : -0.421: 0
: 11242:M 271 PRO 2HB :M 277 ASP OD2 : -0.400: 0

: 11242:M 671 CYS SG :M 666 LEU 2HB : -0.721: 0

```


PSVS Software Environment

: 11242:M 671 CYS SG	:M 684 SER HA	: -0.666:	0
: 11242:M 715 ALA 2HB	:M 671 CYS 1HB	: -0.590:	0
: 11242:M 680 CYS HA	:M 673 SER O	: -0.568:	0
: 11242:M 682 SER 2HB	:M 671 CYS HA	: -0.518:	0
: 11242:M 671 CYS O	:M 680 CYS 2HB	: -0.499:	0
: 11242:M 673 SER 1HB	:M 712 ALA O	: -0.482:	0
: 11242:M 621 ARG 1HH2	:M 704 ASP CG	: -0.464:	0
: 11242:M 712 ALA HA	:M 704 ASP HA	: -0.420:	0
: 11242:M 50 GLU 2HB	:M 237 ARG 1HG	: -0.719:	0
: 11242:M 50 GLU O	:M 233 LYS 1HE	: -0.591:	0
: 11242:M 237 ARG 2HH1	:M 245 ASP CG	: -0.493:	0
: 11242:M 73 ALA 1HB	:M 233 LYS 2HD	: -0.489:	0
: 11242:M 73 ALA 3HB	:M 49 GLY 2HA	: -0.464:	0
: 11242:M 426 MET HA	:M 429 ASP 1HB	: -0.713:	0
: 11242:M 429 ASP CG	:M 341 ARG 1HH2	: -0.461:	0
: 11242:M 547 PRO 1HB	:M 507 LEU 1HD1	: -0.712:	0
: 11242:M 546 PRO 2HD	:M 545 SER HA	: -0.487:	0
: 11242:M 547 PRO 2HD	:M 546 PRO HA	: -0.462:	0
: 11242:M 732 SER HA	:M 735 GLN 2HE2	: -0.703:	0
: 11242:M 732 SER O	:M 735 GLN 1HG	: -0.517:	0
: 11242:M 344 THR 3HG2	:M 361 GLN HA	: -0.688:	0
: 11242:M 256 ILE 1HG1	:M 435 LEU 2HB	: -0.680:	0
: 11242:M 299 ILE 2HG2	:M 414 PHE O	: -0.669:	0
: 11242:M 302 PHE 2HB	:M 299 ILE HA	: -0.628:	0
: 11242:M 413 PHE 1HB	:M 299 ILE HB	: -0.454:	0
: 11242:M 303 ARG 2HG	:M 299 ILE 1HG1	: -0.429:	0
: 11242:M 299 ILE O	:M 303 ARG 2HG	: -0.403:	0
: 11242:M 23 GLU HA	:M 35 LYS 2HD	: -0.667:	0
: 11242:M 35 LYS 1HZ	:M 161 GLU CD	: -0.491:	0
: 11242:M 640 ASN O	:M 605 SER HA	: -0.655:	0
: 11242:M 636 ARG O	:M 640 ASN 1HB	: -0.535:	0
: 11242:M 520 GLU 1HG	:M 515 PRO HA	: -0.651:	0
: 11242:M 564 ASP CG	:M 513 LYS 1HZ	: -0.564:	0
: 11242:M 513 LYS 2HB	:M 523 TYR HA	: -0.515:	0
: 11242:M 520 GLU 2HB	:M 523 TYR OH	: -0.459:	0
: 11242:M 520 GLU CD	:M 513 LYS NZ	: -0.430:	0
: 11242:M 517 THR O	:M 520 GLU 1HB	: -0.412:	0
: 11242:M 262 ALA 3HB	:M 272 ASP HA	: -0.647:	0
: 11242:M 272 ASP HA	:M 262 ALA CB	: -0.455:	0
: 11242:M 635 ARG HA	:M 638 ASP 1HB	: -0.644:	0
: 11242:M 638 ASP HA	:M 607 THR HA	: -0.631:	0
: 11242:M 635 ARG 1HH1	:M 165 GLU CD	: -0.413:	0
: 11242:M 130 GLU CD	:M 235 LYS 1HZ	: -0.641:	0
: 11242:M 129 GLY O	:M 135 ALA 2HB	: -0.581:	0
: 11242:M 132 GLU CD	:M 39 ARG 2HH1	: -0.483:	0
: 11242:M 235 LYS 2HB	:M 132 GLU 1HG	: -0.464:	0
: 11242:M 38 ARG 2HH2	:M 118 ASP 2HB	: -0.459:	0
: 11242:M 118 ASP HA	:M 130 GLU 2HB	: -0.454:	0
: 11242:M 235 LYS 2HG	:M 135 ALA 3HB	: -0.433:	0

PSVS Software Environment

: 11242:M 39 ARG 1HH1	:M 39 ARG 2HD	: -0.419:	0
: 11242:M 455 ILE 2HG1	:M 436 LEU 2HD2	: -0.635:	0
: 11242:M 459 VAL 1HG1	:M 433 VAL 3HG1	: -0.567:	0
: 11242:M 433 VAL 1HG1	:M 455 ILE 2HD1	: -0.517:	0
: 11242:M 461 GLN 1HG	:M 436 LEU 2HB	: -0.492:	0
: 11242:M 436 LEU 2HD1	:M 257 ILE HB	: -0.471:	0
: 11242:M 451 ILE O	:M 455 ILE 1HG1	: -0.456:	0
: 11242:M 454 SER OG	:M 451 ILE HA	: -0.427:	0
: 11242:M 651 ILE 1HD1	:M 643 LEU 1HD1	: -0.629:	0
: 11242:M 657 VAL 2HG2	:M 658 TYR HD1	: -0.445:	0
: 11242:M 657 VAL 3HG1	:M 658 TYR H	: -0.434:	0
: 11242:M 657 VAL HB	:M 651 ILE HB	: -0.419:	0
: 11242:M 658 TYR CE2	:M 569 SER 1HB	: -0.414:	0
: 11242:M 91 GLU CD	:M 234 ARG 2HH2	: -0.626:	0
: 11242:M 234 ARG 2HB	:M 231 PRO O	: -0.475:	0
: 11242:M 76 TRP HZ2	:M 234 ARG 1HD	: -0.413:	0
: 11242:M 234 ARG 1HD	:M 76 TRP CZ2	: -0.403:	0
: 11242:M 633 ILE 2HD1	:M 630 LYS HA	: -0.620:	0
: 11242:M 633 ILE 1HG2	:M 617 ALA HA	: -0.497:	0
: 11242:M 412 VAL 1HG2	:M 419 PRO 2HD	: -0.617:	0
: 11242:M 371 CYS HA	:M 406 ILE O	: -0.613:	0
: 11242:M 371 CYS 1HB	:M 407 MET SD	: -0.533:	0
: 11242:M 371 CYS 2HB	:M 376 TYR H	: -0.451:	0
: 11242:M 393 PRO O	:M 406 ILE HA	: -0.430:	0
: 11242:M 376 TYR 1HB	:M 397 ARG 1HD	: -0.426:	0
: 11242:M 699 TYR HD1	:M 717 PHE HD1	: -0.588:	0
: 11242:M 717 PHE CD1	:M 699 TYR HA	: -0.498:	0
: 11242:M 338 LYS 2HB	:M 333 SER O	: -0.587:	0
: 11242:M 338 LYS HA	:M 254 LYS HA	: -0.504:	0
: 11242:M 254 LYS CA	:M 338 LYS HA	: -0.450:	0
: 11242:M 338 LYS 2HZ	:M 336 GLU CD	: -0.439:	0
: 11242:M 164 GLU CD	:M 179 ARG 1HH2	: -0.584:	0
: 11242:M 179 ARG 2HD	:M 180 PRO 1HD	: -0.418:	0
: 11242:M 724 GLN HA	:M 727 ILE 2HD1	: -0.579:	0
: 11242:M 259 LEU 2HD1	:M 438 VAL 2HG2	: -0.579:	0
: 11242:M 725 GLU CD	:M 746 LYS 1HZ	: -0.511:	0
: 11242:M 724 GLN OE1	:M 746 LYS 2HE	: -0.419:	0
: 11242:M 711 ARG 2HH1	:M 705 GLU CD	: -0.564:	0
: 11242:M 711 ARG CZ	:M 711 ARG 1HB	: -0.420:	0
: 11242:M 270 ILE 2HD1	:M 348 ASP 2HB	: -0.560:	0
: 11242:M 31 GLU CD	:M 31 GLU H	: -0.552:	0
: 11242:M 60 VAL 1HG1	:M 6 ALA 1HB	: -0.549:	0
: 11242:M 321 PHE 1HB	:M 350 LEU 1HD1	: -0.549:	0
: 11242:M 490 CYS HA	:M 497 TYR 2HB	: -0.549:	0

PSVS Software Environment

: 11242:M 60 VAL HB	:M 57 GLU OE2	:	-0.512:	0
: 11242:M 57 GLU 1HG	:M 60 VAL H	:	-0.457:	0
: 11242:M 332 LEU 3HD1	:M 497 TYR HA	:	-0.444:	0
: 11242:M 268 CYS SG	:M 265 SER HA	:	-0.430:	0
: 11242:M 497 TYR O	:M 490 CYS 2HB	:	-0.418:	0
: 11242:M 490 CYS SG	:M 500 LEU 3HD2	:	-0.416:	0
: 11242:M 321 PHE 2HB	:M 268 CYS O	:	-0.414:	0
: 11242:M 224 VAL 3HG2	:M 220 LEU O	:	-0.548:	0
: 11242:M 534 VAL 3HG2	:M 532 LEU O	:	-0.547:	0
: 11242:M 483 ASP 2HB	:M 325 LEU 2HD1	:	-0.547:	0
: 11242:M 483 ASP OD2	:M 324 SER 2HB	:	-0.438:	0
: 11242:M 264 VAL 2HG2	:M 261 GLY O	:	-0.544:	0
: 11242:M 345 GLN 1HB	:M 261 GLY 1HA	:	-0.411:	0
: 11242:M 441 SER 2HB	:M 261 GLY 2HA	:	-0.406:	0
: 11242:M 598 PRO 2HD	:M 597 ASN 2HB	:	-0.541:	0
: 11242:M 516 ARG 2HH2	:M 565 ASP CG	:	-0.541:	0
: 11242:M 7 LEU 1HB	:M 182 ILE HB	:	-0.540:	0
: 11242:M 182 ILE O	:M 4 GLU HA	:	-0.517:	0
: 11242:M 142 TYR HA	:M 182 ILE 3HD1	:	-0.506:	0
: 11242:M 182 ILE CD1	:M 142 TYR HA	:	-0.442:	0
: 11242:M 576 GLU CD	:M 734 LYS 1HZ	:	-0.539:	0
: 11242:M 707 ASP CG	:M 613 ARG 1HH2	:	-0.535:	0
: 11242:M 408 LYS 2HD	:M 372 LEU 1HD2	:	-0.534:	0
: 11242:M 627 ARG 1HB	:M 624 TRP 2HB	:	-0.532:	0
: 11242:M 59 GLU H	:M 59 GLU CD	:	-0.529:	0
: 11242:M 59 GLU CD	:M 58 ARG 1HH1	:	-0.436:	0
: 11242:M 589 GLU CD	:M 58 ARG 1HH2	:	-0.428:	0
: 11242:M 58 ARG H	:M 58 ARG 2HG	:	-0.414:	0
: 11242:M 34 ARG 2HG	:M 134 GLU CD	:	-0.528:	0
: 11242:M 34 ARG 1HH2	:M 144 ASP CG	:	-0.527:	0
: 11242:M 34 ARG 1HH1	:M 34 ARG 2HG	:	-0.477:	0
: 11242:M 248 LYS 1HZ	:M 252 GLU CD	:	-0.526:	0
: 11242:M 248 LYS NZ	:M 252 GLU CD	:	-0.428:	0
: 11242:M 293 PRO 2HB	:M 283 LEU 1HB	:	-0.524:	0
: 11242:M 669 SER 1HB	:M 703 GLU 2HB	:	-0.524:	0
: 11242:M 622 LYS 2HB	:M 619 THR O	:	-0.521:	0
: 11242:M 279 ILE HB	:M 273 PHE HA	:	-0.471:	0
: 11242:M 283 LEU HG	:M 279 ILE O	:	-0.452:	0
: 11242:M 293 PRO HA	:M 290 LEU 3HD1	:	-0.448:	0

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: 11242:M 622 LYS 1HB	:M 703 GLU 1HG	:	-0.448:	0
: 11242:M 622 LYS 1HB	:M 703 GLU CG	:	-0.440:	0
: 11242:M 703 GLU CD	:M 622 LYS 1HE	:	-0.440:	0
: 11242:M 283 LEU HA	:M 286 ASP 1HB	:	-0.433:	0
: 11242:M 622 LYS 1HZ	:M 694 GLU CD	:	-0.427:	0
: 11242:M 697 GLU OE1	:M 622 LYS 2HG	:	-0.423:	0
: 11242:M 702 LEU 3HD2	:M 702 LEU HA	:	-0.420:	0
: 11242:M 702 LEU 2HD1	:M 697 GLU 1HG	:	-0.412:	0
: 11242:M 466 ARG 1HH2	:M 481 ASP CG	:	-0.523:	0
: 11242:M 158 HIS HA	:M 177 THR HB	:	-0.518:	0
: 11242:M 506 LYS 1HB	:M 484 VAL 2HG1	:	-0.517:	0
: 11242:M 512 GLU HA	:M 524 LEU O	:	-0.516:	0
: 11242:M 187 PHE HD2	:M 184 PRO 1HB	:	-0.514:	0
: 11242:M 610 LYS HA	:M 608 GLY O	:	-0.514:	0
: 11242:M 610 LYS 2HB	:M 610 LYS 3HZ	:	-0.506:	0
: 11242:M 610 LYS HA	:M 609 GLU HA	:	-0.505:	0
: 11242:M 609 GLU OE1	:M 610 LYS NZ	:	-0.424:	0
: 11242:M 184 PRO 2HD	:M 183 GLY 1HA	:	-0.415:	0
: 11242:M 232 PRO 1HD	:M 66 GLY O	:	-0.509:	0
: 11242:M 578 LYS NZ	:M 739 ASP CG	:	-0.509:	0
: 11242:M 579 PRO 2HD	:M 578 LYS HA	:	-0.475:	0
: 11242:M 578 LYS 1HZ	:M 739 ASP CG	:	-0.440:	0
: 11242:M 188 VAL 1HG2	:M 205 LEU 1HD2	:	-0.508:	0
: 11242:M 309 PHE HZ	:M 411 ILE 2HD1	:	-0.505:	0
: 11242:M 411 ILE 3HG2	:M 347 ILE 1HG2	:	-0.450:	0
: 11242:M 645 LEU 2HB	:M 660 ASP HA	:	-0.500:	0
: 11242:M 599 ASP O	:M 601 LYS 1HD	:	-0.498:	0
: 11242:M 649 ARG 1HD	:M 648 ASN C	:	-0.455:	0
: 11242:M 599 ASP CG	:M 601 LYS NZ	:	-0.444:	0
: 11242:M 599 ASP CG	:M 649 ARG 1HH2	:	-0.422:	0
: 11242:M 649 ARG 1HD	:M 648 ASN O	:	-0.415:	0
: 11242:M 199 ARG 1HH2	:M 217 ASP CG	:	-0.496:	0
: 11242:M 274 ARG 1HG	:M 280 TYR HD2	:	-0.494:	0
: 11242:M 280 TYR HE1	:M 297 PHE HD1	:	-0.444:	0
: 11242:M 280 TYR CE1	:M 294 GLN HA	:	-0.423:	0
: 11242:M 14 SER 2HB	:M 10 GLN H	:	-0.492:	0
: 11242:M 421 GLN OE1	:M 424 ARG 1HD	:	-0.492:	0
: 11242:M 420 GLU HA	:M 423 HIS HD2	:	-0.453:	0
: 11242:M 11 PRO 1HD	:M 10 GLN 2HB	:	-0.423:	0
: 11242:M 424 ARG 1HH1	:M 424 ARG 1HD	:	-0.416:	0
: 11242:M 424 ARG 2HH1	:M 420 GLU CD	:	-0.415:	0

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: 11242:M 323 PRO 2HD	:M 322 GLN HA	:	-0.482:	0
: 11242:M 323 PRO O	:M 328 LYS NZ	:	-0.417:	0
: 11242:M 529 PRO 2HD	:M 528 PRO HA	:	-0.481:	0
: 11242:M 533 HIS 1HB	:M 504 PRO 1HG	:	-0.481:	0
: 11242:M 330 ILE 2HD1	:M 327 HIS HA	:	-0.476:	0
: 11242:M 114 PRO 2HD	:M 113 GLU HA	:	-0.475:	0
: 11242:M 458 GLU CD	:M 238 LYS 3HZ	:	-0.470:	0
: 11242:M 458 GLU O	:M 238 LYS NZ	:	-0.461:	0
: 11242:M 238 LYS NZ	:M 458 GLU CD	:	-0.436:	0
: 11242:M 78 GLU CD	:M 77 ARG 1HH2	:	-0.469:	0
: 11242:M 430 LYS NZ	:M 431 ASP OD2	:	-0.464:	0
: 11242:M 428 TYR OH	:M 427 LYS NZ	:	-0.463:	0
: 11242:M 366 PHE HE2	:M 313 ALA 1HB	:	-0.461:	0
: 11242:M 366 PHE 1HB	:M 318 PRO 2HG	:	-0.404:	0
: 11242:M 42 PRO 2HB	:M 581 GLU 2HB	:	-0.460:	0
: 11242:M 342 ASN 1HB	:M 339 LEU 1HD2	:	-0.460:	0
: 11242:M 519 LYS NZ	:M 581 GLU CD	:	-0.428:	0
: 11242:M 581 GLU OE2	:M 519 LYS NZ	:	-0.403:	0
: 11242:M 681 GLN 1HG	:M 672 GLY 2HA	:	-0.459:	0
: 11242:M 522 ALA HA	:M 477 GLU 1HB	:	-0.458:	0
: 11242:M 463 LEU 2HB	:M 477 GLU HA	:	-0.428:	0
: 11242:M 695 ILE HA	:M 698 PHE CD2	:	-0.456:	0
: 11242:M 698 PHE HA	:M 714 GLY 1HA	:	-0.443:	0
: 11242:M 698 PHE HD1	:M 668 SER 1HB	:	-0.431:	0
: 11242:M 381 GLU HA	:M 384 ARG 2HD	:	-0.453:	0
: 11242:M 311 LYS HA	:M 390 GLN CD	:	-0.453:	0
: 11242:M 701 GLY O	:M 743 PRO 1HD	:	-0.453:	0
: 11242:M 289 ASP OD1	:M 311 LYS NZ	:	-0.421:	0
: 11242:M 329 PHE 1HB	:M 486 ILE 3HG2	:	-0.451:	0
: 11242:M 326 CYS HA	:M 486 ILE 2HG1	:	-0.416:	0
: 11242:M 300 GLU OE2	:M 304 LYS NZ	:	-0.449:	0
: 11242:M 304 LYS NZ	:M 300 GLU CD	:	-0.411:	0
: 11242:M 548 ASP HA	:M 509 GLU 1HG	:	-0.447:	0
: 11242:M 359 ILE 1HD1	:M 351 GLU 1HB	:	-0.446:	0
: 11242:M 594 GLN 2HB	:M 650 TYR CE1	:	-0.444:	0
: 11242:M 410 GLU OE2	:M 377 LYS NZ	:	-0.442:	0

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: 11242:M 449 ALA 2HB	:M 443 LEU O	: -0.441:	0
: 11242:M 485 ILE 2HD1	:M 482 CYS HA	: -0.440:	0
: 11242:M 356 ILE 1HG1	:M 331 ALA HA	: -0.439:	0
: 11242:M 211 PRO 2HG	:M 202 LEU 1HB	: -0.438:	0
: 11242:M 306 PRO 1HB	:M 310 PHE HE1	: -0.436:	0
: 11242:M 306 PRO 1HD	:M 305 ASP HA	: -0.408:	0
: 11242:M 307 ARG 1HH1	:M 305 ASP CG	: -0.405:	0
: 11242:M 306 PRO 1HB	:M 310 PHE CE1	: -0.401:	0
: 11242:M 733 VAL O	:M 737 VAL 3HG2	: -0.432:	0
: 11242:M 203 LYS NZ	:M 204 ASP OD2	: -0.430:	0
: 11242:M 47 SER OG	:M 51 PRO HA	: -0.428:	0
: 11242:M 214 GLU CD	:M 214 GLU H	: -0.427:	0
: 11242:M 258 VAL HA	:M 437 ILE O	: -0.427:	0
: 11242:M 314 LYS NZ	:M 315 GLU OE2	: -0.426:	0
: 11242:M 590 SER HA	:M 593 GLU CD	: -0.426:	0
: 11242:M 432 GLU CD	:M 255 LYS 3HZ	: -0.426:	0
: 11242:M 95 THR CG2	:M 226 ASN HA	: -0.425:	0
: 11242:M 80 GLU OE1	:M 236 LYS NZ	: -0.425:	0
: 11242:M 226 ASN OD1	:M 95 THR HB	: -0.422:	0
: 11242:M 145 ASN 2HD2	:M 145 ASN C	: -0.424:	0
: 11242:M 207 PRO 1HD	:M 206 LEU HA	: -0.423:	0
: 11242:M 531 PRO 2HD	:M 530 THR HA	: -0.420:	0
: 11242:M 221 TRP HE3	:M 198 PRO 2HG	: -0.420:	0
: 11242:M 150 ASP HA	:M 148 PHE HE2	: -0.419:	0
: 11242:M 148 PHE CE2	:M 150 ASP HA	: -0.405:	0
: 11242:M 68 PRO 2HD	:M 67 CYS HA	: -0.415:	0
: 11242:M 398 CYS SG	:M 374 CYS 1HB	: -0.414:	0
: 11242:M 498 ALA 2HB	:M 494 GLY 1HA	: -0.413:	0
: 11242:M 571 SER HA	:M 574 CYS SG	: -0.412:	0
: 11242:M 181 ARG 2HD	:M 181 ARG 1HH1	: -0.412:	0
: 11242:M 167 ARG 1HH1	:M 167 ARG 2HD	: -0.411:	0
: 11242:M 353 VAL 3HG2	:M 349 THR O	: -0.410:	0
: 11242:M 403 PRO 1HD	:M 402 GLU HA	: -0.409:	0

PSVS Software Environment

```
: 11242:M 656 GLU OE1 :M 572 LYS NZ : -0.408: 0
: 11242:M 320 GLN 2HG :M 317 TYR HD2 : -0.408: 0
: 11242:M 572 LYS 1HZ :M 656 GLU CD : -0.407: 0
: 11242:M 580 GLN OE1 :M 580 GLN HA : -0.407: 0
: 11242:M 360 ILE HB :M 343 TYR CD2 : -0.407: 0
: 11242:M 28 PRO 1HD :M 27 SER 2HB : -0.404: 0
: 11242:M 316 ILE 1HG1 :M 312 PHE O : -0.400: 0
: 11242:M 159 SER OG :M 176 TRP 1HB : -0.400: 0
#sum2 ::23.75 clashscore : 23.75 clashscore B
```

Output from PDB validation software

Summary from PDB validation

Jan. 29, 16:03:16 2017

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.

Chain	Atom	Res	Seq	Chain	Atom	Res	Seq	Symm_Code	Distance
A	C	ARG	235 -	A	N	GLY	68	(1, 5, 5, 5)	Dist = 1.31
A	C	MET	66 -	A	N	CYS	67	(1, 5, 5, 5)	Dist = 1.32
A	O	ARG	235 -	A	N	GLY	68	(1, 5, 5, 5)	Dist = 2.19

PSVS Software Environment

=> 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 0.014 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 2.4 degrees.

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

Deviation	Residue Name	Chain ID	Sequence Number	Model	AT1	-	AT2	-	AT3	Bond Angle	Dictionary Value
-15.2	ARG	A	21	1	CA	-	CB	-	CG	98.9	114.1

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.

Model	Chain	Residue Name	Residue Number	Chiral Center	Chiral Neighbor	Original Atom Name
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PSVS Software Environment

1	A	ILE	164	CB	CG2
1	A	ILE	164	CB	CG1

OTHER IMPORTANT ISSUES

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

==> The following residues are missing:

(Note: The SEQ number starts from 1 for each chain according to SEQRES sequence record.)

RES MOD#C SEQ

```

CYS( 1 A 67 )
GLY( 1 A 68 )
ASP( 1 A 69 )
GLY( 1 A 70 )
CYS( 1 A 71 )
ASN( 1 A 72 )
GLY( 1 A 73 )
GLY( 1 A 74 )
TYR( 1 A 75 )
PRO( 1 A 76 )
ALA( 1 A 77 )
GLU( 1 A 78 )
ALA( 1 A 79 )
TRP( 1 A 80 )
ASN( 1 A 81 )
PHE( 1 A 82 )
TRP( 1 A 83 )
THR( 1 A 84 )
ARG( 1 A 85 )
LYS( 1 A 86 )
GLY( 1 A 87 )
LEU( 1 A 88 )
VAL( 1 A 89 )
SER( 1 A 90 )
GLY( 1 A 91 )
GLY( 1 A 92 )
LEU( 1 A 93 )
TYR( 1 A 94 )
GLU( 1 A 95 )
SER( 1 A 96 )
HIS( 1 A 97 )
VAL( 1 A 98 )
GLY( 1 A 99 )
CYS( 1 A 100 )
ARG( 1 A 101 )
PRO( 1 A 102 )
TYR( 1 A 103 )
SER( 1 A 104 )
ILE( 1 A 105 )
PRO( 1 A 106 )
PRO( 1 A 107 )
CYS( 1 A 108 )
GLU( 1 A 109 )
HIS( 1 A 110 )
HIS( 1 A 111 )
VAL( 1 A 112 )

```

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ASN(1 A 113)
GLY(1 A 114)
SER(1 A 115)
ARG(1 A 116)
PRO(1 A 117)
PRO(1 A 118)
CYS(1 A 119)
THR(1 A 120)
GLY(1 A 121)
GLU(1 A 122)
GLY(1 A 123)
ASP(1 A 124)
THR(1 A 125)
PRO(1 A 126)
LYS(1 A 127)
CYS(1 A 128)
SER(1 A 129)
LYS(1 A 130)
ILE(1 A 131)
CYS(1 A 132)
GLU(1 A 133)
PRO(1 A 134)
GLY(1 A 135)
TYR(1 A 136)
SER(1 A 137)
PRO(1 A 138)
THR(1 A 139)
TYR(1 A 140)
LYS(1 A 141)
GLN(1 A 142)
ASP(1 A 143)
LYS(1 A 144)
HIS(1 A 145)
TYR(1 A 146)
GLY(1 A 147)
TYR(1 A 148)
ASN(1 A 149)
SER(1 A 150)
TYR(1 A 151)
SER(1 A 152)
VAL(1 A 153)
SER(1 A 154)
ASN(1 A 155)
SER(1 A 156)
GLU(1 A 157)
LYS(1 A 158)
ASP(1 A 159)
ILE(1 A 160)
MET(1 A 161)
ALA(1 A 162)
GLU(1 A 163)
ILE(1 A 164)
TYR(1 A 165)
LYS(1 A 166)
ASN(1 A 167)
GLY(1 A 168)
PRO(1 A 169)
VAL(1 A 170)
GLU(1 A 171)
GLY(1 A 172)
ALA(1 A 173)
PHE(1 A 174)

PSVS Software Environment

```
SER( 1 A 175 )
VAL( 1 A 176 )
TYR( 1 A 177 )
SER( 1 A 178 )
ASP( 1 A 179 )
PHE( 1 A 180 )
LEU( 1 A 181 )
LEU( 1 A 182 )
TYR( 1 A 183 )
LYS( 1 A 184 )
SER( 1 A 185 )
GLY( 1 A 186 )
VAL( 1 A 187 )
TYR( 1 A 188 )
GLN( 1 A 189 )
HIS( 1 A 190 )
VAL( 1 A 191 )
THR( 1 A 192 )
GLY( 1 A 193 )
GLU( 1 A 194 )
MET( 1 A 195 )
MET( 1 A 196 )
GLY( 1 A 197 )
GLY( 1 A 198 )
HIS( 1 A 199 )
ALA( 1 A 200 )
ILE( 1 A 201 )
ARG( 1 A 202 )
ILE( 1 A 203 )
LEU( 1 A 204 )
GLY( 1 A 205 )
TRP( 1 A 206 )
GLY( 1 A 207 )
VAL( 1 A 208 )
GLU( 1 A 209 )
ASN( 1 A 210 )
GLY( 1 A 211 )
THR( 1 A 212 )
PRO( 1 A 213 )
TYR( 1 A 214 )
TRP( 1 A 215 )
LEU( 1 A 216 )
VAL( 1 A 217 )
ALA( 1 A 218 )
ASN( 1 A 219 )
SER( 1 A 220 )
TRP( 1 A 221 )
ASN( 1 A 222 )
THR( 1 A 223 )
ASP( 1 A 224 )
TRP( 1 A 225 )
GLY( 1 A 226 )
ASP( 1 A 227 )
ASN( 1 A 228 )
GLY( 1 A 229 )
PHE( 1 A 230 )
PHE( 1 A 231 )
LYS( 1 A 232 )
ILE( 1 A 233 )
LEU( 1 A 234 )
ARG( 1 A 235 )
ARG( 1 A 236 )
```

PSVS Software Environment

```
GLY( 1 A 237 )
GLN( 1 A 238 )
ASP( 1 A 239 )
HIS( 1 A 240 )
CYS( 1 A 241 )
GLY( 1 A 242 )
ILE( 1 A 243 )
GLU( 1 A 244 )
SER( 1 A 245 )
GLU( 1 A 246 )
VAL( 1 A 247 )
VAL( 1 A 248 )
ALA( 1 A 249 )
GLY( 1 A 250 )
ILE( 1 A 251 )
PRO( 1 A 252 )
ARG( 1 A 253 )
THR( 1 A 254 )
ASP( 1 A 255 )
ALA( 2 A 299 )
TRP( 2 A 300 )
TRP( 2 A 301 )
THR( 2 A 302 )
CYS( 2 A 419 )
TYR( 2 A 528 )
LYS( 2 A 529 )
GLN( 2 A 530 )
ILE( 2 A 576 )
TYR( 2 A 577 )
ASN( 2 A 577 )
GLY( 2 A 578 )
PHE( 2 A 599 )
LEU( 2 A 599 )
TYR( 2 A 600 )
SER( 2 A 601 )
TYR( 2 A 603 )
ASN( 2 A 654 )
GLY( 2 A 655 )
THR( 2 A 656 )
PHE( 2 A 698 )
PHE( 2 A 699 )
LYS( 2 A 700 )
ILE( 2 A 701 )
HIS( 2 A 719 )
CYS( 2 A 720 )
VAL( 2 A 732 )
ALA( 2 A 733 )
GLY( 2 A 734 )
ILE( 2 A 735 )
PRO( 2 A 736 )
ARG( 2 A 737 )
```

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MISMATCH: ChainID=A ResNum=1 (... MET)
MISMATCH: ChainID=A ResNum=2 (... ALA)
MISMATCH: ChainID=A ResNum=3 (... ASP)
MISMATCH: ChainID=A ResNum=4 (... GLU)
MISMATCH: ChainID=A ResNum=5 (... ALA)
MISMATCH: ChainID=A ResNum=6 (... ALA)
MISMATCH: ChainID=A ResNum=7 (... LEU)
MISMATCH: ChainID=A ResNum=8 (... ALA)
MISMATCH: ChainID=A ResNum=10 (... GLN)
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PSVS Software Environment

MISMATCH: ChainID=A ResNum=11 (... PRO)
MISMATCH: ChainID=A ResNum=12 (... GLY)
MISMATCH: ChainID=A ResNum=13 (... GLY)
MISMATCH: ChainID=A ResNum=14 (... SER)
MISMATCH: ChainID=A ResNum=16 (... SER)
MISMATCH: ChainID=A ResNum=17 (... ALA)
MISMATCH: ChainID=A ResNum=18 (... ALA)
MISMATCH: ChainID=A ResNum=19 (... GLY)
MISMATCH: ChainID=A ResNum=20 (... ALA)
MISMATCH: ChainID=A ResNum=21 (... ASP)
MISMATCH: ChainID=A ResNum=22 (... ARG)
MISMATCH: ChainID=A ResNum=23 (... GLU)
MISMATCH: ChainID=A ResNum=24 (... ALA)
MISMATCH: ChainID=A ResNum=27 (... SER)
MISMATCH: ChainID=A ResNum=28 (... PRO)
MISMATCH: ChainID=A ResNum=29 (... ALA)
MISMATCH: ChainID=A ResNum=30 (... GLY)
MISMATCH: ChainID=A ResNum=31 (... GLU)
MISMATCH: ChainID=A ResNum=32 (... PRO)
MISMATCH: ChainID=A ResNum=33 (... LEU)
MISMATCH: ChainID=A ResNum=34 (... ARG)
MISMATCH: ChainID=A ResNum=35 (... LYS)
MISMATCH: ChainID=A ResNum=36 (... ARG)
MISMATCH: ChainID=A ResNum=37 (... PRO)
MISMATCH: ChainID=A ResNum=38 (... ARG)
MISMATCH: ChainID=A ResNum=39 (PHE ARG)
MISMATCH: ChainID=A ResNum=41 (... GLY)
MISMATCH: ChainID=A ResNum=42 (... PRO)
MISMATCH: ChainID=A ResNum=43 (... GLY)
MISMATCH: ChainID=A ResNum=44 (... LEU)
MISMATCH: ChainID=A ResNum=45 (... GLU)
MISMATCH: ChainID=A ResNum=46 (... ARG)
MISMATCH: ChainID=A ResNum=47 (... SER)
MISMATCH: ChainID=A ResNum=48 (... PRO)
MISMATCH: ChainID=A ResNum=49 (... GLY)
MISMATCH: ChainID=A ResNum=50 (... GLU)
MISMATCH: ChainID=A ResNum=51 (... PRO)
MISMATCH: ChainID=A ResNum=52 (... GLY)
MISMATCH: ChainID=A ResNum=53 (... GLY)
MISMATCH: ChainID=A ResNum=54 (... ALA)
MISMATCH: ChainID=A ResNum=55 (... ALA)
MISMATCH: ChainID=A ResNum=56 (... PRO)
MISMATCH: ChainID=A ResNum=57 (... GLU)
MISMATCH: ChainID=A ResNum=58 (... ARG)
MISMATCH: ChainID=A ResNum=59 (... GLU)
MISMATCH: ChainID=A ResNum=60 (... VAL)
MISMATCH: ChainID=A ResNum=61 (... PRO)
MISMATCH: ChainID=A ResNum=62 (... ALA)
MISMATCH: ChainID=A ResNum=63 (... ALA)
MISMATCH: ChainID=A ResNum=66 (... GLY)
MISMATCH: ChainID=A ResNum=67 (... CYS)
MISMATCH: ChainID=A ResNum=68 (... PRO)
MISMATCH: ChainID=A ResNum=69 (... GLY)
MISMATCH: ChainID=A ResNum=70 (... ALA)
MISMATCH: ChainID=A ResNum=71 (... ALA)
MISMATCH: ChainID=A ResNum=72 (... ALA)
MISMATCH: ChainID=A ResNum=73 (... ALA)
MISMATCH: ChainID=A ResNum=74 (... ALA)
MISMATCH: ChainID=A ResNum=75 (... LEU)
MISMATCH: ChainID=A ResNum=76 (... TRP)
MISMATCH: ChainID=A ResNum=77 (... ARG)
MISMATCH: ChainID=A ResNum=78 (... GLU)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=79 (... ALA)
MISMATCH: ChainID=A ResNum=80 (... GLU)
MISMATCH: ChainID=A ResNum=81 (... ALA)
MISMATCH: ChainID=A ResNum=82 (... GLU)
MISMATCH: ChainID=A ResNum=83 (... ALA)
MISMATCH: ChainID=A ResNum=84 (... ALA)
MISMATCH: ChainID=A ResNum=85 (... ALA)
MISMATCH: ChainID=A ResNum=86 (... ALA)
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MISMATCH: ChainID=A ResNum=91 (... GLU)
MISMATCH: ChainID=A ResNum=92 (... ALA)
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MISMATCH: ChainID=A ResNum=94 (... ALA)
MISMATCH: ChainID=A ResNum=95 (... THR)
MISMATCH: ChainID=A ResNum=96 (... ALA)
MISMATCH: ChainID=A ResNum=97 (... ALA)
MISMATCH: ChainID=A ResNum=98 (... ALA)
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MISMATCH: ChainID=A ResNum=103 (... ASN)
MISMATCH: ChainID=A ResNum=104 (TRP GLY)
MISMATCH: ChainID=A ResNum=106 (... GLY)
MISMATCH: ChainID=A ResNum=107 (... LEU)
MISMATCH: ChainID=A ResNum=109 (CYS GLY)
MISMATCH: ChainID=A ResNum=111 (... SER)
MISMATCH: ChainID=A ResNum=112 (... ARG)
MISMATCH: ChainID=A ResNum=113 (... GLU)
MISMATCH: ChainID=A ResNum=114 (... PRO)
MISMATCH: ChainID=A ResNum=115 (... PRO)
MISMATCH: ChainID=A ResNum=116 (... LEU)
MISMATCH: ChainID=A ResNum=117 (... ALA)
MISMATCH: ChainID=A ResNum=118 (... ASP)
MISMATCH: ChainID=A ResNum=119 (... ASN)
MISMATCH: ChainID=A ResNum=120 (... LEU)
MISMATCH: ChainID=A ResNum=121 (... TYR)
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MISMATCH: ChainID=A ResNum=123 (... GLU)
MISMATCH: ChainID=A ResNum=124 (... ASP)
MISMATCH: ChainID=A ResNum=125 (... ASP)
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MISMATCH: ChainID=A ResNum=127 (... ASP)
MISMATCH: ChainID=A ResNum=128 (... GLU)
MISMATCH: ChainID=A ResNum=129 (... GLY)
MISMATCH: ChainID=A ResNum=130 (... GLU)
MISMATCH: ChainID=A ResNum=131 (THR GLU)
MISMATCH: ChainID=A ResNum=132 (ILE GLU)
MISMATCH: ChainID=A ResNum=133 (LYS GLU)
MISMATCH: ChainID=A ResNum=135 (... ALA)
MISMATCH: ChainID=A ResNum=136 (... ALA)
MISMATCH: ChainID=A ResNum=137 (... ALA)
MISMATCH: ChainID=A ResNum=138 (... ALA)
MISMATCH: ChainID=A ResNum=139 (... ALA)
MISMATCH: ChainID=A ResNum=141 (... GLY)
MISMATCH: ChainID=A ResNum=142 (... TYR)
MISMATCH: ChainID=A ResNum=145 (... ASN)
MISMATCH: ChainID=A ResNum=146 (... LEU)
MISMATCH: ChainID=A ResNum=147 (... LEU)
MISMATCH: ChainID=A ResNum=148 (... PHE)
MISMATCH: ChainID=A ResNum=149 (... GLY)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=150 (... ASP)
MISMATCH: ChainID=A ResNum=151 (... GLU)
MISMATCH: ChainID=A ResNum=152 (... ILE)
MISMATCH: ChainID=A ResNum=153 (... ILE)
MISMATCH: ChainID=A ResNum=154 (... THR)
MISMATCH: ChainID=A ResNum=155 (GLN ASN)
MISMATCH: ChainID=A ResNum=157 (... PHE)
MISMATCH: ChainID=A ResNum=158 (... HIS)
MISMATCH: ChainID=A ResNum=161 (GLY GLU)
MISMATCH: ChainID=A ResNum=163 (CYS ASP)
MISMATCH: ChainID=A ResNum=164 (TRP GLU)
MISMATCH: ChainID=A ResNum=165 (ALA GLU)
MISMATCH: ChainID=A ResNum=166 (PHE ASP)
MISMATCH: ChainID=A ResNum=167 (GLY ARG)
MISMATCH: ChainID=A ResNum=169 (VAL SER)
MISMATCH: ChainID=A ResNum=170 (GLU HIS)
MISMATCH: ChainID=A ResNum=172 (... SER)
MISMATCH: ChainID=A ResNum=173 (ILE SER)
MISMATCH: ChainID=A ResNum=176 (... TRP)
MISMATCH: ChainID=A ResNum=177 (... THR)
MISMATCH: ChainID=A ResNum=178 (... PRO)
MISMATCH: ChainID=A ResNum=179 (... ARG)
MISMATCH: ChainID=A ResNum=180 (... PRO)
MISMATCH: ChainID=A ResNum=183 (CYS GLY)
MISMATCH: ChainID=A ResNum=184 (ILE PRO)
MISMATCH: ChainID=A ResNum=185 (HIS TYR)
MISMATCH: ChainID=A ResNum=187 (ASN PHE)
MISMATCH: ChainID=A ResNum=189 (... GLN)
MISMATCH: ChainID=A ResNum=190 (... GLN)
MISMATCH: ChainID=A ResNum=191 (... HIS)
MISMATCH: ChainID=A ResNum=192 (... LEU)
MISMATCH: ChainID=A ResNum=193 (... MET)
MISMATCH: ChainID=A ResNum=194 (... ILE)
MISMATCH: ChainID=A ResNum=195 (... GLY)
MISMATCH: ChainID=A ResNum=196 (... THR)
MISMATCH: ChainID=A ResNum=197 (... ASP)
MISMATCH: ChainID=A ResNum=198 (... PRO)
MISMATCH: ChainID=A ResNum=199 (... ARG)
MISMATCH: ChainID=A ResNum=200 (... THR)
MISMATCH: ChainID=A ResNum=201 (... ILE)
MISMATCH: ChainID=A ResNum=202 (... LEU)
MISMATCH: ChainID=A ResNum=203 (... LYS)
MISMATCH: ChainID=A ResNum=204 (... ASP)
MISMATCH: ChainID=A ResNum=205 (... LEU)
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MISMATCH: ChainID=A ResNum=207 (... PRO)
MISMATCH: ChainID=A ResNum=208 (... GLU)
MISMATCH: ChainID=A ResNum=209 (... THR)
MISMATCH: ChainID=A ResNum=210 (... ILE)
MISMATCH: ChainID=A ResNum=211 (... PRO)
MISMATCH: ChainID=A ResNum=212 (SER PRO)
MISMATCH: ChainID=A ResNum=213 (VAL PRO)
MISMATCH: ChainID=A ResNum=215 (... LEU)
MISMATCH: ChainID=A ResNum=216 (... ASP)
MISMATCH: ChainID=A ResNum=217 (... ASP)
MISMATCH: ChainID=A ResNum=218 (... MET)
MISMATCH: ChainID=A ResNum=219 (... THR)
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MISMATCH: ChainID=A ResNum=221 (... TRP)
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MISMATCH: ChainID=A ResNum=223 (... ILE)
MISMATCH: ChainID=A ResNum=225 (... ILE)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=226 (... ASN)
MISMATCH: ChainID=A ResNum=227 (... ILE)
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MISMATCH: ChainID=A ResNum=231 (... PRO)
MISMATCH: ChainID=A ResNum=232 (... PRO)
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MISMATCH: ChainID=A ResNum=234 (... ARG)
MISMATCH: ChainID=A ResNum=235 (... LYS)
MISMATCH: ChainID=A ResNum=236 (... LYS)
MISMATCH: ChainID=A ResNum=237 (... ARG)
MISMATCH: ChainID=A ResNum=238 (... LYS)
MISMATCH: ChainID=A ResNum=239 (... ASP)
MISMATCH: ChainID=A ResNum=240 (... ILE)
MISMATCH: ChainID=A ResNum=241 (... ASN)
MISMATCH: ChainID=A ResNum=242 (... THR)
MISMATCH: ChainID=A ResNum=243 (ALA ILE)
MISMATCH: ChainID=A ResNum=246 (... ALA)
MISMATCH: ChainID=A ResNum=247 (... VAL)
MISMATCH: ChainID=A ResNum=248 (... LYS)
MISMATCH: ChainID=A ResNum=249 (... LEU)
MISMATCH: ChainID=A ResNum=251 (... GLN)
MISMATCH: ChainID=A ResNum=252 (... GLU)
MISMATCH: ChainID=A ResNum=253 (... CYS)
MISMATCH: ChainID=A ResNum=254 (... LYS)
MISMATCH: ChainID=A ResNum=255 (... LYS)
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MISMATCH: ChainID=A ResNum=257 (... ILE)
MISMATCH: ChainID=A ResNum=258 (... VAL)
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MISMATCH: ChainID=A ResNum=262 (CYS ALA)
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MISMATCH: ChainID=A ResNum=266 (... VAL)
MISMATCH: ChainID=A ResNum=267 (MET SER)
MISMATCH: ChainID=A ResNum=270 (... ILE)
MISMATCH: ChainID=A ResNum=271 (... PRO)
MISMATCH: ChainID=A ResNum=273 (... PHE)
MISMATCH: ChainID=A ResNum=274 (... ARG)
MISMATCH: ChainID=A ResNum=275 (GLY SER)
MISMATCH: ChainID=A ResNum=276 (CYS ARG)
MISMATCH: ChainID=A ResNum=277 (ASN ASP)
MISMATCH: ChainID=A ResNum=279 (GLY ILE)
MISMATCH: ChainID=A ResNum=281 (... ALA)
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MISMATCH: ChainID=A ResNum=283 (... LEU)
MISMATCH: ChainID=A ResNum=284 (... ALA)
MISMATCH: ChainID=A ResNum=285 (... VAL)
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MISMATCH: ChainID=A ResNum=287 (... PHE)
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MISMATCH: ChainID=A ResNum=299 (... ILE)
MISMATCH: ChainID=A ResNum=301 (ASN TYR)
MISMATCH: ChainID=A ResNum=305 (... ASP)
MISMATCH: ChainID=A ResNum=306 (... PRO)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=307 (... ARG)
MISMATCH: ChainID=A ResNum=308 (... PRO)
MISMATCH: ChainID=A ResNum=309 (... PHE)
MISMATCH: ChainID=A ResNum=310 (... PHE)
MISMATCH: ChainID=A ResNum=311 (... LYS)
MISMATCH: ChainID=A ResNum=312 (... PHE)
MISMATCH: ChainID=A ResNum=313 (... ALA)
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MISMATCH: ChainID=A ResNum=315 (... GLU)
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MISMATCH: ChainID=A ResNum=317 (... TYR)
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MISMATCH: ChainID=A ResNum=321 (... PHE)
MISMATCH: ChainID=A ResNum=322 (... GLN)
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MISMATCH: ChainID=A ResNum=324 (... SER)
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MISMATCH: ChainID=A ResNum=328 (... LYS)
MISMATCH: ChainID=A ResNum=329 (... PHE)
MISMATCH: ChainID=A ResNum=330 (... ILE)
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MISMATCH: ChainID=A ResNum=334 (... ASP)
MISMATCH: ChainID=A ResNum=335 (... LYS)
MISMATCH: ChainID=A ResNum=336 (... GLU)
MISMATCH: ChainID=A ResNum=338 (GLY LYS)
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MISMATCH: ChainID=A ResNum=345 (... GLN)
MISMATCH: ChainID=A ResNum=346 (... ASN)
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MISMATCH: ChainID=A ResNum=350 (... LEU)
MISMATCH: ChainID=A ResNum=352 (... GLN)
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MISMATCH: ChainID=A ResNum=362 (... CYS)
MISMATCH: ChainID=A ResNum=363 (... HIS)
MISMATCH: ChainID=A ResNum=364 (... GLY)
MISMATCH: ChainID=A ResNum=365 (... SER)
MISMATCH: ChainID=A ResNum=366 (... PHE)
MISMATCH: ChainID=A ResNum=367 (... ALA)
MISMATCH: ChainID=A ResNum=368 (... THR)
MISMATCH: ChainID=A ResNum=369 (... ALA)
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MISMATCH: ChainID=A ResNum=373 (... ILE)
MISMATCH: ChainID=A ResNum=374 (... CYS)
MISMATCH: ChainID=A ResNum=375 (... LYS)
MISMATCH: ChainID=A ResNum=376 (... TYR)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=377 (... LYS)
MISMATCH: ChainID=A ResNum=378 (... VAL)
MISMATCH: ChainID=A ResNum=379 (... ASP)
MISMATCH: ChainID=A ResNum=380 (... CYS)
MISMATCH: ChainID=A ResNum=381 (... GLU)
MISMATCH: ChainID=A ResNum=382 (HIS ALA)
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MISMATCH: ChainID=A ResNum=387 (... ILE)
MISMATCH: ChainID=A ResNum=388 (... PHE)
MISMATCH: ChainID=A ResNum=389 (... ASN)
MISMATCH: ChainID=A ResNum=390 (... GLN)
MISMATCH: ChainID=A ResNum=391 (... VAL)
MISMATCH: ChainID=A ResNum=392 (... VAL)
MISMATCH: ChainID=A ResNum=393 (... PRO)
MISMATCH: ChainID=A ResNum=394 (... ARG)
MISMATCH: ChainID=A ResNum=396 (... PRO)
MISMATCH: ChainID=A ResNum=398 (... CYS)
MISMATCH: ChainID=A ResNum=399 (... PRO)
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MISMATCH: ChainID=A ResNum=405 (SER ALA)
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MISMATCH: ChainID=A ResNum=410 (... GLU)
MISMATCH: ChainID=A ResNum=411 (... ILE)
MISMATCH: ChainID=A ResNum=412 (... VAL)
MISMATCH: ChainID=A ResNum=413 (... PHE)
MISMATCH: ChainID=A ResNum=414 (... PHE)
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MISMATCH: ChainID=A ResNum=416 (... GLU)
MISMATCH: ChainID=A ResNum=417 (... ASN)
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MISMATCH: ChainID=A ResNum=427 (... LYS)
MISMATCH: ChainID=A ResNum=428 (... TYR)
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MISMATCH: ChainID=A ResNum=430 (... LYS)
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MISMATCH: ChainID=A ResNum=432 (... GLU)
MISMATCH: ChainID=A ResNum=433 (... VAL)
MISMATCH: ChainID=A ResNum=434 (... ASP)
MISMATCH: ChainID=A ResNum=435 (... LEU)
MISMATCH: ChainID=A ResNum=436 (... LEU)
MISMATCH: ChainID=A ResNum=437 (HIS ILE)
MISMATCH: ChainID=A ResNum=439 (ASN ILE)
MISMATCH: ChainID=A ResNum=442 (... SER)
MISMATCH: ChainID=A ResNum=443 (... LEU)
MISMATCH: ChainID=A ResNum=444 (... LYS)
MISMATCH: ChainID=A ResNum=445 (... VAL)
MISMATCH: ChainID=A ResNum=448 (... VAL)
MISMATCH: ChainID=A ResNum=449 (... ALA)
MISMATCH: ChainID=A ResNum=450 (... LEU)
MISMATCH: ChainID=A ResNum=451 (... ILE)
MISMATCH: ChainID=A ResNum=452 (... PRO)
MISMATCH: ChainID=A ResNum=453 (... SER)

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MISMATCH: ChainID=A ResNum=454 (... SER)
MISMATCH: ChainID=A ResNum=455 (... ILE)
MISMATCH: ChainID=A ResNum=456 (... PRO)
MISMATCH: ChainID=A ResNum=457 (... HIS)
MISMATCH: ChainID=A ResNum=458 (... GLU)
MISMATCH: ChainID=A ResNum=459 (... VAL)
MISMATCH: ChainID=A ResNum=460 (... PRO)
MISMATCH: ChainID=A ResNum=461 (... GLN)
MISMATCH: ChainID=A ResNum=462 (... ILE)
MISMATCH: ChainID=A ResNum=463 (... LEU)
MISMATCH: ChainID=A ResNum=464 (... ILE)
MISMATCH: ChainID=A ResNum=465 (... ASN)
MISMATCH: ChainID=A ResNum=466 (... ARG)
MISMATCH: ChainID=A ResNum=467 (... GLU)
MISMATCH: ChainID=A ResNum=468 (... PRO)
MISMATCH: ChainID=A ResNum=469 (... LEU)
MISMATCH: ChainID=A ResNum=471 (... HIS)
MISMATCH: ChainID=A ResNum=472 (... LEU)
MISMATCH: ChainID=A ResNum=473 (... HIS)
MISMATCH: ChainID=A ResNum=474 (... PHE)
MISMATCH: ChainID=A ResNum=475 (... ASP)
MISMATCH: ChainID=A ResNum=476 (... VAL)
MISMATCH: ChainID=A ResNum=477 (... GLU)
MISMATCH: ChainID=A ResNum=478 (... LEU)
MISMATCH: ChainID=A ResNum=479 (... LEU)
MISMATCH: ChainID=A ResNum=480 (... GLY)
MISMATCH: ChainID=A ResNum=481 (... ASP)
MISMATCH: ChainID=A ResNum=482 (... CYS)
MISMATCH: ChainID=A ResNum=483 (... ASP)
MISMATCH: ChainID=A ResNum=484 (... VAL)
MISMATCH: ChainID=A ResNum=485 (... ILE)
MISMATCH: ChainID=A ResNum=486 (... ILE)
MISMATCH: ChainID=A ResNum=487 (... ASN)
MISMATCH: ChainID=A ResNum=488 (... GLU)
MISMATCH: ChainID=A ResNum=489 (... LEU)
MISMATCH: ChainID=A ResNum=491 (... HIS)
MISMATCH: ChainID=A ResNum=492 (... ARG)
MISMATCH: ChainID=A ResNum=493 (... LEU)
MISMATCH: ChainID=A ResNum=494 (THR GLY)
MISMATCH: ChainID=A ResNum=497 (... TYR)
MISMATCH: ChainID=A ResNum=498 (... ALA)
MISMATCH: ChainID=A ResNum=499 (... LYS)
MISMATCH: ChainID=A ResNum=500 (... LEU)
MISMATCH: ChainID=A ResNum=501 (GLY CYS)
MISMATCH: ChainID=A ResNum=502 (ASP CYS)
MISMATCH: ChainID=A ResNum=503 (THR ASN)
MISMATCH: ChainID=A ResNum=505 (... VAL)
MISMATCH: ChainID=A ResNum=507 (CYS LEU)
MISMATCH: ChainID=A ResNum=509 (LYS GLU)
MISMATCH: ChainID=A ResNum=511 (CYS THR)
MISMATCH: ChainID=A ResNum=513 (... LYS)
MISMATCH: ChainID=A ResNum=514 (... PRO)
MISMATCH: ChainID=A ResNum=516 (... ARG)
MISMATCH: ChainID=A ResNum=517 (... THR)
MISMATCH: ChainID=A ResNum=518 (... GLN)
MISMATCH: ChainID=A ResNum=519 (... LYS)
MISMATCH: ChainID=A ResNum=520 (... GLU)
MISMATCH: ChainID=A ResNum=521 (... LEU)
MISMATCH: ChainID=A ResNum=522 (GLY ALA)
MISMATCH: ChainID=A ResNum=524 (... LEU)
MISMATCH: ChainID=A ResNum=526 (... GLU)
MISMATCH: ChainID=A ResNum=527 (... LEU)

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MISMATCH: ChainID=A ResNum=528 (... PRO)
MISMATCH: ChainID=A ResNum=531 (ASP PRO)
MISMATCH: ChainID=A ResNum=532 (LYS LEU)
MISMATCH: ChainID=A ResNum=534 (TYR VAL)
MISMATCH: ChainID=A ResNum=535 (GLY SER)
MISMATCH: ChainID=A ResNum=536 (TYR GLU)
MISMATCH: ChainID=A ResNum=537 (ASN ASP)
MISMATCH: ChainID=A ResNum=539 (TYR SER)
MISMATCH: ChainID=A ResNum=541 (... PRO)
MISMATCH: ChainID=A ResNum=542 (... GLU)
MISMATCH: ChainID=A ResNum=543 (... ARG)
MISMATCH: ChainID=A ResNum=544 (... THR)
MISMATCH: ChainID=A ResNum=545 (... SER)
MISMATCH: ChainID=A ResNum=546 (... PRO)
MISMATCH: ChainID=A ResNum=547 (... PRO)
MISMATCH: ChainID=A ResNum=548 (... ASP)
MISMATCH: ChainID=A ResNum=549 (... SER)
MISMATCH: ChainID=A ResNum=550 (... SER)
MISMATCH: ChainID=A ResNum=551 (... VAL)
MISMATCH: ChainID=A ResNum=552 (... ILE)
MISMATCH: ChainID=A ResNum=554 (... THR)
MISMATCH: ChainID=A ResNum=555 (... LEU)
MISMATCH: ChainID=A ResNum=556 (... LEU)
MISMATCH: ChainID=A ResNum=557 (... ASP)
MISMATCH: ChainID=A ResNum=558 (... GLN)
MISMATCH: ChainID=A ResNum=559 (... ALA)
MISMATCH: ChainID=A ResNum=560 (... ALA)
MISMATCH: ChainID=A ResNum=561 (... LYS)
MISMATCH: ChainID=A ResNum=564 (... ASP)
MISMATCH: ChainID=A ResNum=565 (... ASP)
MISMATCH: ChainID=A ResNum=566 (... LEU)
MISMATCH: ChainID=A ResNum=567 (... ASP)
MISMATCH: ChainID=A ResNum=568 (... VAL)
MISMATCH: ChainID=A ResNum=571 (... SER)
MISMATCH: ChainID=A ResNum=573 (ASP GLY)
MISMATCH: ChainID=A ResNum=574 (ILE CYS)
MISMATCH: ChainID=A ResNum=576 (ALA GLU)
MISMATCH: ChainID=A ResNum=580 (VAL GLN)
MISMATCH: ChainID=A ResNum=582 (GLY VAL)
MISMATCH: ChainID=A ResNum=583 (ALA GLN)
MISMATCH: ChainID=A ResNum=584 (PHE THR)
MISMATCH: ChainID=A ResNum=586 (... ARG)
MISMATCH: ChainID=A ResNum=587 (... ASN)
MISMATCH: ChainID=A ResNum=589 (TYR GLU)
MISMATCH: ChainID=A ResNum=591 (... ILE)
MISMATCH: ChainID=A ResNum=592 (... ALA)
MISMATCH: ChainID=A ResNum=593 (... GLU)
MISMATCH: ChainID=A ResNum=594 (... GLN)
MISMATCH: ChainID=A ResNum=595 (... MET)
MISMATCH: ChainID=A ResNum=596 (... GLU)
MISMATCH: ChainID=A ResNum=597 (... ASN)
MISMATCH: ChainID=A ResNum=598 (... PRO)
MISMATCH: ChainID=A ResNum=602 (GLY ASN)
MISMATCH: ChainID=A ResNum=604 (GLN GLY)
MISMATCH: ChainID=A ResNum=605 (HIS SER)
MISMATCH: ChainID=A ResNum=606 (VAL SER)
MISMATCH: ChainID=A ResNum=610 (... LYS)
MISMATCH: ChainID=A ResNum=611 (... ASN)
MISMATCH: ChainID=A ResNum=612 (... GLU)
MISMATCH: ChainID=A ResNum=613 (... ARG)
MISMATCH: ChainID=A ResNum=614 (... THR)
MISMATCH: ChainID=A ResNum=615 (... SER)

PSVS Software Environment

MISMATCH: ChainID=A ResNum=616 (MET VAL)
MISMATCH: ChainID=A ResNum=617 (MET ALA)
MISMATCH: ChainID=A ResNum=619 (... THR)
MISMATCH: ChainID=A ResNum=620 (... VAL)
MISMATCH: ChainID=A ResNum=621 (... ARG)
MISMATCH: ChainID=A ResNum=622 (... LYS)
MISMATCH: ChainID=A ResNum=623 (... CYS)
MISMATCH: ChainID=A ResNum=624 (... TRP)
MISMATCH: ChainID=A ResNum=625 (... PRO)
MISMATCH: ChainID=A ResNum=626 (... ASN)
MISMATCH: ChainID=A ResNum=627 (GLY ARG)
MISMATCH: ChainID=A ResNum=628 (HIS VAL)
MISMATCH: ChainID=A ResNum=630 (... LYS)
MISMATCH: ChainID=A ResNum=631 (... GLU)
MISMATCH: ChainID=A ResNum=632 (... GLN)
MISMATCH: ChainID=A ResNum=634 (... SER)
MISMATCH: ChainID=A ResNum=636 (ILE ARG)
MISMATCH: ChainID=A ResNum=638 (... ASP)
MISMATCH: ChainID=A ResNum=640 (... ASN)
MISMATCH: ChainID=A ResNum=641 (... GLN)
MISMATCH: ChainID=A ResNum=642 (... TYR)
MISMATCH: ChainID=A ResNum=643 (... LEU)
MISMATCH: ChainID=A ResNum=644 (... PHE)
MISMATCH: ChainID=A ResNum=645 (... LEU)
MISMATCH: ChainID=A ResNum=646 (... PRO)
MISMATCH: ChainID=A ResNum=647 (... PRO)
MISMATCH: ChainID=A ResNum=648 (... ASN)
MISMATCH: ChainID=A ResNum=649 (... ARG)
MISMATCH: ChainID=A ResNum=650 (... TYR)
MISMATCH: ChainID=A ResNum=651 (... ILE)
MISMATCH: ChainID=A ResNum=652 (... PHE)
MISMATCH: ChainID=A ResNum=653 (TRP HIS)
MISMATCH: ChainID=A ResNum=655 (VAL ALA)
MISMATCH: ChainID=A ResNum=657 (PRO VAL)
MISMATCH: ChainID=A ResNum=659 (... SER)
MISMATCH: ChainID=A ResNum=660 (... ASP)
MISMATCH: ChainID=A ResNum=661 (... SER)
MISMATCH: ChainID=A ResNum=662 (... GLU)
MISMATCH: ChainID=A ResNum=663 (... ASP)
MISMATCH: ChainID=A ResNum=664 (... ASP)
MISMATCH: ChainID=A ResNum=665 (TRP VAL)
MISMATCH: ChainID=A ResNum=667 (VAL SER)
MISMATCH: ChainID=A ResNum=668 (ALA SER)
MISMATCH: ChainID=A ResNum=669 (ASN SER)
MISMATCH: ChainID=A ResNum=671 (... CYS)
MISMATCH: ChainID=A ResNum=672 (... GLY)
MISMATCH: ChainID=A ResNum=673 (TRP SER)
MISMATCH: ChainID=A ResNum=675 (THR SER)
MISMATCH: ChainID=A ResNum=677 (TRP SER)
MISMATCH: ChainID=A ResNum=679 (... THR)
MISMATCH: ChainID=A ResNum=680 (... CYS)
MISMATCH: ChainID=A ResNum=681 (... GLN)
MISMATCH: ChainID=A ResNum=682 (... SER)
MISMATCH: ChainID=A ResNum=683 (... PRO)
MISMATCH: ChainID=A ResNum=684 (... SER)
MISMATCH: ChainID=A ResNum=685 (... LEU)
MISMATCH: ChainID=A ResNum=686 (... GLU)
MISMATCH: ChainID=A ResNum=687 (... GLU)
MISMATCH: ChainID=A ResNum=688 (... PRO)
MISMATCH: ChainID=A ResNum=689 (... MET)
MISMATCH: ChainID=A ResNum=690 (... GLU)
MISMATCH: ChainID=A ResNum=692 (... GLU)

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MISMATCH: ChainID=A ResNum=693 (... SER)
MISMATCH: ChainID=A ResNum=694 (... GLU)
MISMATCH: ChainID=A ResNum=695 (... ILE)
MISMATCH: ChainID=A ResNum=696 (... GLU)
MISMATCH: ChainID=A ResNum=697 (... GLU)
MISMATCH: ChainID=A ResNum=698 (... PHE)
MISMATCH: ChainID=A ResNum=699 (... TYR)
MISMATCH: ChainID=A ResNum=703 (... GLU)
MISMATCH: ChainID=A ResNum=704 (... ASP)
MISMATCH: ChainID=A ResNum=705 (... GLU)
MISMATCH: ChainID=A ResNum=706 (... PRO)
MISMATCH: ChainID=A ResNum=707 (... ASP)
MISMATCH: ChainID=A ResNum=708 (... VAL)
MISMATCH: ChainID=A ResNum=709 (... PRO)
MISMATCH: ChainID=A ResNum=710 (... GLU)
MISMATCH: ChainID=A ResNum=712 (... ALA)
MISMATCH: ChainID=A ResNum=713 (... GLY)
MISMATCH: ChainID=A ResNum=714 (... GLY)
MISMATCH: ChainID=A ResNum=715 (... ALA)
MISMATCH: ChainID=A ResNum=716 (... GLY)
MISMATCH: ChainID=A ResNum=717 (ARG PHE)
MISMATCH: ChainID=A ResNum=719 (GLN THR)
MISMATCH: ChainID=A ResNum=722 (... ASP)
MISMATCH: ChainID=A ResNum=723 (... ASP)
MISMATCH: ChainID=A ResNum=724 (... GLN)
MISMATCH: ChainID=A ResNum=725 (... GLU)
MISMATCH: ChainID=A ResNum=726 (... ALA)
MISMATCH: ChainID=A ResNum=728 (... ASN)
MISMATCH: ChainID=A ResNum=730 (... ALA)
MISMATCH: ChainID=A ResNum=731 (... ILE)
MISMATCH: ChainID=A ResNum=733 (... VAL)
MISMATCH: ChainID=A ResNum=734 (... LYS)
MISMATCH: ChainID=A ResNum=735 (... GLN)
MISMATCH: ChainID=A ResNum=740 (... MET)
MISMATCH: ChainID=A ResNum=741 (... ASN)
MISMATCH: ChainID=A ResNum=742 (... TYR)
MISMATCH: ChainID=A ResNum=743 (... PRO)
MISMATCH: ChainID=A ResNum=744 (... SER)
MISMATCH: ChainID=A ResNum=745 (... ASN)
MISMATCH: ChainID=A ResNum=746 (... LYS)
MISMATCH: ChainID=A ResNum=747 (... SER)
SEQUENCE WARNING: Residue (A GLU 300 ) and Residue (A TYR 301 ) are linked together
SEQUENCE WARNING: Residue (A PHE 302 ) and Residue (A ARG 303 ) are linked together
SEQUENCE WARNING: Residue (A PRO 419 ) and Residue (A GLU 420 ) are linked together
SEQUENCE WARNING: Residue (A THR 530 ) and Residue (A PRO 531 ) are linked together
SEQUENCE WARNING: Residue (A GLU 577 ) and Residue (A LYS 578 ) are linked together
SEQUENCE WARNING: Residue (A LYS 578 ) and Residue (A PRO 579 ) are linked together
SEQUENCE WARNING: Residue (A ASP 599 ) and Residue (A LEU 600 ) are linked together
SEQUENCE WARNING: Residue (A LEU 600 ) and Residue (A LYS 601 ) are linked together
SEQUENCE WARNING: Residue (A LYS 601 ) and Residue (A ASN 602 ) are linked together
SEQUENCE WARNING: Residue (A VAL 603 ) and Residue (A GLY 604 ) are linked together
SEQUENCE WARNING: Residue (A GLU 656 ) and Residue (A VAL 657 ) are linked together
SEQUENCE WARNING: Residue (A GLY 701 ) and Residue (A LEU 702 ) are linked together
SEQUENCE WARNING: Residue (A ASP 720 ) and Residue (A GLY 721 ) are linked together
SEQUENCE WARNING: Residue (A VAL 737 ) and Residue (A THR 738 ) are linked together
```

There were mismatches between the deposited sequence and sequence in coordinates involving alanines and/or glycines. The residue names have been changed to match the deposited sequence and/or the sequence database unless engineered mutation were specified in the deposition. The missing side chain atoms are listed in remark 470.

PSVS Software Environment

PDB Chain_ID: A

```

1
SEQRES: ... LEU ... PRO
COORDS: met ala asp glu ala ala leu ala LEU gln pro gly gly ser PRO
1 15
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

3 4
SEQRES: ... ALA SER ...
COORDS: ser ala ala gly ala asp arg glu ala ALA SER ser pro ala gly
16 30
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

5 6
SEQRES: ... PHE ASP ...
COORDS: glu pro leu arg lys arg pro arg arg ASP gly pro gly leu glu
31 45
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

SEQRES: ...
COORDS: arg ser pro gly glu pro gly gly ala ala pro glu arg glu val
46 60
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

7 8
SEQRES: ... ALA ARG ...
COORDS: pro ala ala ALA ARG gly cys pro gly ala ala ala ala ala leu
61 75
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

9 10
SEQRES: ... GLU GLN
COORDS: trp arg glu ala glu ala glu ala ala ala ala gly gly GLU GLN
76 90
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

11 12
SEQRES: ... TRP PRO
COORDS: glu ala gln ala thr ala ala ala gly glu gly asp asn gly PRO
91 105
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

13 15
SEQRES: ... GLN CYS PRO ...
COORDS: gly leu GLN gly PRO ser arg glu pro pro leu ala asp asn leu
106 120
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

16 19
SEQRES: ... THR ILE LYS GLU ...
COORDS: tyr asp glu asp asp asp asp glu gly glu glu glu glu GLU ala
121 135
^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

20 22
SEQRES: ... ILE ... ARG ASP ...
COORDS: ala ala ala ala ILE gly tyr ARG ASP asn leu leu phe gly asp
136 150

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PSVS Software Environment

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    ^^^ ^^^ ^^^ ^^^          ^^^ ^^^          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^
                                23                                31
SEQRES: ... .. GLN GLY ... .. SER CYS GLY SER CYS TRP ALA
COORDS: glu ile ile thr asn GLY phe his SER CYS glu SER asp glu glu
151
    ^^^ ^^^ ^^^ ^^^ ^^^          ^^^ ^^^          ^^^ ^^^ ^^^ ^^^

                                32                                40
SEQRES: PHE GLY ALA VAL GLU ALA ... ILE SER ASP ... ..
COORDS: asp arg ALA ser his ALA ser ser SER ASP trp thr pro arg pro
166
    ^^^ ^^^          ^^^ ^^^          ^^^ ^^^          ^^^ ^^^ ^^^ ^^^

                                41                                48
SEQRES: ARG ILE CYS ILE HIS THR ASN VAL ... ..
COORDS: ARG ILE gly pro tyr THR phe VAL gln gln his leu met ile gly
181
    ^^^ ^^^ ^^^          ^^^          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

SEQRES: ... ..
COORDS: thr asp pro arg thr ile leu lys asp leu leu pro glu thr ile
196
    ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                                49                                52
SEQRES: ... SER VAL GLU ... .. VAL ...
COORDS: pro pro pro GLU leu asp asp met thr leu trp gln ile VAL ile
211
    ^^^ ^^^ ^^^          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                                53
SEQRES: ... .. SER ... ..
COORDS: asn ile leu SER glu pro pro lys arg lys lys arg lys asp ile
226
    ^^^ ^^^ ^^^          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                                54                                57
SEQRES: ... .. ALA GLU ASP ... .. LEU ... ..
COORDS: asn thr ile GLU ASP ala val lys leu LEU gln glu cys lys lys
241
    ^^^ ^^^ ^^^          ^^^ ^^^ ^^^ ^^^          ^^^ ^^^ ^^^ ^^^ ^^^

                                58                                66
SEQRES: ... .. LEU THR CYS CYS GLY ... SER ... MET CYS GLY ...
COORDS: ile ile val LEU THR gly ala GLY val SER val ser CYS GLY ile
256
    ^^^ ^^^ ^^^          ^^^ ^^^          ^^^          ^^^ ^^^          ^^^

                                67                                73
SEQRES: ... ASP ... .. GLY CYS ASN GLY GLY TYR ... ..
COORDS: pro ASP phe arg ser arg asp GLY ile TYR ala arg leu ala val
271
    ^^^          ^^^ ^^^ ^^^ ^^^ ^^^          ^^^          ^^^ ^^^ ^^^ ^^^ ^^^

                                74                                76
SEQRES: ... .. PRO ... ALA ... .. GLU
COORDS: asp phe pro asp leu pro asp PRO gln ALA met phe asp ile GLU
286
    ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^          ^^^          ^^^ ^^^ ^^^ ^^^

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77                               84
SEQRES:  ALA TRP ASN PHE TRP THR ARG LYS ... ..
COORDS:  ... .. tyr PHE ... .. ARG LYS asp pro arg pro phe phe lys
          301                                     311
          ^^^                               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               85                               86
SEQRES:  ... .. GLY ... .. LEU ...
COORDS:  phe ala lys glu ile tyr pro GLY gln phe gln pro ser LEU cys
          312                                     326
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               87                               91
SEQRES:  ... .. VAL SER ... .. GLY GLY LEU ... ..
COORDS:  his lys phe ile ala leu SER asp lys glu GLY lys LEU leu arg
          327                                     341
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^ ^^^ ^^^       ^^^ ^^^

                               92                               93
SEQRES:  ... TYR ... .. GLU ... ..
COORDS:  asn TYR thr gln asn ile asp thr leu GLU gln val ala gly ile
          342                                     356
          ^^^       ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^ ^^^ ^^^ ^^^

                               94
SEQRES:  ... .. SER ...
COORDS:  gln arg ile ile gln cys his gly ser phe ala thr ala SER cys
          357                                     371
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               95                               97
SEQRES:  ... .. HIS VAL ... GLY ...
COORDS:  leu ile cys lys tyr lys val asp cys glu ala VAL arg GLY asp
          372                                     386
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^ ^^^

                               98                               99
SEQRES:  ... .. CYS ... ARG ... ..
COORDS:  ile phe asn gln val val pro arg CYS pro ARG cys pro ala asp
          387                                     401
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^       ^^^ ^^^ ^^^ ^^^

                               100                              104
SEQRES:  ... PRO TYR SER ILE ... .. PRO ... ..
COORDS:  glu PRO leu ala ILE met lys PRO glu ile val phe phe gly glu
          402                                     416
          ^^^       ^^^ ^^^       ^^^ ^^^       ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               105                              108
SEQRES:  ... .. PRO CYS GLU ... .. HIS ... ..
COORDS:  asn leu PRO ... GLU gln phe HIS arg ala met lys tyr asp lys
          417                                     430
          ^^^ ^^^       ^^^ ^^^       ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               109                              113
SEQRES:  ... .. HIS VAL ASN GLY SER ... ..
COORDS:  asp glu val asp leu leu ile VAL ile GLY SER ser leu lys val
          431                                     445
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^       ^^^       ^^^ ^^^ ^^^ ^^^

                               114  115
SEQRES:  ARG PRO ... ..

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COORDS: ARG PRO val ala leu ile pro ser ser ile pro his glu val pro
         446                                     460
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               116
SEQRES: ... .. PRO ... ..
COORDS: gln ile leu ile asn arg glu pro leu PRO his leu his phe asp
         461                                     475
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               117
SEQRES: ... .. CYS
COORDS: val glu leu leu gly asp cys asp val ile ile asn glu leu CYS
         476                                     490
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               118                               124
SEQRES: ... .. THR GLY GLU ... .. GLY ASP THR PRO ...
COORDS: his arg leu gly GLY GLU tyr ala lys leu cys cys asn PRO val
         491                                     505
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               125                               132
SEQRES: LYS CYS SER LYS ILE CYS GLU ... .. PRO ... ..
COORDS: LYS leu SER glu ILE thr GLU lys pro PRO arg thr gln lys glu
         506                                     520
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               133                               142
SEQRES: ... GLY TYR ... SER ... .. PRO THR TYR LYS GLN ASP LYS
COORDS: leu ala TYR leu SER glu leu pro PRO THR ... .. pro leu
         521                                     532
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               143                               150
SEQRES: HIS TYR GLY TYR ASN SER TYR SER ... ..
COORDS: HIS val ser glu asp SER ser SER pro glu arg thr ser pro pro
         533                                     547
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               151                               152
SEQRES: ... .. VAL ... .. SER
COORDS: asp ser ser val ile VAL thr leu leu asp gln ala ala lys SER
         548                                     562
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               153                               161
SEQRES: ASN ... .. SER GLU ... LYS ASP ILE MET ALA GLU
COORDS: ASN asp asp leu asp val SER GLU ser LYS gly cys MET glu GLU
         563                                     577
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               162                               174
SEQRES: ILE TYR LYS ASN GLY PRO VAL GLU GLY ALA PHE SER ... .. VAL
COORDS: ... .. LYS ... .. PRO gln GLU val gln thr SER arg asn VAL
         578                                     588
               ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

                               175                               181
SEQRES: TYR SER ... .. ASP PHE LEU LEU TYR
COORDS: glu SER ile ala glu gln met glu asn pro ASP ... LEU ... ..
         589                                     600

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PSVS Software Environment

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      ^^^      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^
182                                192
SEQRES: LYS SER GLY VAL TYR GLN HIS VAL THR GLY GLU ... ..
COORDS: LYS ... asn VAL ... gly ser ser THR GLY GLU lys asn glu arg
601                                613
      ^^^      ^^^ ^^^ ^^^
193                                197
SEQRES: ... .. MET MET GLY ... .. .. .. .. .. GLY HIS
COORDS: thr ser val ala GLY thr val arg lys cys trp pro asn arg val
614                                628
      ^^^ ^^^ ^^^ ^^^      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^
198                                203
SEQRES: ALA ... .. ILE ... ARG ILE LEU ... GLY ... ..
COORDS: ALA lys glu gln ILE ser ARG arg LEU asp GLY asn gln tyr leu
629                                643
      ^^^ ^^^ ^^^      ^^^      ^^^      ^^^      ^^^ ^^^ ^^^ ^^^
204                                209
SEQRES: ... .. .. .. .. .. .. TRP GLY VAL GLU ASN GLY
COORDS: phe leu pro pro asn arg tyr ile phe his GLY ala GLU ... ..
644                                656
      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^      ^^^
210                                218
SEQRES: THR PRO TYR ... .. .. .. .. TRP LEU VAL ALA ASN SER
COORDS: ... val TYR ser asp ser glu asp asp val LEU ser ser ser SER
657                                670
      ^^^      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^      ^^^ ^^^ ^^^
219                                224
SEQRES: ... .. TRP ASN THR ASP TRP GLY ... .. .. .. ..
COORDS: cys gly ser ASN ser ASP ser GLY thr cys gln ser pro ser leu
671                                685
      ^^^ ^^^ ^^^      ^^^      ^^^      ^^^ ^^^ ^^^ ^^^ ^^^
225                                226
SEQRES: ... .. .. .. .. ASP ... .. .. .. .. ASN
COORDS: glu glu pro met glu ASP glu ser glu ile glu glu phe tyr ASN
686                                700
      ^^^ ^^^ ^^^ ^^^ ^^^      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^
227                                233
SEQRES: GLY PHE PHE LYS ILE LEU ... .. .. .. .. ARG
COORDS: GLY ... .. .. .. LEU glu asp glu pro asp val pro glu ARG
701                                711
      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^ ^^^
234                                240
SEQRES: ... .. .. .. .. ARG GLY GLN ASP HIS CYS GLY ... ..
COORDS: ala gly gly ala gly phe GLY thr ASP ... .. GLY asp asp gln
712                                724
      ^^^ ^^^ ^^^ ^^^ ^^^ ^^^      ^^^      ^^^ ^^^ ^^^
241                                247
SEQRES: ... .. ILE ... GLU ... .. SER ... .. GLU VAL VAL ALA
COORDS: glu ala ILE asn GLU ala ile SER val lys gln GLU VAL ... ..
725                                737
      ^^^ ^^^      ^^^      ^^^ ^^^      ^^^ ^^^ ^^^

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PSVS Software Environment

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                248                253
SEQRES:  GLY  ILE  PRO  ARG  THR  ASP  ...  ...  ...  ...  ...  ...  ...  ...
COORDS:  ...  ...  ...  ...  THR  ASP  met  asn  tyr  pro  ser  asn  lys  ser
                738                                747
                ^^^  ^^^  ^^^  ^^^  ^^^  ^^^  ^^^  ^^^

```

=> The following residues have missing atoms:

RES	MOD#	C	SEQ	ATOMS										
ARG	(1 A	235)	N	CA	C	O	CB	CG	CD	NE	CZ	NH1		
			NH2											
MET	(1 B	66)	N	CA	C	O	CB	CG	SD	CE				
ARG	(1 B	235)	N	CA	C	O	CB	CG	CD	NE	CZ	NH1		
			NH2											

DocflSIRT1CathB.pdb: Error: Residues (ARG ARG) have same chain_ID 'A' and residue number '235'

DocflSIRT1CathB.pdb: Missing KEYWDS records

DocflSIRT1CathB.pdb: Missing TITLE record