



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:08 pm GMT

PDB ID : 2HRN  
Title : Solution Structure of Cu(I) P174L-HSco1  
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Deposited on : 2006-07-20

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

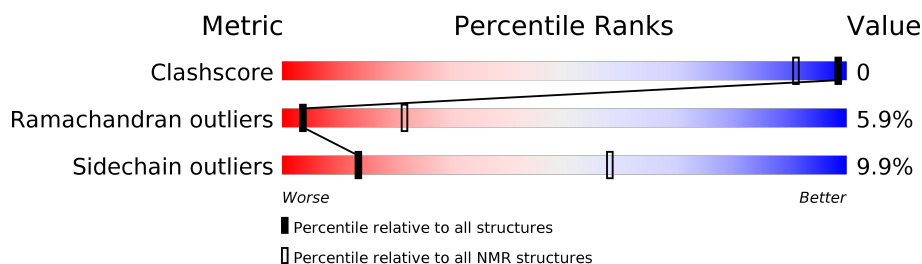
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	173	

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model ? as representative, based on the following criterion: *minimized average structure*.

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:246, A:258-A:298 (150)	0.90	6

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 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2755 atoms, of which 1364 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	173	Total	C	H	N	O	S	0
			2754	891	1364	224	270	5	

There are 4 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
A	174	LEU	PRO	ENGINEERED	UNP O75880

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

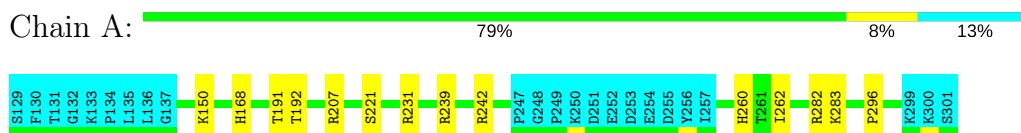
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

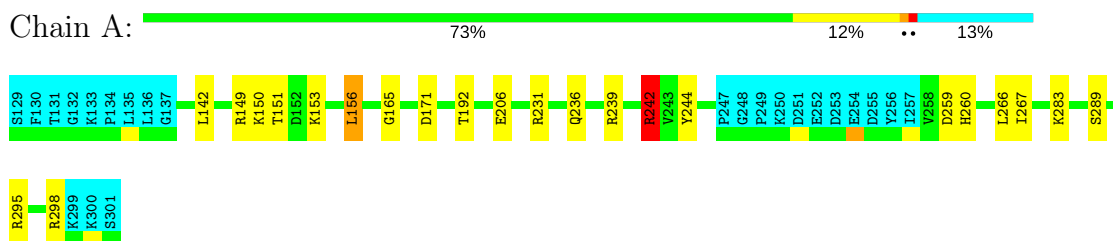


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

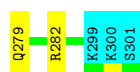
- Molecule 1: SCO1 protein homolog, mitochondrial



#### 4.2.2 Score per residue for model 2

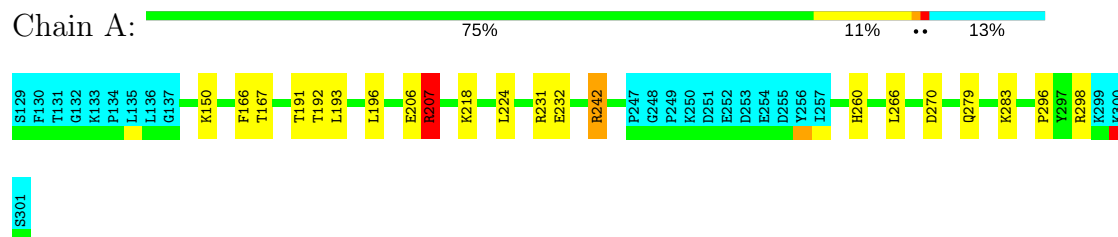
- Molecule 1: SCO1 protein homolog, mitochondrial





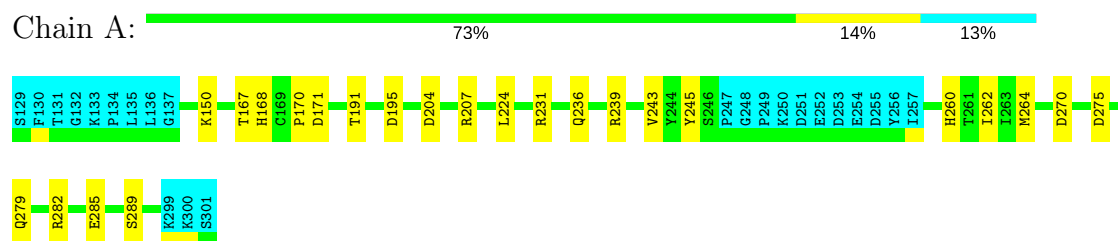
### 4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial



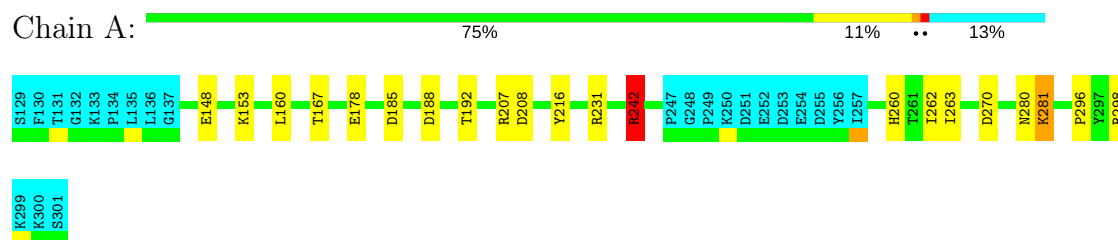
### 4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial



### 4.2.5 Score per residue for model 5

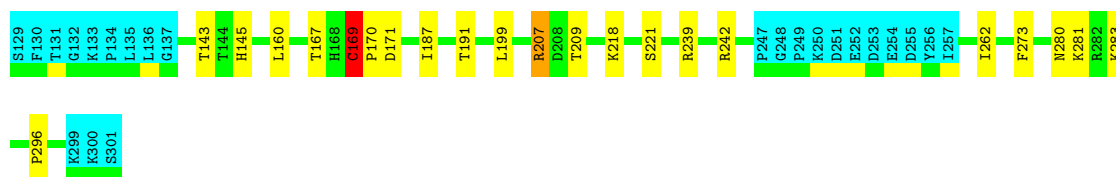
- Molecule 1: SCO1 protein homolog, mitochondrial



### 4.2.6 Score per residue for model 6 (medoid)

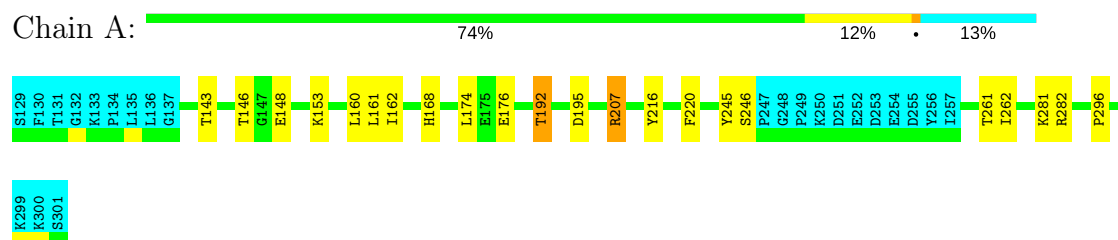
- Molecule 1: SCO1 protein homolog, mitochondrial





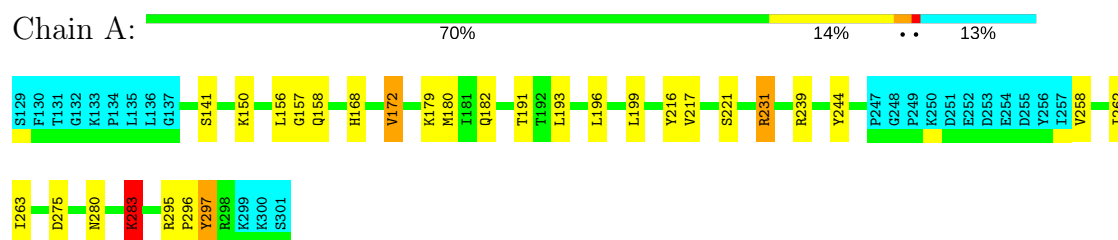
#### 4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial



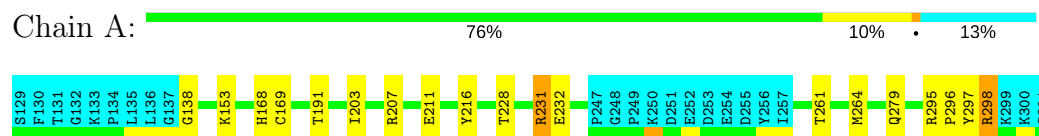
#### 4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial



#### 4.2.9 Score per residue for model 9

- Molecule 1: SCO1 protein homolog, mitochondrial



#### 4.2.10 Score per residue for model 10

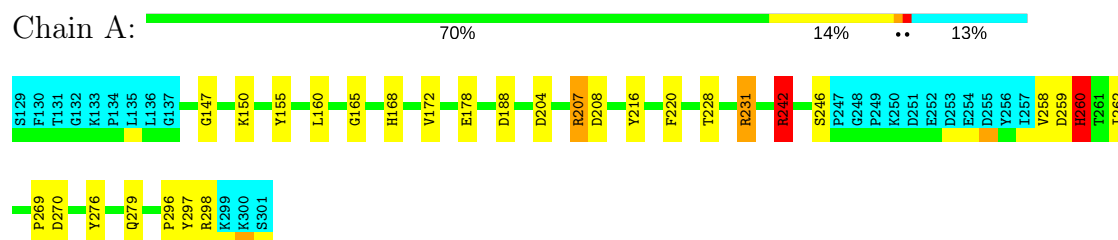
- Molecule 1: SCO1 protein homolog, mitochondrial





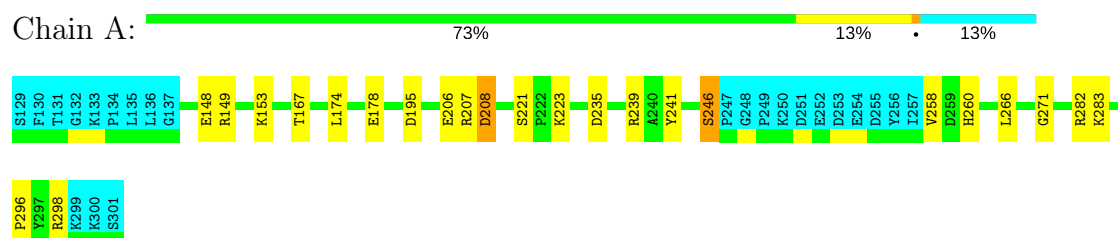
#### 4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



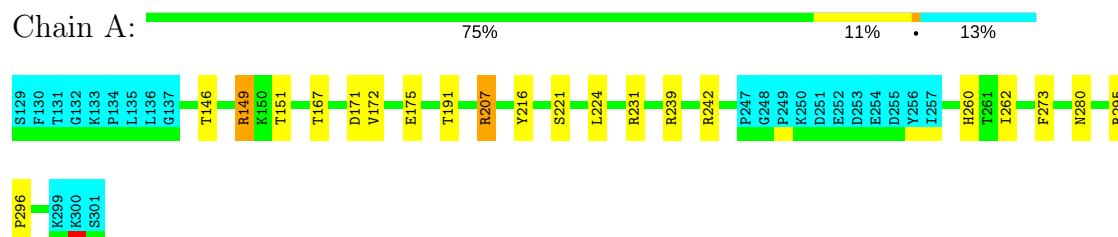
#### 4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



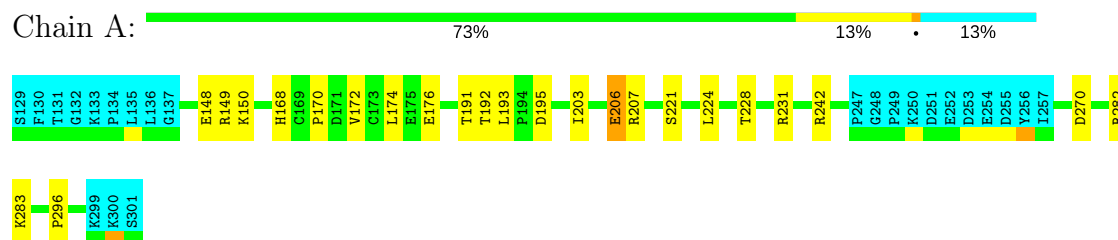
#### 4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial



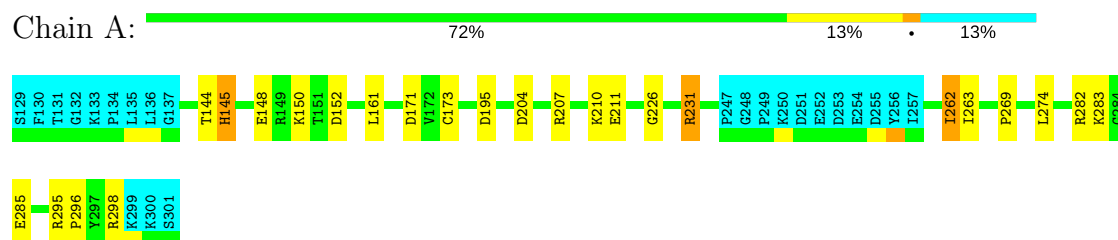
#### 4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



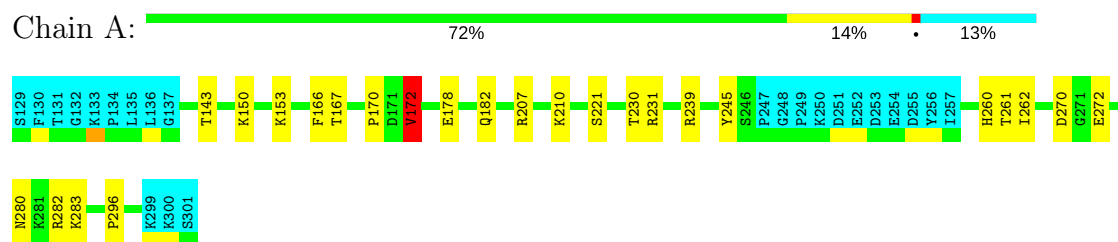
#### 4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



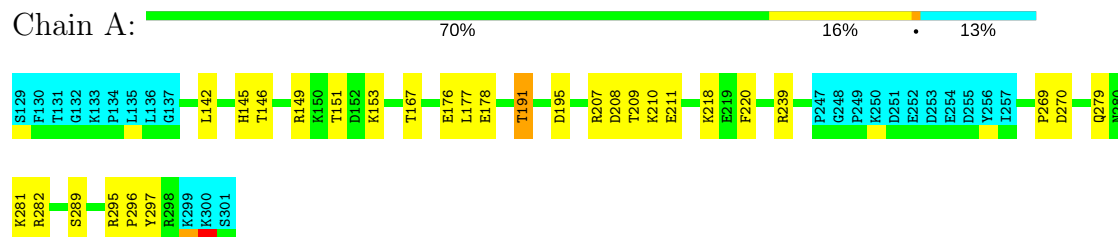
#### 4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



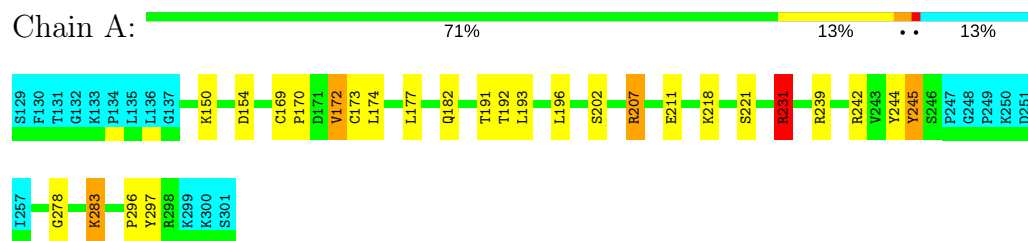
#### 4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



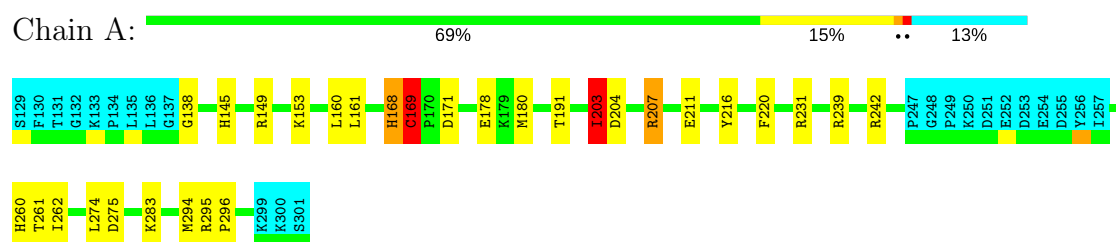
## 4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



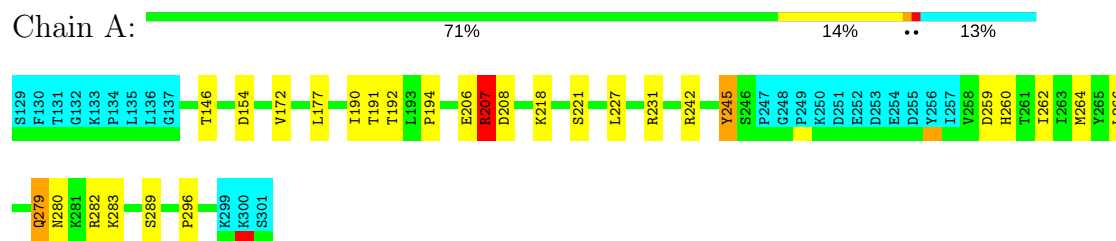
## 4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



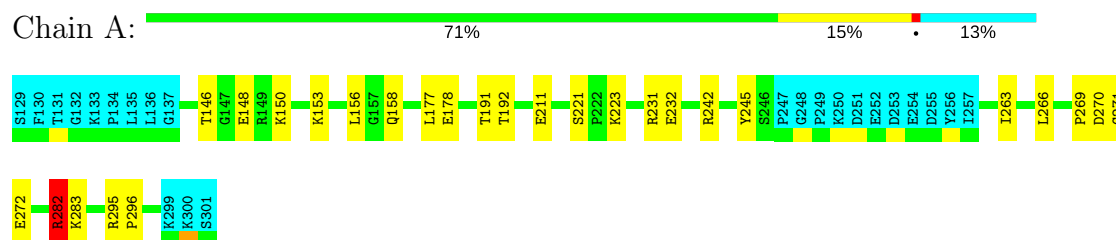
## 4.2.20 Score per residue for model 20

- Molecule 1: SCO1 protein homolog, mitochondrial



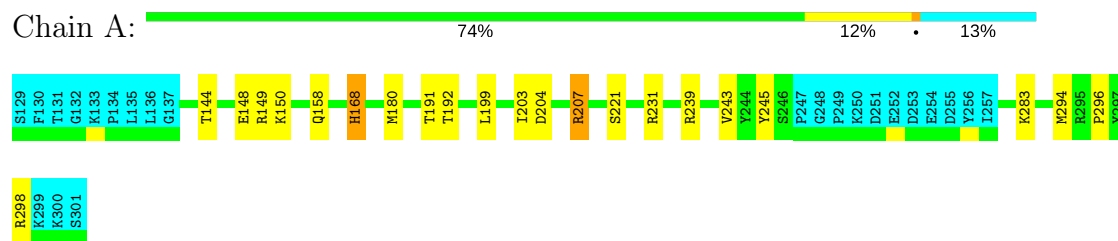
## 4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



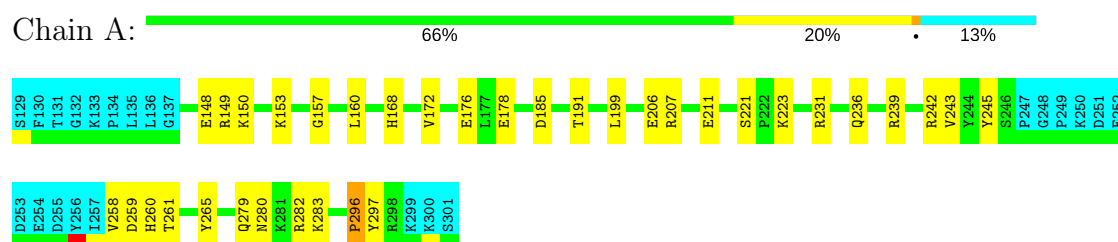
#### 4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



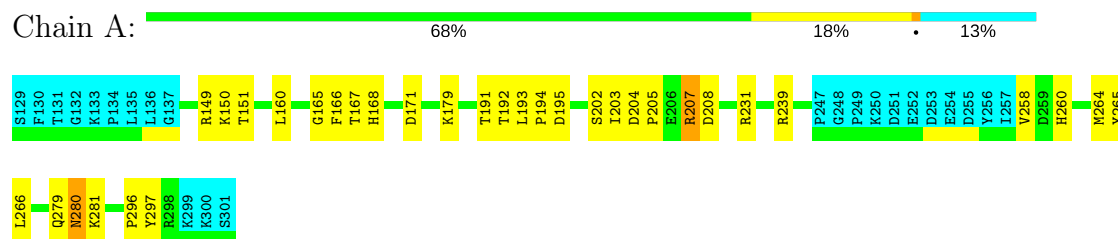
#### 4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



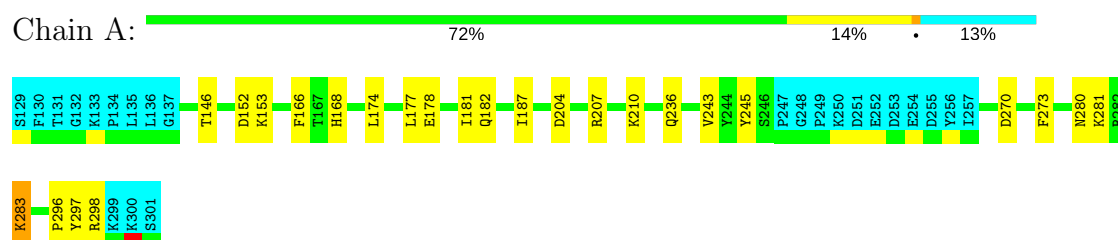
#### 4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



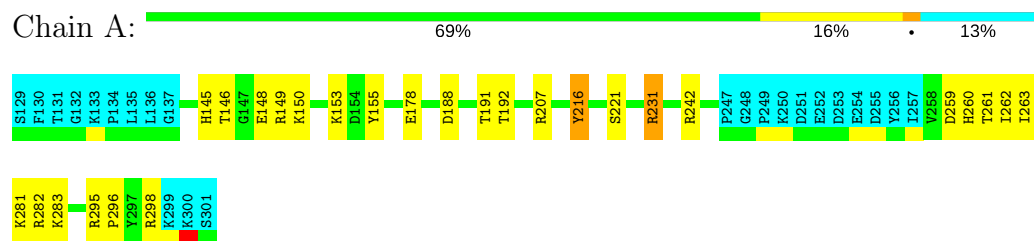
#### 4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



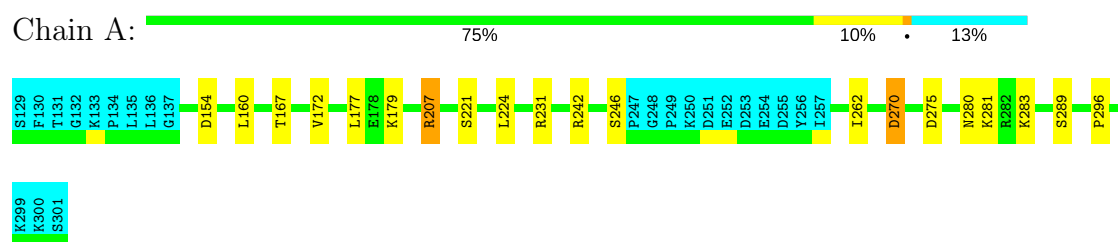
#### 4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



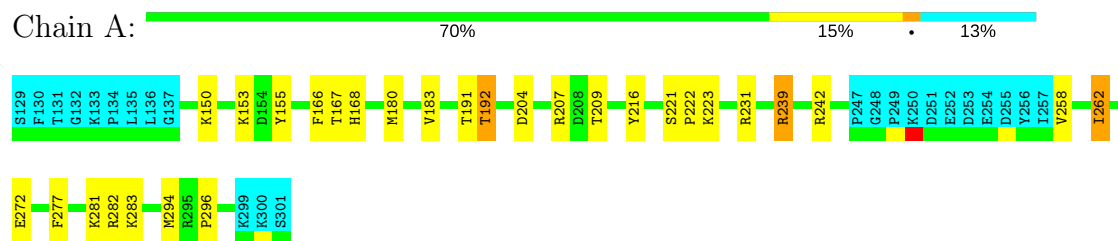
#### 4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



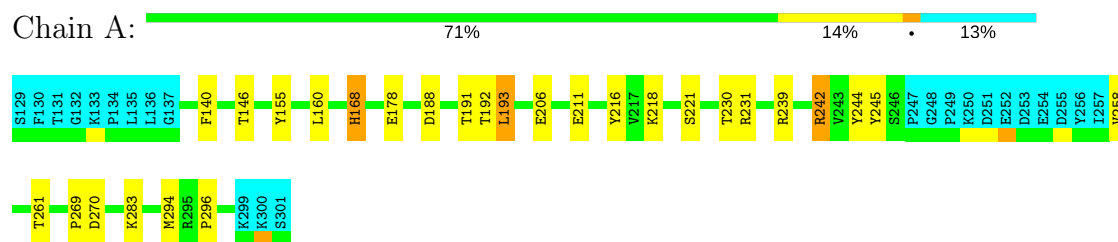
#### 4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial



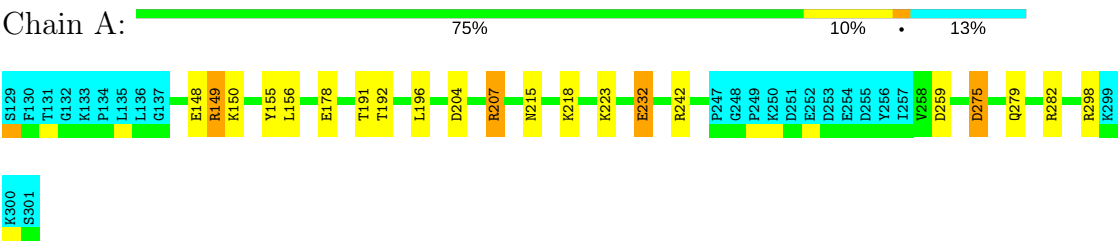
#### 4.2.29 Score per residue for model 29

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.30 Score per residue for model 30

- Molecule 1: SCO1 protein homolog, mitochondrial



## 5 Refinement protocol and experimental data overview ⓘ

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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	0.72±0.01	0±0/1242 (0.0±0.0%)	1.08±0.04	4±2/1688 (0.2±0.1%)
All	All	0.72	0/37260 (0.0%)	1.08	113/50640 (0.2%)

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	2.2±1.2
All	All	0	65

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	207	ARG	NE-CZ-NH1	11.80	126.20	120.30	30	12
1	A	231	ARG	NE-CZ-NH2	-9.96	115.32	120.30	14	8
1	A	231	ARG	NE-CZ-NH1	8.69	124.64	120.30	29	20
1	A	172	VAL	CA-CB-CG2	7.35	121.92	110.90	16	1
1	A	239	ARG	NE-CZ-NH1	7.30	123.95	120.30	28	15
1	A	282	ARG	NE-CZ-NH1	7.06	123.83	120.30	28	8
1	A	149	ARG	NE-CZ-NH1	7.03	123.81	120.30	30	11
1	A	298	ARG	NE-CZ-NH1	6.94	123.77	120.30	12	6
1	A	207	ARG	NE-CZ-NH2	-6.79	116.91	120.30	13	2
1	A	245	TYR	CB-CG-CD2	-6.56	117.07	121.00	18	1
1	A	239	ARG	NE-CZ-NH2	-6.34	117.13	120.30	10	2
1	A	242	ARG	NE-CZ-NH1	6.34	123.47	120.30	30	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	242	ARG	NE-CZ-NH2	-6.33	117.14	120.30	10	2
1	A	231	ARG	CD-NE-CZ	6.32	132.44	123.60	4	3
1	A	155	TYR	CB-CG-CD1	-6.01	117.39	121.00	29	3
1	A	295	ARG	NE-CZ-NH1	5.96	123.28	120.30	15	4
1	A	216	TYR	CB-CG-CD2	-5.91	117.45	121.00	29	1
1	A	216	TYR	CB-CG-CD1	-5.88	117.47	121.00	26	1
1	A	275	ASP	CB-CG-OD1	5.54	123.29	118.30	19	2
1	A	275	ASP	CB-CG-OD2	-5.54	113.31	118.30	19	1
1	A	242	ARG	CD-NE-CZ	5.19	130.87	123.60	10	1
1	A	244	TYR	CB-CG-CD1	-5.17	117.90	121.00	8	1
1	A	297	TYR	CB-CG-CD1	-5.09	117.94	121.00	11	1
1	A	172	VAL	CA-CB-CG1	5.09	118.53	110.90	18	1
1	A	297	TYR	CB-CG-CD2	-5.08	117.95	121.00	8	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	207	ARG	Sidechain,Peptide	6
1	A	269	PRO	Peptide	5
1	A	216	TYR	Sidechain	4
1	A	231	ARG	Sidechain	4
1	A	168	HIS	Peptide	3
1	A	206	GLU	Peptide	3
1	A	282	ARG	Sidechain,Peptide	3
1	A	246	SER	Peptide	2
1	A	295	ARG	Sidechain	2
1	A	169	CYS	Peptide	2
1	A	241	TYR	Sidechain,Peptide	2
1	A	297	TYR	Sidechain	2
1	A	170	PRO	Peptide	2
1	A	242	ARG	Sidechain	2
1	A	138	GLY	Peptide	1
1	A	258	VAL	Peptide	1
1	A	167	THR	Peptide	1
1	A	204	ASP	Peptide	1
1	A	221	SER	Peptide	1
1	A	281	LYS	Peptide	1
1	A	140	PHE	Sidechain	1
1	A	192	THR	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	239	ARG	Sidechain	1
1	A	296	PRO	Peptide	1
1	A	194	PRO	Peptide	1
1	A	203	ILE	Peptide	1
1	A	260	HIS	Sidechain	1
1	A	280	ASN	Peptide	1
1	A	271	GLY	Peptide	1
1	A	165	GLY	Peptide	1
1	A	157	GLY	Peptide	1
1	A	163	TYR	Sidechain	1
1	A	193	LEU	Peptide	1
1	A	156	LEU	Peptide	1
1	A	149	ARG	Sidechain	1
1	A	298	ARG	Sidechain	1
1	A	208	ASP	Peptide	1

## 6.2 Too-close contacts

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	1212	1188	1187	1±1
All	All	36390	35640	35610	17

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:203:ILE:HG23	1:A:204:ASP:H	0.54	1.63	19	1
1:A:211:GLU:CD	1:A:211:GLU:H	0.47	2.13	29	2
1:A:232:GLU:H	1:A:232:GLU:CD	0.46	2.14	30	2
1:A:211:GLU:H	1:A:211:GLU:CD	0.44	2.16	17	1
1:A:172:VAL:CG1	1:A:261:THR:HG21	0.44	2.43	16	1
1:A:180:MET:O	1:A:183:VAL:HG22	0.43	2.13	28	1
1:A:207:ARG:CZ	1:A:207:ARG:HA	0.43	2.44	2	1
1:A:145:HIS:CE1	1:A:226:GLY:H	0.43	2.32	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:GLN:HB3	1:A:283:LYS:HE3	0.43	1.90	25	2
1:A:165:GLY:HA2	1:A:260:HIS:CD2	0.43	2.48	11	1
1:A:232:GLU:CD	1:A:232:GLU:H	0.42	2.17	3	1
1:A:172:VAL:HG12	1:A:261:THR:HG21	0.41	1.91	16	1
1:A:169:CYS:SG	1:A:170:PRO:HD2	0.40	2.56	6	1
1:A:182:GLN:C	1:A:283:LYS:HE3	0.40	2.36	18	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	150/173 (87%)	122±4 (81±3%)	19±3 (13±2%)	9±3 (6±2%)	4	22
All	All	4500/5190 (87%)	3653 (81%)	580 (13%)	267 (6%)	4	22

All 58 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	296	PRO	26
1	A	191	THR	17
1	A	192	THR	14
1	A	221	SER	13
1	A	207	ARG	12
1	A	242	ARG	11
1	A	262	ILE	10
1	A	270	ASP	9
1	A	168	HIS	8
1	A	172	VAL	8
1	A	171	ASP	7
1	A	245	TYR	7
1	A	279	GLN	6
1	A	261	THR	6
1	A	204	ASP	6
1	A	258	VAL	6

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Mol	Chain	Res	Type	Models (Total)
1	A	223	LYS	5
1	A	243	VAL	5
1	A	280	ASN	5
1	A	208	ASP	5
1	A	167	THR	5
1	A	260	HIS	5
1	A	244	TYR	4
1	A	193	LEU	4
1	A	283	LYS	4
1	A	263	ILE	4
1	A	272	GLU	4
1	A	246	SER	3
1	A	195	ASP	3
1	A	281	LYS	3
1	A	259	ASP	3
1	A	203	ILE	3
1	A	145	HIS	3
1	A	170	PRO	3
1	A	282	ARG	2
1	A	169	CYS	2
1	A	274	LEU	2
1	A	220	PHE	2
1	A	209	THR	2
1	A	298	ARG	2
1	A	206	GLU	1
1	A	165	GLY	1
1	A	194	PRO	1
1	A	152	ASP	1
1	A	228	THR	1
1	A	271	GLY	1
1	A	146	THR	1
1	A	273	PHE	1
1	A	166	PHE	1
1	A	231	ARG	1
1	A	148	GLU	1
1	A	147	GLY	1
1	A	222	PRO	1
1	A	156	LEU	1
1	A	278	GLY	1
1	A	205	PRO	1
1	A	138	GLY	1
1	A	157	GLY	1

### 6.3.2 Protein sidechains ⓘ

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	133/153 (87%)	120±3 (90±2%)	13±3 (10±2%)	13	58
All	All	3990/4590 (87%)	3596 (90%)	394 (10%)	13	58

All 100 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	17
1	A	283	LYS	17
1	A	153	LYS	15
1	A	178	GLU	14
1	A	207	ARG	11
1	A	148	GLU	11
1	A	160	LEU	10
1	A	260	HIS	9
1	A	242	ARG	8
1	A	177	LEU	8
1	A	262	ILE	7
1	A	146	THR	7
1	A	218	LYS	7
1	A	174	LEU	6
1	A	280	ASN	6
1	A	281	LYS	6
1	A	279	GLN	6
1	A	266	LEU	6
1	A	168	HIS	5
1	A	289	SER	5
1	A	211	GLU	5
1	A	167	THR	5
1	A	196	LEU	5
1	A	297	TYR	5
1	A	195	ASP	5
1	A	231	ARG	5
1	A	216	TYR	5
1	A	224	LEU	5
1	A	180	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	210	LYS	4
1	A	188	ASP	4
1	A	282	ARG	4
1	A	169	CYS	4
1	A	206	GLU	4
1	A	199	LEU	4
1	A	172	VAL	4
1	A	176	GLU	4
1	A	166	PHE	4
1	A	179	LYS	4
1	A	275	ASP	4
1	A	270	ASP	4
1	A	294	MET	4
1	A	245	TYR	4
1	A	191	THR	4
1	A	151	THR	4
1	A	264	MET	4
1	A	236	GLN	4
1	A	154	ASP	3
1	A	161	LEU	3
1	A	239	ARG	3
1	A	149	ARG	3
1	A	143	THR	3
1	A	202	SER	3
1	A	158	GLN	3
1	A	259	ASP	3
1	A	295	ARG	3
1	A	156	LEU	3
1	A	298	ARG	3
1	A	273	PHE	3
1	A	228	THR	2
1	A	223	LYS	2
1	A	203	ILE	2
1	A	193	LEU	2
1	A	144	THR	2
1	A	187	ILE	2
1	A	142	LEU	2
1	A	235	ASP	2
1	A	221	SER	2
1	A	219	GLU	2
1	A	185	ASP	2
1	A	220	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	285	GLU	2
1	A	173	CYS	2
1	A	232	GLU	2
1	A	274	LEU	2
1	A	265	TYR	2
1	A	230	THR	2
1	A	145	HIS	2
1	A	155	TYR	2
1	A	152	ASP	1
1	A	213	ILE	1
1	A	175	GLU	1
1	A	141	SER	1
1	A	272	GLU	1
1	A	171	ASP	1
1	A	190	ILE	1
1	A	182	GLN	1
1	A	276	TYR	1
1	A	192	THR	1
1	A	162	ILE	1
1	A	263	ILE	1
1	A	267	ILE	1
1	A	204	ASP	1
1	A	209	THR	1
1	A	227	LEU	1
1	A	217	VAL	1
1	A	215	ASN	1
1	A	277	PHE	1
1	A	208	ASP	1
1	A	181	ILE	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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

No chemical shift data were provided