



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2022 – 12:07 AM EST

PDB ID : 2RLI  
Title : Solution structure of Cu(I) human Sco2  
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Deposited on : 2007-07-11

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

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The following versions of software and data (see [references ⓘ](#)) 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

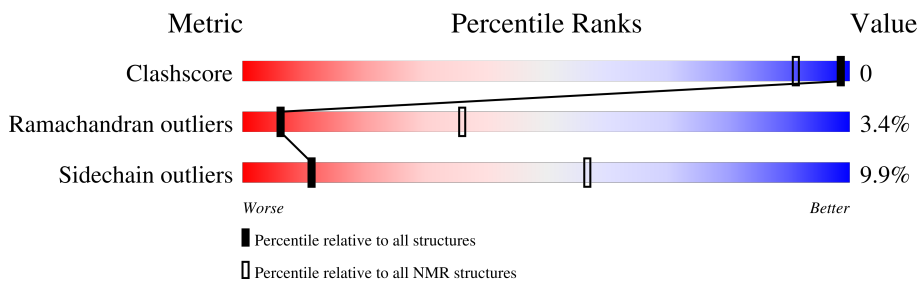
# 1 Overall quality at a glance

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  $\geq 3$ , 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	171	 76% 11% 13% .

## 2 Ensemble composition and analysis i

This entry contains 31 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:103-A:210, A:222-A:261 (148)	0.97	3

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 5 clusters and 12 single-model clusters were found.

Cluster number	Models
1	5, 6, 12, 13, 20, 23, 29
2	3, 4, 7, 11, 14
3	10, 15, 18
4	1, 27
5	9, 31
Single-model clusters	2; 8; 16; 17; 19; 21; 22; 24; 25; 26; 28; 30

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2677 atoms, of which 1306 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SCO2 protein homolog, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	170	2676	864	1306	243	257	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP O43819
A	97	SER	-	expression tag	UNP O43819
A	98	PHE	-	expression tag	UNP O43819
A	99	THR	-	expression tag	UNP O43819

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

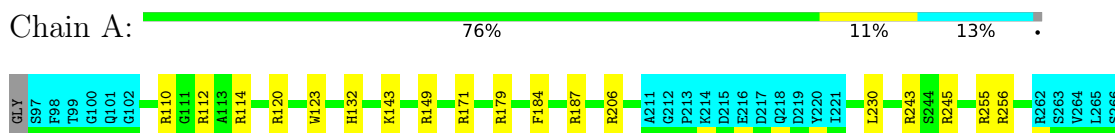
Mol	Chain	Residues	Atoms	
			Total	Cu
2	A	1	1	1

## 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: SCO2 protein homolog, mitochondrial

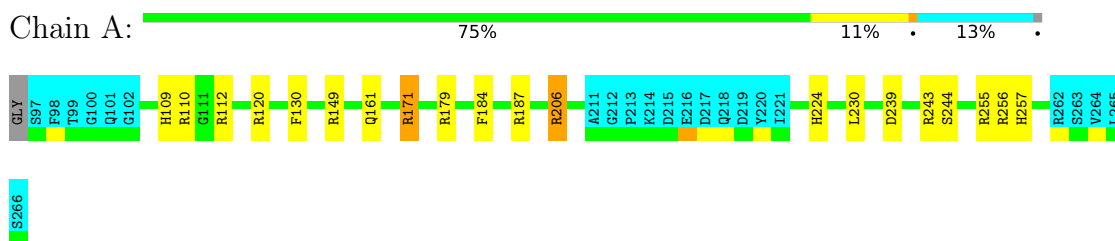


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

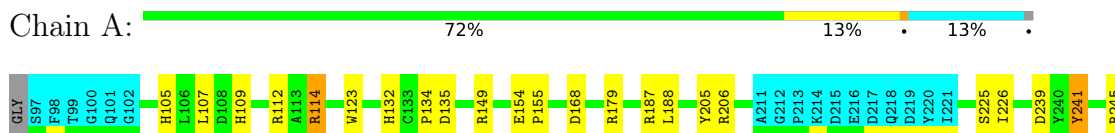
#### 4.2.1 Score per residue for model 1

- Molecule 1: SCO2 protein homolog, mitochondrial



#### 4.2.2 Score per residue for model 2

- Molecule 1: SCO2 protein homolog, mitochondrial

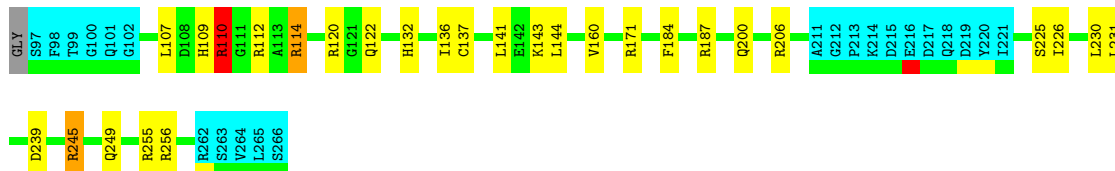




### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: SCO2 protein homolog, mitochondrial

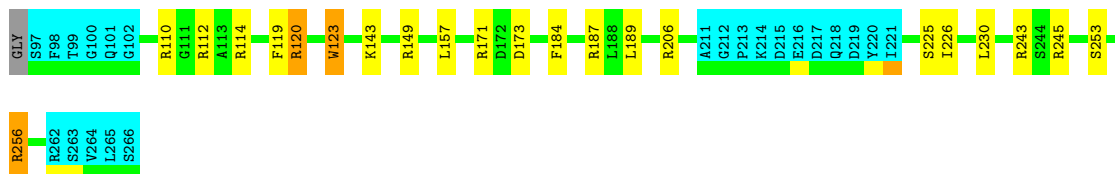
Chain A: 70% 15% 13%



### 4.2.4 Score per residue for model 4

- Molecule 1: SCO2 protein homolog, mitochondrial

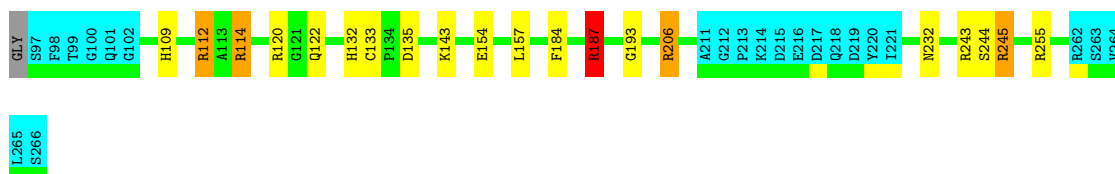
Chain A: 74% 11% 13%



### 4.2.5 Score per residue for model 5

- Molecule 1: SCO2 protein homolog, mitochondrial

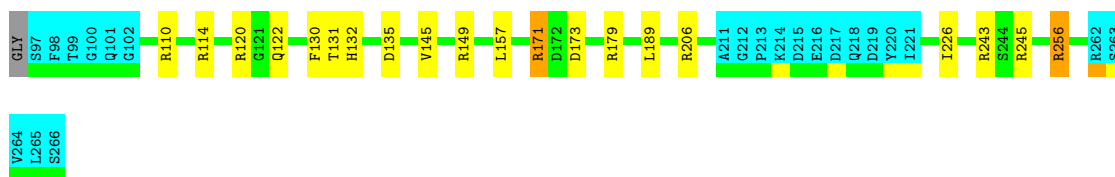
Chain A: 75% 9% 13%



### 4.2.6 Score per residue for model 6

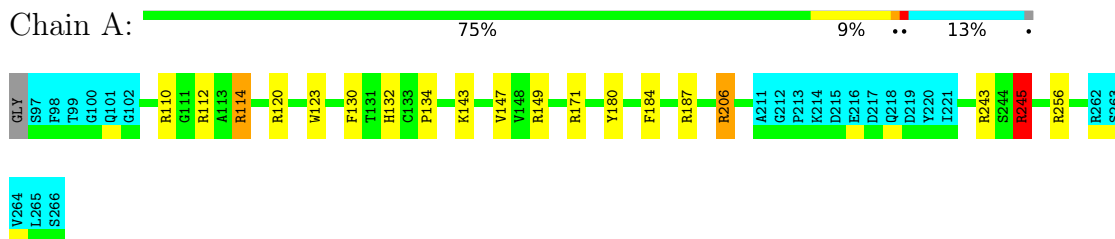
- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 75% 11% 13%



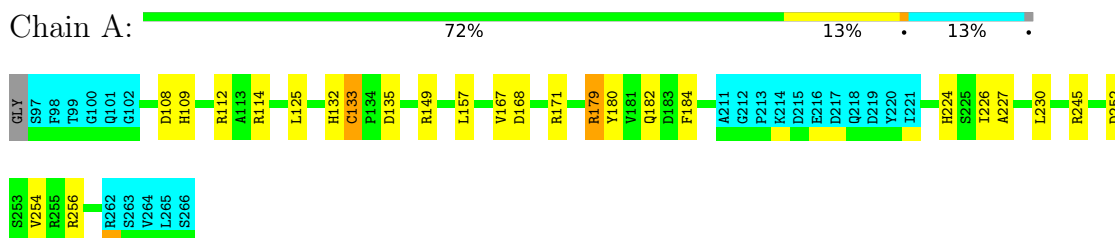
#### 4.2.7 Score per residue for model 7

- Molecule 1: SCO2 protein homolog, mitochondrial



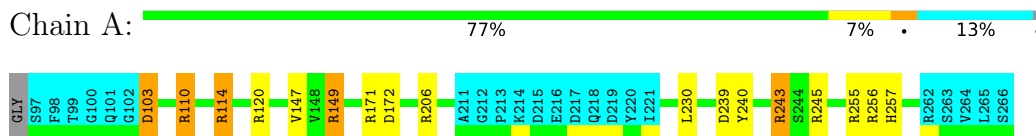
#### 4.2.8 Score per residue for model 8

- Molecule 1: SCO2 protein homolog, mitochondrial



#### 4.2.9 Score per residue for model 9

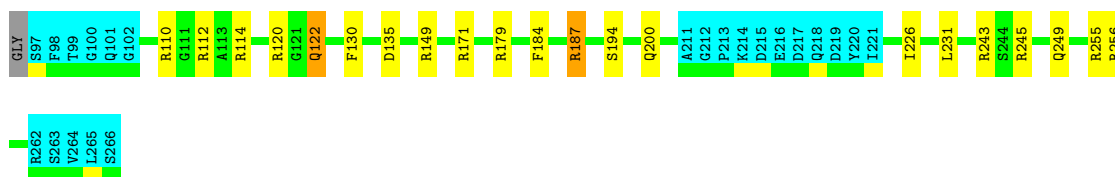
- Molecule 1: SCO2 protein homolog, mitochondrial



#### 4.2.10 Score per residue for model 10

- Molecule 1: SCO2 protein homolog, mitochondrial

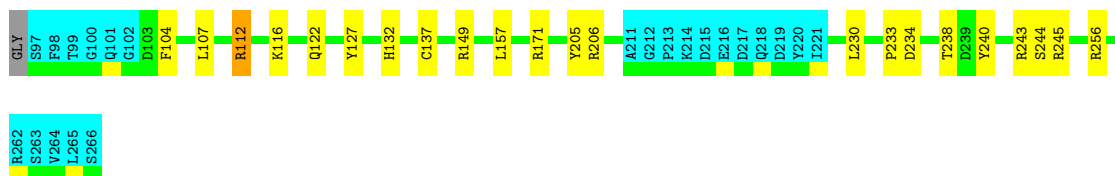




#### 4.2.11 Score per residue for model 11

- Molecule 1: SCO2 protein homolog, mitochondrial

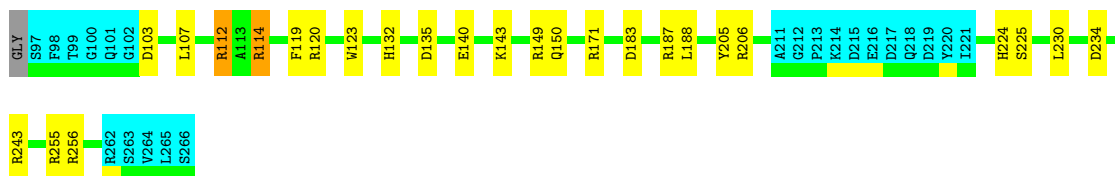
Chain A: 74% 12% 13%



#### 4.2.12 Score per residue for model 12

- Molecule 1: SCO2 protein homolog, mitochondrial

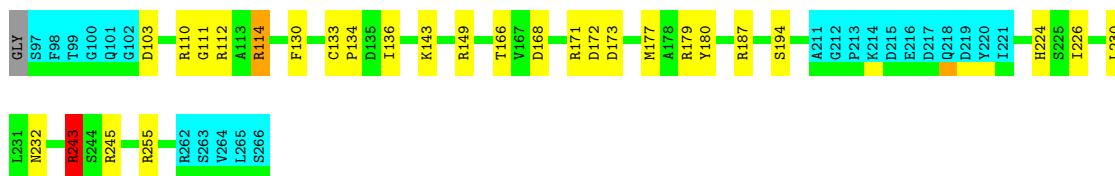
Chain A: 71% 14% 13%



#### 4.2.13 Score per residue for model 13

- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 70% 15% 13%

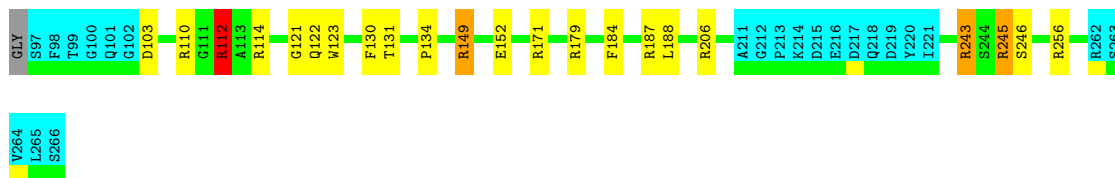


#### 4.2.14 Score per residue for model 14

- Molecule 1: SCO2 protein homolog, mitochondrial



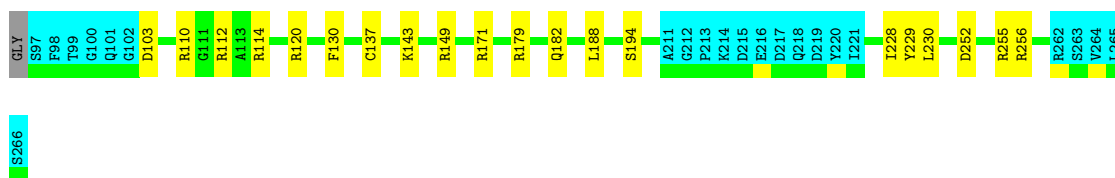
Chain A:  74% 11% 13%



#### 4.2.15 Score per residue for model 15

- Molecule 1: SCO2 protein homolog, mitochondrial

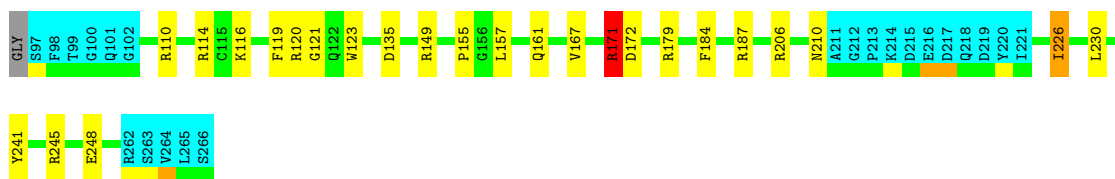
Chain A:  75% 12% 13%



#### 4.2.16 Score per residue for model 16

- Molecule 1: SCO2 protein homolog, mitochondrial

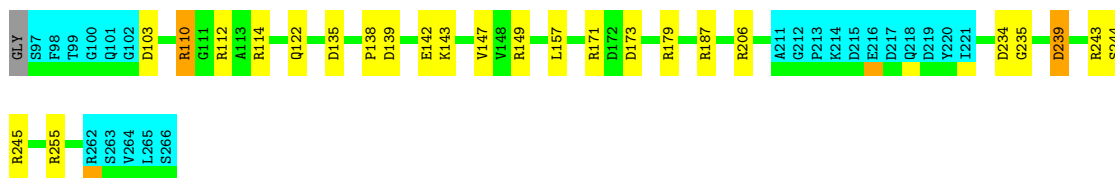
Chain A:  72% 13% 13%



#### 4.2.17 Score per residue for model 17

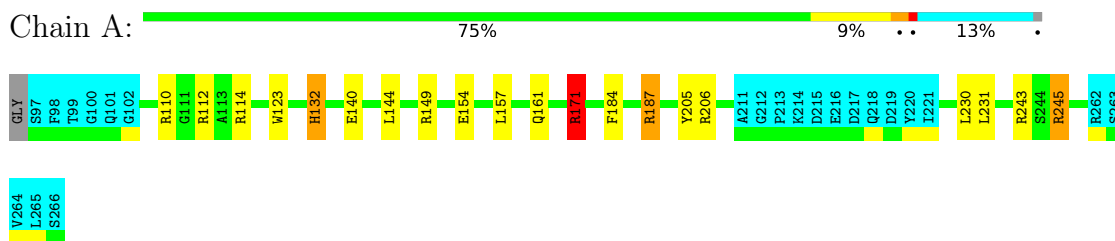
- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A:  72% 13% 13%



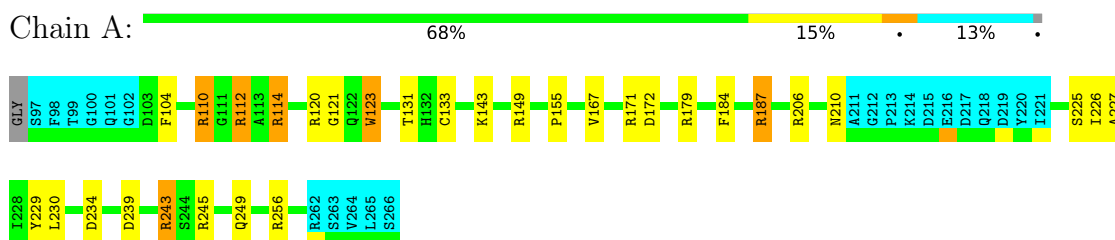
#### 4.2.18 Score per residue for model 18

- Molecule 1: SCO2 protein homolog, mitochondrial



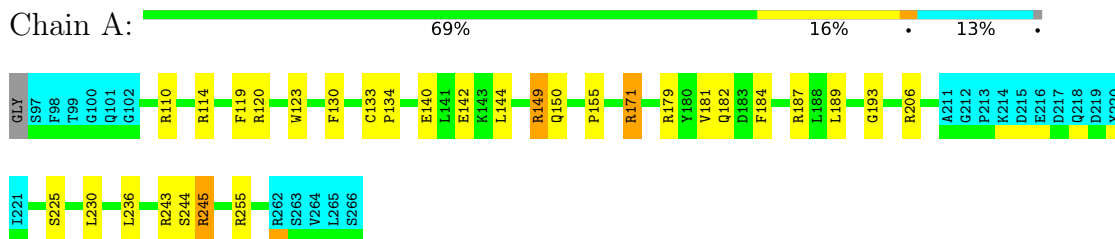
#### 4.2.19 Score per residue for model 19

- Molecule 1: SCO2 protein homolog, mitochondrial



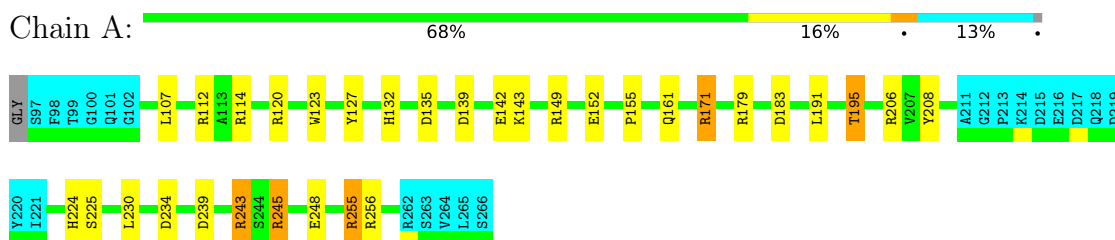
#### 4.2.20 Score per residue for model 20

- Molecule 1: SCO2 protein homolog, mitochondrial



#### 4.2.21 Score per residue for model 21

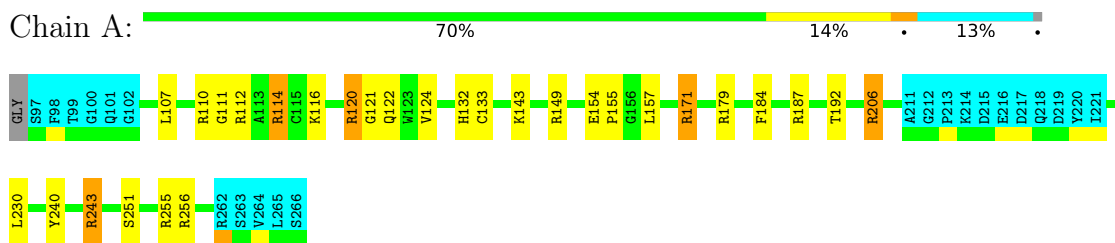
- Molecule 1: SCO2 protein homolog, mitochondrial





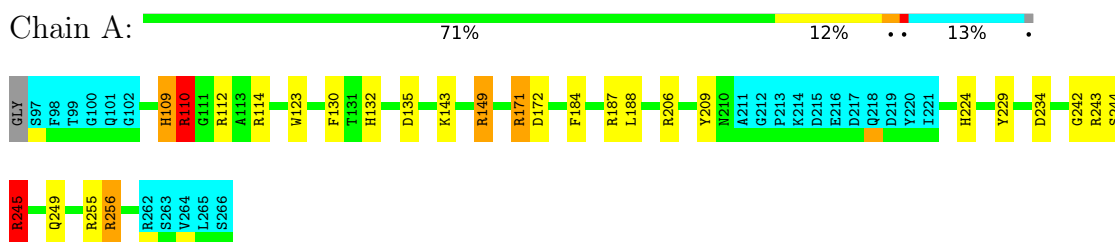
#### 4.2.26 Score per residue for model 26

- Molecule 1: SCO2 protein homolog, mitochondrial



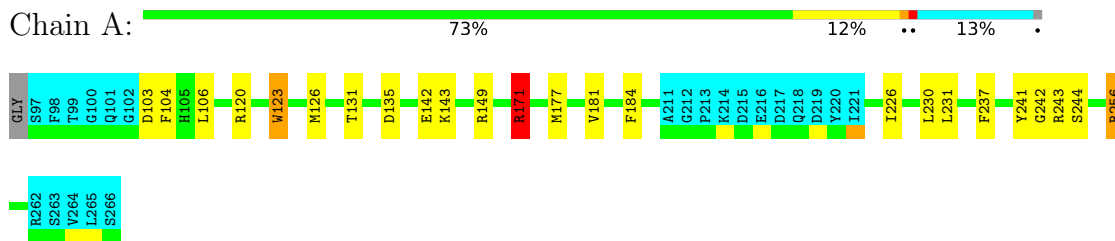
#### 4.2.27 Score per residue for model 27

- Molecule 1: SCO2 protein homolog, mitochondrial



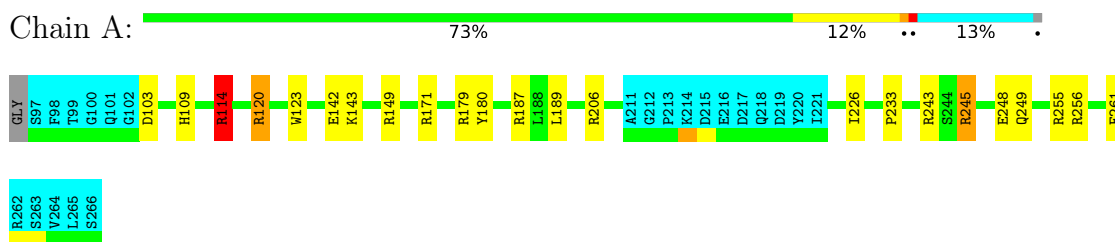
#### 4.2.28 Score per residue for model 28

- Molecule 1: SCO2 protein homolog, mitochondrial



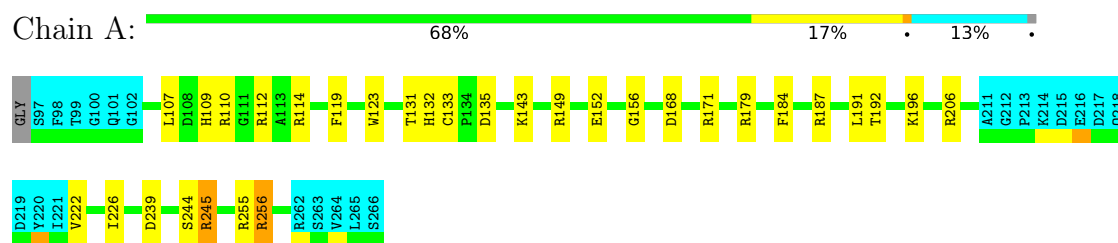
#### 4.2.29 Score per residue for model 29

- Molecule 1: SCO2 protein homolog, mitochondrial



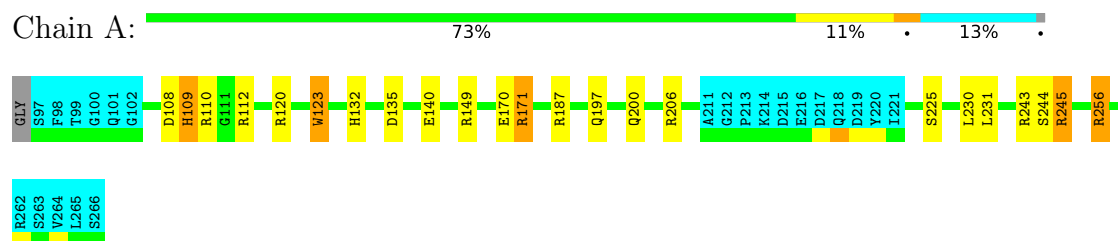
### 4.2.30 Score per residue for model 30

- Molecule 1: SCO2 protein homolog, mitochondrial



### 4.2.31 Score per residue for model 31

- Molecule 1: SCO2 protein homolog, mitochondrial



## 5 Refinement protocol and experimental data overview

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

Of the 350 calculated structures, 31 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

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	0.73±0.01	0±0/1237 ( 0.0± 0.0%)	1.14±0.03	10±3/1681 ( 0.6± 0.2%)
All	All	0.73	0/38347 ( 0.0%)	1.14	313/52111 ( 0.6%)

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	1.2±1.2
All	All	0	38

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	149	ARG	NE-CZ-NH1	9.12	124.86	120.30	30	27
1	A	245	ARG	NE-CZ-NH1	9.09	124.85	120.30	22	19
1	A	179	ARG	NE-CZ-NH1	9.05	124.82	120.30	2	18
1	A	112	ARG	NE-CZ-NH1	8.79	124.69	120.30	5	22
1	A	256	ARG	NE-CZ-NH1	8.59	124.60	120.30	27	20
1	A	120	ARG	NE-CZ-NH1	8.48	124.54	120.30	20	19
1	A	243	ARG	NE-CZ-NH1	8.39	124.49	120.30	6	22
1	A	171	ARG	NE-CZ-NH1	8.11	124.36	120.30	8	22
1	A	114	ARG	NE-CZ-NH2	-7.98	116.31	120.30	26	7
1	A	110	ARG	NE-CZ-NH1	7.93	124.27	120.30	22	18
1	A	187	ARG	NE-CZ-NH1	7.91	124.26	120.30	5	18
1	A	114	ARG	NE-CZ-NH1	7.74	124.17	120.30	9	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	206	ARG	NE-CZ-NH1	7.35	123.98	120.30	9	17
1	A	255	ARG	NE-CZ-NH1	7.20	123.90	120.30	17	18
1	A	255	ARG	NE-CZ-NH2	-6.81	116.90	120.30	9	3
1	A	256	ARG	NE-CZ-NH2	-6.80	116.90	120.30	6	9
1	A	110	ARG	NE-CZ-NH2	-6.74	116.93	120.30	9	4
1	A	243	ARG	NE-CZ-NH2	-6.64	116.98	120.30	14	3
1	A	179	ARG	NE-CZ-NH2	-6.56	117.02	120.30	1	5
1	A	112	ARG	NE-CZ-NH2	-6.16	117.22	120.30	30	3
1	A	205	TYR	CB-CG-CD2	-6.11	117.34	121.00	12	2
1	A	120	ARG	NE-CZ-NH2	-6.05	117.27	120.30	26	2
1	A	171	ARG	NE-CZ-NH2	-5.90	117.35	120.30	31	2
1	A	245	ARG	NE-CZ-NH2	-5.79	117.40	120.30	7	2
1	A	245	ARG	CD-NE-CZ	5.70	131.57	123.60	7	1
1	A	149	ARG	NE-CZ-NH2	-5.69	117.46	120.30	8	3
1	A	256	ARG	CD-NE-CZ	5.62	131.47	123.60	8	1
1	A	187	ARG	NE-CZ-NH2	-5.60	117.50	120.30	17	5
1	A	206	ARG	NE-CZ-NH2	-5.51	117.55	120.30	12	1
1	A	243	ARG	CD-NE-CZ	5.41	131.18	123.60	6	1
1	A	179	ARG	CD-NE-CZ	5.25	130.95	123.60	20	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	241	TYR	Sidechain	3
1	A	114	ARG	Sidechain	3
1	A	245	ARG	Sidechain	3
1	A	110	ARG	Sidechain,Peptide	2
1	A	171	ARG	Peptide,Sidechain	2
1	A	256	ARG	Sidechain	2
1	A	243	ARG	Sidechain	2
1	A	112	ARG	Sidechain	2
1	A	103	ASP	Peptide	2
1	A	132	HIS	Peptide,Sidechain	2
1	A	154	GLU	Peptide	1
1	A	205	TYR	Sidechain	1
1	A	157	LEU	Peptide	1
1	A	244	SER	Peptide	1
1	A	133	CYS	Peptide	1
1	A	180	TYR	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	138	PRO	Peptide	1
1	A	121	GLY	Peptide	1
1	A	227	ALA	Peptide	1
1	A	179	ARG	Sidechain	1
1	A	149	ARG	Sidechain	1
1	A	240	TYR	Sidechain	1
1	A	109	HIS	Peptide	1
1	A	156	GLY	Peptide	1
1	A	187	ARG	Sidechain	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	1203	1154	1153	0±0
All	All	37324	35774	35743	4

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:166:THR:HG22	1:A:168:ASP:H	0.53	1.63	13	1
1:A:136:ILE:HG23	1:A:137:CYS:H	0.50	1.65	3	1
1:A:132:HIS:CG	1:A:133:CYS:H	0.45	2.29	8	1
1:A:166:THR:HG21	1:A:172:ASP:CB	0.41	2.46	13	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	148/171 (87%)	125±4 (85±3%)	18±4 (12±2%)	5±2 (3±2%)	6	36
All	All	4588/5301 (87%)	3883 (85%)	551 (12%)	154 (3%)	6	36

All 49 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	135	ASP	11
1	A	226	ILE	10
1	A	244	SER	8
1	A	132	HIS	8
1	A	109	HIS	7
1	A	134	PRO	7
1	A	245	ARG	7
1	A	155	PRO	6
1	A	225	SER	6
1	A	171	ARG	6
1	A	187	ARG	5
1	A	110	ARG	5
1	A	243	ARG	5
1	A	122	GLN	4
1	A	123	TRP	4
1	A	121	GLY	4
1	A	168	ASP	3
1	A	131	THR	3
1	A	233	PRO	3
1	A	157	LEU	3
1	A	154	GLU	3
1	A	120	ARG	2
1	A	206	ARG	2
1	A	193	GLY	2
1	A	103	ASP	2
1	A	111	GLY	2
1	A	133	CYS	2
1	A	167	VAL	2
1	A	242	GLY	2
1	A	130	PHE	1
1	A	227	ALA	1
1	A	136	ILE	1
1	A	194	SER	1
1	A	172	ASP	1
1	A	235	GLY	1
1	A	239	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	112	ARG	1
1	A	181	VAL	1
1	A	236	LEU	1
1	A	195	THR	1
1	A	234	ASP	1
1	A	248	GLU	1
1	A	174	VAL	1
1	A	208	TYR	1
1	A	139	ASP	1
1	A	205	TYR	1
1	A	237	PHE	1
1	A	261	PHE	1
1	A	222	VAL	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	129/147 (88%)	116±3 (90±2%)	13±3 (10±2%)	11	57
All	All	3999/4557 (88%)	3605 (90%)	394 (10%)	11	57

All 93 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	184	PHE	19
1	A	230	LEU	18
1	A	143	LYS	18
1	A	123	TRP	16
1	A	114	ARG	15
1	A	171	ARG	13
1	A	245	ARG	11
1	A	130	PHE	10
1	A	206	ARG	9
1	A	239	ASP	9
1	A	132	HIS	8
1	A	107	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	188	LEU	7
1	A	157	LEU	7
1	A	224	HIS	6
1	A	231	LEU	6
1	A	119	PHE	6
1	A	112	ARG	6
1	A	133	CYS	6
1	A	182	GLN	6
1	A	161	GLN	5
1	A	249	GLN	5
1	A	189	LEU	5
1	A	256	ARG	5
1	A	187	ARG	5
1	A	122	GLN	5
1	A	180	TYR	5
1	A	103	ASP	5
1	A	149	ARG	5
1	A	234	ASP	5
1	A	140	GLU	5
1	A	243	ARG	5
1	A	142	GLU	5
1	A	109	HIS	4
1	A	110	ARG	4
1	A	200	GLN	4
1	A	226	ILE	4
1	A	173	ASP	4
1	A	172	ASP	4
1	A	116	LYS	4
1	A	144	LEU	3
1	A	135	ASP	3
1	A	120	ARG	3
1	A	147	VAL	3
1	A	252	ASP	3
1	A	240	TYR	3
1	A	104	PHE	3
1	A	127	TYR	3
1	A	152	GLU	3
1	A	229	TYR	3
1	A	248	GLU	3
1	A	139	ASP	3
1	A	257	HIS	2
1	A	246	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	253	SER	2
1	A	141	LEU	2
1	A	225	SER	2
1	A	232	ASN	2
1	A	108	ASP	2
1	A	167	VAL	2
1	A	194	SER	2
1	A	137	CYS	2
1	A	205	TYR	2
1	A	238	THR	2
1	A	150	GLN	2
1	A	183	ASP	2
1	A	177	MET	2
1	A	131	THR	2
1	A	210	ASN	2
1	A	191	LEU	2
1	A	208	TYR	2
1	A	197	GLN	2
1	A	192	THR	2
1	A	105	HIS	1
1	A	241	TYR	1
1	A	160	VAL	1
1	A	154	GLU	1
1	A	145	VAL	1
1	A	125	LEU	1
1	A	179	ARG	1
1	A	254	VAL	1
1	A	228	ILE	1
1	A	195	THR	1
1	A	255	ARG	1
1	A	124	VAL	1
1	A	251	SER	1
1	A	209	TYR	1
1	A	106	LEU	1
1	A	126	MET	1
1	A	181	VAL	1
1	A	196	LYS	1
1	A	170	GLU	1
1	A	244	SER	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](#)

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