Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 04:04 PM EST

PDB ID	:	2GT5
Title	:	Solution structure of apo Human Sco1
Authors	:	Banci, L.; Bertini, I.; Calderone, V.; Ciofi-Baffoni, S.; Mangani, S.; Palumaa, P.; Martinelli, M.; Wang, S.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2006-04-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

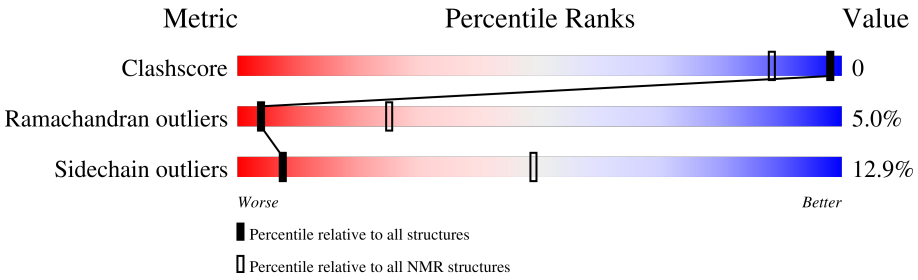
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	173	73% 9% 18%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 20 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:138-A:167, A:173-A:245, A:263-A:301 (142)	1.05	20

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 10, 14, 15, 16, 18, 20, 24, 25, 26, 29
2	4, 11, 12, 13, 17, 19, 21, 23
3	9, 30
4	27, 28
Single-model clusters	22

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2751 atoms, of which 1362 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SCO1 protein homolog, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	173	2751	890	1362	224	270	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	cloning artifact	UNP O75880
A	130	PHE	-	cloning artifact	UNP O75880
A	131	THR	-	cloning artifact	UNP O75880

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 73% 9% 18%

S129 F130 T131 G132 K133 P134 L135 L136 G137 R149 K150 H168 C169 P170 D171 V172 T191 I203 D204 P205 E206 R207 K218 R231 R239 R242 S246 P247 G248 P249 K250 D251 E252 D253 E254 D255 Y256 I257 V258 D259 H260 T261 I262 K283 R298 K299 K300 S301

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 66% 13% • 18%

S129 F130 T131 G132 K133 P134 L135 L136 G137 S141 E148 R149 K150 L156 G157 Q158 Y163 H168 C169 P170 D171 V172 C173 I181 P194 D204 P205 E206 R207 S221 R231 R242 V243 Y244 Y245 S246 P247 G248 P249 K250 D251 E252 D253 E254 D255 Y256 I257 V258 D259

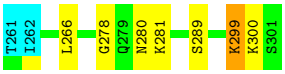
H260 T261 I262 I263 M264 L274 N280 K281 R282 K283 R295 P296 K300 S301

4.2.2 Score per residue for model 2

• Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 69% 11% • 18%

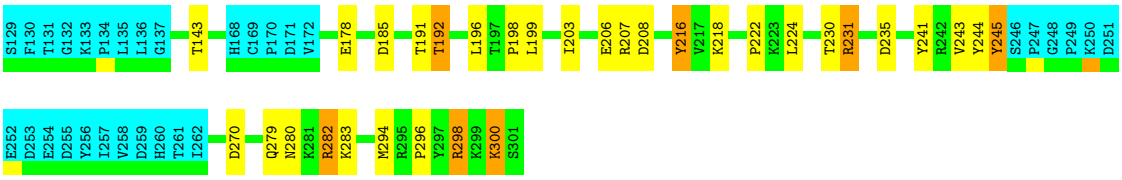
S129 F130 T131 G132 K133 P134 L135 L136 G137 T146 G147 E148 R149 D152 H168 C169 P170 D171 V172 E175 M180 T191 S202 R207 K210 K218 E219 F220 L224 R239 R242 S246 P247 G248 P249 K250 D251 E252 D253 E254 D255 Y256 I257 V258 D259 H260



4.2.3 Score per residue for model 3

• Molecule 1: SCO1 protein homolog, mitochondrial

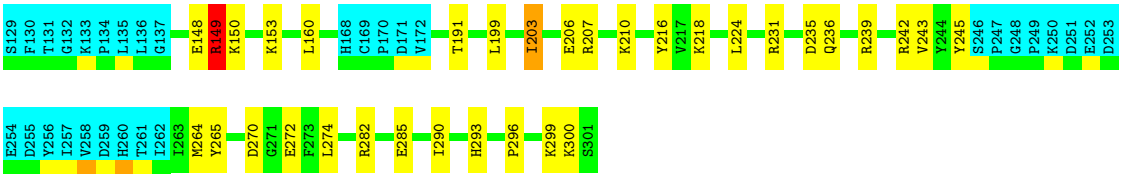
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: SCO1 protein homolog, mitochondrial

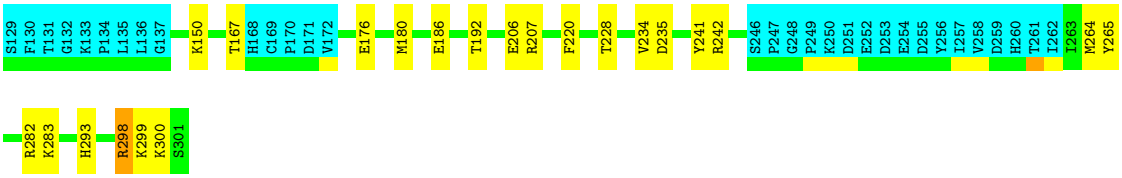
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: SCO1 protein homolog, mitochondrial

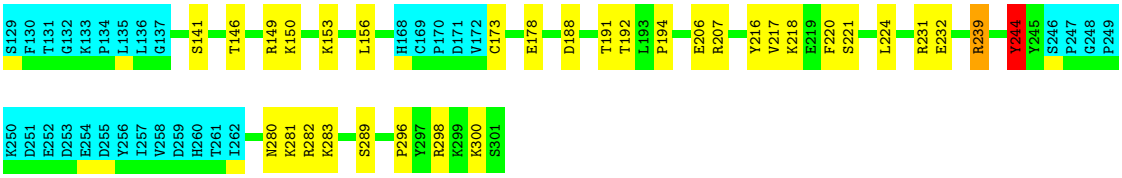
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: SCO1 protein homolog, mitochondrial

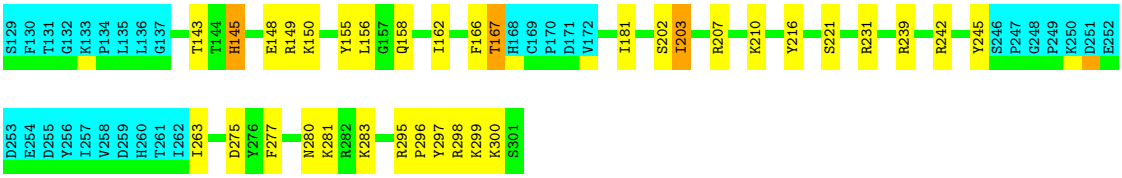
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial

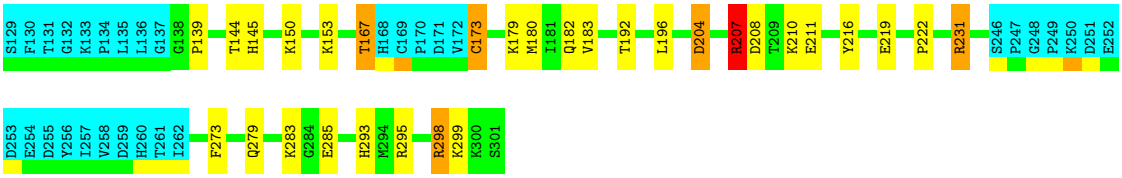
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A:

4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 68% 13% • 18%

S129 F130 T131 G132 K133 P134 L135 L136 G137 T143 T144 H145 T146 R149 K150 K153 Q158 T167 H168 C169 P170 D171 V172 T191 L199 I203 D204 P205 K210 K218 E219 L224 L227 R231 R242 S246 P247 G248 P249 K250 D251 E252 D253 E254 D255

Y256 I257 V258 D259 H260 T261 I262 I263 M264 I267 K281 Y297 R298 S301

4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 64% 15% • 18%

S129 F130 T131 G132 K133 P134 L135 L136 G137 L142 H145 K150 L160 T167 H168 C169 P170 D171 V172 C173 M180 V184 S189 I190 T191 T192 L199 I203 D204 P205 E206 R207 K218 E219 T228 G229 T230 R231 V237 R242 S246 P247 G248 P249 K250

D251 E252 D253 E254 D255 Y256 I257 V258 D259 H260 T261 I262 I263 G268 G271 E272 N280 K283 S289 K300 S301

4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 64% 16% • 18%

S129 F130 T131 G132 K133 P134 L135 L136 G137 T144 E148 R149 K150 Q158 W159 L160 H168 C169 P170 D171 V172 C173 P174 T191 S202 I203 D204 R207 D208 T209 K210 E211 K218 S221 T230 R231 V234 D235 Q236 V237 A238 R239 A240 Y241 R242 V243 S246 P247

G248 P249 K250 D251 E252 D253 E254 D255 Y256 I257 V258 D259 H260 T261 I262 K281 E285 H293 M294 R295 P296 Y297 K300 S301

4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 68% 12% • 18%

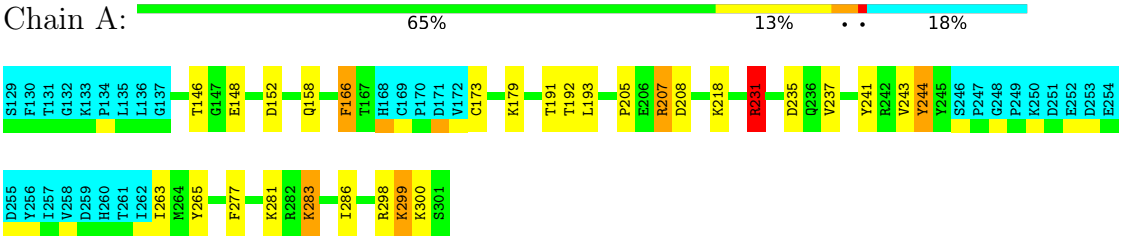
S129 F130 T131 G132 K133 P134 L135 L136 G137 H145 R149 K153 D154 Y155 L156 F166 T167 H168 C169 P170 D171 V172 T191 T192 I203 R207 K210 L224 R231 D235 Q236 V237 A238 R239 A240 Y241 R242 V243 S246 P247 G248 P249 K250 D251 E252 D253 E254 D255

Y256 I257 V258 D259 H260 T261 I262 Y265 L266 L274 P296 K299 K300 S301

4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial

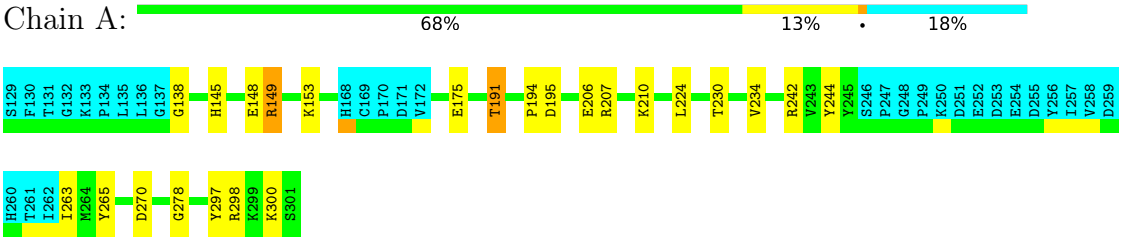
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial

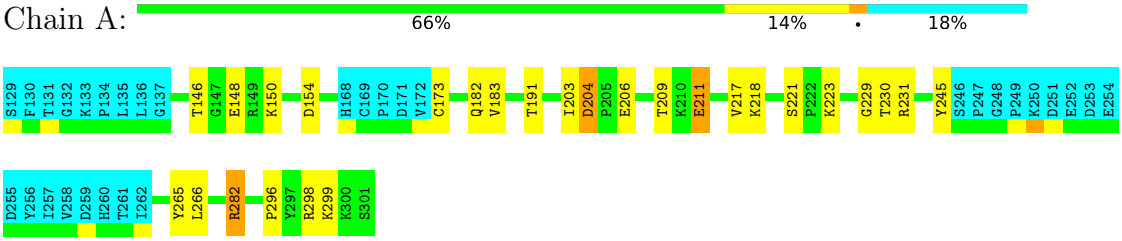
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial

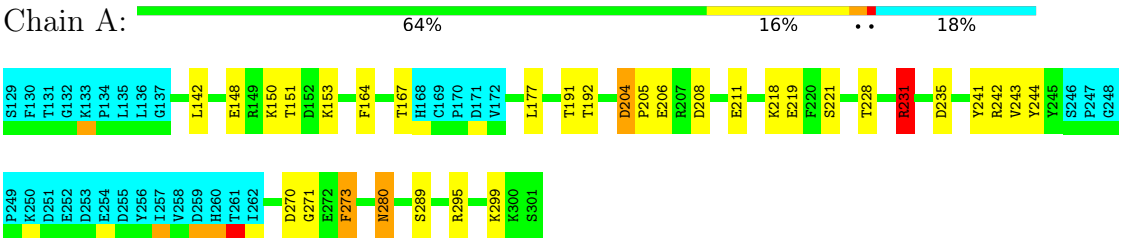
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial

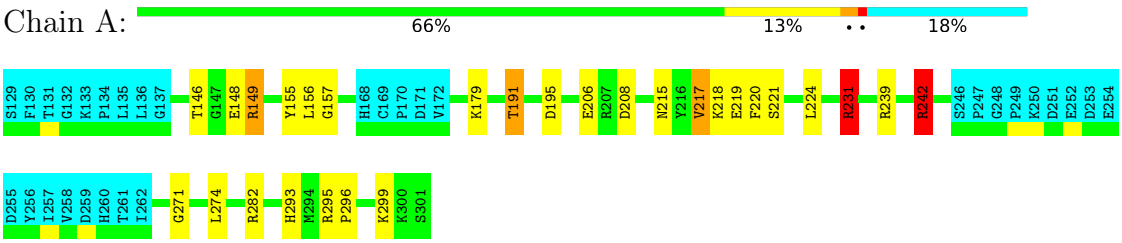
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial

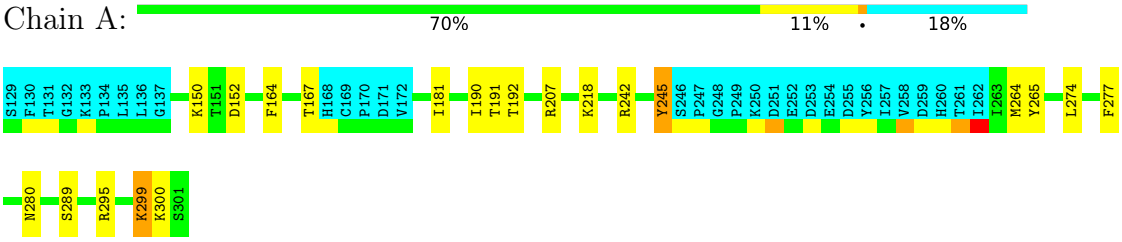
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial

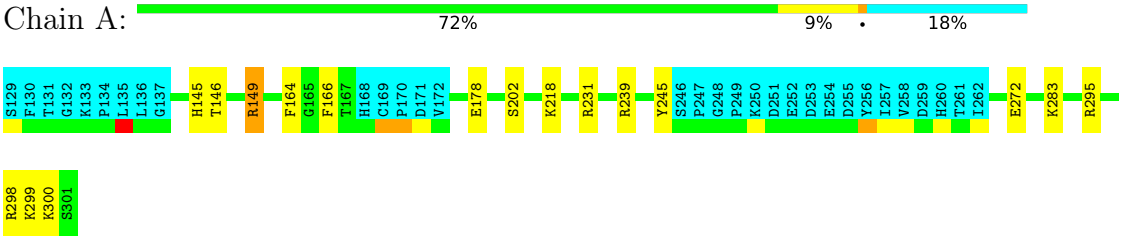
Chain A:



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: SCO1 protein homolog, mitochondrial

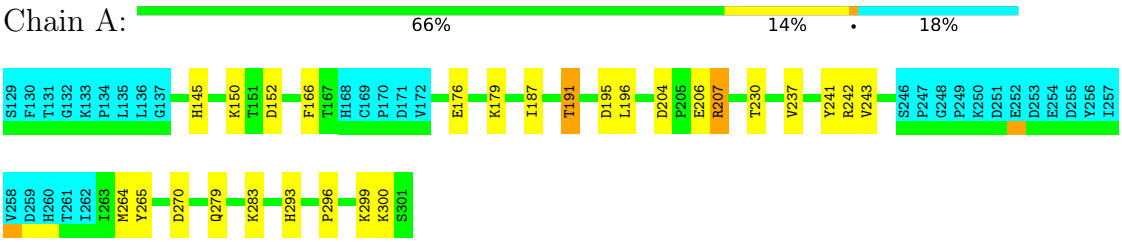
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial

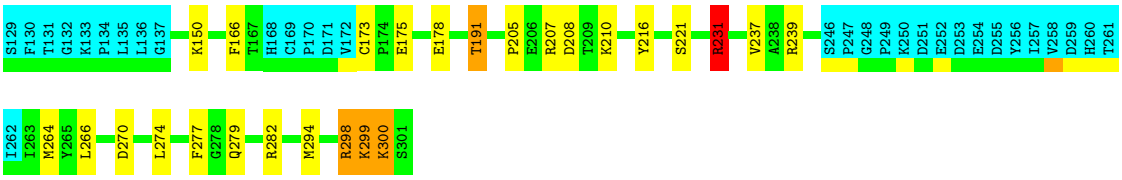
Chain A:



4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial

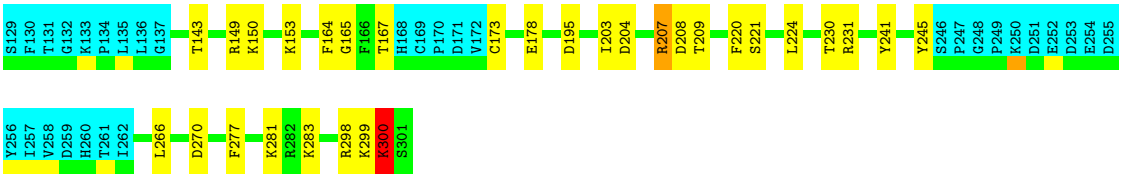
Chain A: 67% 12% • • 18%



4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial

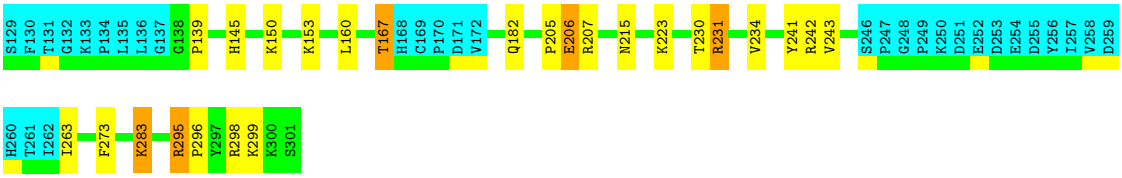
Chain A: 65% 16% • • 18%



4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial

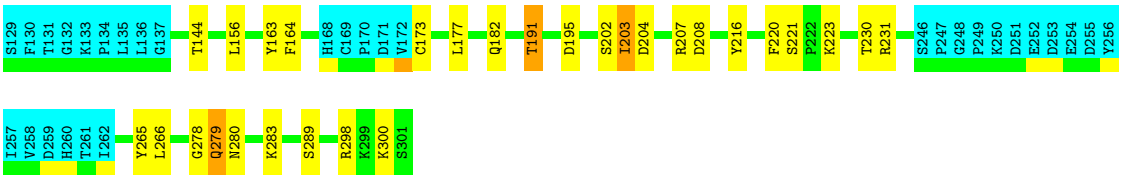
Chain A: 68% 12% • 18%



4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial

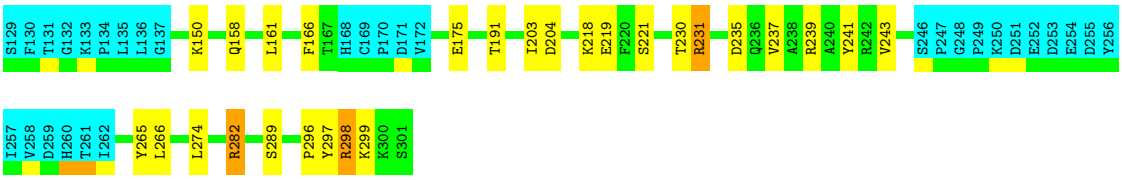
Chain A: 65% 15% • 18%



4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial

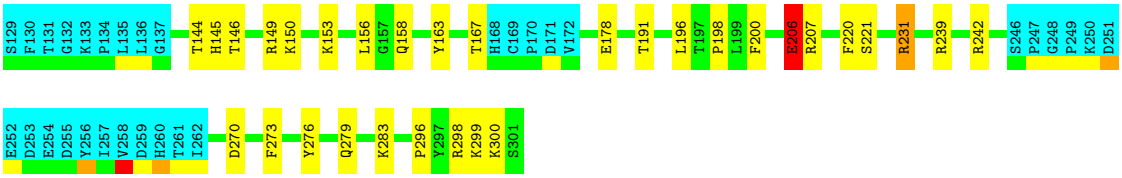
Chain A: 66% 14% • 18%



4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial

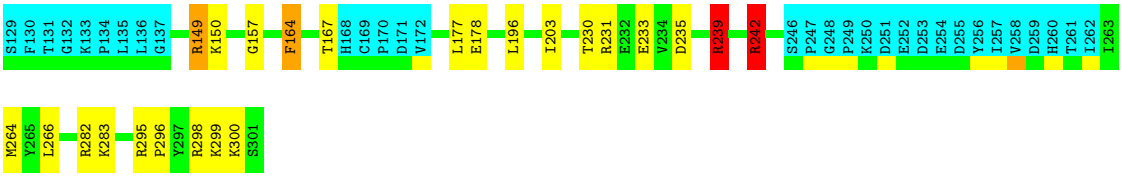
Chain A: 64% 17% •• 18%



4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial

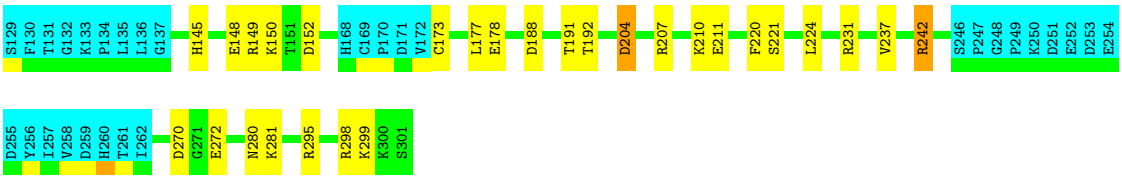
Chain A: 68% 12% •• 18%



4.2.29 Score per residue for model 29

- Molecule 1: SCO1 protein homolog, mitochondrial

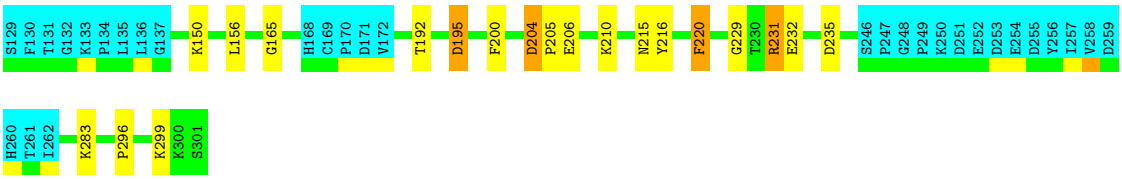
Chain A: 66% 15% • 18%



4.2.30 Score per residue for model 30

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 350 calculated structures, 30 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	8.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/1179 (0.0± 0.0%)	1.13±0.04	4±2/1594 (0.3± 0.1%)
All	All	0.73	0/35370 (0.0%)	1.13	121/47820 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.7±1.7
All	All	0	112

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	298	ARG	NE-CZ-NH1	12.74	126.67	120.30	22	12
1	A	207	ARG	NE-CZ-NH1	12.15	126.37	120.30	21	10
1	A	242	ARG	NE-CZ-NH1	10.77	125.68	120.30	28	10
1	A	231	ARG	NE-CZ-NH1	9.72	125.16	120.30	27	22
1	A	231	ARG	NE-CZ-NH2	-9.25	115.67	120.30	4	8
1	A	149	ARG	NE-CZ-NH1	8.39	124.49	120.30	2	8
1	A	149	ARG	NE-CZ-NH2	8.30	124.45	120.30	23	3
1	A	282	ARG	NE-CZ-NH1	7.20	123.90	120.30	22	6
1	A	166	PHE	CB-CG-CD2	-7.05	115.86	120.80	14	1
1	A	207	ARG	NE-CZ-NH2	-6.86	116.87	120.30	4	3
1	A	239	ARG	NE-CZ-NH2	6.82	123.71	120.30	28	4
1	A	207	ARG	CD-NE-CZ	6.60	132.84	123.60	21	1
1	A	239	ARG	NE-CZ-NH1	6.52	123.56	120.30	4	8
1	A	298	ARG	CD-NE-CZ	6.48	132.68	123.60	22	1
1	A	231	ARG	CD-NE-CZ	6.48	132.68	123.60	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	244	TYR	CB-CG-CD2	-6.42	117.14	121.00	6	1
1	A	242	ARG	CD-NE-CZ	6.32	132.45	123.60	28	1
1	A	282	ARG	NE-CZ-NH2	-6.13	117.23	120.30	3	1
1	A	295	ARG	NE-CZ-NH1	6.09	123.35	120.30	12	5
1	A	166	PHE	CB-CG-CD1	6.06	125.04	120.80	14	1
1	A	216	TYR	CB-CG-CD2	-5.87	117.48	121.00	3	1
1	A	149	ARG	CD-NE-CZ	5.57	131.40	123.60	2	1
1	A	155	TYR	CB-CG-CD2	-5.55	117.67	121.00	18	1
1	A	298	ARG	NE-CZ-NH2	-5.46	117.57	120.30	22	2
1	A	242	ARG	NE-CZ-NH2	-5.46	117.57	120.30	4	1
1	A	166	PHE	CA-CB-CG	5.45	126.97	113.90	14	1
1	A	280	ASN	C-N-CA	5.32	135.01	121.70	2	1
1	A	282	ARG	CD-NE-CZ	5.29	131.01	123.60	3	1
1	A	242	ARG	CA-CB-CG	5.27	125.00	113.40	28	1
1	A	191	THR	CA-CB-CG2	5.17	119.64	112.40	21	1
1	A	278	GLY	C-N-CA	5.16	134.59	121.70	25	1
1	A	245	TYR	CB-CG-CD2	-5.04	117.98	121.00	1	1
1	A	164	PHE	CB-CG-CD2	-5.03	117.28	120.80	28	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	204	ASP	Peptide	10
1	A	207	ARG	Sidechain,Peptide	6
1	A	220	PHE	Peptide,Sidechain	6
1	A	300	LYS	Peptide	5
1	A	206	GLU	Peptide	5
1	A	231	ARG	Sidechain	4
1	A	203	ILE	Peptide	4
1	A	167	THR	Peptide	4
1	A	239	ARG	Sidechain,Peptide	4
1	A	298	ARG	Sidechain,Peptide	4
1	A	245	TYR	Peptide	3
1	A	229	GLY	Peptide	3
1	A	195	ASP	Peptide	3
1	A	242	ARG	Sidechain,Peptide	3
1	A	164	PHE	Peptide,Sidechain	3
1	A	163	TYR	Sidechain	2
1	A	278	GLY	Peptide	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	149	ARG	Peptide,Sidechain	2
1	A	202	SER	Peptide	2
1	A	139	PRO	Peptide	2
1	A	191	THR	Peptide	2
1	A	166	PHE	Peptide	2
1	A	299	LYS	Peptide	2
1	A	157	GLY	Peptide	2
1	A	208	ASP	Peptide	2
1	A	165	GLY	Peptide	2
1	A	194	PRO	Peptide	1
1	A	243	VAL	Peptide	1
1	A	216	TYR	Sidechain	1
1	A	241	TYR	Sidechain	1
1	A	228	THR	Peptide	1
1	A	235	ASP	Peptide	1
1	A	275	ASP	Peptide	1
1	A	297	TYR	Sidechain	1
1	A	222	PRO	Peptide	1
1	A	151	THR	Peptide	1
1	A	182	GLN	Peptide	1
1	A	205	PRO	Peptide	1
1	A	158	GLN	Peptide	1
1	A	265	TYR	Sidechain	1
1	A	244	TYR	Peptide	1
1	A	282	ARG	Peptide	1
1	A	217	VAL	Peptide	1
1	A	271	GLY	Peptide	1
1	A	277	PHE	Peptide	1
1	A	146	THR	Peptide	1
1	A	295	ARG	Sidechain	1
1	A	280	ASN	Peptide	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1152	1141	1141	1±1
All	All	34560	34230	34230	19

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:LEU:H	1:A:196:LEU:HD23	0.48	1.67	21	2
1:A:231:ARG:H	1:A:231:ARG:CD	0.48	2.20	14	1
1:A:149:ARG:HH12	1:A:233:GLU:CD	0.47	2.12	28	1
1:A:180:MET:O	1:A:183:VAL:HG22	0.47	2.09	8	1
1:A:159:TRP:CZ3	1:A:293:HIS:CE1	0.45	3.04	12	1
1:A:200:PHE:CE2	1:A:216:TYR:CE1	0.45	3.04	30	1
1:A:195:ASP:CG	1:A:223:LYS:HZ2	0.44	2.15	9	1
1:A:143:THR:HG23	1:A:210:LYS:HE2	0.43	1.90	7	1
1:A:277:PHE:CE1	1:A:281:LYS:HE3	0.43	2.48	7	1
1:A:146:THR:HG23	1:A:147:GLY:H	0.43	1.74	2	1
1:A:210:LYS:HE3	1:A:211:GLU:OE2	0.42	2.15	12	1
1:A:218:LYS:HZ2	1:A:219:GLU:CD	0.42	2.18	11	1
1:A:181:ILE:HD12	1:A:222:PRO:CG	0.42	2.44	9	1
1:A:203:ILE:HD13	1:A:203:ILE:H	0.42	1.75	13	1
1:A:277:PHE:CZ	1:A:286:ILE:HG23	0.42	2.49	14	1
1:A:182:GLN:CB	1:A:283:LYS:HE3	0.41	2.46	24	1
1:A:143:THR:HB	1:A:210:LYS:HE2	0.40	1.92	10	1
1:A:211:GLU:H	1:A:211:GLU:CD	0.40	2.20	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	141/173 (82%)	115±4 (82±3%)	19±3 (13±2%)	7±3 (5±2%)	4 25
All	All	4230/5190 (82%)	3454 (82%)	566 (13%)	210 (5%)	4 25

All 54 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	191	THR	21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	296	PRO	14
1	A	221	SER	12
1	A	192	THR	11
1	A	173	CYS	9
1	A	243	VAL	9
1	A	207	ARG	8
1	A	241	TYR	8
1	A	204	ASP	6
1	A	299	LYS	6
1	A	205	PRO	6
1	A	206	GLU	5
1	A	281	LYS	5
1	A	242	ARG	5
1	A	245	TYR	4
1	A	231	ARG	4
1	A	270	ASP	4
1	A	167	THR	4
1	A	283	LYS	4
1	A	203	ILE	4
1	A	156	LEU	3
1	A	282	ARG	3
1	A	145	HIS	3
1	A	195	ASP	3
1	A	273	PHE	3
1	A	280	ASN	3
1	A	300	LYS	3
1	A	158	GLN	2
1	A	198	PRO	2
1	A	208	ASP	2
1	A	244	TYR	2
1	A	272	GLU	2
1	A	220	PHE	2
1	A	194	PRO	2
1	A	217	VAL	2
1	A	219	GLU	2
1	A	263	ILE	2
1	A	271	GLY	2
1	A	152	ASP	2
1	A	279	GLN	2
1	A	222	PRO	1
1	A	166	PHE	1
1	A	147	GLY	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	268	GLY	1
1	A	174	PRO	1
1	A	298	ARG	1
1	A	138	GLY	1
1	A	228	THR	1
1	A	190	ILE	1
1	A	146	THR	1
1	A	237	VAL	1
1	A	224	LEU	1
1	A	274	LEU	1
1	A	264	MET	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	125/153 (82%)	109±3 (87±3%)	16±3 (13±3%)	7 49
All	All	3750/4590 (82%)	3268 (87%)	482 (13%)	7 49

All 104 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	150	LYS	22
1	A	299	LYS	18
1	A	300	LYS	15
1	A	218	LYS	15
1	A	283	LYS	14
1	A	148	GLU	11
1	A	230	THR	10
1	A	153	LYS	10
1	A	231	ARG	10
1	A	210	LYS	9
1	A	224	LEU	9
1	A	235	ASP	9
1	A	298	ARG	9
1	A	265	TYR	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	145	HIS	9
1	A	280	ASN	8
1	A	295	ARG	8
1	A	266	LEU	8
1	A	178	GLU	8
1	A	242	ARG	7
1	A	264	MET	7
1	A	149	ARG	7
1	A	289	SER	7
1	A	207	ARG	7
1	A	203	ILE	7
1	A	237	VAL	7
1	A	274	LEU	6
1	A	216	TYR	6
1	A	293	HIS	6
1	A	206	GLU	6
1	A	167	THR	6
1	A	244	TYR	5
1	A	279	GLN	5
1	A	146	THR	5
1	A	156	LEU	5
1	A	179	LYS	5
1	A	208	ASP	5
1	A	219	GLU	5
1	A	270	ASP	5
1	A	173	CYS	4
1	A	152	ASP	4
1	A	175	GLU	4
1	A	199	LEU	4
1	A	160	LEU	4
1	A	234	VAL	4
1	A	144	THR	4
1	A	204	ASP	4
1	A	211	GLU	4
1	A	158	GLN	4
1	A	297	TYR	4
1	A	166	PHE	4
1	A	191	THR	4
1	A	177	LEU	4
1	A	181	ILE	3
1	A	180	MET	3
1	A	202	SER	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	196	LEU	3
1	A	245	TYR	3
1	A	282	ARG	3
1	A	285	GLU	3
1	A	281	LYS	3
1	A	155	TYR	3
1	A	263	ILE	3
1	A	182	GLN	3
1	A	273	PHE	3
1	A	220	PHE	3
1	A	223	LYS	3
1	A	215	ASN	3
1	A	164	PHE	3
1	A	141	SER	2
1	A	239	ARG	2
1	A	143	THR	2
1	A	192	THR	2
1	A	294	MET	2
1	A	176	GLU	2
1	A	188	ASP	2
1	A	232	GLU	2
1	A	142	LEU	2
1	A	209	THR	2
1	A	195	ASP	2
1	A	277	PHE	2
1	A	272	GLU	2
1	A	185	ASP	1
1	A	236	GLN	1
1	A	290	ILE	1
1	A	186	GLU	1
1	A	162	ILE	1
1	A	227	LEU	1
1	A	267	ILE	1
1	A	184	VAL	1
1	A	189	SER	1
1	A	228	THR	1
1	A	193	LEU	1
1	A	154	ASP	1
1	A	183	VAL	1
1	A	217	VAL	1
1	A	151	THR	1
1	A	187	ILE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	221	SER	1
1	A	241	TYR	1
1	A	163	TYR	1
1	A	161	LEU	1
1	A	200	PHE	1
1	A	276	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided