



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:00 pm GMT

PDB ID : 2GQM
Title : Solution structure of Human Cu(I)-Sco1
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Deposited on : 2006-04-21

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

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

with specific help available everywhere you see the ⓘ symbol.

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

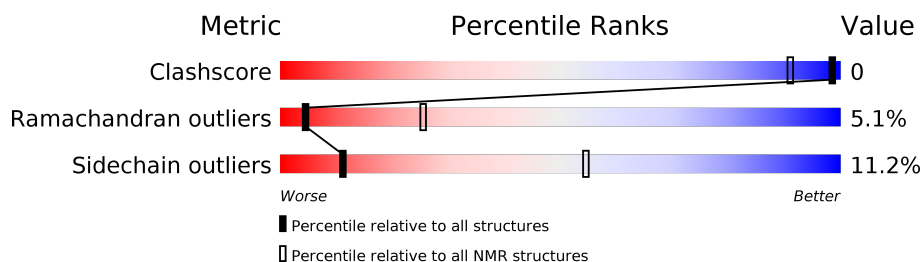
1 Overall quality at a glance

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 ≥ 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	 80% 8% • 11%

2 Ensemble composition and analysis

This entry contains 30 models. Model 13 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:248, A:256-A:298 (154)	0.77	13

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 6 clusters and 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2750 atoms, of which 1360 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
			2749	890	1360	224	270	5	

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

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

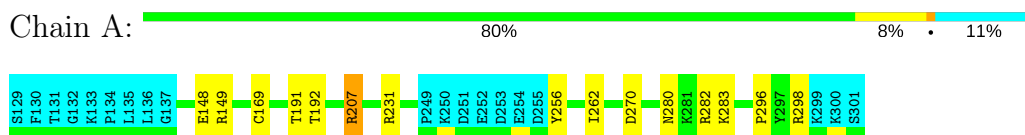
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

4 Residue-property plots [i](#)

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

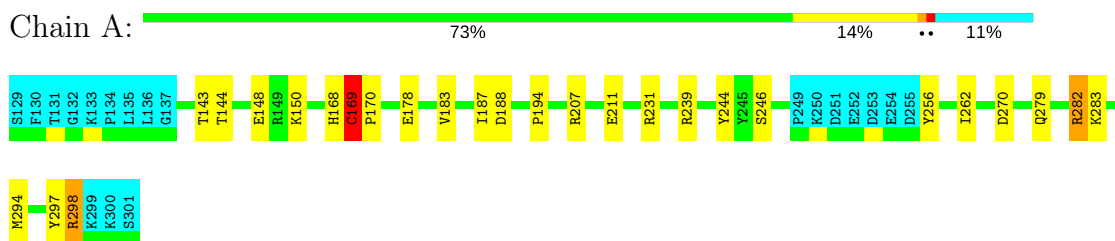


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

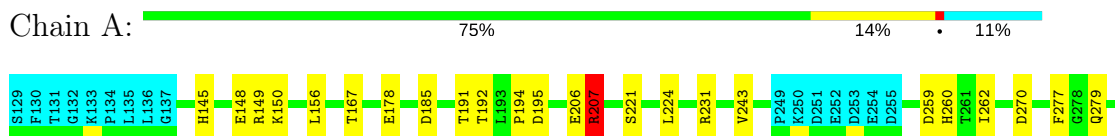
4.2.1 Score per residue for model 1

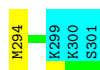
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.2 Score per residue for model 2

- Molecule 1: SCO1 protein homolog, mitochondrial

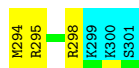




4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 74% 14% 11%



4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 75% 13% 11%



4.2.5 Score per residue for model 5

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 71% 16% 11%



4.2.6 Score per residue for model 6

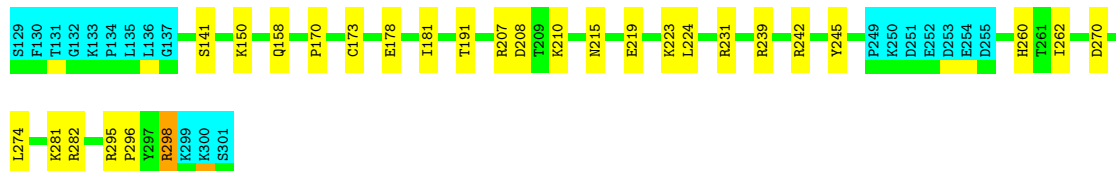
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 77% 12% 11%



4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial



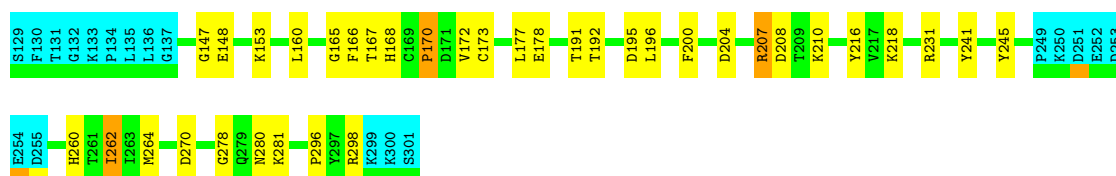
4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial



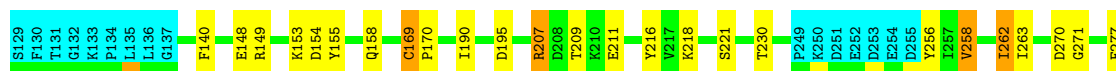
4.2.9 Score per residue for model 9

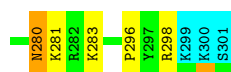
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.10 Score per residue for model 10

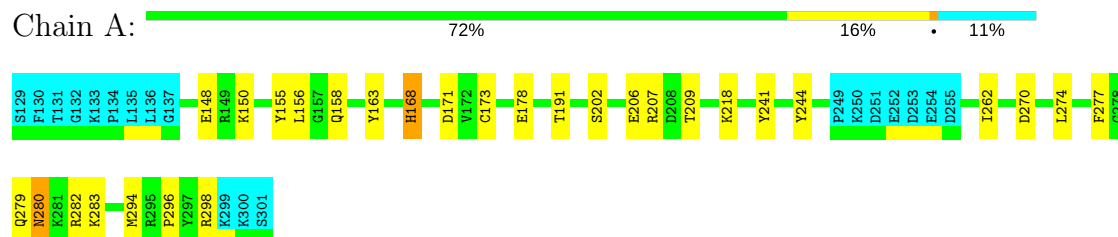
- Molecule 1: SCO1 protein homolog, mitochondrial





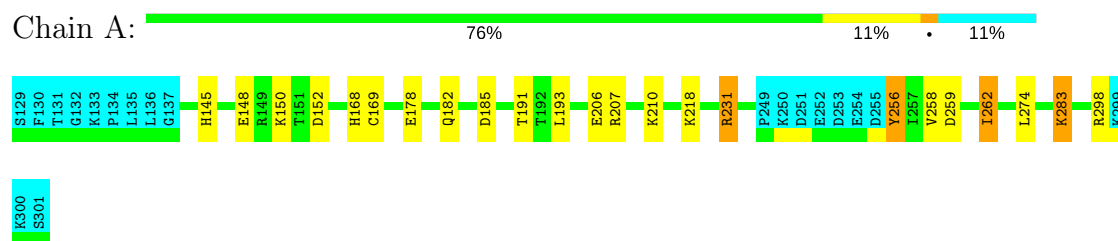
4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



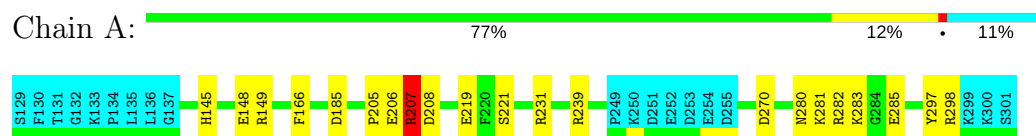
4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



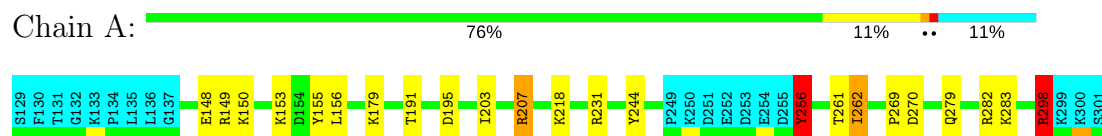
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: SCO1 protein homolog, mitochondrial



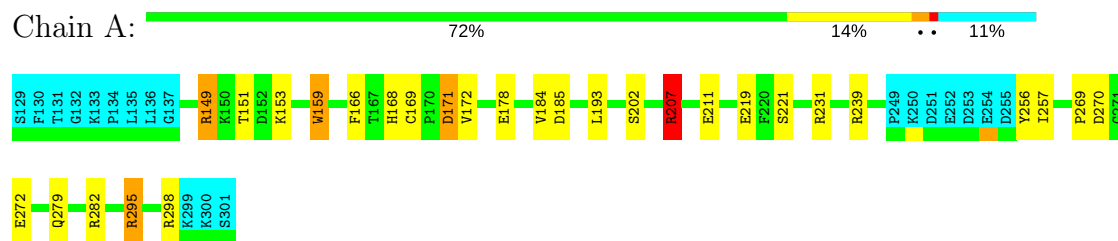
4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



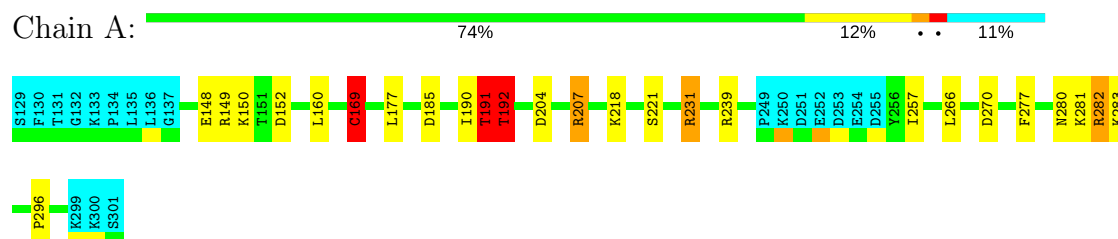
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



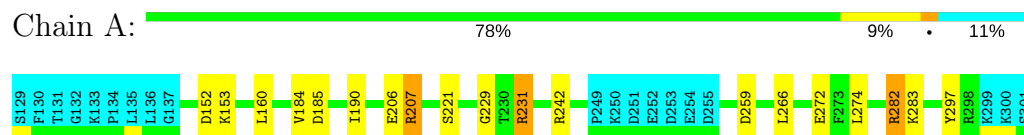
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



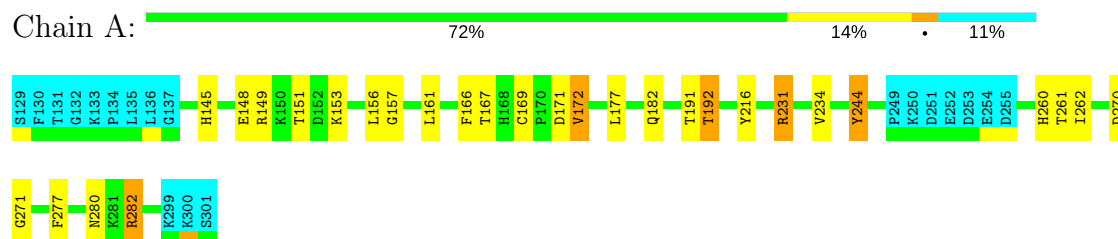
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



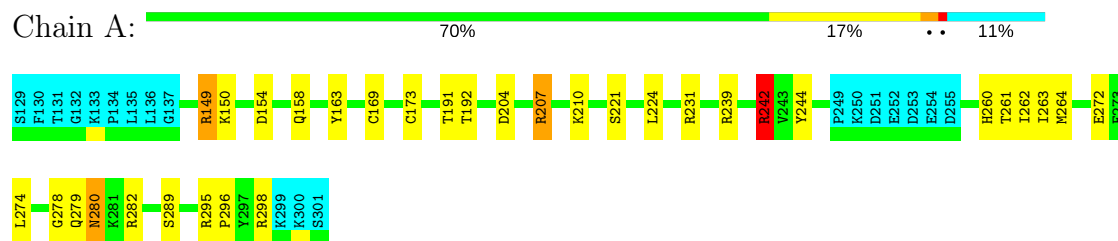
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



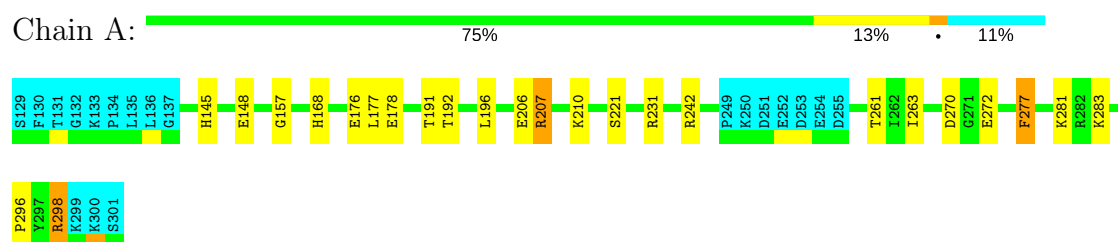
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



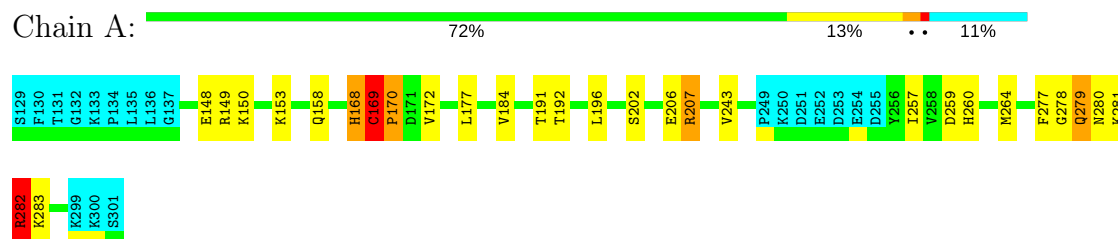
4.2.20 Score per residue for model 20

- Molecule 1: SCO1 protein homolog, mitochondrial



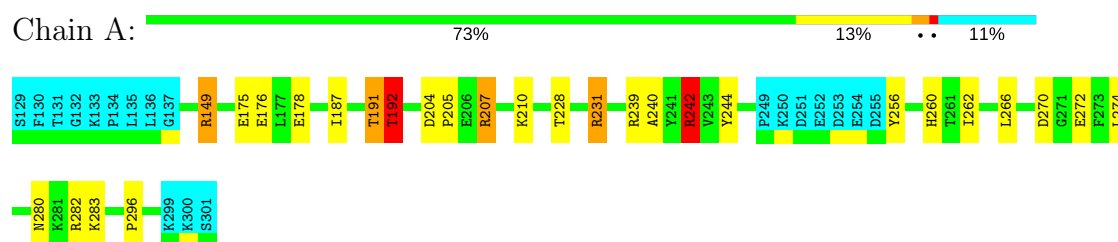
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



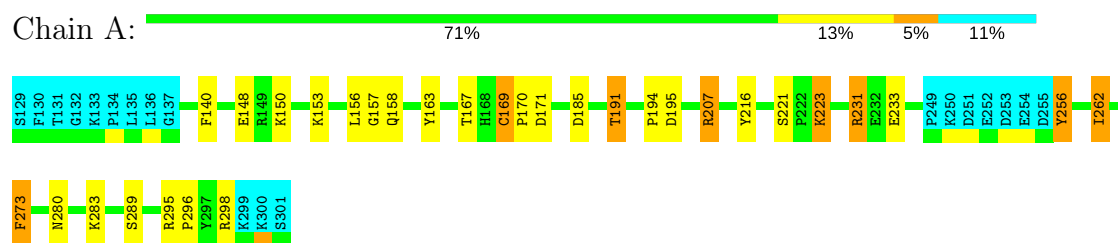
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



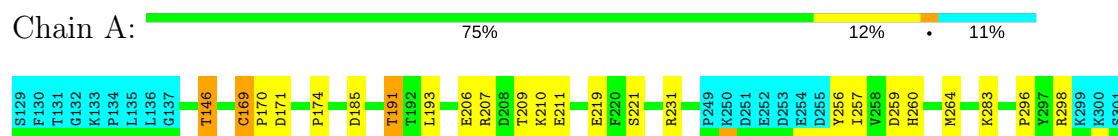
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



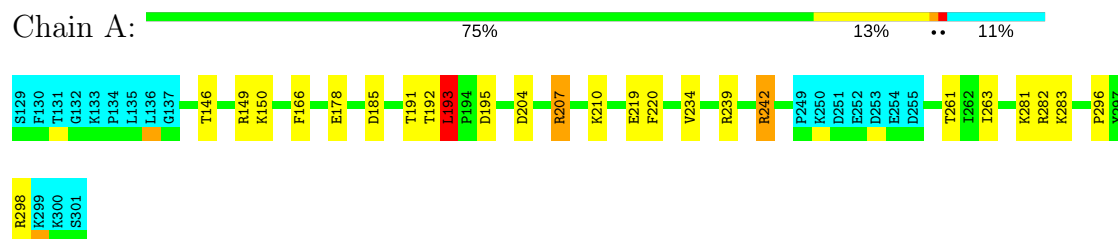
4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



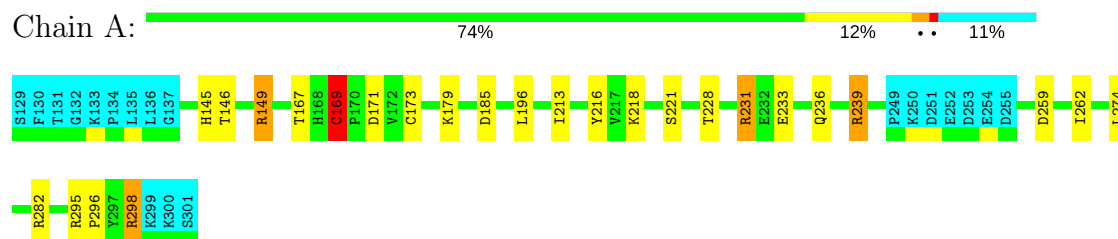
4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



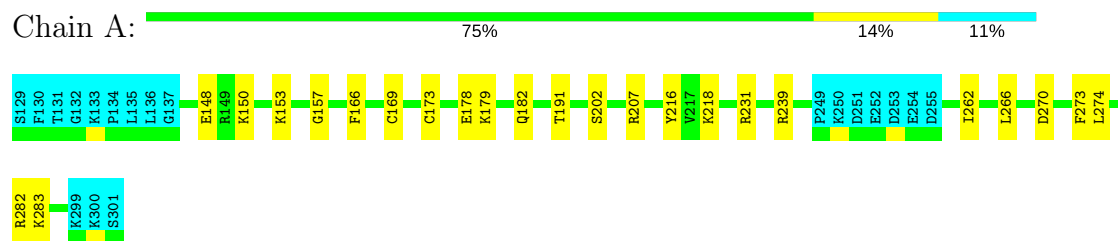
4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



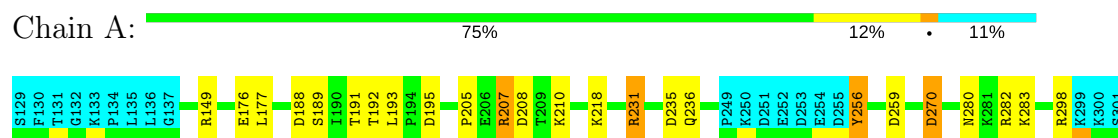
4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



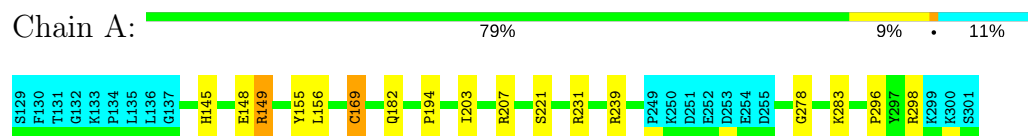
4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial



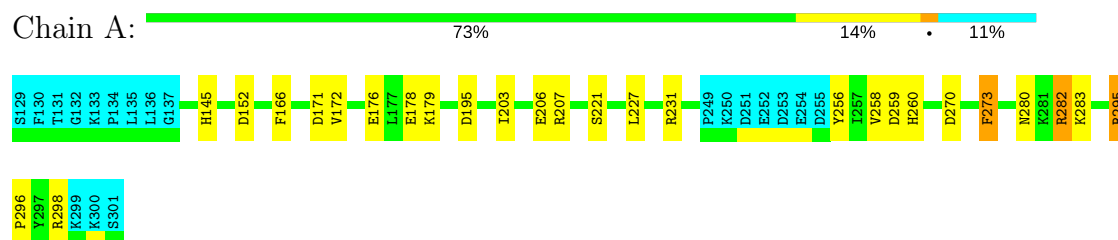
4.2.29 Score per residue for model 29

- 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 (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±0.00	0±0/1275 (0.0±0.0%)	1.09±0.03	4±2/1735 (0.2±0.1%)
All	All	0.73	0/38250 (0.0%)	1.09	125/52050 (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	2.7±1.7
All	All	0	81

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	9.96	125.28	120.30	22	8
1	A	231	ARG	NE-CZ-NH2	-9.84	115.38	120.30	16	7
1	A	207	ARG	NE-CZ-NH1	8.37	124.48	120.30	1	16
1	A	298	ARG	NE-CZ-NH1	8.24	124.42	120.30	26	17
1	A	282	ARG	NE-CZ-NH1	8.05	124.33	120.30	16	13
1	A	242	ARG	NE-CZ-NH1	8.02	124.31	120.30	22	1
1	A	231	ARG	NE-CZ-NH1	7.96	124.28	120.30	23	16
1	A	282	ARG	NE-CZ-NH2	-7.74	116.43	120.30	17	3
1	A	298	ARG	NE-CZ-NH2	-7.35	116.63	120.30	10	3
1	A	216	TYR	CB-CG-CD2	-7.09	116.74	121.00	23	1
1	A	239	ARG	NE-CZ-NH1	6.65	123.63	120.30	3	9
1	A	295	ARG	NE-CZ-NH2	-6.61	116.99	120.30	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	297	TYR	CB-CG-CD2	-6.42	117.15	121.00	13	1
1	A	295	ARG	NE-CZ-NH1	6.41	123.50	120.30	8	4
1	A	207	ARG	NE-CZ-NH2	-6.31	117.14	120.30	28	3
1	A	192	THR	CA-CB-CG2	6.28	121.19	112.40	16	2
1	A	191	THR	CA-CB-CG2	6.00	120.80	112.40	3	2
1	A	149	ARG	NE-CZ-NH2	-5.99	117.31	120.30	28	1
1	A	256	TYR	CB-CG-CD2	-5.98	117.42	121.00	5	4
1	A	231	ARG	CD-NE-CZ	5.91	131.88	123.60	14	4
1	A	282	ARG	CD-NE-CZ	5.69	131.57	123.60	17	2
1	A	241	TYR	CB-CG-CD2	-5.68	117.59	121.00	11	1
1	A	242	ARG	NE-CZ-NH2	-5.46	117.57	120.30	19	2
1	A	278	GLY	C-N-CA	5.01	134.24	121.70	19	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	169	CYS	Peptide	7
1	A	216	TYR	Sidechain	5
1	A	269	PRO	Peptide	4
1	A	207	ARG	Sidechain	4
1	A	149	ARG	Sidechain	4
1	A	244	TYR	Sidechain	3
1	A	280	ASN	Peptide	3
1	A	259	ASP	Peptide	3
1	A	205	PRO	Peptide	3
1	A	231	ARG	Sidechain	3
1	A	163	TYR	Sidechain	3
1	A	157	GLY	Peptide	3
1	A	140	PHE	Peptide	2
1	A	242	ARG	Sidechain,Peptide	2
1	A	241	TYR	Sidechain	2
1	A	261	THR	Peptide	2
1	A	193	LEU	Peptide	2
1	A	191	THR	Peptide	2
1	A	190	ILE	Peptide	2
1	A	278	GLY	Peptide	2
1	A	192	THR	Peptide	2
1	A	170	PRO	Peptide	2
1	A	295	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	194	PRO	Peptide	1
1	A	271	GLY	Peptide	1
1	A	195	ASP	Peptide	1
1	A	208	ASP	Peptide	1
1	A	296	PRO	Peptide	1
1	A	172	VAL	Peptide	1
1	A	279	GLN	Peptide	1
1	A	229	GLY	Peptide	1
1	A	298	ARG	Peptide	1
1	A	182	GLN	Peptide	1
1	A	282	ARG	Sidechain	1
1	A	202	SER	Peptide	1
1	A	167	THR	Peptide	1
1	A	245	TYR	Sidechain	1
1	A	243	VAL	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	1242	1214	1213	0±1
All	All	37290	36420	36390	13

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:184:VAL:HG23	1:A:196:LEU:H	0.50	1.66	21	1
1:A:169:CYS:HB3	1:A:171:ASP:H	0.46	1.70	26	1
1:A:182:GLN:HB3	1:A:283:LYS:HE3	0.46	1.88	29	1
1:A:277:PHE:CE1	1:A:281:LYS:HE2	0.45	2.46	21	1
1:A:182:GLN:CB	1:A:283:LYS:HE3	0.44	2.43	5	1
1:A:169:CYS:SG	1:A:170:PRO:HD2	0.44	2.53	21	1
1:A:150:LYS:HE2	1:A:155:TYR:CE2	0.43	2.48	14	1
1:A:159:TRP:CD1	1:A:269:PRO:HD3	0.43	2.48	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:PHE:CE2	1:A:258:VAL:HG11	0.43	2.48	30	1
1:A:159:TRP:CD1	1:A:193:LEU:HD23	0.43	2.48	15	1
1:A:190:ILE:O	1:A:191:THR:HG23	0.42	2.14	16	1
1:A:182:GLN:C	1:A:283:LYS:HE3	0.42	2.35	12	1
1:A:165:GLY:HA3	1:A:173:CYS:SG	0.40	2.56	9	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	154/173 (89%)	129±4 (83±2%)	18±4 (11±2%)	8±3 (5±2%)	4	25
All	All	4620/5190 (89%)	3857 (83%)	529 (11%)	234 (5%)	4	25

All 53 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	18
1	A	270	ASP	17
1	A	296	PRO	16
1	A	221	SER	14
1	A	262	ILE	12
1	A	206	GLU	12
1	A	192	THR	11
1	A	168	HIS	9
1	A	169	CYS	9
1	A	170	PRO	8
1	A	280	ASN	8
1	A	207	ARG	7
1	A	279	GLN	6
1	A	195	ASP	6
1	A	204	ASP	5
1	A	171	ASP	5
1	A	194	PRO	5

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Mol	Chain	Res	Type	Models (Total)
1	A	203	ILE	4
1	A	283	LYS	4
1	A	167	THR	4
1	A	263	ILE	4
1	A	244	TYR	3
1	A	172	VAL	3
1	A	298	ARG	3
1	A	273	PHE	3
1	A	282	ARG	3
1	A	256	TYR	2
1	A	147	GLY	2
1	A	272	GLU	2
1	A	242	ARG	2
1	A	158	GLN	2
1	A	223	LYS	2
1	A	281	LYS	2
1	A	261	THR	2
1	A	155	TYR	1
1	A	193	LEU	1
1	A	228	THR	1
1	A	209	THR	1
1	A	157	GLY	1
1	A	196	LEU	1
1	A	278	GLY	1
1	A	243	VAL	1
1	A	271	GLY	1
1	A	174	PRO	1
1	A	208	ASP	1
1	A	146	THR	1
1	A	257	ILE	1
1	A	277	PHE	1
1	A	258	VAL	1
1	A	220	PHE	1
1	A	240	ALA	1
1	A	152	ASP	1
1	A	159	TRP	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	136/153 (89%)	121±3 (89±2%)	15±3 (11±2%)	11	54
All	All	4080/4590 (89%)	3624 (89%)	456 (11%)	11	54

All 103 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	207	ARG	21
1	A	148	GLU	18
1	A	178	GLU	15
1	A	283	LYS	15
1	A	150	LYS	12
1	A	153	LYS	11
1	A	231	ARG	11
1	A	260	HIS	11
1	A	262	ILE	11
1	A	149	ARG	10
1	A	256	TYR	10
1	A	185	ASP	10
1	A	218	LYS	10
1	A	274	LEU	9
1	A	210	LYS	9
1	A	177	LEU	8
1	A	298	ARG	8
1	A	145	HIS	8
1	A	156	LEU	8
1	A	282	ARG	7
1	A	259	ASP	7
1	A	166	PHE	7
1	A	169	CYS	7
1	A	280	ASN	6
1	A	211	GLU	6
1	A	277	PHE	6
1	A	179	LYS	6
1	A	242	ARG	6
1	A	219	GLU	6
1	A	281	LYS	6
1	A	257	ILE	5
1	A	266	LEU	5
1	A	173	CYS	5
1	A	270	ASP	5
1	A	191	THR	5
1	A	239	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	294	MET	5
1	A	224	LEU	4
1	A	193	LEU	4
1	A	264	MET	4
1	A	152	ASP	4
1	A	295	ARG	4
1	A	192	THR	4
1	A	202	SER	4
1	A	176	GLU	4
1	A	158	GLN	4
1	A	208	ASP	4
1	A	160	LEU	4
1	A	187	ILE	3
1	A	155	TYR	3
1	A	196	LEU	3
1	A	146	THR	3
1	A	233	GLU	3
1	A	272	GLU	3
1	A	297	TYR	3
1	A	245	TYR	3
1	A	230	THR	2
1	A	236	GLN	2
1	A	209	THR	2
1	A	188	ASP	2
1	A	195	ASP	2
1	A	175	GLU	2
1	A	204	ASP	2
1	A	171	ASP	2
1	A	154	ASP	2
1	A	184	VAL	2
1	A	289	SER	2
1	A	168	HIS	2
1	A	151	THR	2
1	A	273	PHE	2
1	A	244	TYR	2
1	A	258	VAL	2
1	A	144	THR	2
1	A	172	VAL	2
1	A	223	LYS	2
1	A	234	VAL	2
1	A	261	THR	2
1	A	183	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	232	GLU	1
1	A	221	SER	1
1	A	142	LEU	1
1	A	279	GLN	1
1	A	143	THR	1
1	A	227	LEU	1
1	A	285	GLU	1
1	A	237	VAL	1
1	A	141	SER	1
1	A	189	SER	1
1	A	182	GLN	1
1	A	246	SER	1
1	A	180	MET	1
1	A	220	PHE	1
1	A	215	ASN	1
1	A	200	PHE	1
1	A	161	LEU	1
1	A	216	TYR	1
1	A	228	THR	1
1	A	243	VAL	1
1	A	181	ILE	1
1	A	235	ASP	1
1	A	167	THR	1
1	A	276	TYR	1
1	A	213	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