



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:07 AM UTC

PDB ID : 2RLI / pdb_00002rli
Title : Solution structure of Cu(I) human Sco2
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Deposited on : 2007-07-11

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

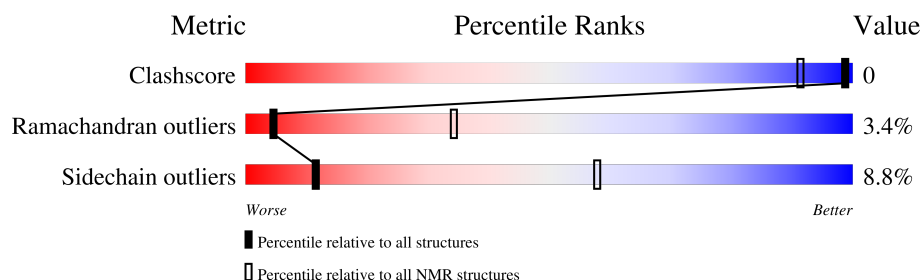
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	171	 80% 6% 13% .

2 Ensemble composition and analysis

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)	1.68	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
1	A	170	Total	C	H	N	O	S	0
			2676	864	1306	243	257	6	

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 (CCD ID: CU1) (formula: Cu).

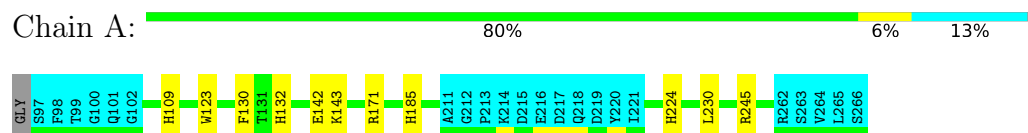
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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

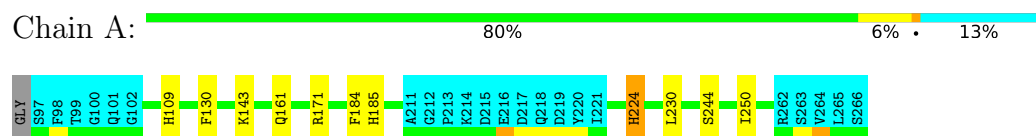


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

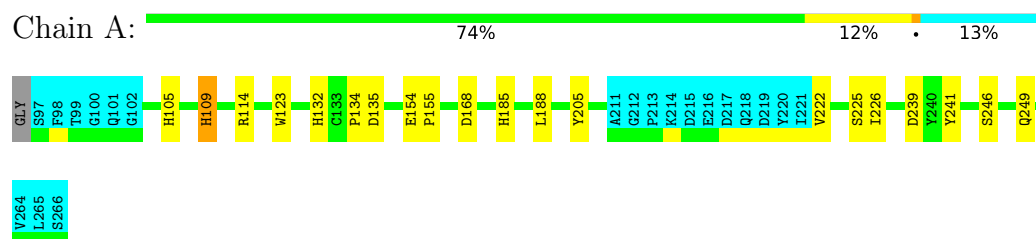
4.2.1 Score per residue for model 1

- Molecule 1: SCO2 protein homolog, mitochondrial



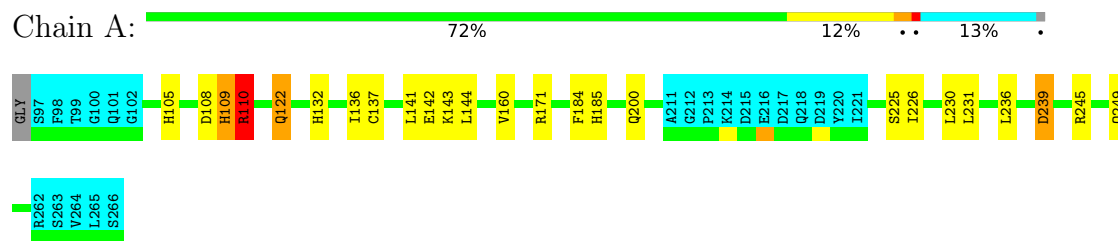
4.2.2 Score per residue for model 2

- Molecule 1: SCO2 protein homolog, mitochondrial



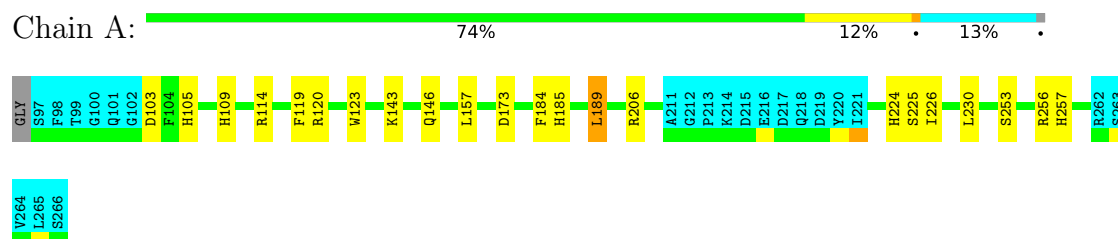
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: SCO2 protein homolog, mitochondrial



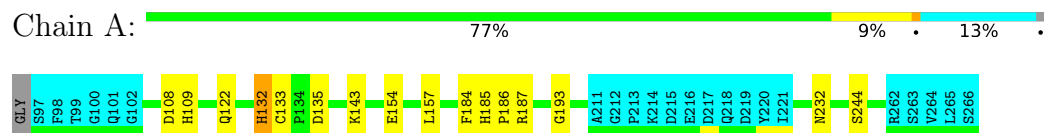
4.2.4 Score per residue for model 4

- Molecule 1: SCO2 protein homolog, mitochondrial



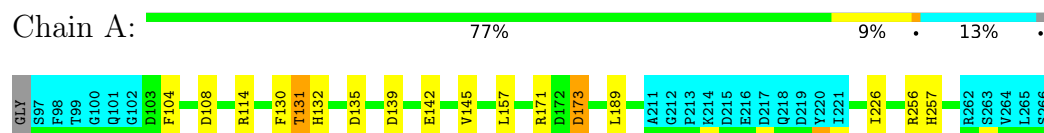
4.2.5 Score per residue for model 5

- Molecule 1: SCO2 protein homolog, mitochondrial



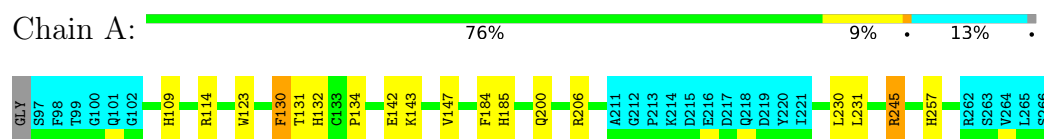
4.2.6 Score per residue for model 6

- Molecule 1: SCO2 protein homolog, mitochondrial



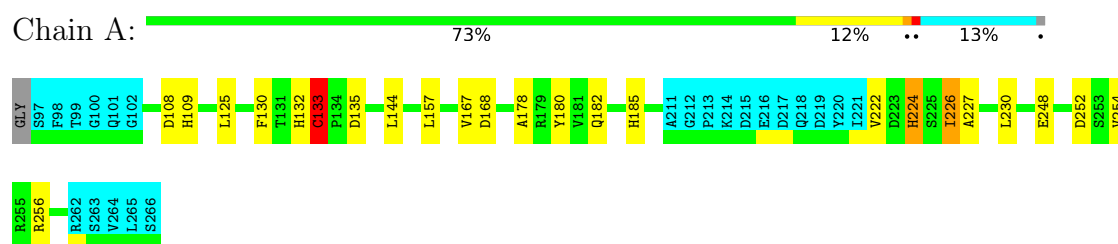
4.2.7 Score per residue for model 7

- Molecule 1: SCO2 protein homolog, mitochondrial



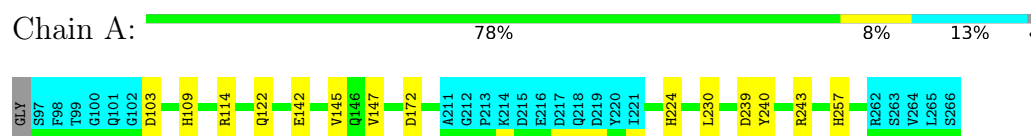
4.2.8 Score per residue for model 8

- Molecule 1: SCO2 protein homolog, mitochondrial



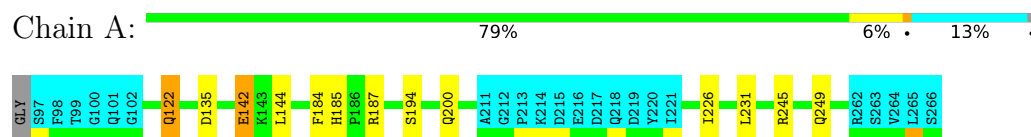
4.2.9 Score per residue for model 9

- 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





4.2.12 Score per residue for model 12

- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 73% 13% 13%



4.2.13 Score per residue for model 13

- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 74% 11% 13%



4.2.14 Score per residue for model 14

- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 75% 11% 13%



4.2.15 Score per residue for model 15

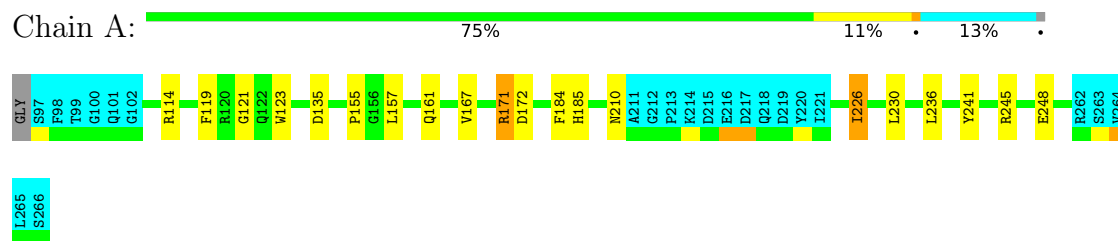
- Molecule 1: SCO2 protein homolog, mitochondrial

Chain A: 78% 8% 13%



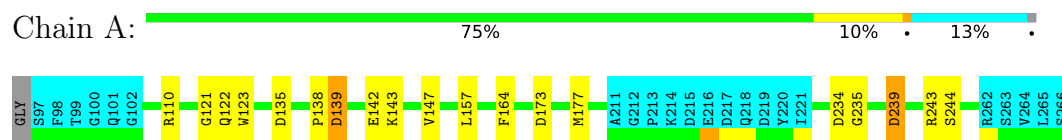
4.2.16 Score per residue for model 16

- Molecule 1: SCO2 protein homolog, mitochondrial



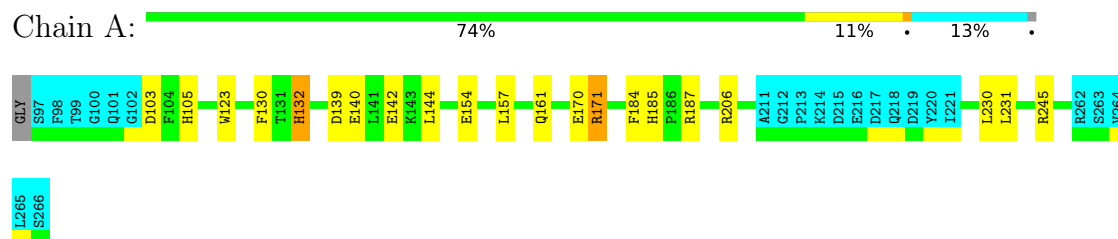
4.2.17 Score per residue for model 17

- Molecule 1: SCO2 protein homolog, mitochondrial



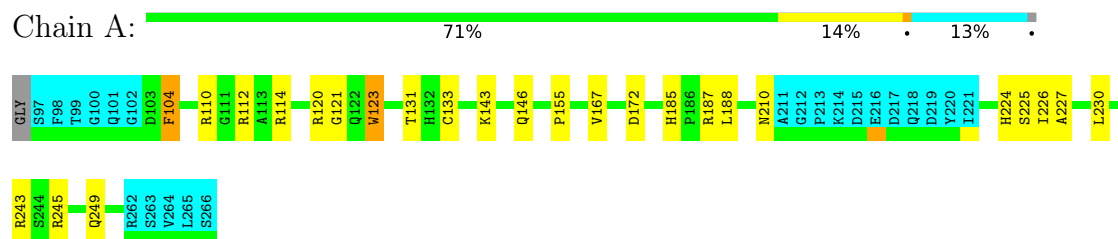
4.2.18 Score per residue for model 18

- Molecule 1: SCO2 protein homolog, mitochondrial



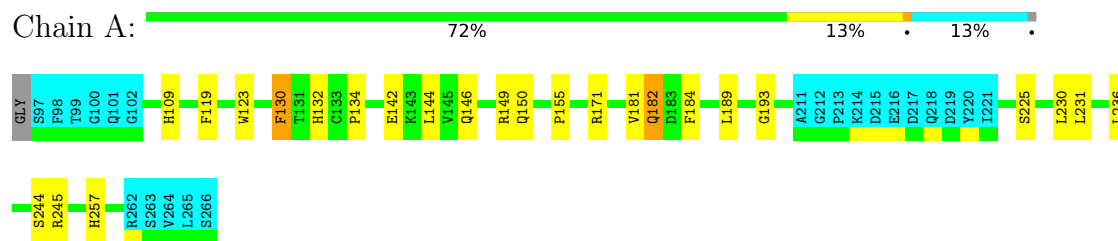
4.2.19 Score per residue for model 19

- Molecule 1: SCO2 protein homolog, mitochondrial



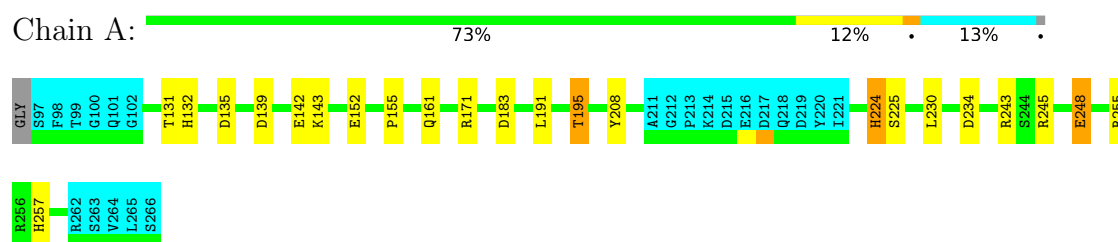
4.2.20 Score per residue for model 20

- Molecule 1: SCO2 protein homolog, mitochondrial



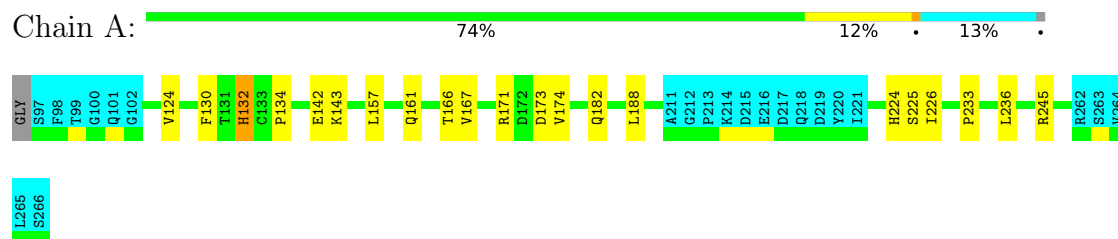
4.2.21 Score per residue for model 21

- Molecule 1: SCO2 protein homolog, mitochondrial



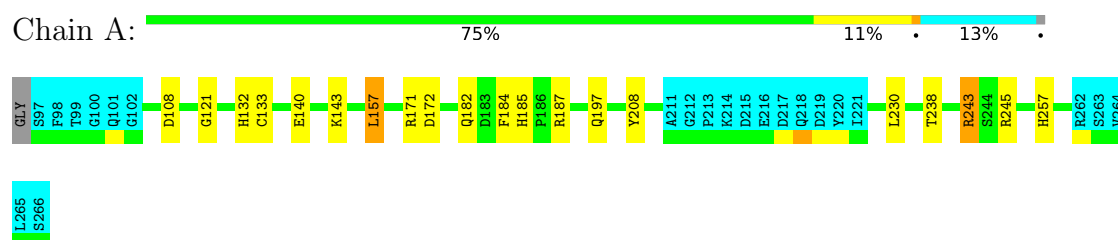
4.2.22 Score per residue for model 22

- Molecule 1: SCO2 protein homolog, mitochondrial



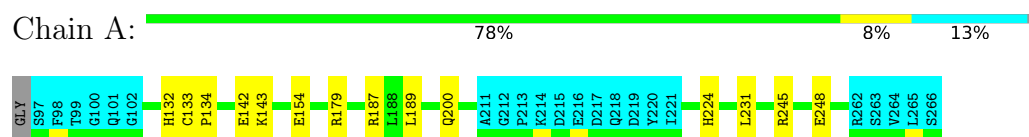
4.2.23 Score per residue for model 23

- Molecule 1: SCO2 protein homolog, mitochondrial



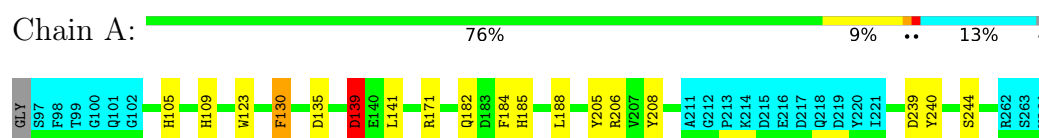
4.2.24 Score per residue for model 24

- Molecule 1: SCO2 protein homolog, mitochondrial



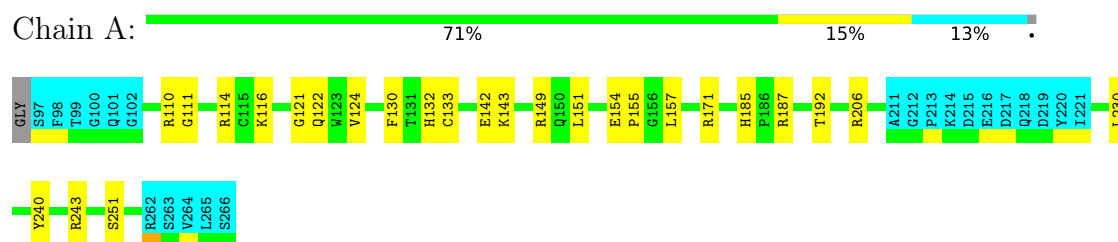
4.2.25 Score per residue for model 25

- Molecule 1: SCO2 protein homolog, mitochondrial



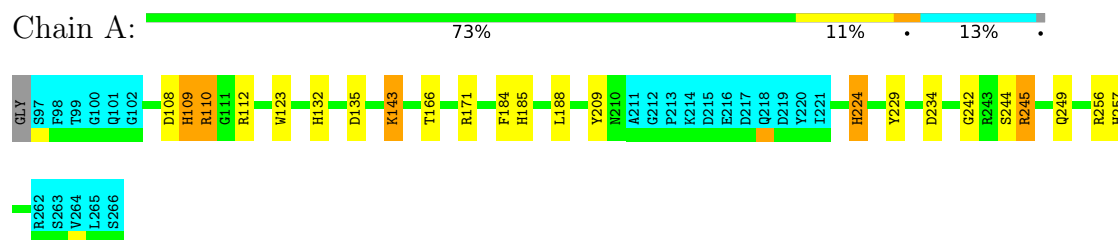
4.2.26 Score per residue for model 26

- Molecule 1: SCO2 protein homolog, mitochondrial



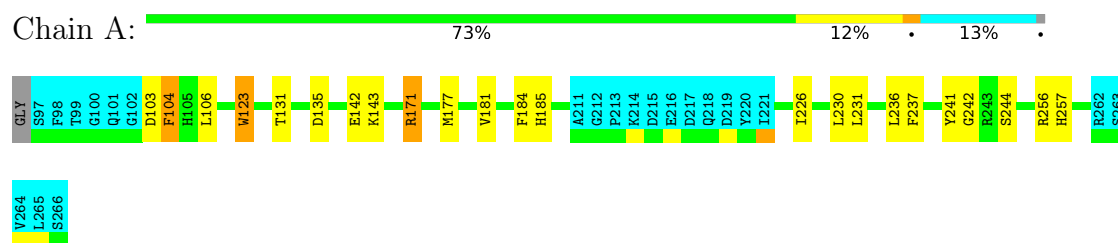
4.2.27 Score per residue for model 27

- Molecule 1: SCO2 protein homolog, mitochondrial



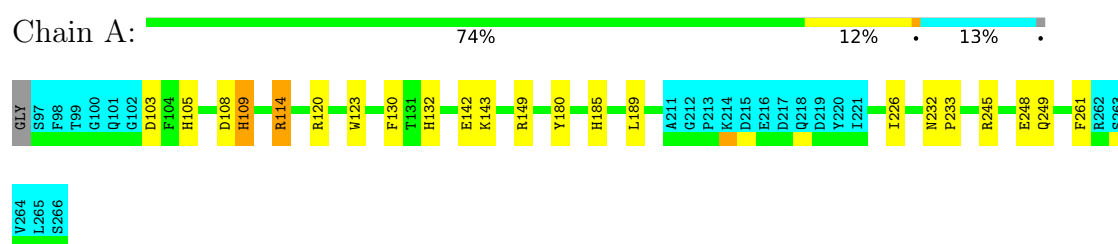
4.2.28 Score per residue for model 28

- Molecule 1: SCO2 protein homolog, mitochondrial



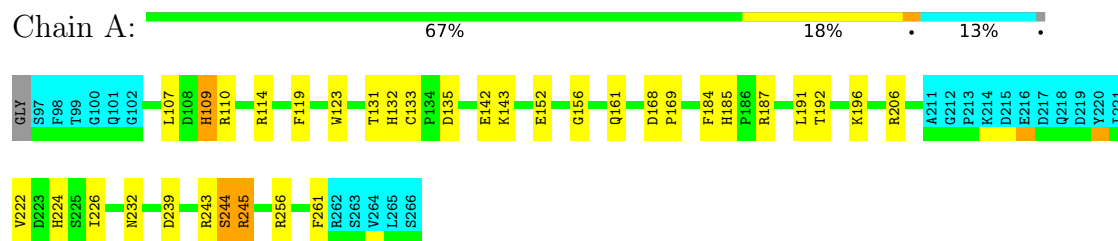
4.2.29 Score per residue for model 29

- Molecule 1: SCO2 protein homolog, mitochondrial



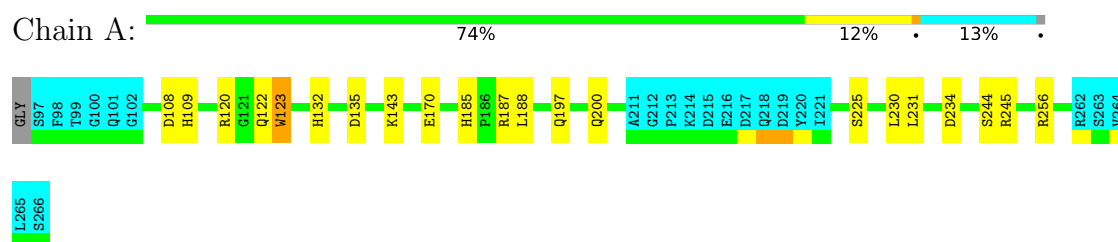
4.2.30 Score per residue for model 30

- 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

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	0.90±0.01	0±0/1237 (0.0± 0.0%)	1.46±0.03	6±3/1681 (0.3± 0.2%)
All	All	0.90	0/38347 (0.0%)	1.46	180/52111 (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	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	103	ASP	CA-CB-CG	7.75	120.35	112.60	4	1
1	A	104	PHE	CA-CB-CG	7.26	121.06	113.80	11	6
1	A	130	PHE	CA-CB-CG	6.68	120.48	113.80	25	9
1	A	244	SER	CA-C-N	6.61	134.16	121.54	30	1
1	A	244	SER	C-N-CA	6.61	134.16	121.54	30	1
1	A	178	ALA	CA-C-N	6.45	129.40	120.63	8	1
1	A	178	ALA	C-N-CA	6.45	129.40	120.63	8	1
1	A	185	HIS	CB-CG-CD2	-6.40	122.88	131.20	7	23
1	A	224	HIS	CA-CB-CG	6.34	120.14	113.80	1	2
1	A	108	ASP	CA-CB-CG	6.18	118.78	112.60	27	6
1	A	206	ARG	CA-C-N	6.04	128.01	121.97	18	1
1	A	206	ARG	C-N-CA	6.04	128.01	121.97	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	173	ASP	CA-C-N	5.99	132.75	121.97	22	1
1	A	173	ASP	C-N-CA	5.99	132.75	121.97	22	1
1	A	261	PHE	CA-CB-CG	5.91	119.71	113.80	30	1
1	A	142	GLU	CA-C-N	5.84	128.11	120.28	7	9
1	A	142	GLU	C-N-CA	5.84	128.11	120.28	7	9
1	A	224	HIS	CB-CG-CD2	-5.83	123.62	131.20	30	9
1	A	139	ASP	CA-C-N	5.81	128.34	120.38	11	4
1	A	139	ASP	C-N-CA	5.81	128.34	120.38	11	4
1	A	239	ASP	CA-CB-CG	5.80	118.40	112.60	3	1
1	A	139	ASP	CA-CB-CG	-5.79	106.81	112.60	17	1
1	A	109	HIS	CA-C-N	5.71	132.44	121.54	30	2
1	A	109	HIS	C-N-CA	5.71	132.44	121.54	30	2
1	A	234	ASP	CA-CB-CG	5.70	118.30	112.60	31	1
1	A	109	HIS	CB-CG-CD2	-5.69	123.80	131.20	29	7
1	A	257	HIS	CB-CG-CD2	-5.67	123.83	131.20	28	8
1	A	121	GLY	CA-C-N	5.67	132.37	121.54	17	1
1	A	121	GLY	C-N-CA	5.67	132.37	121.54	17	1
1	A	232	ASN	CA-C-N	5.63	126.88	119.84	12	3
1	A	232	ASN	C-N-CA	5.63	126.88	119.84	12	3
1	A	170	GLU	CA-C-N	5.59	132.22	121.54	18	1
1	A	170	GLU	C-N-CA	5.59	132.22	121.54	18	1
1	A	226	ILE	CA-C-N	5.58	132.20	121.54	8	1
1	A	226	ILE	C-N-CA	5.58	132.20	121.54	8	1
1	A	105	HIS	CB-CG-CD2	-5.57	123.95	131.20	12	6
1	A	131	THR	CA-C-N	5.57	132.18	121.54	21	3
1	A	131	THR	C-N-CA	5.57	132.18	121.54	21	3
1	A	133	CYS	N-CA-CB	-5.56	105.56	111.29	8	1
1	A	145	VAL	CA-C-N	5.54	127.97	120.38	9	1
1	A	145	VAL	C-N-CA	5.54	127.97	120.38	9	1
1	A	143	LYS	CA-C-N	5.50	128.12	120.63	27	1
1	A	143	LYS	C-N-CA	5.50	128.12	120.63	27	1
1	A	243	ARG	CA-C-N	5.47	132.00	121.54	30	1
1	A	243	ARG	C-N-CA	5.47	132.00	121.54	30	1
1	A	169	PRO	CA-C-N	5.44	131.93	121.54	30	1
1	A	169	PRO	C-N-CA	5.44	131.93	121.54	30	1
1	A	157	LEU	N-CA-C	5.43	113.11	108.22	23	1
1	A	136	ILE	CB-CA-C	5.39	115.85	111.05	15	1
1	A	146	GLN	OE1-CD-NE2	-5.38	117.22	122.60	4	3
1	A	186	PRO	CA-C-N	5.34	131.74	121.54	5	1
1	A	186	PRO	C-N-CA	5.34	131.74	121.54	5	1
1	A	182	GLN	OE1-CD-NE2	-5.33	117.27	122.60	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	245	ARG	CA-C-N	5.30	131.66	121.54	19	1
1	A	245	ARG	C-N-CA	5.30	131.66	121.54	19	1
1	A	132	HIS	CB-CG-CD2	-5.30	124.31	131.20	5	1
1	A	189	LEU	CA-C-N	5.24	125.80	122.18	4	1
1	A	189	LEU	C-N-CA	5.24	125.80	122.18	4	1
1	A	169	PRO	N-CA-CB	5.24	105.86	102.92	12	1
1	A	122	GLN	CA-C-N	5.24	131.55	121.54	31	1
1	A	122	GLN	C-N-CA	5.24	131.55	121.54	31	1
1	A	132	HIS	CA-CB-CG	5.22	119.03	113.80	20	1
1	A	173	ASP	CA-CB-CG	-5.18	107.42	112.60	6	1
1	A	107	LEU	CA-C-N	5.18	128.83	121.42	11	1
1	A	107	LEU	C-N-CA	5.18	128.83	121.42	11	1
1	A	225	SER	CA-C-N	5.17	131.27	121.97	22	1
1	A	225	SER	C-N-CA	5.17	131.27	121.97	22	1
1	A	119	PHE	CA-CB-CG	5.14	118.94	113.80	20	1
1	A	245	ARG	CD-NE-CZ	5.12	131.57	124.40	7	1
1	A	236	LEU	CA-C-N	5.12	131.31	121.54	28	1
1	A	236	LEU	C-N-CA	5.12	131.31	121.54	28	1
1	A	200	GLN	OE1-CD-NE2	-5.11	117.50	122.60	7	1
1	A	257	HIS	CA-CB-CG	5.09	118.89	113.80	4	1
1	A	122	GLN	OE1-CD-NE2	-5.09	117.51	122.60	9	1
1	A	184	PHE	CA-CB-CG	5.05	118.85	113.80	20	1
1	A	256	ARG	CD-NE-CZ	5.05	131.47	124.40	8	1
1	A	134	PRO	CA-C-N	5.01	131.10	121.54	12	1
1	A	134	PRO	C-N-CA	5.01	131.10	121.54	12	1
1	A	103	ASP	N-CA-C	5.00	114.89	108.34	18	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

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Mol	Chain	Res	Type	Group	Models (Total)
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
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

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±1
All	All	37324	35774	35743	6

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:108:ASP:C	1:A:110:ARG:H	0.42	2.22	3	1
1:A:164:PHE:CD1	1:A:177:MET:HE1	0.41	2.51	17	1
1:A:166:THR:HG21	1:A:172:ASP:CB	0.41	2.46	13	1

6.3 Torsion angles

6.3.1 Protein backbone

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%)	4	34
All	All	4588/5301 (87%)	3883 (85%)	551 (12%)	154 (3%)	4	34

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

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Mol	Chain	Res	Type	Models (Total)
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
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 ⓘ

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%)	118±3 (91±2%)	11±3 (9±2%)	11	58
All	All	3999/4557 (88%)	3647 (91%)	352 (9%)	11	58

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	143	LYS	20
1	A	230	LEU	19
1	A	123	TRP	15

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Mol	Chain	Res	Type	Models (Total)
1	A	184	PHE	14
1	A	171	ARG	10
1	A	114	ARG	9
1	A	188	LEU	9
1	A	132	HIS	9
1	A	130	PHE	8
1	A	224	HIS	8
1	A	231	LEU	8
1	A	245	ARG	8
1	A	142	GLU	8
1	A	157	LEU	7
1	A	161	GLN	6
1	A	239	ASP	6
1	A	249	GLN	6
1	A	182	GLN	6
1	A	122	GLN	5
1	A	144	LEU	5
1	A	189	LEU	5
1	A	133	CYS	5
1	A	248	GLU	5
1	A	200	GLN	4
1	A	226	ILE	4
1	A	173	ASP	4
1	A	256	ARG	4
1	A	206	ARG	4
1	A	152	GLU	4
1	A	109	HIS	3
1	A	141	LEU	3
1	A	236	LEU	3
1	A	119	PHE	3
1	A	135	ASP	3
1	A	232	ASN	3
1	A	147	VAL	3
1	A	172	ASP	3
1	A	240	TYR	3
1	A	187	ARG	3
1	A	104	PHE	3
1	A	107	LEU	3
1	A	103	ASP	3
1	A	112	ARG	3
1	A	140	GLU	3
1	A	234	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	243	ARG	3
1	A	139	ASP	3
1	A	222	VAL	2
1	A	246	SER	2
1	A	253	SER	2
1	A	110	ARG	2
1	A	225	SER	2
1	A	108	ASP	2
1	A	125	LEU	2
1	A	167	VAL	2
1	A	252	ASP	2
1	A	194	SER	2
1	A	116	LYS	2
1	A	137	CYS	2
1	A	238	THR	2
1	A	183	ASP	2
1	A	177	MET	2
1	A	180	TYR	2
1	A	131	THR	2
1	A	229	TYR	2
1	A	210	ASN	2
1	A	120	ARG	2
1	A	149	ARG	2
1	A	191	LEU	2
1	A	208	TYR	2
1	A	124	VAL	2
1	A	166	THR	2
1	A	197	GLN	2
1	A	192	THR	2
1	A	250	ILE	1
1	A	105	HIS	1
1	A	160	VAL	1
1	A	154	GLU	1
1	A	145	VAL	1
1	A	254	VAL	1
1	A	205	TYR	1
1	A	228	ILE	1
1	A	150	GLN	1
1	A	195	THR	1
1	A	255	ARG	1
1	A	151	LEU	1
1	A	251	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	209	TYR	1
1	A	106	LEU	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 oligosaccharides 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