

Protein Structure Validation Suite (PSVS)

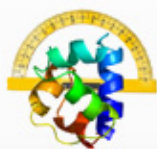


PSVS report for DoccytocSirt1

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PSVS report for DoccytocSirt1



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 order residues.

Procheck analysis,RMSD calculation and structure superimposition are based on: Dihedral angle order parameter, with $S(\phi)+S(\psi)\geq 1.8$

NESG ID: NAME

PDB ID:

Deposition date:

Common Name:

Class:

Length (a.a.): 537

Organism:

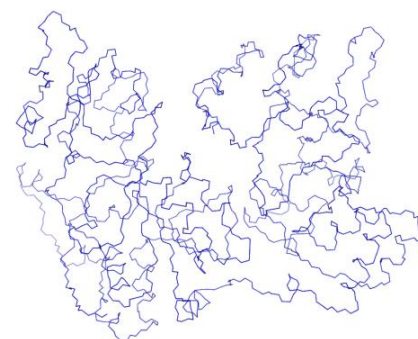
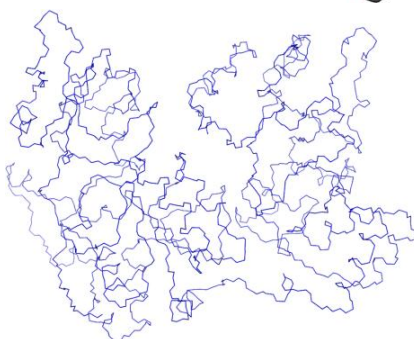
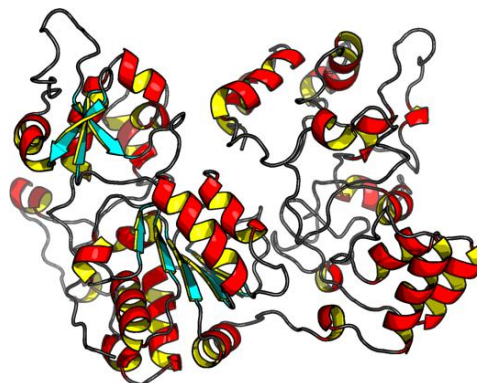
SwissProt /

TrEMBL ID:

models: 2

Oligomerization: monomer

Molecular weight: 58785



Secondary Structure Elements:

alpha helices: 4A-8A, 19A-25A, 35A-38A, 66A-69A, 77A-84A, 128A-132A, 139A-144A, 163A-166A, 185A-194A, 198A-205A, 217A-229A, 243A-252A, 279A-286A, 299A-304A, 307A-316A, 325A-336A, 350A-354A, 381A-388A, 420A-429A, 451A-454A, 482A-493A, 495A-500A, 518A-522A
beta strands: 359A-361A, 339A-344A, 256A-260A, 435A-439A, 461A-465A, 476A-479A, 377A-379A, 364A-371A, 407A-411A

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	6.0 Å	4.1 Å	4.1 Å
All heavy atoms	5.9 Å	4.1 Å	4.1 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
91.7%	8.3%	0.0%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
95.1%	3.3%	1.6%		

Global quality scores

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

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-Raw score	0.36	0.54	-0.24	-0.23	20.67
Z-score ¹	-1.61	-0.45	-0.63	-1.36	-2.02

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: 2.8 °

RMS deviation for bond lengths: 0.012 Å

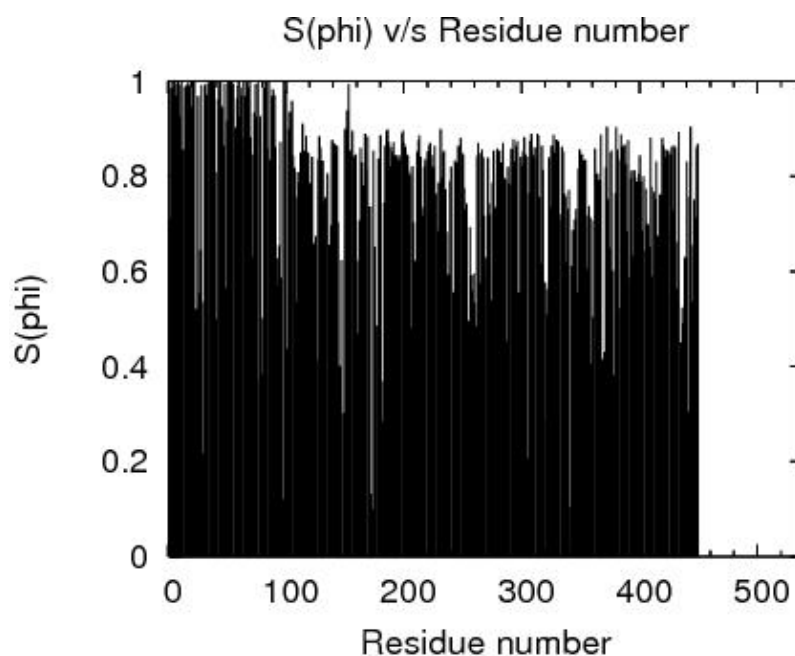
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28; a positive value indicates a 'better' score

²Order residues:

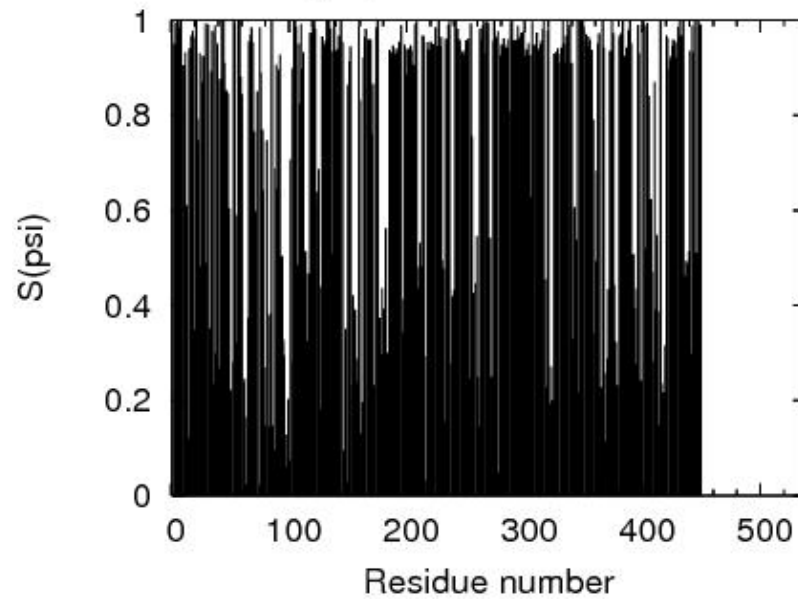
4A-10A,15A-18A,43A-45A,57A-59A,66A-69A,103A-106A,262A-264A,293A-296A,348A-351A,380A-382A

³Selected residues:

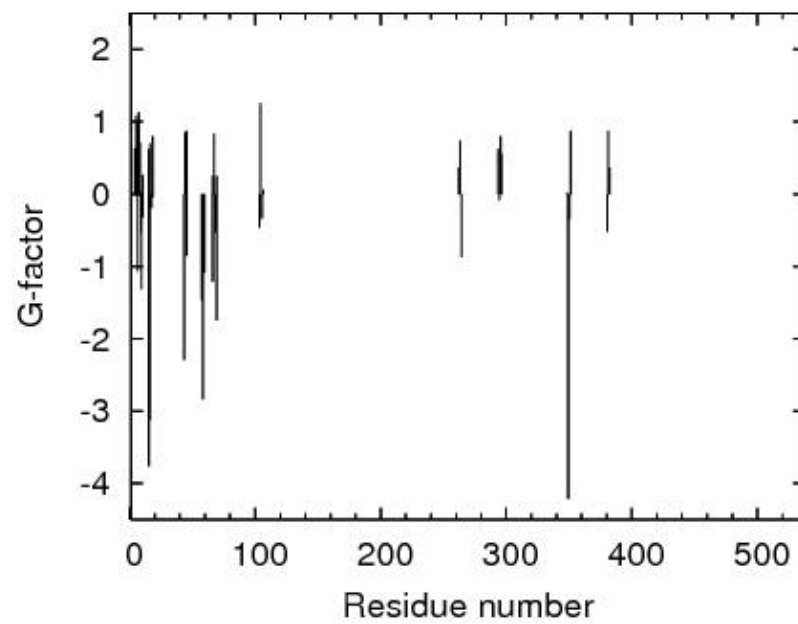
4A-10A,15A-18A,43A-45A,57A-59A,66A-69A,103A-106A,262A-264A,293A-296A,348A-351A,380A-382A



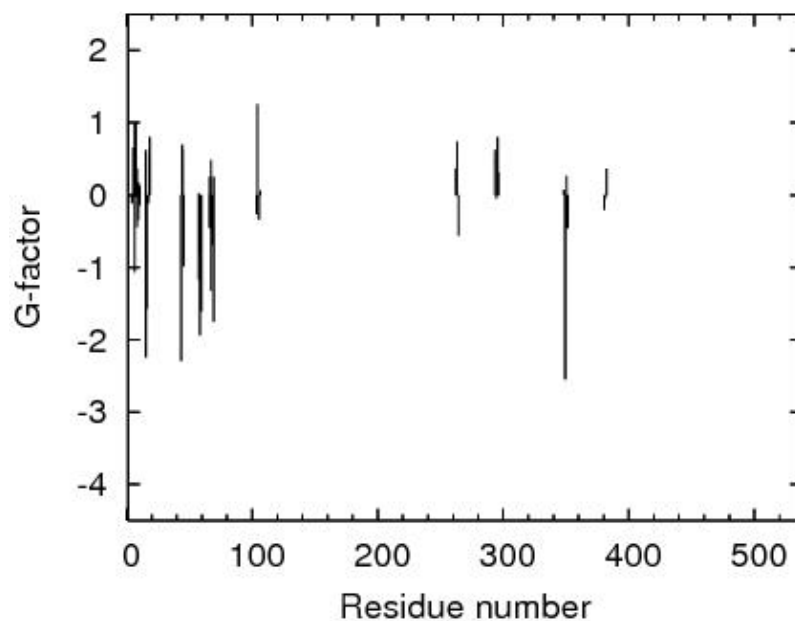
S(psi) v/s Residue number



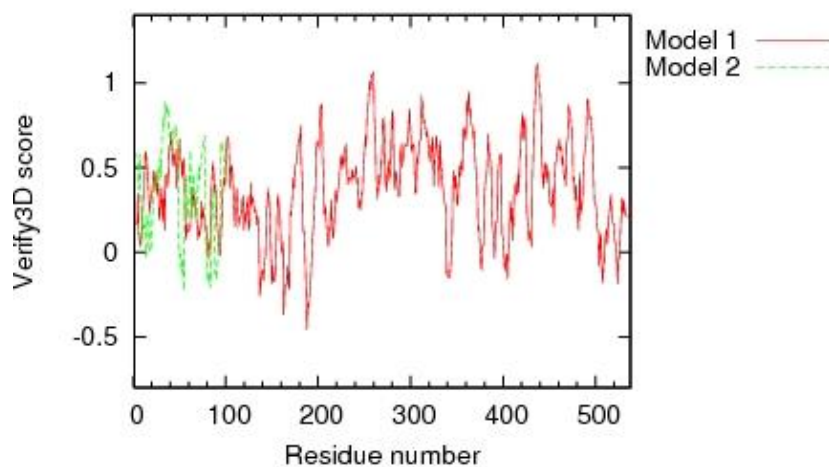
Procheck G-factor for phi-psi



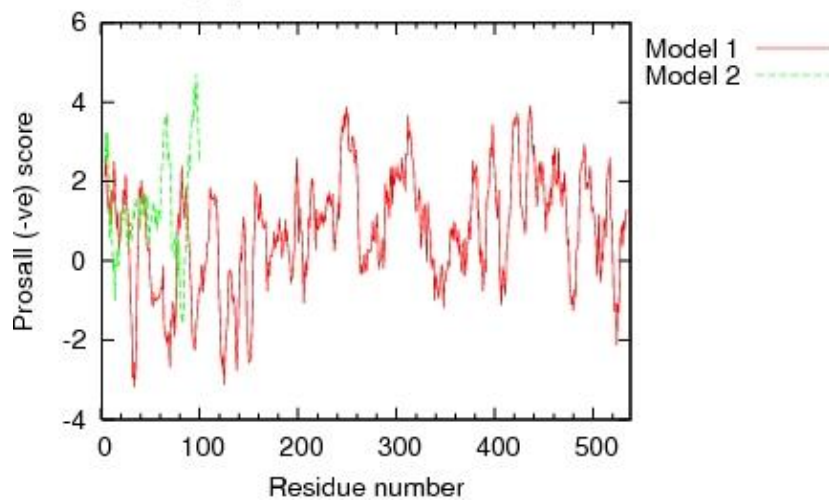
Procheck G-factor for all dihedral angles



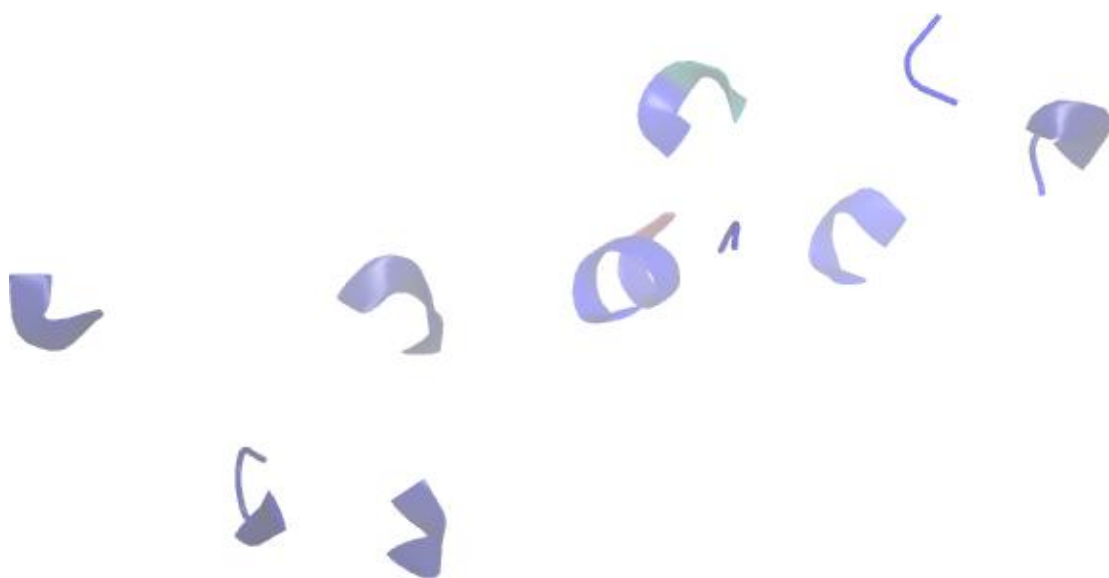
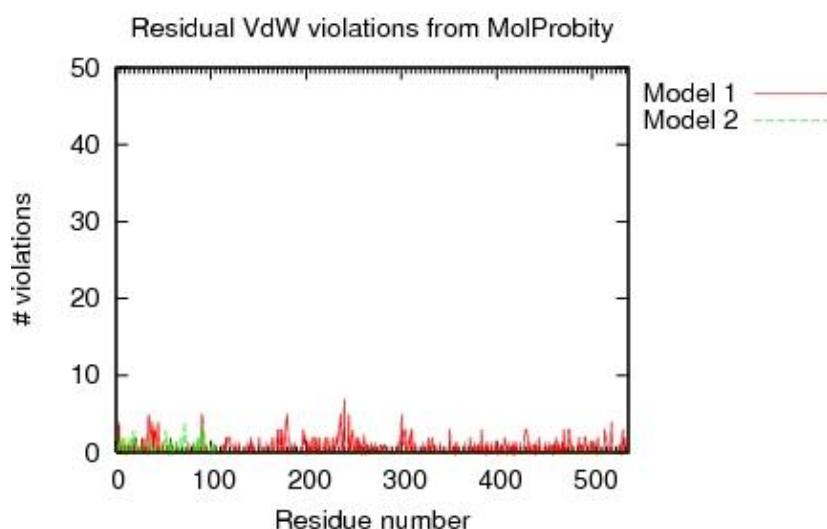
Verify3D score over window of 7 residues



ProsaII (-ve) score over window of 7 residues



PSVS Software Environment



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

References:

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17. Bagaria, A., Jaravine, V., Huang, Y.J., Montelione, G.T., and Guntert, P. "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

Summary of structure quality factors

Analyses performed for order residues.

Total structures computed	currently unknown		
Number of structures used	2		
RMSD Values			
	all	ordered ^e	Selected ^f
All backbone atoms	6.0 Å	4.1 Å	4.1 Å
All heavy atoms	5.9 Å	4.1 Å	4.1 Å
Structure Quality Factors - overall statistics			
	Mean score	SD	Z-score ^g
Procheck G-factor ^e (phi / psi only)	-0.24	N/A	-0.63
Procheck G-factor ^e (all dihedral angles)	-0.23	N/A	-1.36
Verify3D	0.36	0.0141	-1.61
ProsaII (-ve)	0.54	0.2263	-0.45
MolProbity clashscore	20.67	0.2121	-2.02
Ramachandran Plot Summary from Procheck ^f			
Most favoured regions	91.7%		
Additionally allowed regions	8.3%		
Generously allowed regions	0.0%		
Disallowed regions	0.0%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	95.1%		
Allowed regions	3.3%		
Disallowed regions	1.6%		

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

Ordered residue ranges:

4A-10A,15A-18A,43A-45A,57A-59A,66A-69A,103A-106A,262A-264A,293A-296A,348A-351A,380A-382A

^f Residues selected based on: Dihedral angle order parameter, with S(phi)+S(psi)>=1.8

Selected residue ranges:

4A-10A,15A-18A,43A-45A,57A-59A,66A-69A,103A-106A,262A-264A,293A-296A,348A-351A,380A-382A

^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 DoccytocSirt1 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
#	-----											
	MET	A	1		0.710							
	ALA	A	2	0.985	0.950	706.094	706.264				2	2
	ASP	A	3	0.940	0.217	1.000						
	GLU	A	4	0.997	0.994	0.917	0.398	0.331			4	4
	ALA	A	5	1.000	1.000	706.419	706.280	706.766	706.896		5	5
	ALA	A	6	0.969	0.983						6	6
	LEU	A	7	0.994	0.996	0.550	0.999	706.879	705.949		7	7
	ALA	A	8	0.997	1.000	706.076	706.034	706.286	706.165		8	8
	LEU	A	9	0.991	0.902	1.000	0.995				9	9
	GLN	A	10	0.925	0.905	0.613	0.771				10	10
	PRO	A	11	1.000	0.018	0.968	0.391					
	GLY	A	12	0.033	0.932	706.216	706.067	706.879				
	GLY	A	13	0.856	0.610	705.921	706.807	706.051	705.968			
	SER	A	14	0.987	0.121	0.991						
	PRO	A	15	0.991	0.939	0.199					15	15
	SER	A	16	0.916	0.941	0.959	706.153	706.741			16	16
	ALA	A	17	0.995	0.967	706.296					17	17
	ALA	A	18	0.988	0.976	706.249	706.028				18	18
	GLY	A	19	0.946	0.348	706.896						
	ALA	A	20	1.000	0.964	706.265					20	20
	ASP	A	21	0.998	0.999	0.815	0.986	706.168			21	21
	ARG	A	22	0.999	0.792	0.913	0.405	0.492	0.451			
	GLU	A	23	0.520	0.747							
	ALA	A	24	0.294	0.930							
	ALA	A	25	0.968	0.482	705.954	706.140	706.261	706.056			
	SER	A	26	0.554	0.869	0.735	706.814					
	SER	A	27	0.644	0.924	0.042	705.904	706.150	706.029			
	PRO	A	28	0.991	0.806	1.000						28
	ALA	A	29	0.535	0.992							
	GLY	A	30	0.216	0.489	706.869	706.478					
	GLU	A	31	0.992	0.990	0.863	0.887				31	31
	PRO	A	32	0.971	0.202	0.420	0.721					
	LEU	A	33	0.467	0.351	0.984	0.943					
	ARG	A	34	0.996	0.892							34
	LYS	A	35	0.847	0.976	0.985	0.497					35
	ARG	A	36	1.000	0.235	0.423	0.978					
	PRO	A	37	0.304	0.988							
	ARG	A	38	1.000	0.300	0.999	0.914	0.511	0.065	0.999		
	ARG	A	39	0.992	0.950	0.668	0.728	0.477	0.976		39	39
	ASP	A	40	0.498	0.268	0.398						
	GLY	A	41	0.808	0.876							41
	PRO	A	42	0.961	0.087	0.429	0.525	706.777				
	GLY	A	43	0.997	0.998						43	43
	LEU	A	44	0.997	1.000	0.205	0.680				44	44
	GLU	A	45	0.947	0.910						45	45
	ARG	A	46	0.944	0.416	0.476	0.581					

[illegible]

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GLY	A	109	0.534	0.824						
PRO	A	110	0.808	0.991	0.987	0.893	706.560	706.759	706.759	110
SER	A	111	0.786	0.896	0.987					
ARG	A	112	0.849	0.932	0.875	0.162	0.412	0.695	0.999	112
GLU	A	113	0.469	0.266	0.815	0.686	0.373	706.839	706.562	
PRO	A	114	0.910	0.513	0.952	0.938				
PRO	A	115	0.853	0.325	0.957	0.991	706.554	706.759	706.759	
LEU	A	116	0.845	0.467	0.194	0.890				
ALA	A	117	0.885	0.349						
ASP	A	118	0.849	0.973	0.935	0.947	706.831	706.851	706.553	118
ASN	A	119	0.848	0.971	0.893	0.617				119
LEU	A	120	0.785	0.992	0.789	0.173	706.545	706.759	706.759	
TYR	A	121	0.758	1.000	0.800	0.748				
ASP	A	122	0.840	0.982	0.798	0.809				122
GLU	A	123	0.485	0.638	0.071	0.646	0.867	706.835	706.537	
ASP	A	124	0.658	0.614	0.434	0.992				
ASP	A	125	0.673	0.686	0.096	0.993	706.535	706.759	706.759	
ASP	A	126	0.415	0.180	0.388	0.794				
ASP	A	127	0.834	0.439	0.187	0.952				
GLU	A	128	0.884	0.965	0.135	0.823	0.999	706.840	706.566	128
GLY	A	129	0.860	0.948						129
GLU	A	130	0.828	0.944	0.810	0.832	0.945	706.759	706.759	130
GLU	A	131	0.832	0.956	0.592	0.825	0.890			131
GLU	A	132	0.746	1.000	0.405	0.854	0.769			
GLU	A	133	0.755	0.996	0.453	0.828	0.920	706.850	706.568	
GLU	A	134	0.746	0.999	0.876	0.556	0.595			
ALA	A	135	0.805	0.982	706.828	706.855	706.572	706.759	706.759	135
ALA	A	136	0.498	0.508						
ALA	A	137	0.655	0.934						
ALA	A	138	0.696	0.999			706.834	706.851	706.586	
ALA	A	139	0.875	0.907						139
ILE	A	140	0.799	0.935	0.837	0.213	706.579	706.759	706.759	
GLY	A	141	0.868	0.939						141
TYR	A	142	0.767	0.967	0.843	0.998				
ARG	A	143	0.863	0.958	0.809	0.398	0.819	0.594	0.985	143
ASP	A	144	0.703	0.997	0.875	0.977				
ASN	A	145	0.400	0.953	0.726	0.669	706.565	706.759	706.759	
LEU	A	146	0.158	0.095	0.899	0.700				
LEU	A	147	0.623	0.062	0.868	0.051				
PHE	A	148	0.302	0.350	0.135	0.814	706.847	706.859	706.572	
GLY	A	149	0.077	0.028						
ASP	A	150	0.899	0.863	0.101	0.920	706.566	706.759	706.759	150
GLU	A	151	0.780	0.913	0.931	0.795	0.998			
ILE	A	152	0.938	0.944	0.846	0.126				152
ILE	A	153	0.993	0.231	0.290	0.892	706.847	706.854	706.597	
THR	A	154	0.854	0.421	0.759					
ASN	A	155	0.798	0.377	0.649	0.879	706.594	706.759	706.759	
GLY	A	156	0.895	0.391						
PHE	A	157	0.588	0.237	0.868	0.611				
HIS	A	158	0.842	0.288	0.046	0.409	706.836	706.860	706.612	
SER	A	159	0.845	0.987	0.970					159
CYS	A	160	0.468	0.831	0.891	706.861	706.621	706.759	706.759	
GLU	A	161	0.622	0.131	0.068	0.748	0.947			
SER	A	162	0.706	0.196	0.970					
ASP	A	163	0.859	0.921	0.351	0.575	706.833	706.857	706.607	163
GLU	A	164	0.828	0.964	0.918	0.037	0.697			164
GLU	A	165	0.720	0.981	0.666	0.762	0.849	706.759	706.759	
ASP	A	166	0.781	0.842	0.052	0.777				
ARG	A	167	0.889	0.959	0.883	0.011	0.130	0.471	0.979	167
ALA	A	168	0.814	0.127			706.822	706.858	706.610	
SER	A	169	0.883	0.959	0.824					169
HIS	A	170	0.483	0.759	0.759	0.453	706.615	706.759	706.759	

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ALA	A	171	0.736	0.866						
SER	A	172	0.132	0.232	0.980					
SER	A	173	0.100	0.045	1.000	706.810	706.854	706.630		
SER	A	174	0.854	0.983	0.976					174
ASP	A	175	0.651	0.999	0.923	0.585	706.608	706.759	706.759	
TRP	A	176	0.248	0.164	0.713	0.850				
THR	A	177	0.485	0.373	0.949					
PRO	A	178	0.836	0.297	0.969	0.948	706.804	706.852	706.623	
ARG	A	179	0.693	0.436	0.001	0.070	0.827	0.421	0.998	
PRO	A	180	0.886	0.392	0.991	0.885	706.627	706.759	706.759	
ARG	A	181	0.284	0.019	0.923	0.164	0.208	0.678	0.997	
ILE	A	182	0.368	0.562	0.790	0.852				
GLY	A	183	0.744	0.057			706.826	706.850	706.610	
PRO	A	184	0.864	0.300	0.980	0.956				
TYR	A	185	0.895	0.937	0.105	0.843	706.602	706.759	706.759	185
THR	A	186	0.898	0.931	0.959					186
PHE	A	187	0.872	0.928	0.799	1.000				187
VAL	A	188	0.819	0.946	0.022		706.822	706.842	706.618	188
GLN	A	189	0.862	0.940	0.057	0.865	0.788			189
GLN	A	190	0.851	0.928	0.789	0.270	0.698	706.759	706.759	190
HIS	A	191	0.871	0.932	0.728	0.822				191
LEU	A	192	0.843	0.940	0.813	0.116				192
MET	A	193	0.817	0.954	0.836	0.028	0.819	706.839	706.629	193
ILE	A	194	0.844	0.931	0.810	0.067				194
GLY	A	195	0.496	0.988	706.821	706.833	706.627	706.759	706.759	
THR	A	196	0.833	0.413	0.937					
ASP	A	197	0.844	0.342	0.802	0.562				
PRO	A	198	0.890	0.948	0.970	0.947	706.821	706.831	706.634	198
ARG	A	199	0.896	0.885	0.174	0.122	0.876	0.293	1.000	199
THR	A	200	0.869	0.939	0.957	706.841	706.603	706.759	706.759	200
ILE	A	201	0.861	0.938	0.870	0.024				201
LEU	A	202	0.845	0.940	0.047	0.904				202
LYS	A	203	0.843	0.946	0.842	0.026	0.154	0.145	706.597	203
ASP	A	204	0.809	0.936	0.064	0.840				204
LEU	A	205	0.802	0.906	0.771	0.159	706.585	706.759	706.759	205
LEU	A	206	0.481	0.657	0.862	0.046				
PRO	A	207	0.820	0.991	0.982	0.962				207
GLU	A	208	0.703	0.999	0.343	0.654	0.824	706.851	706.583	
THR	A	209	0.541	0.480	0.917					
ILE	A	210	0.622	0.436	0.737	0.741	706.577	706.759	706.759	
PRO	A	211	0.852	0.531	0.982	0.953				
PRO	A	212	0.876	0.482	0.978	0.950				
PRO	A	213	0.886	0.967	0.982	0.969	706.797	706.849	706.568	213
GLU	A	214	0.840	0.966	0.891	0.820	0.339			214
LEU	A	215	0.734	0.293	0.812	0.173	706.570	706.759	706.759	
ASP	A	216	0.716	0.032	0.723	0.893				
ASP	A	217	0.819	0.953	0.720	0.941				217
MET	A	218	0.835	0.938	0.828	0.862	0.837	706.856	706.562	218
THR	A	219	0.831	0.924	0.885					219
LEU	A	220	0.851	0.954	0.809	0.202	706.598	706.759	706.759	220
TRP	A	221	0.863	0.915	0.030	0.810				221
GLN	A	222	0.869	0.949	0.835	0.089	0.778			222
ILE	A	223	0.843	0.905	0.854	0.029	706.805	706.833	706.608	223
VAL	A	224	0.819	0.984	0.895					224
ILE	A	225	0.764	0.937	0.805	0.788	706.613	706.759	706.759	
ASN	A	226	0.864	0.945	0.599	0.689				226
ILE	A	227	0.762	1.000	0.844	0.029				
LEU	A	228	0.684	0.945	0.831	0.091	706.795	706.826	706.607	
SER	A	229	0.786	0.964	0.967					
GLU	A	230	0.369	0.494	0.314	0.765	0.957	706.759	706.759	
PRO	A	231	0.899	0.477	0.973	0.951				
PRO	A	232	0.797	0.157	0.963	0.947				

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LYS	A	233	0.850	0.960	0.829	0.029	0.873	0.226	706.614	233
ARG	A	234	0.854	0.909	0.729	0.011	0.207	0.415	1.000	234
LYS	A	235	0.772	0.990	0.121	0.969	0.109	0.302	706.759	
LYS	A	236	0.682	1.000	0.625	0.070	0.016	0.326		
ARG	A	237	0.593	0.277	0.626	0.009	0.047	0.628	1.000	
LYS	A	238	0.490	0.419	0.881	0.845	0.268	0.767	706.613	
ASP	A	239	0.789	0.049	0.943	0.968				
ILE	A	240	0.819	0.433	0.885	0.137	706.611	706.759	706.759	
ASN	A	241	0.556	0.999	0.733	0.546				
THR	A	242	0.186	0.145	0.869					
ILE	A	243	0.833	0.981	0.034	0.129	706.819	706.807	706.604	243
GLU	A	244	0.828	0.959	0.972	0.880	0.861			244
ASP	A	245	0.794	0.956	0.828	0.881	706.619	706.759	706.759	
ALA	A	246	0.864	0.934						246
VAL	A	247	0.840	0.932	0.072					247
LYS	A	248	0.880	0.926	0.840	0.194	0.017	0.290	706.617	248
LEU	A	249	0.850	0.936	0.698	0.888				249
LEU	A	250	0.845	0.957	0.758	0.171	706.617	706.759	706.759	250
GLN	A	251	0.775	0.951	0.853	0.099	0.976			
GLU	A	252	0.730	0.961	0.786	0.536	0.895			
CYS	A	253	0.742	0.245	0.887		706.807	706.794	706.602	
LYS	A	254	0.495	0.992	0.828	0.764	0.063	0.033		
LYS	A	255	0.442	0.755	0.915	0.019	0.415	0.034	706.759	
ILE	A	256	0.692	0.421	0.908	0.056				
ILE	A	257	0.591	0.426	0.834	0.029				
VAL	A	258	0.560	0.446	0.039		706.802	706.805	706.602	
LEU	A	259	0.595	0.545	0.894	0.009				
THR	A	260	0.534	0.249	0.973	706.803	706.592	706.759	706.759	
GLY	A	261	0.484	0.145						
ALA	A	262	0.842	0.981						262
GLY	A	263	0.870	0.959			706.803	706.798	706.576	263
VAL	A	264	0.848	0.988	0.894					264
SER	A	265	0.574	0.999	0.924	706.808	706.589	706.759	706.759	
VAL	A	266	0.856	0.930	0.076					266
SER	A	267	0.839	0.993	0.992					267
CYS	A	268	0.717	0.998	0.953		706.785	706.806	706.604	
GLY	A	269	0.628	0.993						
ILE	A	270	0.602	0.542	0.874	0.088	706.588	706.759	706.759	
PRO	A	271	0.838	0.249	0.974	0.955				
ASP	A	272	0.742	0.065	0.780	0.846				
PHE	A	273	0.718	0.956	0.828	0.728	706.780	706.807	706.580	
ARG	A	274	0.540	0.999	0.728	0.114	0.040	0.194	0.999	
SER	A	275	0.786	0.076	0.979	706.805	706.591	706.759	706.759	
ARG	A	276	0.854	0.964	0.916	0.066	0.089	0.227	1.000	276
ASP	A	277	0.589	0.976	0.813	0.840				
GLY	A	278	0.734	0.047			706.815	706.806	706.577	
ILE	A	279	0.857	0.926	0.841	0.020				279
TYR	A	280	0.841	0.948	0.764	0.972	706.577	706.759	706.759	280
ALA	A	281	0.853	0.925						281
ARG	A	282	0.828	0.961	0.884	0.065	0.188	0.223	0.999	282
LEU	A	283	0.820	0.947	0.844	0.025	706.819	706.811	706.579	283
ALA	A	284	0.870	0.941						284
VAL	A	285	0.796	0.908	0.100	706.812	706.572	706.759	706.759	
ASP	A	286	0.792	0.959	0.867	0.977				
PHE	A	287	0.453	0.808	0.921	0.565				
PRO	A	288	0.819	0.996	0.962	0.947	706.833	706.808	706.586	288
ASP	A	289	0.691	0.998	0.911	0.994				
LEU	A	290	0.783	0.327	0.745	0.098	706.594	706.759	706.759	
PRO	A	291	0.858	0.957	0.981	0.957				291
ASP	A	292	0.187	0.141	0.566	0.794				
PRO	A	293	0.878	0.958	0.971	0.946	706.832	706.804	706.602	293
GLN	A	294	0.830	0.987	0.895	0.117	0.392			294

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ALA	A	295	0.864	0.961	706.830	706.799	706.592	706.759	706.759	295
MET	A	296	0.874	0.967	0.021	0.846	0.829			296
PHE	A	297	0.548	0.973	0.906	0.576				
ASP	A	298	0.555	0.453	0.181	0.912	706.817	706.795	706.587	
ILE	A	299	0.840	0.975	0.161	0.887				299
GLU	A	300	0.823	0.924	0.548	0.805	0.800	706.759	706.759	300
TYR	A	301	0.851	0.938	0.046	0.783				301
PHE	A	302	0.882	0.913	0.010	0.723				302
ARG	A	303	0.846	0.951	0.845	0.024	0.778	0.476	0.972	303
LYS	A	304	0.840	0.926	0.850	0.040	0.067	0.864		304
ASP	A	305	0.206	0.627	0.035	1.000	706.599	706.759	706.759	
PRO	A	306	0.764	0.996	0.956	0.946				
ARG	A	307	0.874	0.919	0.900	0.151	0.070	0.580	0.997	307
PRO	A	308	0.889	0.947	0.969	0.942	706.830	706.792	706.601	308
PHE	A	309	0.843	0.912	0.000	0.838				309
PHE	A	310	0.813	0.973	0.761	0.603	706.607	706.759	706.759	310
LYS	A	311	0.859	0.914	0.903	0.124	0.058	0.101		311
PHE	A	312	0.836	0.939	0.100	0.897				312
ALA	A	313	0.889	0.948			706.828	706.776	706.608	313
LYS	A	314	0.886	0.956	0.052	0.054	0.134	0.025		314
GLU	A	315	0.756	0.981	0.931	0.867	0.998	706.759	706.759	
ILE	A	316	0.615	0.998	0.871	0.006				
TYR	A	317	0.864	0.455	0.058	0.747				
PRO	A	318	0.813	0.228	0.968	0.950	706.805	706.779	706.573	
GLY	A	319	0.290	0.978						
GLN	A	320	0.576	1.000	0.930	0.077	0.692	706.759	706.759	
PHE	A	321	0.509	0.193	0.853	0.646				
GLN	A	322	0.562	0.271	0.820	0.866	0.858			
PRO	A	323	0.839	0.200	0.971	0.952	706.798	706.778	706.578	
SER	A	324	0.735	0.062	0.988					
LEU	A	325	0.864	0.929	0.213	0.891	706.574	706.759	706.759	325
CYS	A	326	0.860	0.932	0.866					326
HIS	A	327	0.887	0.924	0.706	0.503				327
LYS	A	328	0.849	0.940	0.017	0.014	0.900	0.072	706.586	328
PHE	A	329	0.877	0.910	0.014	0.737				329
ILE	A	330	0.847	0.928	0.880	0.108	706.586	706.759	706.759	330
ALA	A	331	0.874	0.942						331
LEU	A	332	0.707	0.998	0.852	0.256				
SER	A	333	0.720	0.950	0.888		706.773	706.774	706.580	
ASP	A	334	0.861	0.911	0.048	0.853				334
LYS	A	335	0.851	0.967	0.856	0.879	0.277	0.254	706.759	335
GLU	A	336	0.763	0.997	0.073	0.142	0.967			
GLY	A	337	0.757	0.984						
LYS	A	338	0.618	0.989	0.828	0.490	0.303	0.865	706.559	
LEU	A	339	0.731	0.514	0.025	0.835				
LEU	A	340	0.771	0.910	0.071	0.901	706.548	706.759	706.759	
ARG	A	341	0.105	0.328	0.209	0.740	0.867	0.412	0.992	
ASN	A	342	0.611	0.606	0.059	0.945				
TYR	A	343	0.686	0.537	0.793	0.737	706.803	706.792	706.532	
THR	A	344	0.514	0.332	0.256					
GLN	A	345	0.708	0.999	0.831	0.024	0.802	706.759	706.759	
ASN	A	346	0.731	0.215	0.767	0.986				
ILE	A	347	0.555	0.999	0.857	0.007				
ASP	A	348	0.815	0.996	0.859	1.000	706.792	706.796	706.545	348
THR	A	349	0.856	0.998	0.934					349
LEU	A	350	0.836	0.986	0.826	0.046	706.536	706.759	706.759	350
GLU	A	351	0.846	0.955	0.997	0.810	1.000			351
GLN	A	352	0.765	0.970	0.840	0.174	0.843			
VAL	A	353	0.832	0.944	0.053		706.787	706.798	706.555	353
ALA	A	354	0.834	0.965						354
GLY	A	355	0.605	0.958	706.779	706.797	706.553	706.759	706.759	
ILE	A	356	0.717	0.544	0.888	0.023				

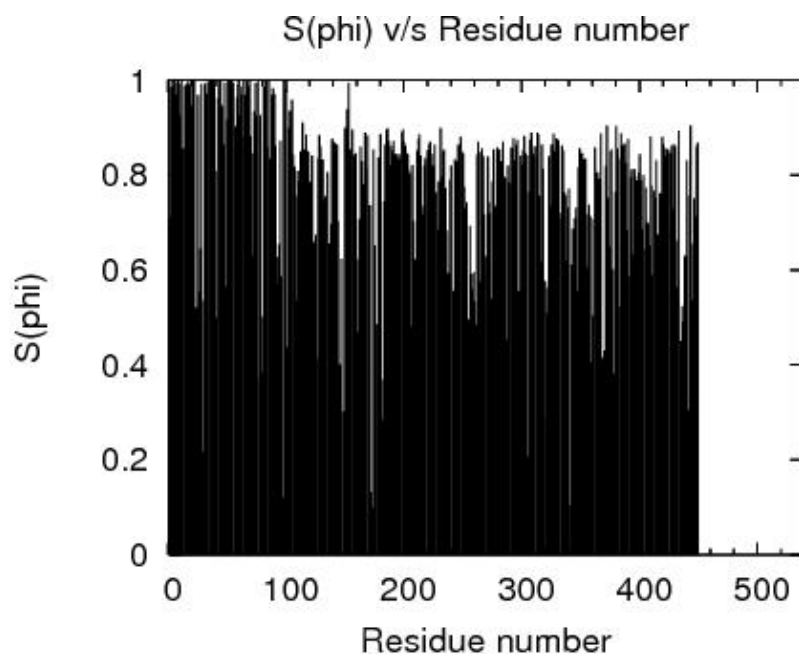
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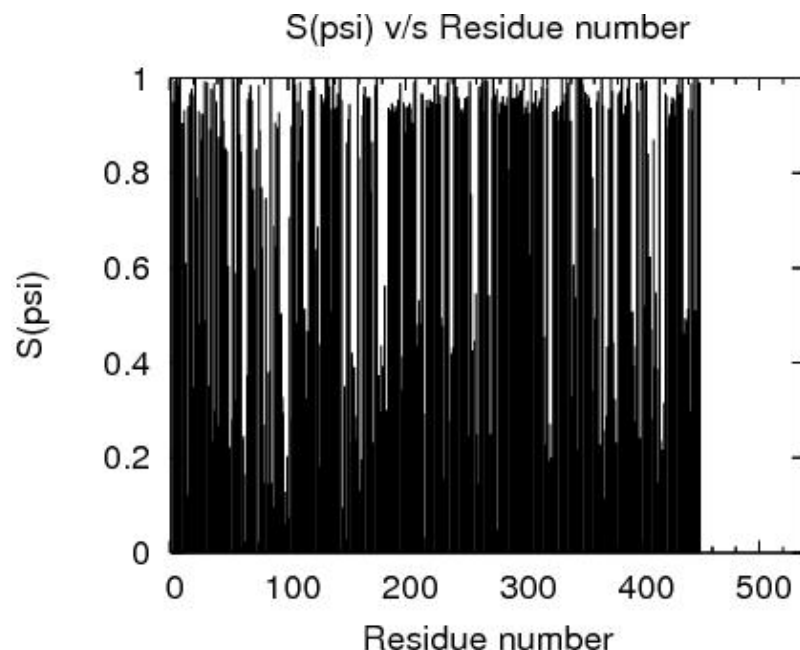
GLN	A	357	0.737	0.937	0.917	0.002	0.273			
ARG	A	358	0.712	0.790	0.694	0.191	0.810	0.040	0.998	
ILE	A	359	0.405	0.341	0.051	0.445				
ILE	A	360	0.504	0.493	0.800	0.816	706.558	706.759	706.759	
GLN	A	361	0.706	0.682	0.729	0.019	0.962			
CYS	A	362	0.857	0.950	0.911					362
HIS	A	363	0.569	0.971	0.825	0.669	706.786	706.806	706.519	
GLY	A	364	0.805	0.227						
SER	A	365	0.064	0.054	0.972	706.810	706.523	706.759	706.759	
PHE	A	366	0.791	1.000	0.774	0.683				
ALA	A	367	0.887	0.942						367
THR	A	368	0.415	0.114	0.964		706.784	706.802	706.508	
ALA	A	369	0.341	0.258						
SER	A	370	0.430	0.288	0.890	706.807	706.498	706.759	706.759	
CYS	A	371	0.818	0.434	0.099					
LEU	A	372	0.904	0.935	0.088	0.858				372
ILE	A	373	0.751	0.874	0.870	0.842	706.792	706.810	706.496	372
CYS	A	374	0.648	0.999	0.925					
LYS	A	375	0.850	0.972	0.866	0.273	0.340	0.065	706.759	375
TYR	A	376	0.854	0.443	0.012	0.792				
LYS	A	377	0.601	0.323	0.834	0.011	0.171	0.882		
VAL	A	378	0.381	0.157	0.861		706.782	706.818	706.514	
ASP	A	379	0.764	0.231	0.904	0.691				
CYS	A	380	0.903	0.964	0.883	706.819	706.521	706.759	706.759	380
GLU	A	381	0.855	0.969	0.925	0.710	0.892			380
ALA	A	382	0.834	0.974						381
VAL	A	383	0.521	0.998	0.870		706.776	706.825	706.537	382
ARG	A	384	0.888	0.925	0.029	0.099	0.866	0.537	1.000	384
GLY	A	385	0.861	0.922	706.774	706.822	706.547	706.759	706.759	385
ASP	A	386	0.856	0.942	0.819	0.967				386
ILE	A	387	0.866	0.921	0.838	0.020				387
PHE	A	388	0.824	0.978	0.794	0.998				388
ASN	A	389	0.683	0.999	0.815	0.905				
GLN	A	390	0.875	0.951	0.823	0.279	0.903			390
VAL	A	391	0.586	0.379	0.085					
VAL	A	392	0.795	0.507	0.051					
PRO	A	393	0.811	0.395	0.971	0.957				
ARG	A	394	0.632	0.277	0.783	0.804	0.196	0.182	0.994	
CYS	A	395	0.812	0.435	0.022					
PRO	A	396	0.798	0.989	0.964	0.949				
ARG	A	397	0.728	0.930	0.007	0.014	0.026	0.106	1.000	
CYS	A	398	0.788	0.242	0.931					
PRO	A	399	0.805	0.199	0.961	0.944				
ALA	A	400	0.844	0.989						400
ASP	A	401	0.789	0.995	0.957	0.707				
GLU	A	402	0.685	0.519	0.093	0.864	0.798			
PRO	A	403	0.799	0.988	0.967	0.949				
LEU	A	404	0.643	0.993	0.856	0.032				
ALA	A	405	0.773	0.840						
ILE	A	406	0.611	0.421	0.895	0.097				
MET	A	407	0.699	0.623	0.856	0.886	0.845			
LYS	A	408	0.651	0.470	0.106	0.213	0.814	0.294		
PRO	A	409	0.881	0.282	0.975	0.952				
GLU	A	410	0.777	0.869	0.897	0.234	0.638			
ILE	A	411	0.589	0.390	0.881	0.066				
VAL	A	412	0.766	0.548	0.004					
PHE	A	413	0.751	0.147	0.765	0.855				
PHE	A	414	0.830	0.387	0.869	0.317				
GLY	A	415	0.674	0.999						
GLU	A	416	0.627	0.235	0.834	0.030	0.990			
ASN	A	417	0.761	0.216	0.007	0.872				
LEU	A	418	0.742	0.128	0.820	0.198				

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PRO	A	419	0.880	0.315	0.971	0.949				
GLU	A	420	0.863	0.967	0.908	0.057	0.915			420
GLN	A	421	0.839	0.962	0.346	0.951	0.888			421
PHE	A	422	0.856	0.897	0.073	0.772				422
HIS	A	423	0.842	0.916	0.875	0.842				423
ARG	A	424	0.854	0.924	0.814	0.026	0.020	0.591	0.996	424
ALA	A	425	0.845	0.945						425
MET	A	426	0.813	0.958	0.173	0.829	0.594			426
LYS	A	427	0.862	0.956	0.830	0.004	0.003	0.029		427
TYR	A	428	0.727	0.920	0.901	0.455				
ASP	A	429	0.864	0.952	0.828	0.995				429
LYS	A	430	0.859	0.985	0.846	0.182	0.031	0.959		430
ASP	A	431	0.661	1.000	0.831	0.981				
GLU	A	432	0.563	0.967	0.719	0.795	0.725			
VAL	A	433	0.893	0.373	0.875					
ASP	A	434	0.450	0.999	0.875	0.987				
LEU	A	435	0.148	0.405	0.012	0.881				
LEU	A	436	0.523	0.461	0.051	0.798				
ILE	A	437	0.490	0.493	0.890	0.030				
VAL	A	438	0.629	0.487	0.017					
ILE	A	439	0.483	0.513	0.935	0.025				
GLY	A	440	0.830	0.935						440
SER	A	441	0.304	0.298	0.098					
SER	A	442	0.756	0.988	0.990					
LEU	A	443	0.904	0.932	0.810	0.022			443	443
LYS	A	444	0.654	1.000	0.281	0.076	0.053	0.043		
VAL	A	445	0.536	0.510	0.024					
ARG	A	446	0.750	0.237	0.875	0.067	0.804	0.236	0.999	
PRO	A	447	0.712	1.000	0.948	0.950				
VAL	A	448	0.860	0.940	0.029					448
ALA	A	449	0.868	0.990						449

JPEG image of S(phi)~Residue_number Plot



JPEG image of S(psi)~Residue_number Plot**Table of Backbone and Heavy Atom RMSD****Text report of backbone and heavy atom RMSD for ordered regions**

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>
> Kabsch RMSD data for family `DoccytocSirt1.pdb'
>
> Kabsch RMSD of backbone atoms in res. A[2..2],A[4..10],A[15..18],A[20..21],A[31..31],A[39..39]
> Kabsch RMSD of backbone atoms in res. A[2..2],A[4..10],A[15..18],A[20..21],A[31..31],A[39..39]
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[2..2],[4..10],[15..18],[20..21],[31..31],[39..39]
> Range of RMSD values to reference struct. is 1.397 to 6.274

> Kabsch RMSD of heavy atoms in res. A[2..2],A[4..10],A[15..18],A[20..21],A[31..31],A[39..39],A[45..45],A[46..46],A[47..47],A[48..48],A[49..49],A[50..50]
> Kabsch RMSD of heavy atoms in res. A[2..2],A[4..10],A[15..18],A[20..21],A[31..31],A[39..39],A[45..45],A[46..46],A[47..47],A[48..48],A[49..49],A[50..50]
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[2..2],[4..10],[15..18],[20..21],[31..31],[39..39],[45..45],[46..46],[47..47],[48..48],[49..49],[50..50]
> Range of RMSD values to reference struct. is 1.810 to 7.089
```

Text report of backbone RMSD for entire protein

```
> Kabsch RMSD of backb atoms in res. *[1..537],for model 1 is: 1.288 (*)
> Kabsch RMSD of backb atoms in res. *[1..537],for model 2 is: 10.725
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[1..537], is: 6.006
> Range of RMSD values to reference struct. is 1.288 to 10.725
```

Text report of heavy atom RMSD for entire protein

```
> Kabsch RMSD of heavy atoms in res. *[1..537],for model 1 is: 1.234 (*)
> Kabsch RMSD of heavy atoms in res. *[1..537],for model 2 is: 10.658
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[1..537], is: 5.946
> Range of RMSD values to reference struct. is 1.234 to 10.658
```

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	6.0	4.1	4.1
All heavy atoms	5.9	4.1	4.1

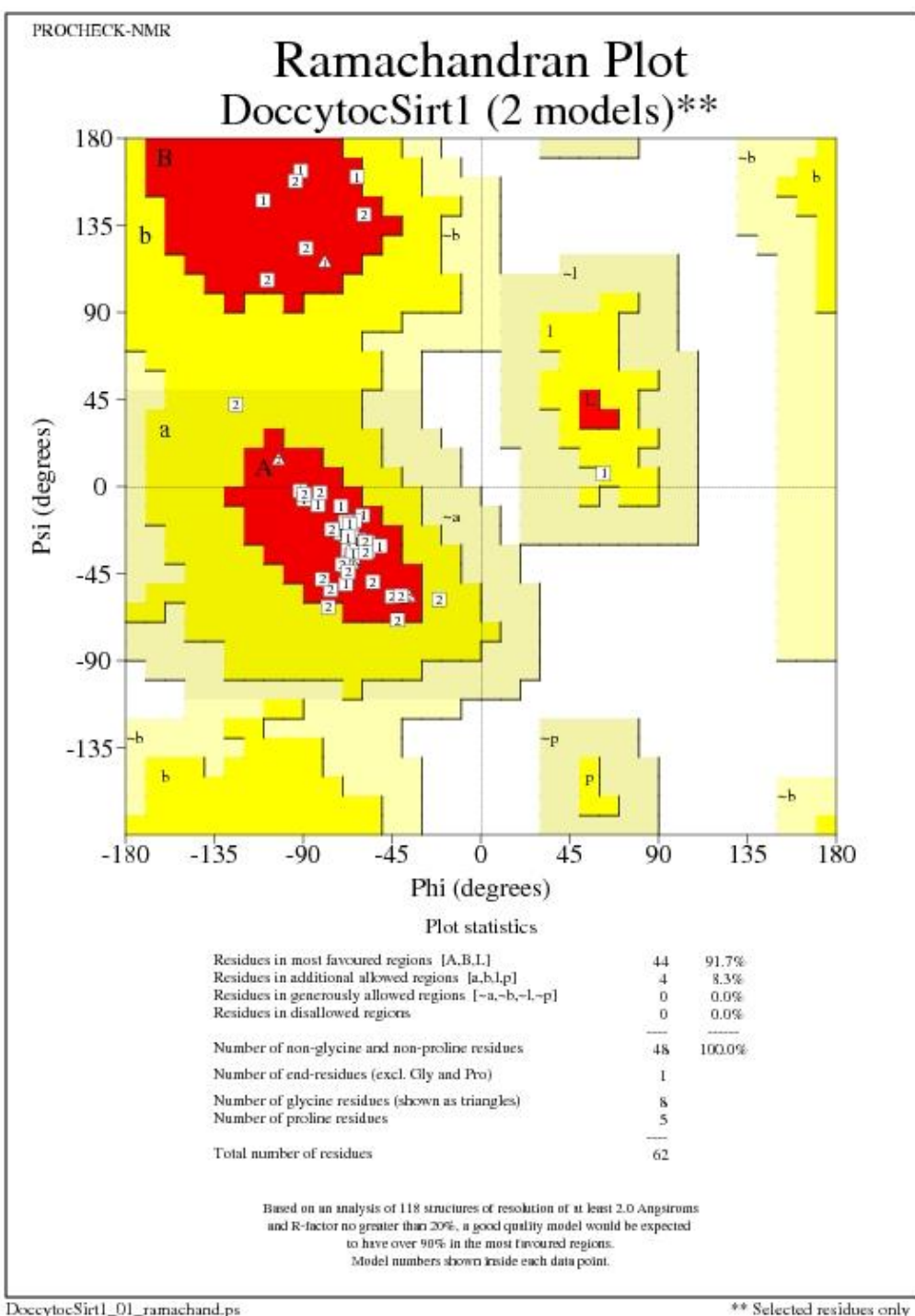
Output from PROCHECK

Ramachandran Plot for all models

Text summary of Ramachandran Plot

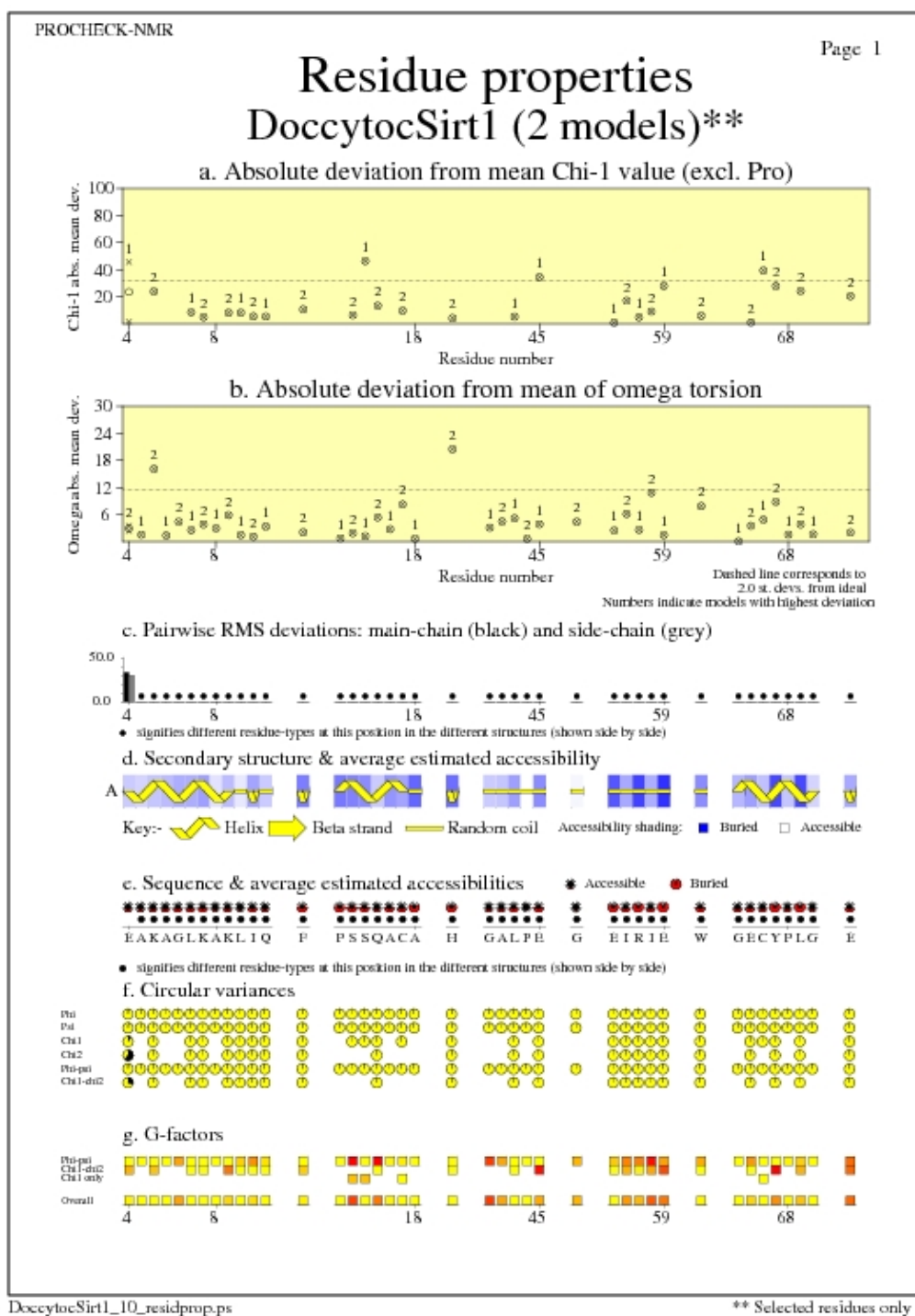
```
+-----<<< P R O C H E C K      S U M M A R Y >>>-----+
|
| DoccytocSirt1_002.rin    0.0                                62 residues |
|
| Ramachandran plot:    91.7% core    8.3% allow    0.0% gener    0.0% disall |
|
*| All Ramachandrans:    3 labelled residues (out of 61)
| Chi1-chi2 plots:      0 labelled residues (out of 33)
|
```

JPEG image for all model Ramachandran Plot

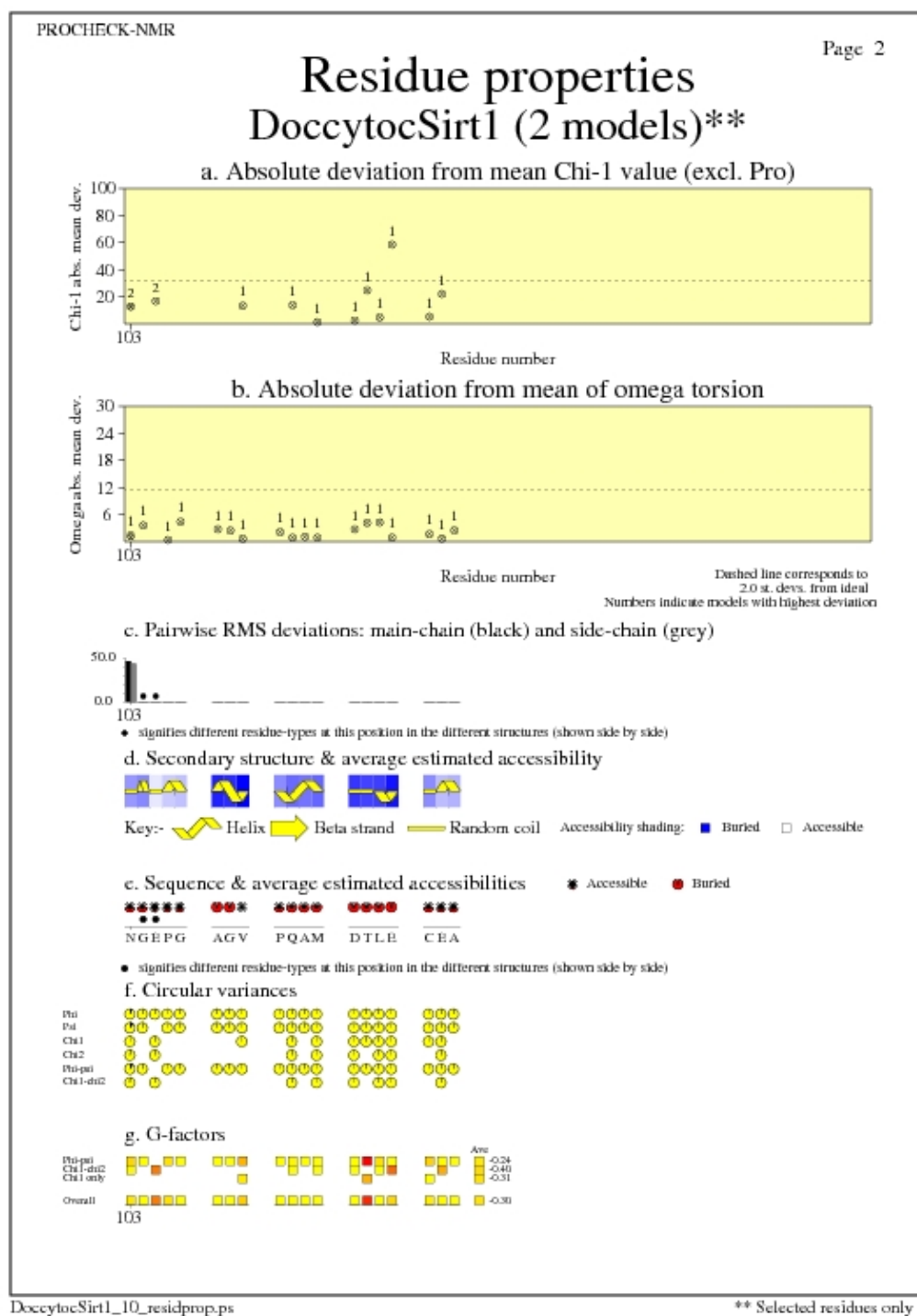


Residue Properties for all models

JPEG for all model Residue Properties - page \$num_n

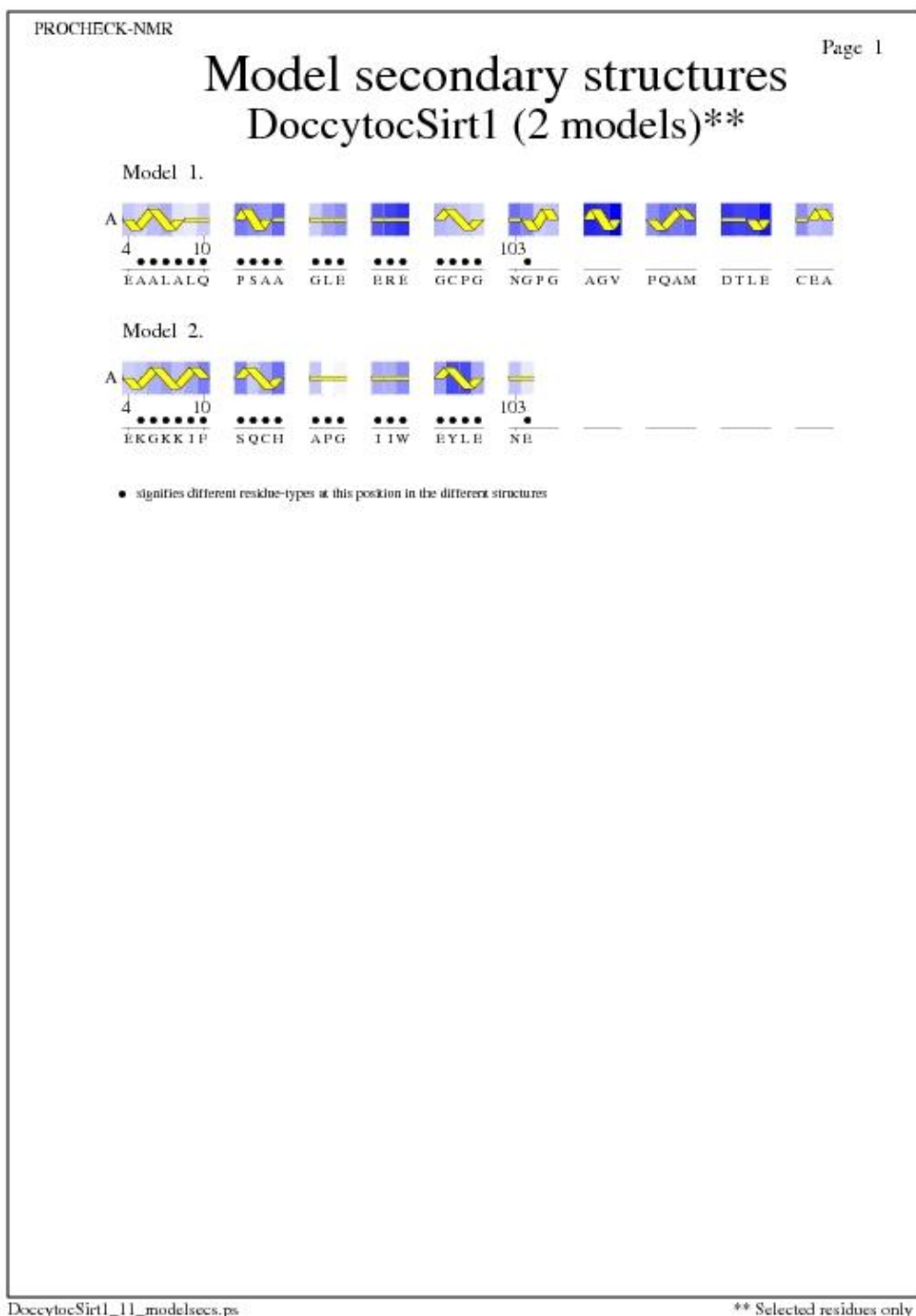


JPEG for all model Residue Properties - page \$num_n



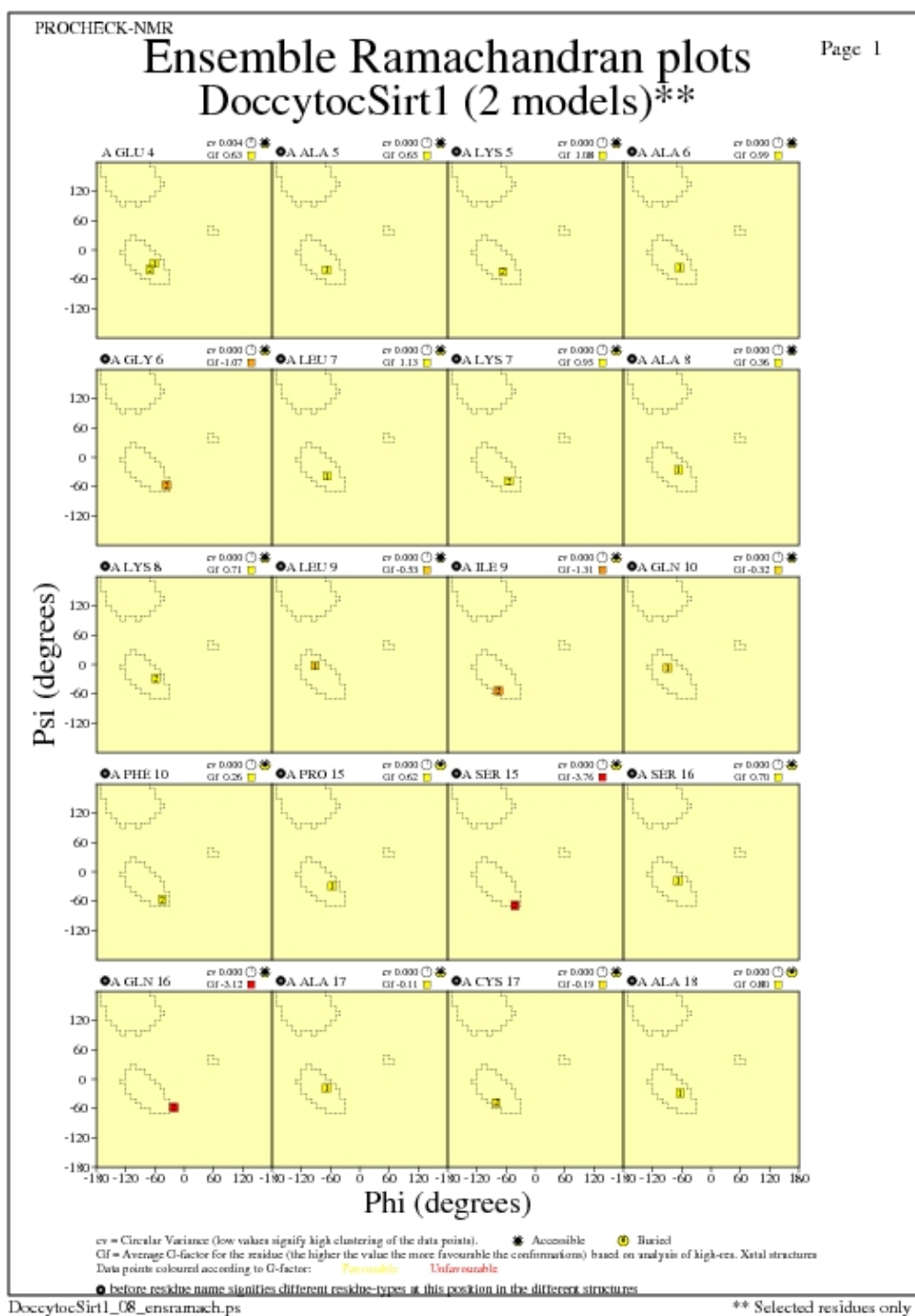
Model Secondary Structures from Procheck

JPEG for Model Secondary Structures

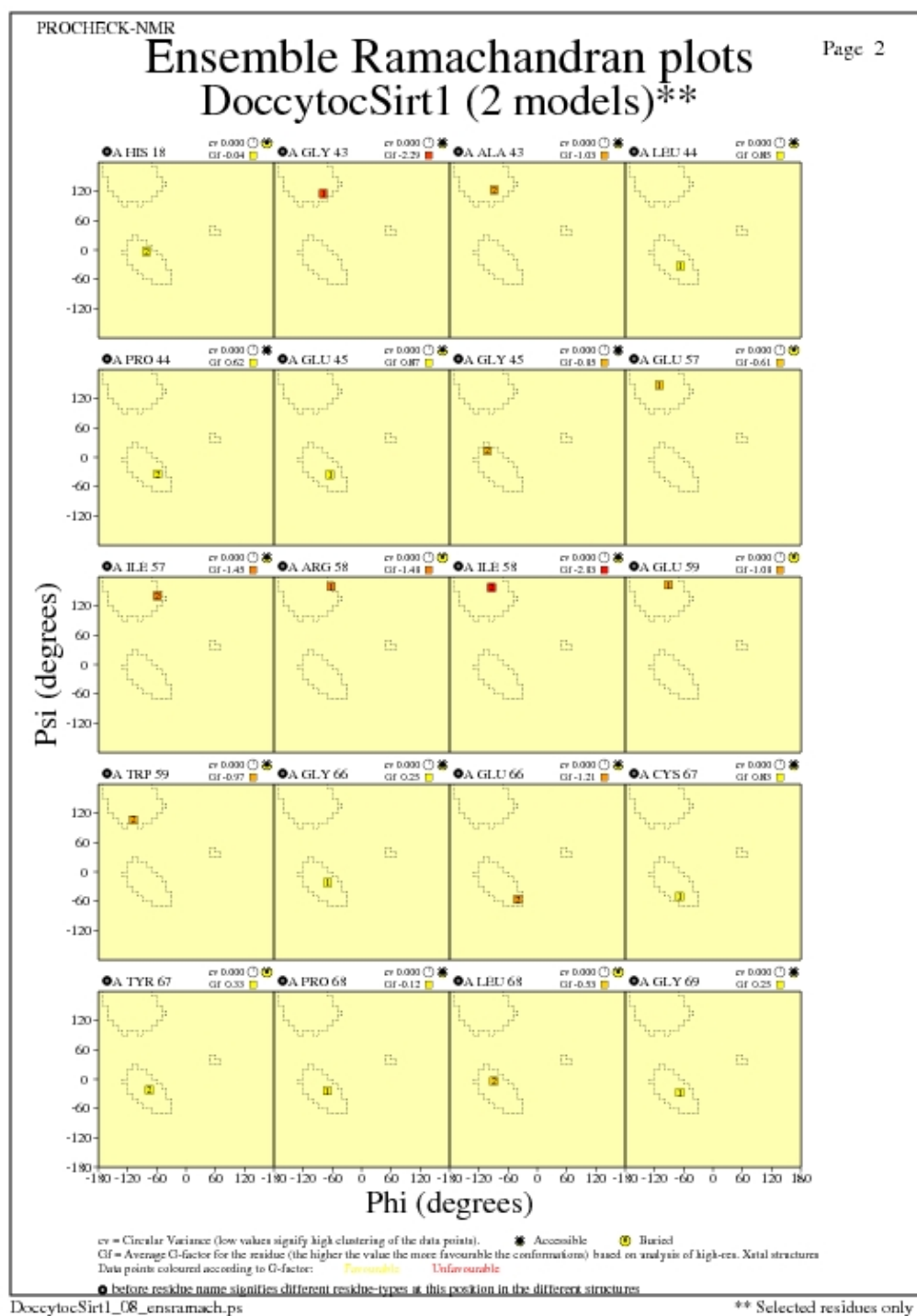


Ramachandran Plots for each residue

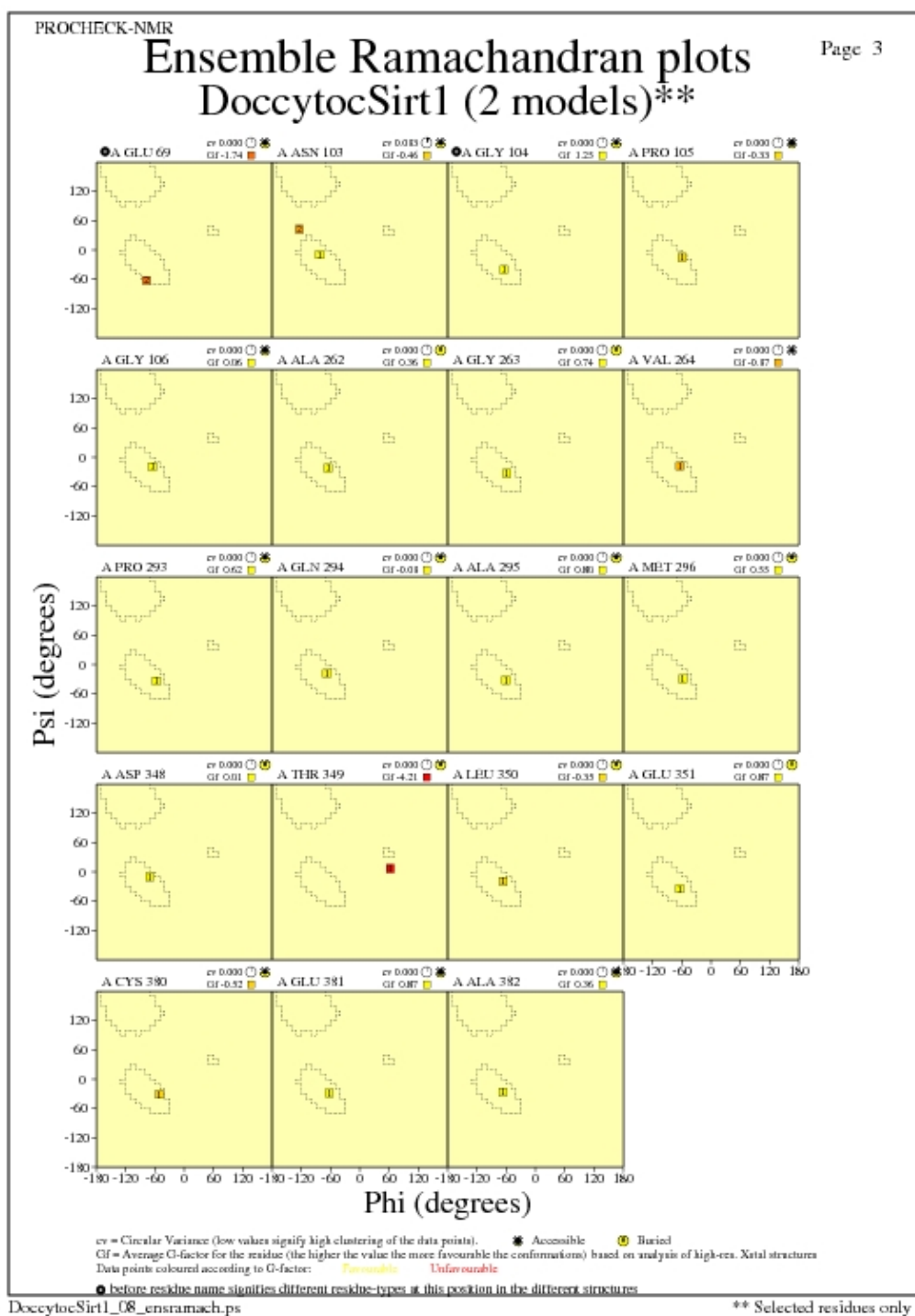
JPEG for residue Ramachandran Plots - page \$num_n



JPEG for residue Ramachandran Plots - page \$num_n



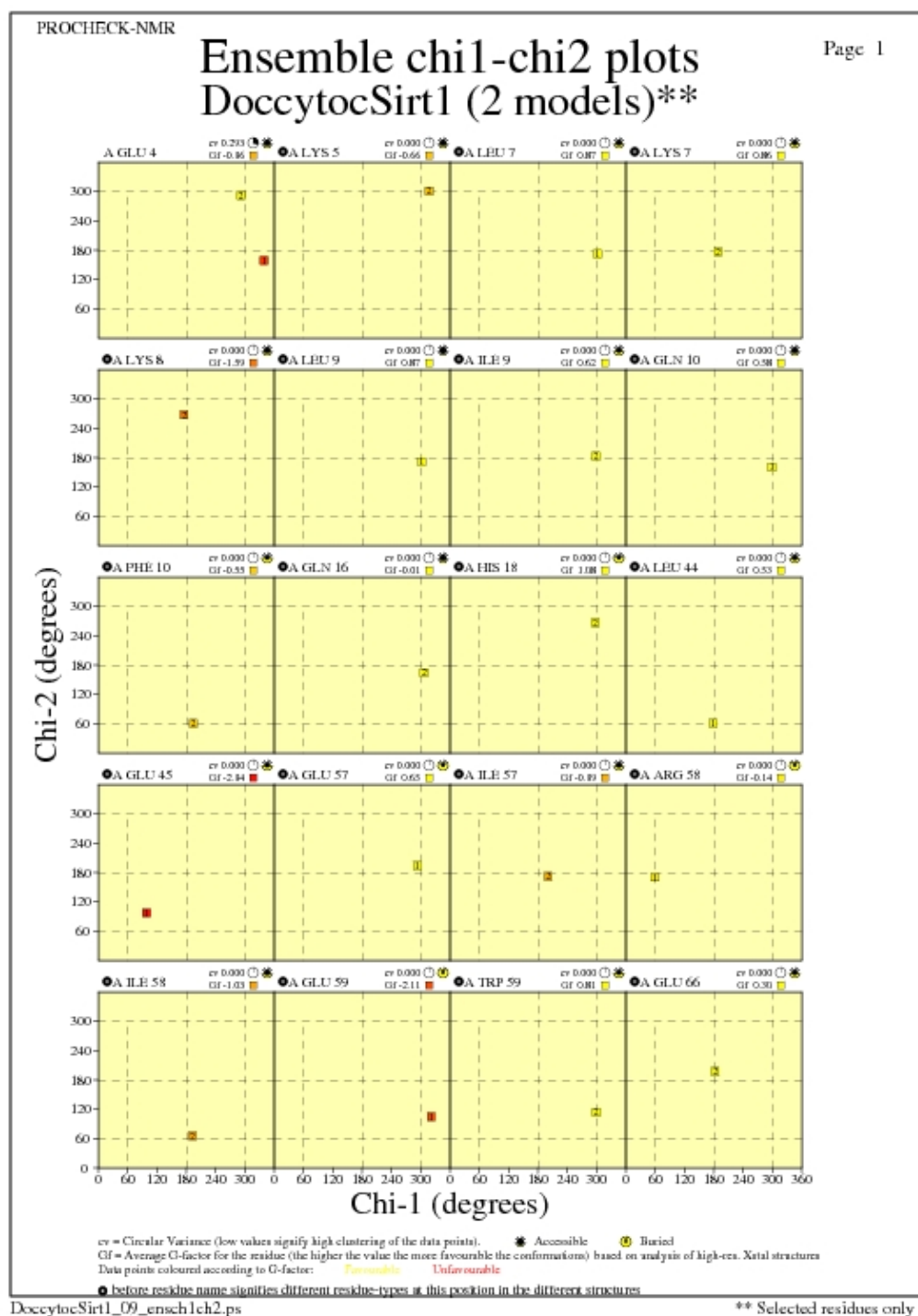
JPEG for residue Ramachandran Plots - page \$num_n



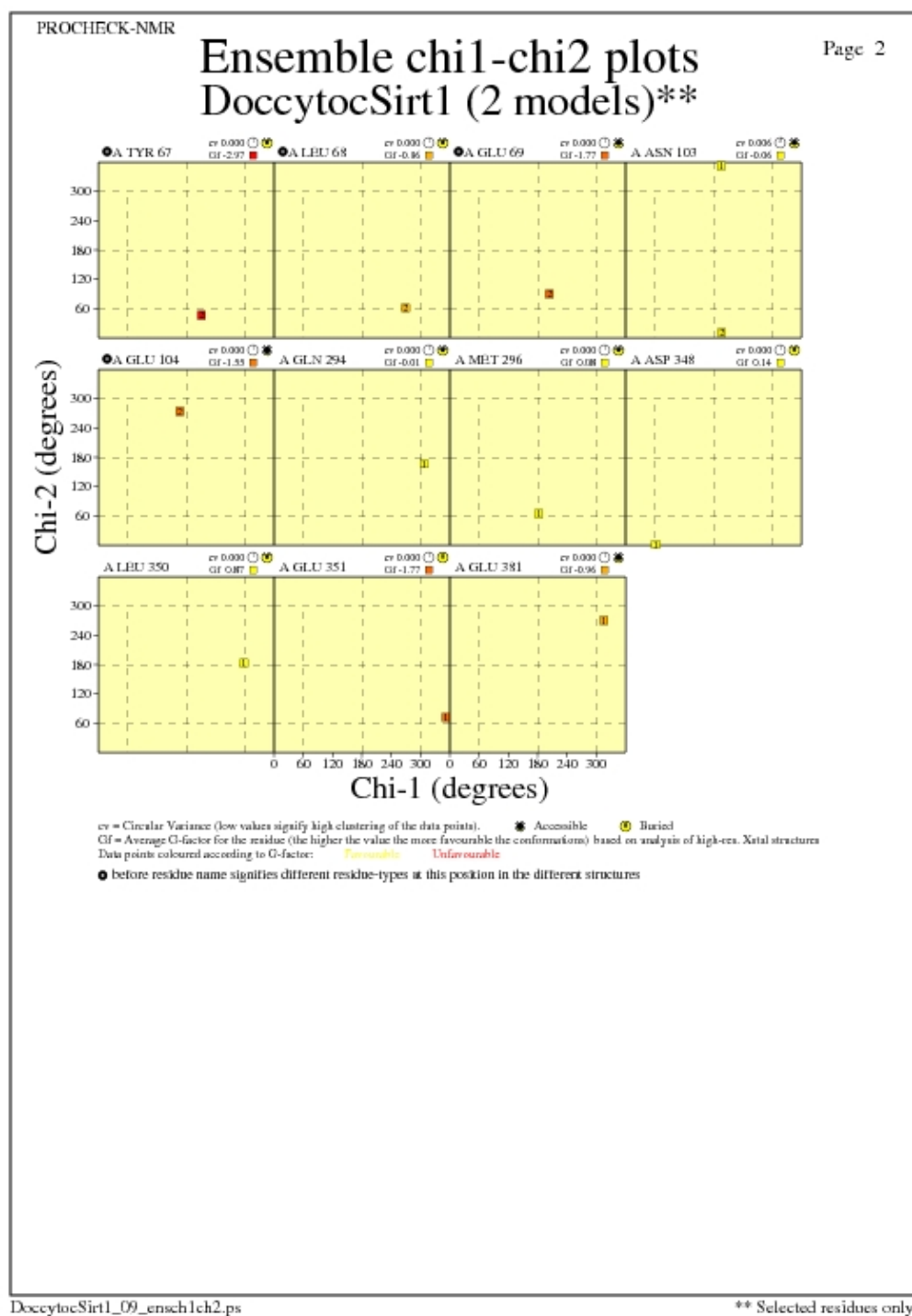
Ramachandran analysis for each residue from Molprobitry

Chi1-Chi2 Plots for each residue

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



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



Procheck G-factors for phi-psi for each residue

JPEG image for residue phi-psi G-factors

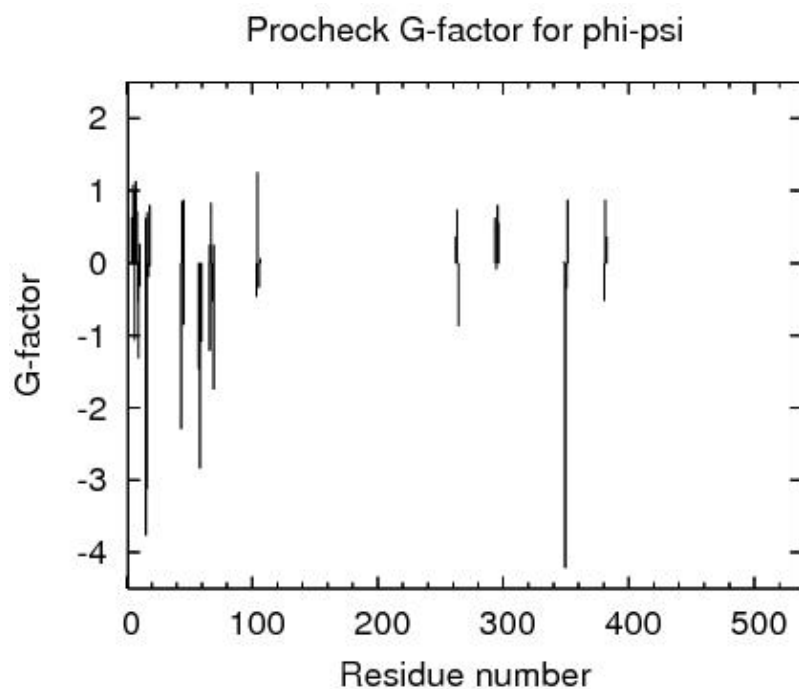


Table of Procheck G-factors for phi-psi for ordered residues

```
#phipsi_gfactor
#Residue\Model  average
4      0.63
5      0.65      1.08
6      0.99     -1.07
7      1.13      0.95
8      0.36      0.71
9     -0.53     -1.31
10     -0.32      0.26
15     0.62     -3.76
16     0.70     -3.12
17     -0.11     -0.19
18     0.80     -0.04
43     -2.29     -1.03
44     0.85      0.62
45     0.87     -0.85
57     -0.61     -1.45
58     -1.48     -2.83
59     -1.08     -0.97
66     0.25     -1.21
67     0.83      0.33
68     -0.12     -0.53
69     0.25     -1.74
103    -0.46
104     1.25
105    -0.33
106     0.06
262     0.36
263     0.74
264    -0.87
293     0.62
294    -0.08
295     0.80
296     0.55
348     0.01
```

```

349      -4.21
350      -0.35
351       0.87
380      -0.52
381       0.87
382       0.36
#Reported_Model_Average -0.239
#Overall_Average_Reported      -0.239

```

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

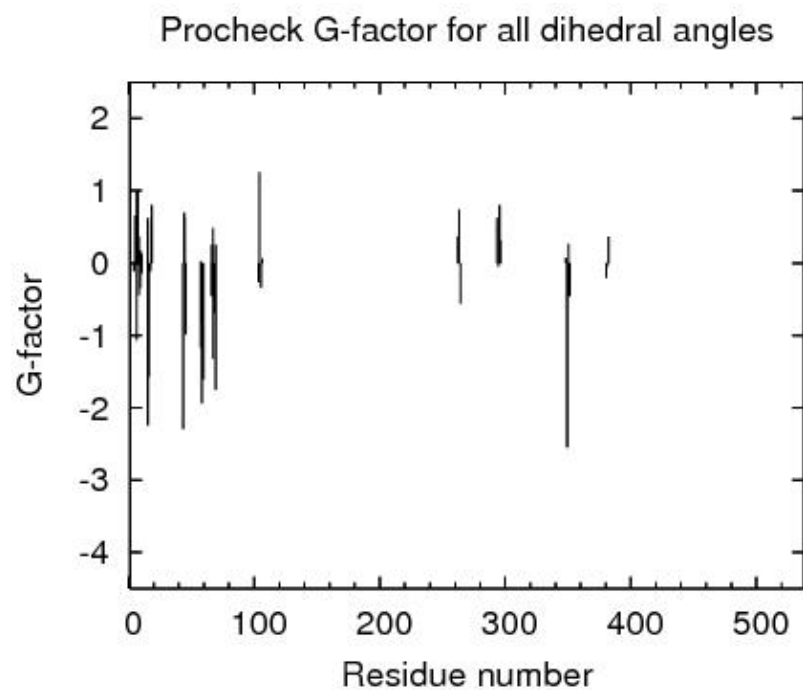


Table of Procheck G-factors for all dihedrals for ordered residues

```

#alldih_gfactor
#Residue\Model  average
4      -0.11
5       0.65    0.21
6       0.99   -1.07
7       1.00    0.90
8       0.36   -0.44
9       0.17   -0.34
10      0.13   -0.14
15      0.62   -2.24
16     -0.01   -1.56
17     -0.11   -0.03
18      0.80    0.52
43     -2.29   -1.03
44      0.69    0.62
45     -0.98   -0.85
57      0.02   -1.17
58     -0.81   -1.93
59     -1.60   -0.08
66      0.25   -0.45

```



```

67      0.48      -1.32
68      -0.12     -0.69
69      0.25      -1.75
103     -0.26
104      1.25     -1.55
105     -0.33
106      0.06
262      0.36
263      0.74
264     -0.56
293      0.62
294     -0.04
295      0.80
296      0.31
348      0.07
349     -2.54
350      0.26
351     -0.45
380     -0.20
381     -0.04
382      0.36
#Reported_Model_Average -0.227
#Overall_Average_Reported -0.227

```

Output from Verify3D

Verify3D Score over a window of \$wsize_s residues

JPEG image for Verify3D Score

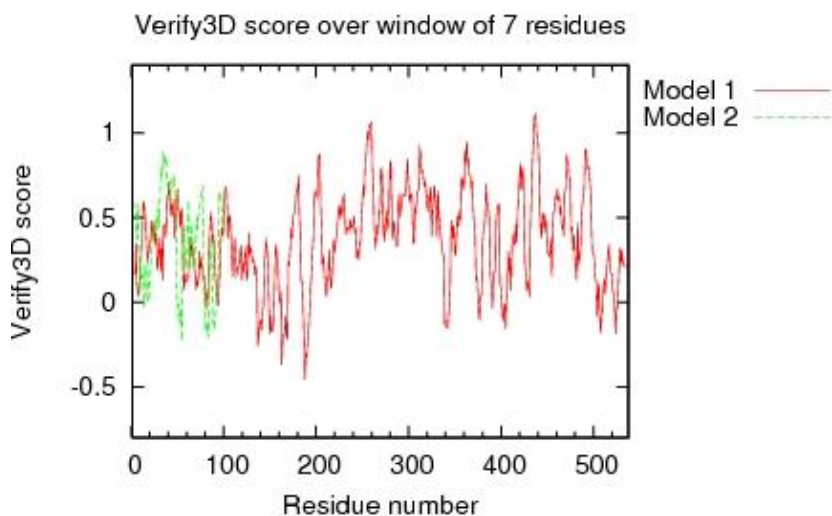


Table of Verify3D scores for ordered residues across all models

```

#verify3d
#Residue\Model  1      2
4      0.62      0.62
5      0.44      0.66
6      0.44      0.63
7     -0.46      0.66
8      0.44      0.66
9     -1.14     -0.54
10     0.10      1.40

```

PSVS Software Environment

15	0.64	0.59
16	0.34	-0.03
17	0.14	-0.35
18	-0.25	-0.61
43	1.10	0.49
44	0.29	0.25
45	0.28	1.10
57	0.28	-0.54
58	0.71	-0.94
59	-0.46	1.62
66	0.63	-0.43
67	-0.17	0.27
68	-0.41	1.30
69	0.63	-0.43
103	0.51	0.51
104	1.10	0.28
105	0.44	
106	1.10	
262	0.49	
263	1.10	
264	-0.40	
293	0.64	
294	0.10	
295	0.49	
296	0.91	
348	0.34	
349	0.08	
350	0.71	
351	0.09	
380	-0.35	
381	0.62	
382	0.44	
#Reported_Model_Average 0.323 0.312		
#Overall_Average_Reported 0.318		

Output from Prosall

Prosall Score over a window of \$winsize_s residues

JPEG image for Prosall Score

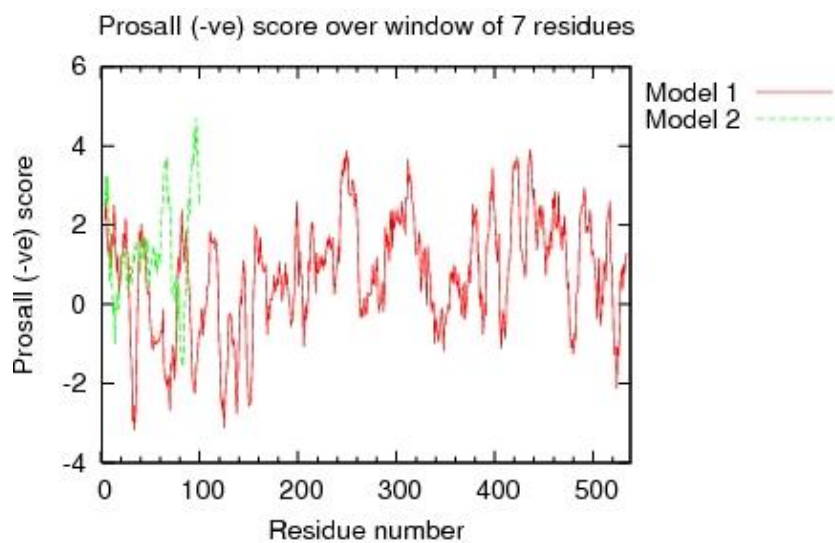


Table of Verify3D scores for ordered residues across all models

```

#verify3d
#Residue\Model  1      2
4      0.62     0.62
5      0.44     0.66
6      0.44     0.63
7      -0.46    0.66
8      0.44     0.66
9      -1.14    -0.54
10     0.10     1.40
15     0.64     0.59
16     0.34    -0.03
17     0.14    -0.35
18     -0.25   -0.61
43     1.10     0.49
44     0.29     0.25
45     0.28     1.10
57     0.28    -0.54
58     0.71    -0.94
59     -0.46    1.62
66     0.63    -0.43
67     -0.17    0.27
68     -0.41    1.30
69     0.63    -0.43
103    0.51     0.51
104    1.10     0.28
105    0.44
106    1.10
262    0.49
263    1.10
264    -0.40
293    0.64
294    0.10
295    0.49
296    0.91
348    0.34
349    0.08
350    0.71
351    0.09
380    -0.35
381    0.62
382    0.44
#Reported_Model_Average 0.323  0.312
#Overall_Average_Reported      0.318

```

Output from MolProbity**VdW violations from MAGE****JPEG image for MAGE VdW violation**

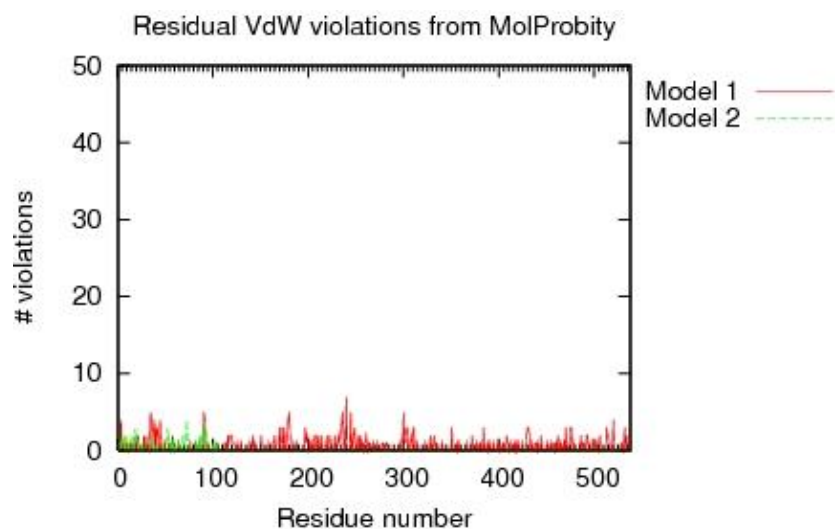


Table of MAGE VdW violations for ordered residues across all models

#mage_clash			
#Residue\Model	1	2	
4.000	4	0	
5.000	0	2	
6.000	0	2	
7.000	1	2	
8.000	0	0	
9.000	0	2	
10.000	1	0	
15.000	1	2	
16.000	0	0	
17.000	0	0	
18.000	0	0	
43.000	0	0	
44.000	1	0	
45.000	4	0	
57.000	0	1	
58.000	2	0	
59.000	1	1	
66.000	0	0	
67.000	0	0	
68.000	0	0	
69.000	0	2	
103.000	0	0	
104.000	1	1	
105.000	1	0	
106.000	0	0	
262.000	1	0	
263.000	0	0	
264.000	1	0	
293.000	0	0	
294.000	0	0	
295.000	0	0	
296.000	1	0	
348.000	0	0	
349.000	0	0	
350.000	0	0	
351.000	3	0	
380.000	1	0	
381.000	1	0	
382.000	0	0	

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#Reported_Model_Average 0.641 0.385

#Overall_Average_Reported 0.513

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

/farm/software/bin/probe

:	8167:A	175	ASP	HA	:	A	470	PRO	O	:	-1.054:	0
:	8167:A	175	ASP	CA	:	A	470	PRO	O	:	-0.751:	0
:	8167:A	159	SER	O	:	A	175	ASP	O	:	-0.627:	0
:	8167:A	468	PRO	O	:	A	470	PRO	2HD	:	-0.501:	0
:	8167:A	207	PRO	1HD	:	A	180	PRO	HA	:	-1.032:	0
:	8167:A	205	LEU	O	:	A	181	ARG	O	:	-0.996:	0
:	8167:A	235	LYS	2HD	:	A	181	ARG	HA	:	-0.730:	0
:	8167:A	235	LYS	CD	:	A	181	ARG	HA	:	-0.646:	0
:	8167:A	180	PRO	HA	:	A	207	PRO	CD	:	-0.638:	0
:	8167:A	235	LYS	2HD	:	A	180	PRO	O	:	-0.580:	0
:	8167:A	208	GLU	1HB	:	A	180	PRO	2HD	:	-0.525:	0
:	8167:A	208	GLU	CD	:	A	234	ARG	1HH2	:	-0.508:	0
:	8167:A	180	PRO	1HB	:	A	234	ARG	2HB	:	-0.492:	0
:	8167:A	45	GLU	1HG	:	A	118	ASP	1HB	:	-0.744:	0
:	8167:A	45	GLU	2HG	:	A	46	ARG	2HG	:	-0.640:	0
:	8167:A	119	ASN	HA	:	A	45	GLU	2HB	:	-0.513:	0
:	8167:A	119	ASN	2HD2	:	A	117	ALA	1HB	:	-0.498:	0
:	8167:A	45	GLU	1HG	:	A	118	ASP	CB	:	-0.463:	0
:	8167:A	418	LEU	3HD2	:	A	412	VAL	1HG1	:	-0.718:	0
:	8167:A	390	GLN	1HG	:	A	311	LYS	HA	:	-0.699:	0
:	8167:A	311	LYS	2HG	:	A	307	ARG	O	:	-0.483:	0
:	8167:A	311	LYS	CD	:	A	308	PRO	HA	:	-0.441:	0
:	8167:A	308	PRO	1HG	:	A	301	TYR	OH	:	-0.430:	0
:	8167:A	122	ASP	CG	:	A	38	ARG	2HH2	:	-0.695:	0
:	8167:A	50	GLU	CD	:	A	38	ARG	1HH2	:	-0.657:	0
:	8167:A	92	ALA	HA	:	A	91	GLU	2HB	:	-0.657:	0
:	8167:A	92	ALA	3HB	:	A	35	LYS	2HD	:	-0.641:	0
:	8167:A	35	LYS	2HD	:	A	92	ALA	CB	:	-0.613:	0
:	8167:A	91	GLU	2HB	:	A	92	ALA	CA	:	-0.596:	0
:	8167:A	21	ASP	1HB	:	A	22	ARG	NH1	:	-0.530:	0
:	8167:A	19	GLY	1HA	:	A	91	GLU	OE2	:	-0.527:	0
:	8167:A	39	ARG	2HG	:	A	35	LYS	O	:	-0.527:	0
:	8167:A	91	GLU	CD	:	A	22	ARG	1HH2	:	-0.492:	0
:	8167:A	82	GLU	CD	:	A	120	LEU	1HD1	:	-0.485:	0
:	8167:A	39	ARG	1HG	:	A	44	LEU	1HB	:	-0.480:	0
:	8167:A	91	GLU	CD	:	A	19	GLY	1HA	:	-0.478:	0
:	8167:A	39	ARG	1HH1	:	A	39	ARG	2HD	:	-0.445:	0
:	8167:A	35	LYS	NZ	:	A	120	LEU	1HD2	:	-0.425:	0
:	8167:A	38	ARG	1HG	:	A	35	LYS	HA	:	-0.402:	0
:	8167:A	248	LYS	1HD	:	A	245	ASP	HA	:	-0.675:	0
:	8167:A	240	ILE	CG2	:	A	476	VAL	HB	:	-0.644:	0
:	8167:A	240	ILE	O	:	A	475	ASP	O	:	-0.637:	0
:	8167:A	240	ILE	H	:	A	475	ASP	2HB	:	-0.630:	0
:	8167:A	245	ASP	1HB	:	A	240	ILE	3HG2	:	-0.620:	0
:	8167:A	245	ASP	CB	:	A	240	ILE	3HG2	:	-0.597:	0
:	8167:A	240	ILE	CG2	:	A	245	ASP	1HB	:	-0.510:	0
:	8167:A	245	ASP	OD1	:	A	248	LYS	NZ	:	-0.500:	0
:	8167:A	462	ILE	1HG1	:	A	476	VAL	2HG1	:	-0.461:	0
:	8167:A	239	ASP	1HB	:	A	475	ASP	2HB	:	-0.436:	0

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: 8167:A 462 ILE HA	:A 476 VAL 2HG1	: -0.429:	0
: 8167:A 240 ILE 1HD1	:A 460 PRO 1HB	: -0.410:	0
: 8167:A 534 VAL 3HG1	:A 332 LEU 1HD2	: -0.658:	0
: 8167:A 534 VAL 3HG1	:A 332 LEU CD2	: -0.456:	0
: 8167:A 176 TRP O	:A 173 SER O	: -0.655:	0
: 8167:A 151 GLU 2HG	:A 173 SER 1HB	: -0.509:	0
: 8167:A 173 SER CB	:A 151 GLU 2HG	: -0.457:	0
: 8167:A 58 ARG 2HH1	:A 123 GLU CD	: -0.631:	0
: 8167:A 58 ARG 2HB	:A 33 LEU 2HB	: -0.475:	0
: 8167:A 283 LEU HG	:A 279 ILE O	: -0.622:	0
: 8167:A 130 GLU 1HG	:A 127 ASP 2HB	: -0.618:	0
: 8167:A 89 GLU 1HB	:A 36 ARG 1HB	: -0.617:	0
: 8167:A 36 ARG 2HB	:A 90 GLN 1HG	: -0.465:	0
: 8167:A 36 ARG 1HH1	:A 36 ARG 1HD	: -0.409:	0
: 8167:A 532 LEU 3HD1	:A 328 LYS 1HB	: -0.611:	0
: 8167:A 500 LEU 2HB	:A 328 LYS 2HE	: -0.583:	0
: 8167:A 323 PRO 1HG	:A 532 LEU 2HD1	: -0.519:	0
: 8167:A 532 LEU 3HD2	:A 531 PRO O	: -0.412:	0
: 8167:A 202 LEU 2HB	:A 211 PRO 2HG	: -0.610:	0
: 8167:A 356 ILE 2HD1	:A 351 GLU 2HB	: -0.610:	0
: 8167:A 211 PRO 2HD	:A 210 ILE HA	: -0.470:	0
: 8167:A 351 GLU CD	:A 351 GLU H	: -0.411:	0
: 8167:A 366 PHE O	:A 380 CYS 2HB	: -0.609:	0
: 8167:A 439 ILE HB	:A 260 THR 2HG2	: -0.602:	0
: 8167:A 41 GLY H	:A 42 PRO 1HD	: -0.601:	0
: 8167:A 42 PRO CD	:A 41 GLY N	: -0.531:	0
: 8167:A 42 PRO 1HD	:A 41 GLY N	: -0.486:	0
: 8167:A 95 THR OG1	:A 121 TYR HA	: -0.589:	0
: 8167:A 179 ARG H	:A 163 ASP 2HB	: -0.580:	0
: 8167:A 454 SER OG	:A 451 ILE HA	: -0.580:	0
: 8167:A 164 GLU OE1	:A 179 ARG 1HD	: -0.545:	0
: 8167:A 179 ARG 1HH1	:A 179 ARG 1HD	: -0.422:	0
: 8167:A 409 PRO O	:A 408 LYS 2HE	: -0.578:	0
: 8167:A 416 GLU OE1	:A 408 LYS NZ	: -0.453:	0
: 8167:A 236 LYS 2HE	:A 231 PRO 1HB	: -0.577:	0
: 8167:A 300 GLU CD	:A 304 LYS 3HZ	: -0.577:	0
: 8167:A 232 PRO O	:A 236 LYS 1HB	: -0.490:	0
: 8167:A 304 LYS NZ	:A 300 GLU CD	: -0.475:	0

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: 8167:A 236 LYS NZ	:A 230 GLU OE1	: -0.464:	0
: 8167:A 236 LYS N	:A 232 PRO O	: -0.433:	0
: 8167:A 300 GLU OE1	:A 304 LYS NZ	: -0.430:	0
: 8167:A 233 LYS HA	:A 236 LYS 1HB	: -0.429:	0
: 8167:A 300 GLU OE2	:A 300 GLU HA	: -0.425:	0
: 8167:A 105 PRO 1HD	:A 104 GLY N	: -0.556:	0
: 8167:A 372 LEU 1HD2	:A 303 ARG 1HG	: -0.551:	0
: 8167:A 432 GLU O	:A 255 LYS 1HD	: -0.551:	0
: 8167:A 255 LYS NZ	:A 432 GLU OE2	: -0.458:	0
: 8167:A 303 ARG 1HH1	:A 303 ARG 2HD	: -0.454:	0
: 8167:A 372 LEU 3HD2	:A 404 LEU 2HB	: -0.439:	0
: 8167:A 142 TYR 1HB	:A 170 HIS HE1	: -0.535:	0
: 8167:A 170 HIS NE2	:A 139 ALA HA	: -0.478:	0
: 8167:A 170 HIS CE1	:A 142 TYR 1HB	: -0.417:	0
: 8167:A 257 ILE 1HD1	:A 429 ASP 2HB	: -0.529:	0
: 8167:A 341 ARG 1HH2	:A 429 ASP CG	: -0.415:	0
: 8167:A 249 LEU 2HD1	:A 253 CYS SG	: -0.523:	0
: 8167:A 253 CYS 2HB	:A 434 ASP OD1	: -0.459:	0
: 8167:A 249 LEU HA	:A 249 LEU 3HD1	: -0.434:	0
: 8167:A 394 ARG 2HD	:A 405 ALA O	: -0.521:	0
: 8167:A 144 ASP O	:A 200 THR 2HG2	: -0.518:	0
: 8167:A 214 GLU CD	:A 214 GLU H	: -0.513:	0
: 8167:A 335 LYS 1HG	:A 331 ALA O	: -0.507:	0
: 8167:A 165 GLU OE2	:A 165 GLU HA	: -0.499:	0
: 8167:A 506 LYS 1HD	:A 503 ASN OD1	: -0.496:	0
: 8167:A 505 VAL O	:A 506 LYS 1HB	: -0.422:	0
: 8167:A 384 ARG 1HH1	:A 384 ARG 2HD	: -0.492:	0
: 8167:A 381 GLU CD	:A 384 ARG 2HH2	: -0.472:	0
: 8167:A 59 GLU CD	:A 34 ARG 2HH2	: -0.490:	0
: 8167:A 430 LYS 3HZ	:A 431 ASP CG	: -0.481:	0
: 8167:A 431 ASP CG	:A 430 LYS NZ	: -0.450:	0
: 8167:A 431 ASP OD2	:A 430 LYS NZ	: -0.429:	0
: 8167:A 472 LEU HG	:A 471 HIS CD2	: -0.477:	0
: 8167:A 515 PRO HA	:A 520 GLU OE1	: -0.476:	0
: 8167:A 31 GLU OE2	:A 28 PRO 1HD	: -0.476:	0
: 8167:A 513 LYS NZ	:A 520 GLU CD	: -0.463:	0
: 8167:A 31 GLU 1HB	:A 28 PRO O	: -0.452:	0

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: 8167:A 520 GLU OE2	:A 513 LYS NZ	: -0.417:	0
: 8167:A 514 PRO O	:A 516 ARG 2HG	: -0.416:	0
: 8167:A 513 LYS 3HZ	:A 520 GLU CD	: -0.413:	0
: 8167:A 515 PRO 2HD	:A 514 PRO HA	: -0.406:	0
: 8167:A 264 VAL 2HG2	:A 261 GLY O	: -0.471:	0
: 8167:A 441 SER 2HB	:A 261 GLY 2HA	: -0.436:	0
: 8167:A 420 GLU CD	:A 424 ARG 2HH2	: -0.466:	0
: 8167:A 492 ARG 1HH2	:A 488 GLU CD	: -0.464:	0
: 8167:A 244 GLU CD	:A 492 ARG 2HH1	: -0.456:	0
: 8167:A 185 TYR CD1	:A 228 LEU 3HD1	: -0.461:	0
: 8167:A 228 LEU 1HD1	:A 188 VAL 1HG2	: -0.451:	0
: 8167:A 4 GLU CD	:A 444 LYS NZ	: -0.458:	0
: 8167:A 296 MET SD	:A 309 PHE HA	: -0.458:	0
: 8167:A 4 GLU H	:A 4 GLU 2HG	: -0.457:	0
: 8167:A 4 GLU OE2	:A 444 LYS NZ	: -0.425:	0
: 8167:A 3 ASP O	:A 7 LEU HG	: -0.455:	0
: 8167:A 377 LYS NZ	:A 410 GLU OE2	: -0.453:	0
: 8167:A 458 GLU 2HB	:A 237 ARG NH2	: -0.451:	0
: 8167:A 237 ARG 1HH1	:A 237 ARG 2HD	: -0.411:	0
: 8167:A 299 ILE 2HD1	:A 302 PHE 2HB	: -0.450:	0
: 8167:A 358 ARG NH2	:A 334 ASP O	: -0.449:	0
: 8167:A 529 PRO 2HD	:A 528 PRO HA	: -0.447:	0
: 8167:A 197 ASP CG	:A 199 ARG 1HH2	: -0.446:	0
: 8167:A 116 LEU 2HD1	:A 116 LEU HA	: -0.446:	0
: 8167:A 197 ASP OD2	:A 199 ARG 2HB	: -0.433:	0
: 8167:A 198 PRO 2HD	:A 197 ASP HA	: -0.409:	0
: 8167:A 64 ALA HA	:A 77 ARG 1HB	: -0.441:	0
: 8167:A 259 LEU 2HD1	:A 438 VAL 2HG2	: -0.441:	0
: 8167:A 223 ILE 2HD1	:A 220 LEU 3HD2	: -0.439:	0
: 8167:A 496 GLU OE2	:A 499 LYS NZ	: -0.439:	0
: 8167:A 220 LEU O	:A 224 VAL 3HG1	: -0.438:	0
: 8167:A 219 THR O	:A 223 ILE 2HG1	: -0.426:	0
: 8167:A 265 SER HA	:A 268 CYS SG	: -0.438:	0
: 8167:A 314 LYS 1HD	:A 388 PHE HA	: -0.432:	0
: 8167:A 247 VAL 3HG1	:A 493 LEU 3HD2	: -0.429:	0
: 8167:A 493 LEU HG	:A 489 LEU O	: -0.410:	0
: 8167:A 54 ALA 2HB	:A 457 HIS ND1	: -0.428:	0

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```

: 8167:A 11 PRO CD :A 10 GLN N : -0.427: 0
: 8167:A 282 ARG 2HG :A 278 GLY O : -0.420: 0
: 8167:A 401 ASP OD2 :A 399 PRO 1HB : -0.417: 0
: 8167:A 15 PRO 2HD :A 14 SER HA : -0.414: 0
: 8167:A 113 GLU HA :A 114 PRO 2HD : -0.413: 0
: 8167:A 272 ASP 1HB :A 262 ALA 3HB : -0.408: 0
: 8167:A 56 PRO 2HD :A 55 ALA HA : -0.406: 0
: 8167:A 465 ASN O :A 479 LEU HA : -0.402: 0
: 8167:A 486 ILE 3HD1 :A 486 ILE HA : -0.402: 0
#sum2 ::20.82 clashscore : 20.82 clashscore B

```

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

/farm/software/bin/probe

```

: 1657:A 6 GLY 1HA :A 93 ASP 2HB : -0.754: 0
: 1657:A 90 GLU O :A 94 LEU HG : -0.436: 0
: 1657:A 93 ASP 2HB :A 6 GLY CA : -0.430: 0
: 1657:A 93 ASP 1HB :A 9 ILE 2HD1 : -0.424: 0
: 1657:A 90 GLU HA :A 9 ILE 3HD1 : -0.412: 0
: 1657:A 90 GLU H :A 89 GLU CD : -0.401: 0

: 1657:A 73 LYS HA :A 73 LYS NZ : -0.670: 0
: 1657:A 73 LYS 3HZ :A 73 LYS HA : -0.569: 0

: 1657:A 26 HIS 2HB :A 31 ASN 1HB : -0.649: 0

: 1657:A 32 LEU HG :A 35 LEU 2HD2 : -0.619: 0

: 1657:A 22 LYS H :A 19 THR HB : -0.618: 0
: 1657:A 15 SER O :A 19 THR 3HG2 : -0.473: 0
: 1657:A 19 THR 1HG2 :A 22 LYS 1HB : -0.445: 0
: 1657:A 11 ILE HA :A 15 SER CB : -0.409: 0

: 1657:A 21 GLU CD :A 21 GLU H : -0.582: 0

: 1657:A 48 TYR 2HB :A 41 GLY H : -0.546: 0

: 1657:A 33 HIS HA :A 20 VAL 2HG1 : -0.528: 0

: 1657:A 61 GLU HA :A 36 PHE HE2 : -0.527: 0
: 1657:A 36 PHE HD1 :A 102 THR OG1 : -0.470: 0

: 1657:A 53 LYS 2HZ :A 53 LYS 2HB : -0.525: 0
: 1657:A 54 ASN OD1 :A 53 LYS NZ : -0.477: 0

: 1657:A 83 VAL 3HG1 :A 86 LYS 1HE : -0.478: 0
: 1657:A 84 GLY O :A 86 LYS 2HD : -0.465: 0

: 1657:A 88 LYS NZ :A 69 GLU OE2 : -0.444: 0
: 1657:A 69 GLU OE1 :A 88 LYS NZ : -0.414: 0

```

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```
: 1657:A 7 LYS 1HE :A 7 LYS 2HB : -0.433: 0
: 1657:A 2 ASP OD1 :A 5 LYS NZ : -0.428: 0
: 1657:A 5 LYS 1HG :A 2 ASP CG : -0.401: 0
: 1657:A 57 ILE 1HG2 :A 52 ASN 2HD2 : -0.426: 0
: 1657:A 74 TYR CZ :A 55 LYS NZ : -0.424: 0
: 1657:A 76 PRO 1HD :A 75 ILE HA : -0.415: 0
: 1657:A 14 CYS H :A 13 LYS 2HB : -0.414: 0
: 1657:A 59 TRP 2HB :A 64 LEU 1HD1 : -0.408: 0
: 1657:A 104 GLU OE1 :A 100 LYS NZ : -0.405: 0
#sum2 ::20.52 clashscore : 20.52 clashscore B
```

Output from PDB validation software

Summary from PDB validation

Jan. 29, 14:13:33 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	O	ARG	181 -	A	O	LEU	205	(1, 5, 5, 5)	Dist = 1.79
A	O	SER	173 -	A	O	TRP	176	(1, 5, 5, 5)	Dist = 2.14
A	O	ILE	240 -	A	O	ASP	475	(1, 5, 5, 5)	Dist = 2.15

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A O SER 159 - A O ASP 175 (1, 5, 5, 5) Dist = 2.17

=> 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 0.012 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 2.8 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
30.0	SER	A	27	1	C	-	N	-	CA	151.7	121.7
-21.3	GLU	A	91	1	CA	-	C	-	O	99.5	120.8
-43.1	ALA	A	92	1	CA	-	C	-	O	77.7	120.8
22.1	ALA	A	92	1	C	-	N	-	CA	143.8	121.7
39.3	ALA	A	92	1	CA	-	C	-	N	155.5	116.2
-42.1	ALA	A	92	1	O	-	C	-	N	80.9	123.0
26.7	GLN	A	93	1	C	-	N	-	CA	148.4	121.7
-17.2	GLY	A	109	1	C	-	N	-	CA	103.4	120.6
-45.5	GLU	A	113	1	CA	-	C	-	O	75.3	120.8
-34.6	GLU	A	113	1	CA	-	C	-	N	82.3	116.9
32.1	GLU	A	113	1	O	-	C	-	N	154.1	122.0
-46.9	PHE	A	148	1	CA	-	C	-	O	73.9	120.8
-31.2	PHE	A	148	1	O	-	C	-	N	91.8	123.0
28.0	ARG	A	167	1	C	-	N	-	CA	149.7	121.7

TORSION ANGLES

The torsion angle distributions have been checked. The postscript file of the

PSVS Software Environment

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.

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

```
MET(  2 A -17 )
ALA(  2 A -16 )
ASP(  2 A -15 )
GLU(  2 A -14 )
ALA(  2 A -13 )
ALA(  2 A -12 )
LEU(  2 A -11 )
ALA(  2 A -10 )
LEU(  2 A  -9 )
GLN(  2 A  -8 )
PRO(  2 A  -7 )
GLY(  2 A  -6 )
GLY(  2 A  -5 )
SER(  2 A  -4 )
PRO(  2 A  -3 )
SER(  2 A  -2 )
ALA(  2 A  -1 )
ALA(  2 A   0 )
ALA(  2 A   1 )
ALA(  2 A  -6 )
ALA(  2 A  -5 )
SER(  2 A  -4 )
SER(  2 A  -3 )
PRO(  2 A  -2 )
ALA(  2 A  -1 )
GLY(  2 A   0 )
GLU(  2 A   1 )
PRO(  2 A   2 )
LEU(  2 A   3 )
ARG(  2 A   4 )
ARG(  2 A -10 )
PRO(  2 A  -9 )
ARG(  2 A  -8 )
ARG(  2 A  -7 )
ASP(  2 A  -6 )
GLY(  2 A  -5 )
PRO(  2 A  -4 )
```

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```
GLY( 2 A -3 )
LEU( 2 A -2 )
GLU( 2 A -1 )
ARG( 2 A 0 )
SER( 2 A 1 )
PRO( 2 A 2 )
GLY( 2 A 3 )
GLU( 2 A 4 )
PRO( 2 A 5 )
GLY( 2 A 0 )
ALA( 2 A 1 )
ALA( 2 A 2 )
PRO( 2 A 3 )
GLU( 2 A 4 )
ARG( 2 A 5 )
GLU( 2 A 6 )
PRO( 2 A -6 )
GLY( 2 A -5 )
ALA( 2 A -4 )
ALA( 2 A -3 )
ALA( 2 A -2 )
ALA( 2 A -1 )
ALA( 2 A 0 )
LEU( 2 A 1 )
TRP( 2 A 2 )
ARG( 2 A 3 )
GLU( 2 A 4 )
ALA( 2 A 5 )
GLU( 2 A 6 )
ALA( 2 A 7 )
GLU( 2 A 8 )
ALA( 2 A 9 )
ALA( 2 A 10 )
ALA( 2 A 11 )
ALA( 2 A 12 )
GLY( 2 A 13 )
GLY( 2 A 14 )
GLU( 2 A 15 )
ALA( 2 A 16 )
ALA( 2 A 17 )
ALA( 2 A 18 )
ALA( 2 A 19 )
ASP( 2 A 22 )
ASN( 2 A 23 )
SER( 2 A 23 )
ARG( 2 A 24 )
GLU( 2 A 25 )
PRO( 2 A 26 )
PRO( 2 A 27 )
LEU( 2 A 28 )
ALA( 2 A 29 )
ASP( 2 A 30 )
TYR( 2 A 14 )
ASP( 2 A 15 )
GLU( 2 A 16 )
ASP( 2 A 17 )
ASP( 2 A 18 )
ASP( 2 A 19 )
ASP( 2 A 20 )
GLU( 2 A 21 )
GLY( 2 A 22 )
GLU( 2 A 23 )
```

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GLU (2 A 24)
GLU (2 A 25)
GLU (2 A 26)
GLU (2 A 27)
ALA (2 A 28)
ALA (2 A 29)
ALA (2 A 30)
ALA (2 A 31)
ALA (2 A 32)
TYR (2 A 30)
ARG (2 A 31)
ASP (2 A 32)
ASN (2 A 33)
LEU (2 A 34)
ASP (2 A 36)
GLU (2 A 37)
ASN (2 A 40)
PHE (2 A 29)
HIS (2 A 30)
SER (2 A 31)
CYS (2 A 32)
GLU (2 A 33)
SER (2 A 34)
ASP (2 A 35)
GLU (2 A 36)
GLU (2 A 37)
ASP (2 A 38)
ARG (2 A 39)
ALA (2 A 40)
SER (2 A 41)
SER (2 A 36)
SER (2 A 37)
SER (2 A 38)
ASP (2 A 39)
TRP (2 A 40)
THR (2 A 41)
PRO (2 A 42)
ARG (2 A 43)
ARG (2 A 43)
ILE (2 A 44)
PHE (2 A 13)
VAL (2 A 14)
GLN (2 A 15)
GLN (2 A 16)
HIS (2 A 17)
LEU (2 A 18)
MET (2 A 19)
ILE (2 A 20)
GLY (2 A 21)
THR (2 A 22)
ASP (2 A 23)
PRO (2 A 24)
ARG (2 A 25)
THR (2 A 26)
ILE (2 A 27)
LEU (2 A 28)
LYS (2 A 29)
ASP (2 A 30)
LEU (2 A 31)
LEU (2 A 32)
PRO (2 A 33)
GLU (2 A 34)

PSVS Software Environment

```
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ILE( 2 A 36 )
PRO( 2 A 37 )
PRO( 2 A 38 )
PRO( 2 A 39 )
GLU( 2 A 40 )
LEU( 2 A 41 )
ASP( 2 A 42 )
ASP( 2 A 43 )
MET( 2 A 44 )
THR( 2 A 45 )
LEU( 2 A 46 )
TRP( 2 A 47 )
GLN( 2 A 48 )
ILE( 2 A 49 )
ILE( 2 A 44 )
LEU( 2 A 45 )
SER( 2 A 46 )
GLU( 2 A 47 )
PRO( 2 A 48 )
PRO( 2 A 49 )
LYS( 2 A 50 )
ARG( 2 A 51 )
LYS( 2 A 52 )
ASN( 2 A 56 )
THR( 2 A 57 )
ALA( 2 A 49 )
VAL( 2 A 50 )
LYS( 2 A 51 )
LEU( 2 A 52 )
LEU( 2 A 53 )
GLN( 2 A 54 )
GLU( 2 A 55 )
CYS( 2 A 56 )
LYS( 2 A 57 )
LYS( 2 A 58 )
ILE( 2 A 59 )
ILE( 2 A 60 )
VAL( 2 A 61 )
LEU( 2 A 62 )
GLY( 2 A 35 )
ALA( 2 A 36 )
GLY( 2 A 37 )
VAL( 2 A 38 )
SER( 2 A 39 )
VAL( 2 A 40 )
SER( 2 A 41 )
CYS( 2 A 42 )
GLY( 2 A 43 )
ILE( 2 A 44 )
PRO( 2 A 45 )
ASP( 2 A 46 )
PHE( 2 A 47 )
ARG( 2 A 48 )
SER( 2 A 49 )
ARG( 2 A 50 )
ASP( 2 A 51 )
GLY( 2 A 52 )
ILE( 2 A 53 )
TYR( 2 A 54 )
ALA( 2 A 55 )
ARG( 2 A 56 )
```

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```
LEU(  2 A  57 )
ALA(  2 A  58 )
VAL(  2 A  59 )
ASP(  2 A  60 )
PHE(  2 A  61 )
PRO(  2 A  62 )
ASP(  2 A  63 )
PRO(  2 A  60 )
ASP(  2 A  61 )
PRO(  2 A  62 )
GLN(  2 A  63 )
ALA(  2 A  64 )
PHE(  2 A  63 )
ASP(  2 A  64 )
ILE(  2 A  65 )
PHE(  2 A  65 )
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LYS(  2 A  67 )
PHE(  2 A  70 )
PHE(  2 A  71 )
PHE(  2 A  71 )
ALA(  2 A  72 )
TYR(  2 A  75 )
GLN(  2 A  54 )
PHE(  2 A  55 )
GLN(  2 A  56 )
PRO(  2 A  57 )
SER(  2 A  58 )
LEU(  2 A  59 )
CYS(  2 A  60 )
HIS(  2 A  61 )
LYS(  2 A  62 )
PHE(  2 A  63 )
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LEU(  2 A  66 )
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GLU(  2 A  70 )
GLY(  2 A  71 )
LYS(  2 A  72 )
LEU(  2 A  73 )
LEU(  2 A  74 )
ARG(  2 A  75 )
ASN(  2 A  76 )
TYR(  2 A  77 )
ASP(  2 A  78 )
THR(  2 A  79 )
LEU(  2 A  80 )
GLU(  2 A  81 )
ALA(  2 A  83 )
GLN(  2 A  68 )
ARG(  2 A  69 )
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ILE(  2 A  71 )
GLN(  2 A  72 )
CYS(  2 A  73 )
HIS(  2 A  74 )
GLY(  2 A  75 )
SER(  2 A  76 )
PHE(  2 A  77 )
```


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```
ALA( 2 A 78 )
THR( 2 A 79 )
ALA( 2 A 80 )
SER( 2 A 81 )
CYS( 2 A 82 )
LEU( 2 A 83 )
ILE( 2 A 84 )
CYS( 2 A 85 )
TYR( 2 A 86 )
VAL( 2 A 58 )
ASP( 2 A 59 )
CYS( 2 A 60 )
GLU( 2 A 61 )
ALA( 2 A 62 )
VAL( 2 A 63 )
ARG( 2 A 64 )
GLY( 2 A 65 )
ASP( 2 A 66 )
ILE( 2 A 67 )
PHE( 2 A 68 )
ASN( 2 A 69 )
GLN( 2 A 70 )
VAL( 2 A 71 )
VAL( 2 A 72 )
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ARG( 2 A 74 )
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PRO( 2 A 76 )
ARG( 2 A 77 )
CYS( 2 A 78 )
PRO( 2 A 79 )
ALA( 2 A 80 )
ASP( 2 A 81 )
GLU( 2 A 82 )
PRO( 2 A 83 )
LEU( 2 A 84 )
ALA( 2 A 85 )
ILE( 2 A 86 )
MET( 2 A 87 )
PRO( 2 A 82 )
GLU( 2 A 83 )
ILE( 2 A 84 )
VAL( 2 A 85 )
PHE( 2 A 86 )
PHE( 2 A 87 )
GLY( 2 A 88 )
ASN( 2 A 87 )
LEU( 2 A 88 )
PRO( 2 A 89 )
GLN( 2 A 88 )
PHE( 2 A 89 )
HIS( 2 A 90 )
MET( 2 A 85 )
LYS( 2 A 86 )
TYR( 2 A 87 )
ASP( 2 A 88 )
LYS( 2 A 89 )
ASP( 2 A 90 )
GLU( 2 A 91 )
VAL( 2 A 92 )
LEU( 2 A 92 )
ILE( 2 A 93 )
```

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VAL(2 A 94)
GLY(2 A 87)
SER(2 A 88)
SER(2 A 89)
LEU(2 A 90)
LYS(2 A 91)
VAL(2 A 92)
ARG(2 A 93)
PRO(2 A 94)
VAL(2 A 95)
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ILE(2 A 51)
PRO(2 A 52)
SER(2 A 53)
SER(2 A 54)
ILE(2 A 55)
PRO(2 A 56)
HIS(2 A 57)
GLU(2 A 58)
VAL(2 A 59)
PRO(2 A 60)
GLN(2 A 61)
ILE(2 A 62)
LEU(2 A 63)
ILE(2 A 64)
ASN(2 A 65)
ARG(2 A 66)
GLU(2 A 67)
PRO(2 A 68)
LEU(2 A 69)
PRO(2 A 70)
HIS(2 A 71)
LEU(2 A 72)
HIS(2 A 73)
PHE(2 A 74)
ASP(2 A 75)
VAL(2 A 76)
GLU(2 A 77)
LEU(2 A 78)
LEU(2 A 79)
GLY(2 A 80)
ASP(2 A 81)
CYS(2 A 82)
ASP(2 A 83)
VAL(2 A 84)
ILE(2 A 85)
ILE(2 A 86)
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GLU(2 A 88)
LEU(2 A 89)
CYS(2 A 90)
HIS(2 A 91)
ARG(2 A 92)
LEU(2 A 93)
GLY(2 A 94)
GLY(2 A 95)
GLU(2 A 96)
ALA(2 A 89)
LYS(2 A 90)
LEU(2 A 91)
CYS(2 A 92)
CYS(2 A 93)

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```

ASN(  2 A  94 )
PRO(  2 A  95 )
VAL(  2 A  96 )
LYS(  2 A  97 )
SER(  2 A  94 )
GLU(  2 A  95 )
ILE(  2 A  96 )
THR(  2 A  97 )
GLU(  2 A  98 )
PRO(  2 A  95 )
PRO(  2 A  96 )
ARG(  2 A  97 )
THR(  2 A  98 )
GLN(  2 A  99 )
GLU(  2 A  99 )
LEU(  2 A 100 )
TYR(  2 A  95 )
LEU(  2 A  96 )
SER(  2 A  97 )
GLU(  2 A  98 )
LEU(  2 A  99 )
PRO(  2 A 100 )
PRO(  2 A 101 )
PRO(  2 A  99 )
LEU(  2 A 100 )
HIS(  2 A 101 )
VAL(  2 A 102 )
ASP(  2 A 105 )

```

```

MISMATCH: ChainID=A ResNum=3  (ARG  VAL)
MISMATCH: ChainID=A ResNum=7  (VAL  LYS)
MISMATCH: ChainID=A ResNum=8  (PRO  LYS)
MISMATCH: ChainID=A ResNum=9  (ALA  ILE)
MISMATCH: ChainID=A ResNum=10 (ALA  PHE)
MISMATCH: ChainID=A ResNum=11 (ALA  ILE)
MISMATCH: ChainID=A ResNum=12 (ARG  MET)
MISMATCH: ChainID=A ResNum=13 (GLY  LYS)
MISMATCH: ChainID=A ResNum=15 (GLU  SER)
MISMATCH: ChainID=A ResNum=17 (GLN  CYS)
MISMATCH: ChainID=A ResNum=18 (ALA  HIS)
MISMATCH: ChainID=A ResNum=20 (GLY  VAL)
MISMATCH: ChainID=A ResNum=22 (...  LYS)
MISMATCH: ChainID=A ResNum=25 (PRO  LYS)
MISMATCH: ChainID=A ResNum=26 (GLY  HIS)
MISMATCH: ChainID=A ResNum=27 (LEU  LYS)
MISMATCH: ChainID=A ResNum=28 (GLN  THR)
MISMATCH: ChainID=A ResNum=33 (ILE  HIS)
MISMATCH: ChainID=A ResNum=38 (ILE  ARG)
MISMATCH: ChainID=A ResNum=39 (ILE  LYS)
MISMATCH: ChainID=A ResNum=42 (HIS  GLN)
MISMATCH: ChainID=A ResNum=46 (...  TYR)
MISMATCH: ChainID=A ResNum=47 (PRO  SER)
MISMATCH: ChainID=A ResNum=50 (VAL  ALA)
MISMATCH: ChainID=A ResNum=51 (ILE  ALA)
MISMATCH: ChainID=A ResNum=54 (ARG  ASN)
MISMATCH: ChainID=A ResNum=56 (ASP  GLY)
MISMATCH: ChainID=A ResNum=59 (...  TRP)
MISMATCH: ChainID=A ResNum=60 (...  GLY)
MISMATCH: ChainID=A ResNum=68 (ASP  LEU)
MISMATCH: ChainID=A ResNum=69 (PRO  GLU)
MISMATCH: ChainID=A ResNum=70 (ARG  ASN)

```

PSVS Software Environment

MISMATCH: ChainID=A ResNum=74 (GLU TYR)
MISMATCH: ChainID=A ResNum=79 (GLN LYS)
MISMATCH: ChainID=A ResNum=80 (ASN MET)
MISMATCH: ChainID=A ResNum=82 (GLN PHE)
MISMATCH: ChainID=A ResNum=103 (SER ASN)
SEQUENCE WARNING: Residue (A GLY 1) and Residue (A ASP 2) are linked together
SEQUENCE WARNING: Residue (A GLU 4) and Residue (A LYS 5) are linked together
SEQUENCE WARNING: Residue (A LYS 5) and Residue (A GLY 6) are linked together
SEQUENCE WARNING: Residue (A GLY 6) and Residue (A LYS 7) are linked together
SEQUENCE WARNING: Residue (A CYS 14) and Residue (A SER 15) are linked together
SEQUENCE WARNING: Residue (A GLN 16) and Residue (A CYS 17) are linked together
SEQUENCE WARNING: Residue (A THR 19) and Residue (A VAL 20) are linked together
SEQUENCE WARNING: Residue (A GLY 23) and Residue (A GLY 24) are linked together
SEQUENCE WARNING: Residue (A PRO 30) and Residue (A ASN 31) are linked together
SEQUENCE WARNING: Residue (A LEU 32) and Residue (A HIS 33) are linked together
SEQUENCE WARNING: Residue (A GLY 34) and Residue (A LEU 35) are linked together
SEQUENCE WARNING: Residue (A GLY 37) and Residue (A ARG 38) are linked together
SEQUENCE WARNING: Residue (A THR 40) and Residue (A GLY 41) are linked together
SEQUENCE WARNING: Residue (A GLY 41) and Residue (A GLN 42) are linked together
SEQUENCE WARNING: Residue (A ALA 43) and Residue (A PRO 44) are linked together
SEQUENCE WARNING: Residue (A PRO 44) and Residue (A GLY 45) are linked together
SEQUENCE WARNING: Residue (A THR 49) and Residue (A ALA 50) are linked together
SEQUENCE WARNING: Residue (A ASN 52) and Residue (A LYS 53) are linked together
SEQUENCE WARNING: Residue (A ILE 57) and Residue (A ILE 58) are linked together
SEQUENCE WARNING: Residue (A ASP 62) and Residue (A THR 63) are linked together
SEQUENCE WARNING: Residue (A THR 63) and Residue (A LEU 64) are linked together
SEQUENCE WARNING: Residue (A LEU 64) and Residue (A MET 65) are linked together
SEQUENCE WARNING: Residue (A MET 65) and Residue (A GLU 66) are linked together
SEQUENCE WARNING: Residue (A TYR 67) and Residue (A LEU 68) are linked together
SEQUENCE WARNING: Residue (A PRO 71) and Residue (A LYS 72) are linked together
SEQUENCE WARNING: Residue (A LYS 72) and Residue (A LYS 73) are linked together
SEQUENCE WARNING: Residue (A ILE 75) and Residue (A PRO 76) are linked together
SEQUENCE WARNING: Residue (A GLY 77) and Residue (A THR 78) are linked together
SEQUENCE WARNING: Residue (A ILE 81) and Residue (A PHE 82) are linked together
SEQUENCE WARNING: Residue (A VAL 83) and Residue (A GLY 84) are linked together
SEQUENCE WARNING: Residue (A ILE 85) and Residue (A LYS 86) are linked together
SEQUENCE WARNING: Residue (A LYS 86) and Residue (A LYS 87) are linked together
SEQUENCE WARNING: Residue (A LYS 87) and Residue (A LYS 88) are linked together
SEQUENCE WARNING: Residue (A LYS 88) and Residue (A GLU 89) are linked together
SEQUENCE WARNING: Residue (A GLU 89) and Residue (A GLU 90) are linked together
SEQUENCE WARNING: Residue (A GLU 90) and Residue (A ARG 91) are linked together
SEQUENCE WARNING: Residue (A ALA 92) and Residue (A ASP 93) are linked together
SEQUENCE WARNING: Residue (A LEU 94) and Residue (A ILE 95) are linked together
SEQUENCE WARNING: Residue (A ILE 95) and Residue (A ALA 96) are linked together
SEQUENCE WARNING: Residue (A ALA 96) and Residue (A TYR 97) are linked together
SEQUENCE WARNING: Residue (A TYR 97) and Residue (A LEU 98) are linked together
SEQUENCE WARNING: Residue (A LEU 98) and Residue (A LYS 99) are linked together
SEQUENCE WARNING: Residue (A LYS 99) and Residue (A LYS 100) are linked together
SEQUENCE WARNING: Residue (A LYS 100) and Residue (A ALA 101) are linked together
SEQUENCE WARNING: Residue (A ALA 101) and Residue (A THR 102) are linked together
SEQUENCE WARNING: Residue (A THR 102) and Residue (A ASN 103) 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.

PDB Chain_ID: A

PSVS Software Environment

```

1
SEQRES: MET ALA ASP GLU ALA ALA LEU ALA LEU GLN PRO GLY GLY SER PRO
COORDS: ... .. 15

16
SEQRES: SER ALA ALA GLY ALA ASP ARG GLU ALA ALA SER SER PRO ALA GLY
COORDS: ... .. 30
          1          4
          ^^^

31
SEQRES: GLU PRO LEU ARG LYS ARG PRO ARG ARG ASP GLY PRO GLY LEU GLU
COORDS: ... .. 45
          5

46
SEQRES: ARG SER PRO GLY GLU PRO GLY GLY ALA ALA PRO GLU ARG GLU VAL
COORDS: ... .. 60
          6          7
          ^^^

61
SEQRES: PRO ALA ALA ALA ARG GLY CYS PRO GLY ALA ALA ALA ALA ALA LEU
COORDS: lys ile phe ile met lys CYS ... .. 75
          8          14
          ^^^ ^^^ ^^^ ^^^ ^^^ ^^^

76
SEQRES: TRP ARG GLU ALA GLU ALA GLU ALA ALA ALA ALA GLY GLY GLU GLN
COORDS: ... .. 90
          15 16
          ^^^

91
SEQRES: GLU ALA GLN ALA THR ALA ALA ALA GLY GLU ... GLY ASP ASN GLY
COORDS: ... .. 104
          cys his THR ... .. val GLU lys GLY ... .. GLY
          17          24
          ^^^ ^^^          ^^^ ^^^

105
SEQRES: PRO GLY LEU GLN GLY PRO SER ARG GLU PRO PRO LEU ALA ASP ASN
COORDS: lys his lys thr GLY PRO ... .. 119
          25          31
          ^^^ ^^^ ^^^ ^^^

120
SEQRES: LEU TYR ASP GLU ASP ASP ASP ASP GLU GLY GLU GLU GLU GLU
COORDS: LEU ... .. 134
          32

135
SEQRES: ALA ALA ALA ALA ALA ILE GLY TYR ARG ASP ASN LEU LEU PHE GLY
COORDS: ... .. 149
          his GLY ... .. LEU PHE GLY
          33          37
          ^^^

150
SEQRES: ASP GLU ILE ILE THR ASN GLY PHE HIS SER CYS GLU SER ASP GLU
COORDS: ... .. 164
          arg lys THR ... GLY ... ..
          38          41
          ^^^ ^^^

```

PSVS Software Environment

```

165                                     179
SEQRES:  GLU ASP ARG ALA SER HIS ALA SER SER SER ASP TRP THR PRO ARG
COORDS:  ... .. gln ALA ... .. 42 43
          ^^^

```

```

180                                     193
SEQRES:  PRO ARG ILE GLY ... PRO TYR THR PHE VAL GLN GLN HIS LEU MET
COORDS:  PRO ... .. GLY tyr ser TYR THR ... .. 44 49
          ^^^ ^^^

```

```

194                                     208
SEQRES:  ILE GLY THR ASP PRO ARG THR ILE LEU LYS ASP LEU LEU PRO GLU
COORDS:  ... .. 44 49

```

```

209                                     223
SEQRES:  THR ILE PRO PRO PRO GLU LEU ASP ASP MET THR LEU TRP GLN ILE
COORDS:  ... .. 50 55
          ^^^ ^^^

```

```

224                                     238
SEQRES:  VAL ILE ASN ILE LEU SER GLU PRO PRO LYS ARG LYS LYS ARG LYS
COORDS:  ala ala ASN ... .. 50 55
          ^^^ ^^^

```

```

239                                     251
SEQRES:  ASP ILE ASN THR ILE ... .. GLU ASP ALA VAL LYS LEU LEU GLN
COORDS:  gly ILE ... .. ILE trp gly GLU ASP ... .. 56 62
          ^^^ ^^^

```

```

252                                     266
SEQRES:  GLU CYS LYS LYS ILE ILE VAL LEU THR GLY ALA GLY VAL SER VAL
COORDS:  ... .. 63

```

```

267                                     281
SEQRES:  SER CYS GLY ILE PRO ASP PHE ARG SER ARG ASP GLY ILE TYR ALA
COORDS:  ... .. 64 65

```

```

282                                     296
SEQRES:  ARG LEU ALA VAL ASP PHE PRO ASP LEU PRO ASP PRO GLN ALA MET
COORDS:  ... .. 64 65

```

```

297                                     311
SEQRES:  PHE ASP ILE GLU TYR PHE ARG LYS ASP PRO ARG PRO PHE PHE LYS
COORDS:  ... .. 66 72
          ^^^ ^^^ ^^^

```

```

312                                     326
SEQRES:  PHE ALA LYS GLU ILE TYR PRO GLY GLN PHE GLN PRO SER LEU CYS
COORDS:  ... .. 73 77
          ^^^

```

PSVS Software Environment

```

327                                     341
SEQRES: HIS LYS PHE ILE ALA LEU SER ASP LYS GLU GLY LYS LEU LEU ARG
COORDS: ... .. ... .. ... .. ... .. ... .. ... .. ... .. ...

```

```

342                                     356
SEQRES: ASN TYR THR GLN ASN ILE ASP THR LEU GLU GLN VAL ALA GLY ILE
COORDS: ... .. THR lys met ILE ... .. ... .. phe VAL ... GLY ILE
              78                                     85
              ^^^ ^^^                               ^^^

```

```

357                                     371
SEQRES: GLN ARG ILE ILE GLN CYS HIS GLY SER PHE ALA THR ALA SER CYS
COORDS: ... .. ... .. ... .. ... .. ... .. ... .. ... .. ...

```

```

372                                     386
SEQRES: LEU ILE CYS LYS TYR LYS VAL ASP CYS GLU ALA VAL ARG GLY ASP
COORDS: ... .. ... LYS ... LYS ... .. ... .. ... .. ... .. ...
              86             87

```

```

387                                     401
SEQRES: ILE PHE ASN GLN VAL VAL PRO ARG CYS PRO ARG CYS PRO ALA ASP
COORDS: ... .. ... .. ... .. ... .. ... .. ... .. ... .. ...

```

```

402                                     416
SEQRES: GLU PRO LEU ALA ILE MET LYS PRO GLU ILE VAL PHE PHE GLY GLU
COORDS: ... .. ... .. ... .. LYS ... .. ... .. ... .. ... GLU
              88                                     89

```

```

417                                     431
SEQRES: ASN LEU PRO GLU GLN PHE HIS ARG ALA MET LYS TYR ASP LYS ASP
COORDS: ... .. ... GLU ... .. ... ARG ALA ... .. ... .. ...
              90             92

```

```

432                                     446
SEQRES: GLU VAL ASP LEU LEU ILE VAL ILE GLY SER SER LEU LYS VAL ARG
COORDS: ... .. ASP LEU ... .. ... ILE ... .. ... .. ... ..
              93             95

```

```

447                                     461
SEQRES: PRO VAL ALA LEU ILE PRO SER SER ILE PRO HIS GLU VAL PRO GLN
COORDS: ... .. ALA ... .. ... .. ... .. ... .. ... .. ...
              96

```

```

462                                     476
SEQRES: ILE LEU ILE ASN ARG GLU PRO LEU PRO HIS LEU HIS PHE ASP VAL
COORDS: ... .. ... .. ... .. ... .. ... .. ... .. ... .. ...

```

```

477                                     491
SEQRES: GLU LEU LEU GLY ASP CYS ASP VAL ILE ILE ASN GLU LEU CYS HIS
COORDS: ... .. ... .. ... .. ... .. ... .. ... .. ... .. ...

```

```

492                                     506
SEQRES: ARG LEU GLY GLY GLU TYR ALA LYS LEU CYS CYS ASN PRO VAL LYS
COORDS: ... .. ... .. ... TYR ... .. ... .. ... .. ... .. ...
              97

```

```

507                                     521

```

PSVS Software Environment

```
SEQRES: LEU SER GLU ILE THR GLU LYS PRO PRO ARG THR GLN LYS GLU LEU
COORDS: LEU ... .. LYS ... .. LYS ... ..
          98                               100
```

```
          522                               536
SEQRES: ALA TYR LEU SER GLU LEU PRO PRO THR PRO LEU HIS VAL SER GLU
COORDS: ALA ... .. THR ... .. asn GLU
          101                               104
                                   ^^^
```

```
          537
SEQRES: ASP
COORDS: ...
```

DoccytocSirt1.pdb: Missing KEYWDS records

DoccytocSirt1.pdb: Missing TITLE record