



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2GQM / pdb_00002gqm
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

<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

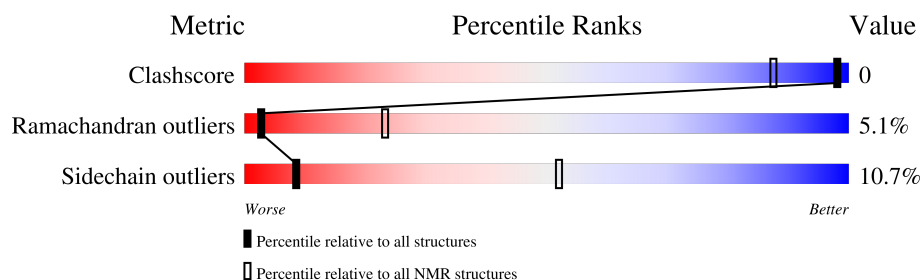
1 Overall quality at a glance

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	173	82% 7% 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)	1.32	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 (CCD ID: CU1) (formula: Cu).

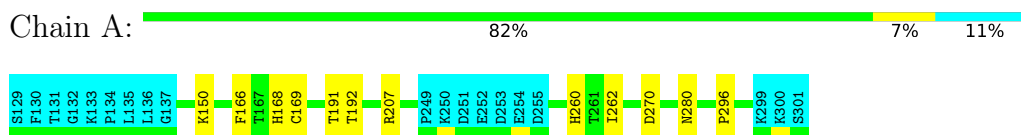
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

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: SCO1 protein homolog, mitochondrial

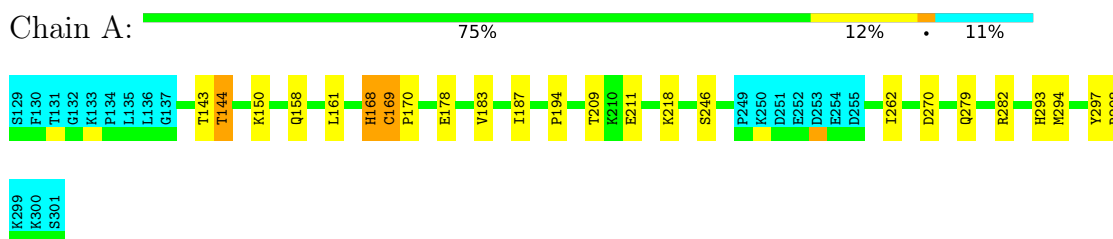


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

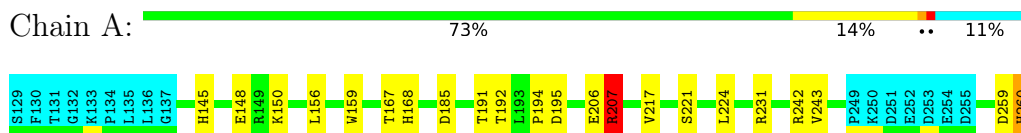
4.2.1 Score per residue for model 1

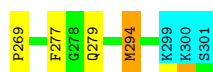
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.2 Score per residue for model 2

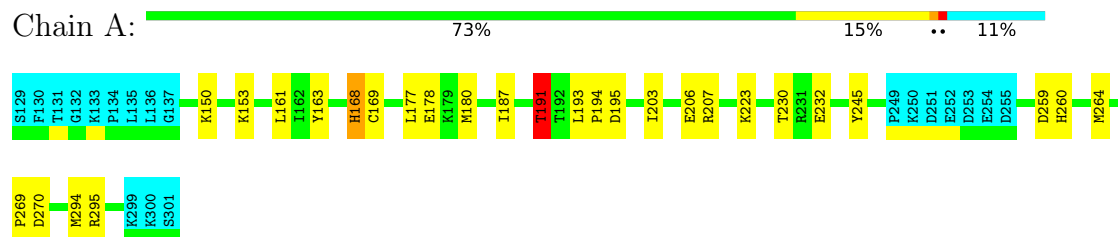
- Molecule 1: SCO1 protein homolog, mitochondrial





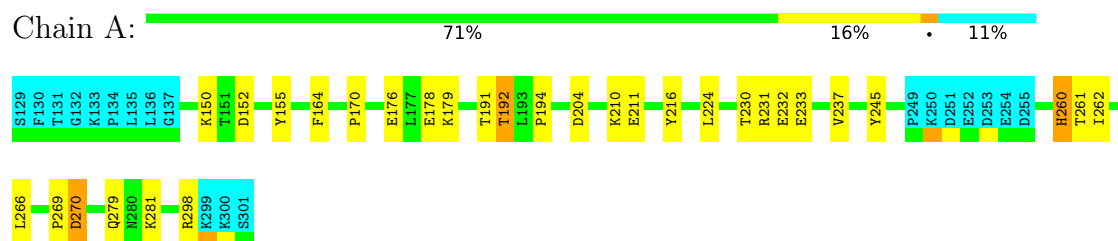
4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial



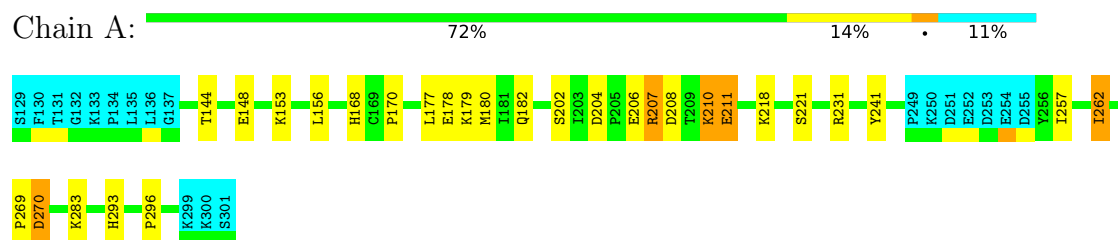
4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.5 Score per residue for model 5

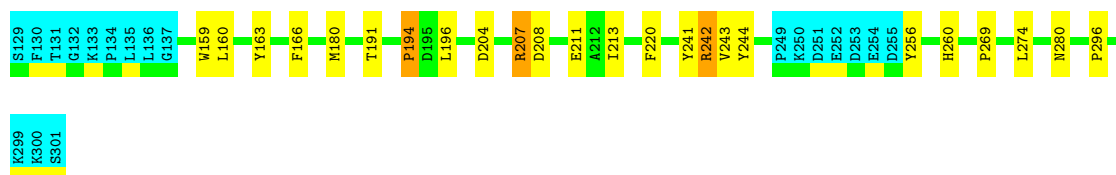
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.6 Score per residue for model 6

- Molecule 1: SCO1 protein homolog, mitochondrial

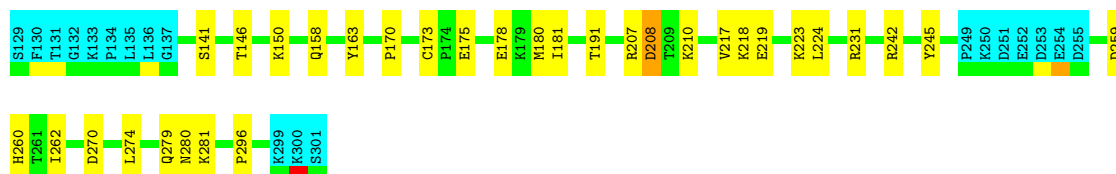




4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial

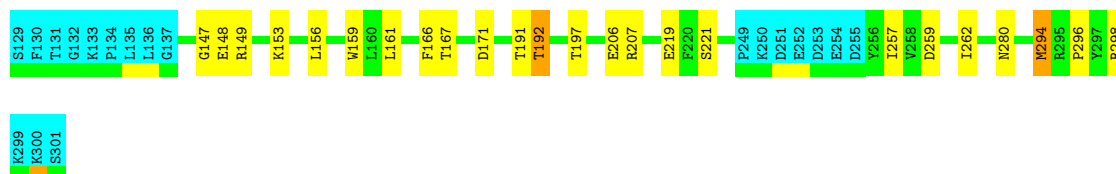
Chain A: 71% 18% 11%



4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial

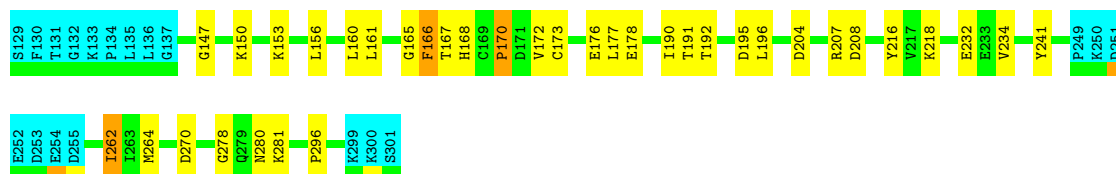
Chain A: 75% 13% 11%



4.2.9 Score per residue for model 9

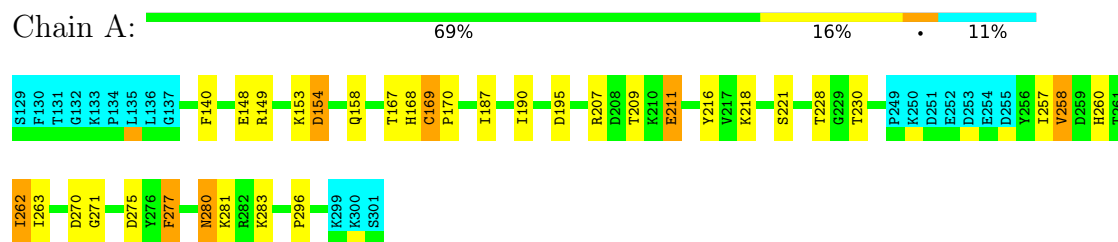
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 68% 19% 11%



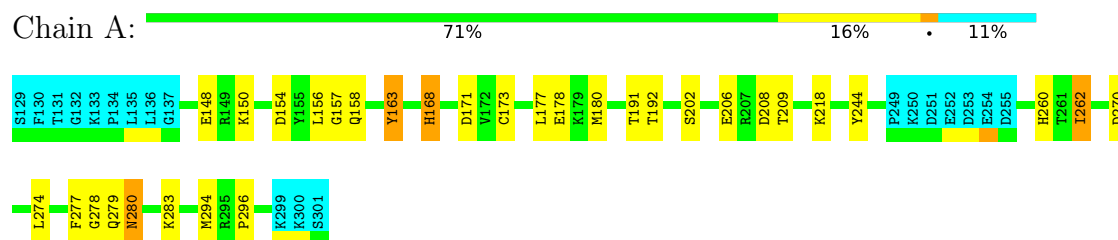
4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial



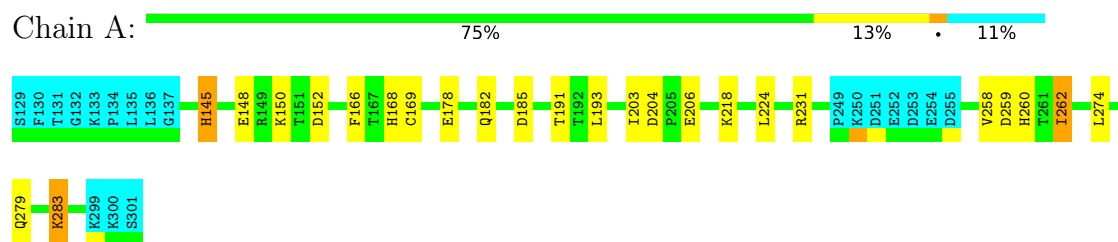
4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



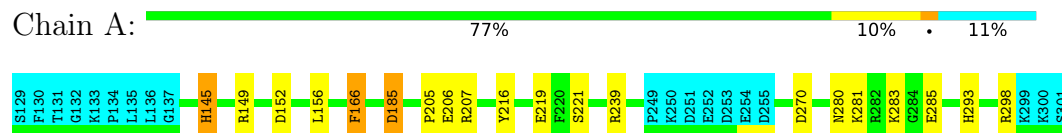
4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



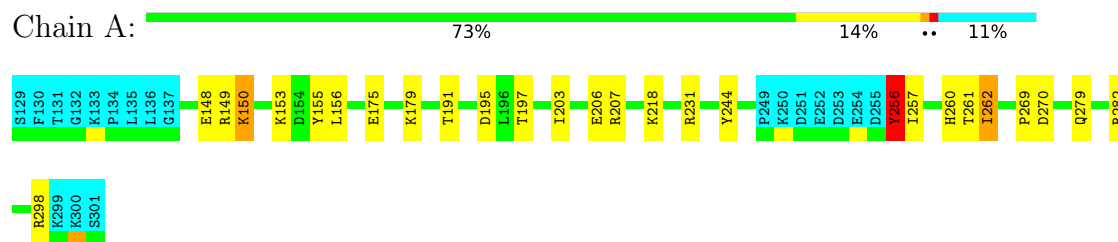
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: SCO1 protein homolog, mitochondrial



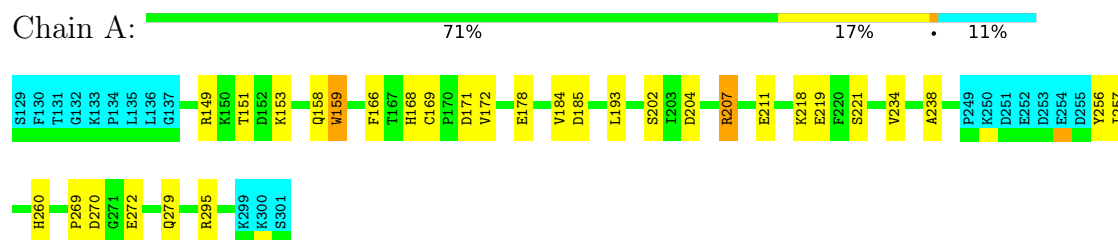
4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



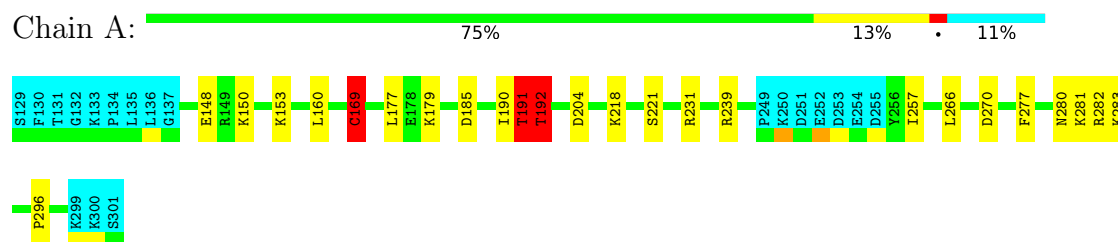
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



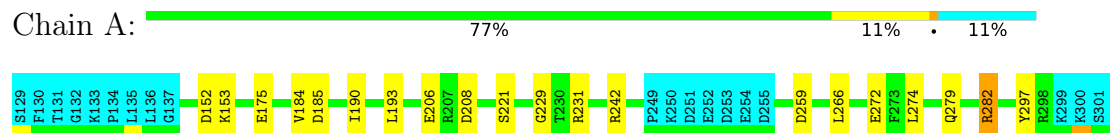
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



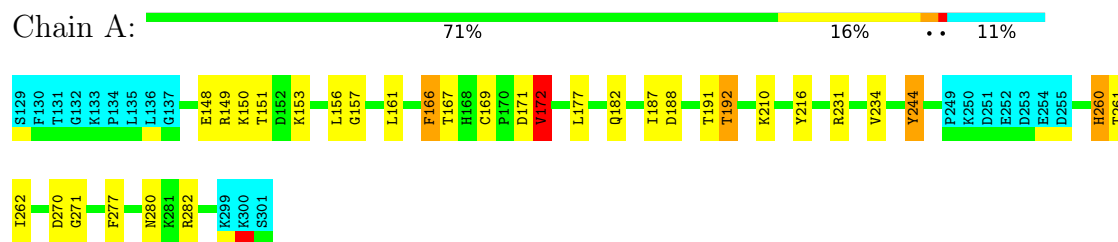
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



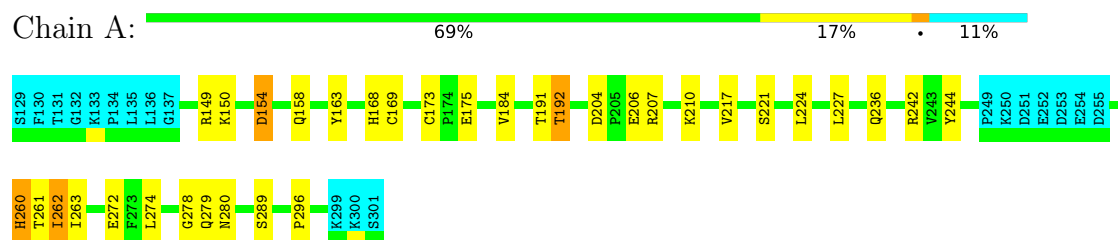
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



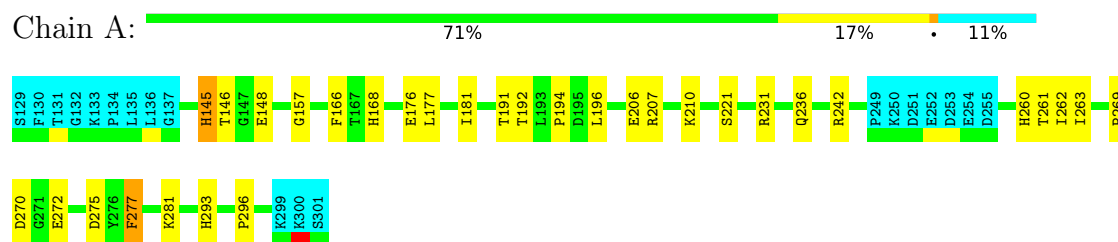
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



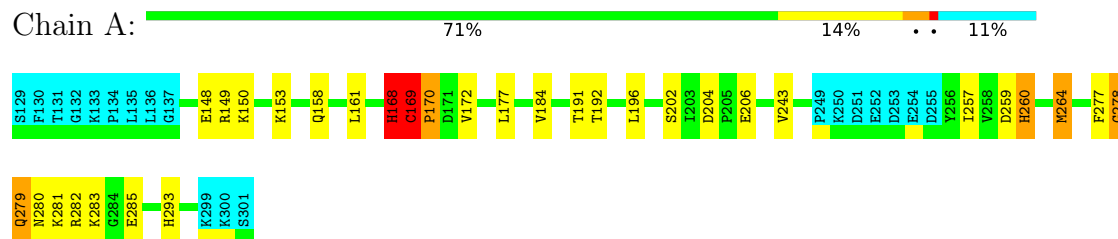
4.2.20 Score per residue for model 20

- Molecule 1: SCO1 protein homolog, mitochondrial



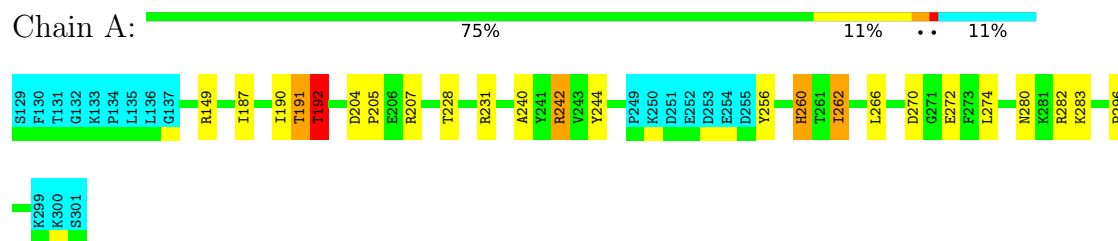
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



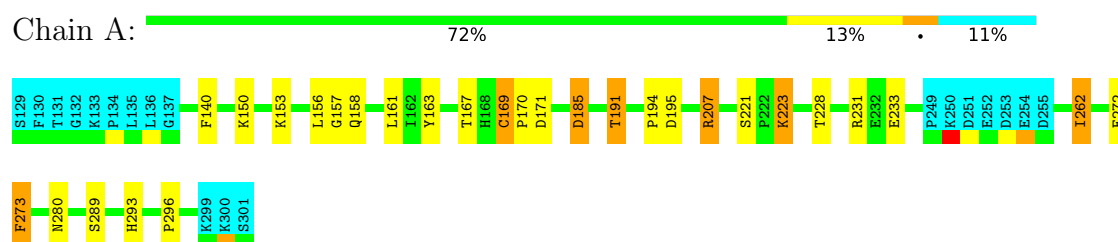
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



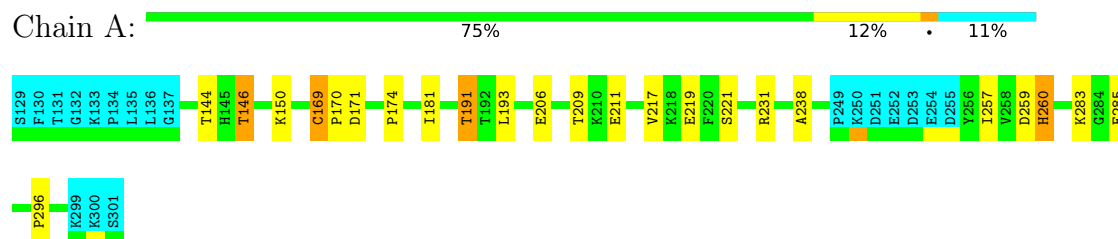
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



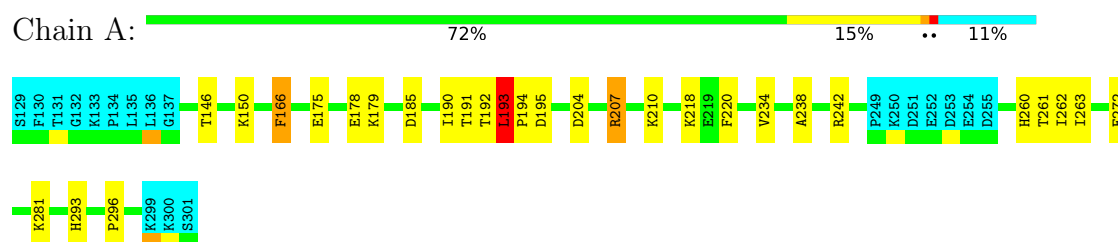
4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



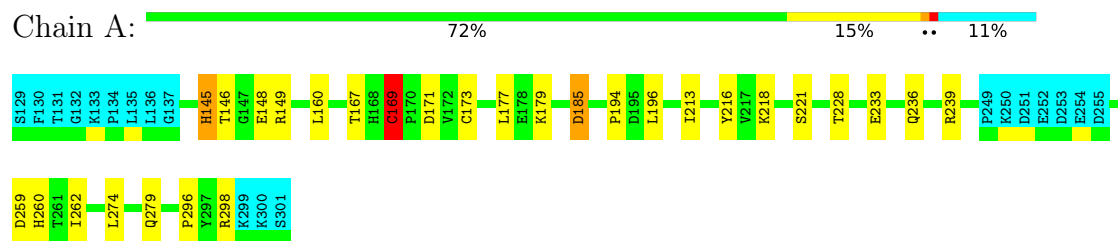
4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



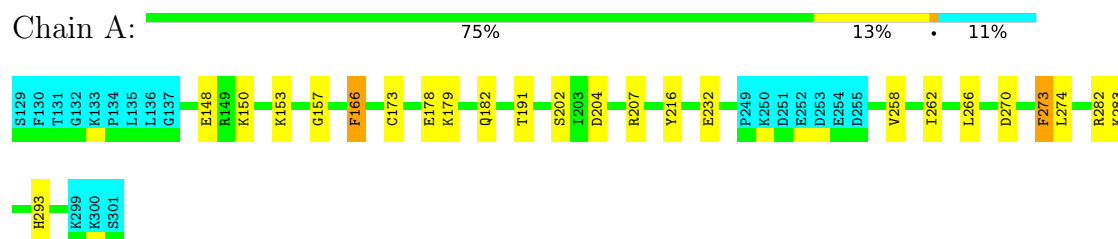
4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



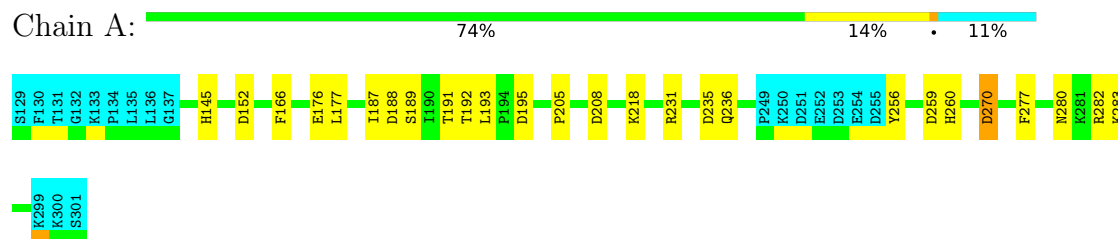
4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



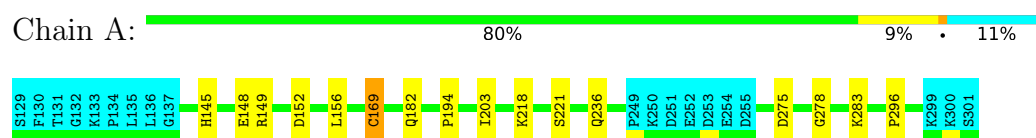
4.2.28 Score per residue for model 28

- 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

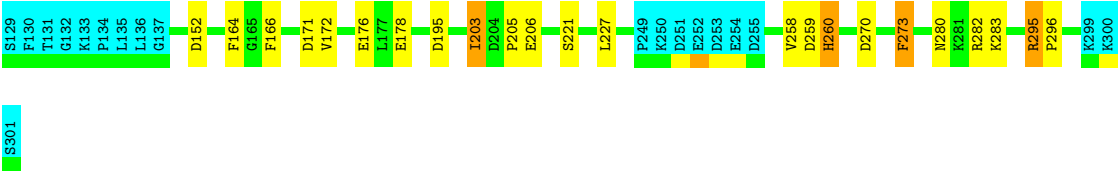
Chain A:

76%

11%

•

11%



S301

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.

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	0.86±0.01	0±0/1275 (0.0± 0.0%)	1.45±0.03	6±3/1735 (0.4± 0.1%)
All	All	0.86	0/38250 (0.0%)	1.46	184/52050 (0.4%)

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	260	HIS	CB-CG-CD2	-7.34	121.66	131.20	25	18
1	A	166	PHE	CA-CB-CG	7.33	121.13	113.80	12	8
1	A	154	ASP	CA-CB-CG	7.29	119.89	112.60	11	3
1	A	152	ASP	CA-CB-CG	7.20	119.80	112.60	13	3
1	A	277	PHE	CA-CB-CG	6.96	120.75	113.80	10	1
1	A	194	PRO	CA-C-N	6.82	132.30	122.21	20	4
1	A	194	PRO	C-N-CA	6.82	132.30	122.21	20	4
1	A	164	PHE	CA-C-N	6.78	128.21	122.17	4	2
1	A	164	PHE	C-N-CA	6.78	128.21	122.17	4	2
1	A	278	GLY	CA-C-N	6.65	134.24	121.54	19	3
1	A	278	GLY	C-N-CA	6.65	134.24	121.54	19	3
1	A	208	ASP	CA-CB-CG	6.46	119.06	112.60	17	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	273	PHE	CA-CB-CG	6.41	120.21	113.80	27	1
1	A	236	GLN	OE1-CD-NE2	-6.41	116.19	122.60	19	2
1	A	293	HIS	CA-CB-CG	6.39	120.19	113.80	23	5
1	A	208	ASP	CA-C-N	6.34	133.65	121.54	11	1
1	A	208	ASP	C-N-CA	6.34	133.65	121.54	11	1
1	A	192	THR	CA-CB-CG2	6.29	121.19	110.50	16	2
1	A	260	HIS	CA-CB-CG	6.07	119.87	113.80	25	2
1	A	150	LYS	CA-C-N	6.07	132.73	121.62	14	2
1	A	150	LYS	C-N-CA	6.07	132.73	121.62	14	2
1	A	190	ILE	CA-C-N	6.06	133.12	121.54	22	3
1	A	190	ILE	C-N-CA	6.06	133.12	121.54	22	3
1	A	191	THR	CA-CB-CG2	6.06	120.80	110.50	3	2
1	A	256	TYR	N-CA-C	6.02	116.50	108.38	6	1
1	A	210	LYS	CA-C-N	6.00	128.80	120.29	18	1
1	A	210	LYS	C-N-CA	6.00	128.80	120.29	18	1
1	A	275	ASP	CA-CB-CG	5.97	118.57	112.60	10	3
1	A	269	PRO	CA-C-N	5.94	128.73	120.29	2	3
1	A	269	PRO	C-N-CA	5.94	128.73	120.29	2	3
1	A	238	ALA	CA-C-N	5.93	128.15	120.44	24	3
1	A	238	ALA	C-N-CA	5.93	128.15	120.44	24	3
1	A	157	GLY	CA-C-N	5.92	132.84	121.54	11	1
1	A	157	GLY	C-N-CA	5.92	132.84	121.54	11	1
1	A	184	VAL	CA-C-N	5.85	128.12	120.28	19	1
1	A	184	VAL	C-N-CA	5.85	128.12	120.28	19	1
1	A	204	ASP	CA-CB-CG	5.80	118.40	112.60	12	4
1	A	168	HIS	CB-CG-CD2	-5.76	123.71	131.20	1	6
1	A	279	GLN	CA-C-N	5.73	128.23	120.38	7	1
1	A	279	GLN	C-N-CA	5.73	128.23	120.38	7	1
1	A	241	TYR	CA-C-N	5.69	132.41	121.54	6	1
1	A	241	TYR	C-N-CA	5.69	132.41	121.54	6	1
1	A	272	GLU	CA-C-N	5.67	132.37	121.54	23	1
1	A	272	GLU	C-N-CA	5.67	132.37	121.54	23	1
1	A	194	PRO	N-CA-CB	5.62	106.50	102.79	6	1
1	A	277	PHE	CA-C-N	5.62	128.19	120.72	28	1
1	A	277	PHE	C-N-CA	5.62	128.19	120.72	28	1
1	A	188	ASP	CA-CB-CG	5.59	118.19	112.60	18	1
1	A	158	GLN	CA-C-N	5.57	132.19	121.54	15	1
1	A	158	GLN	C-N-CA	5.57	132.19	121.54	15	1
1	A	262	ILE	CA-C-N	5.55	131.96	121.97	20	2
1	A	262	ILE	C-N-CA	5.55	131.96	121.97	20	2
1	A	187	ILE	CA-C-N	5.51	127.66	120.28	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	187	ILE	C-N-CA	5.51	127.66	120.28	18	1
1	A	231	ARG	CA-C-N	5.46	127.87	120.44	5	3
1	A	231	ARG	C-N-CA	5.46	127.87	120.44	5	3
1	A	279	GLN	OE1-CD-NE2	-5.46	117.14	122.60	26	3
1	A	262	ILE	CB-CA-C	5.44	120.21	111.29	19	2
1	A	293	HIS	CA-C-N	5.42	127.55	120.28	5	1
1	A	293	HIS	C-N-CA	5.42	127.55	120.28	5	1
1	A	171	ASP	CA-C-N	5.41	127.85	120.77	8	1
1	A	171	ASP	C-N-CA	5.41	127.85	120.77	8	1
1	A	144	THR	CA-C-N	5.40	128.26	120.38	1	1
1	A	144	THR	C-N-CA	5.40	128.26	120.38	1	1
1	A	145	HIS	CB-CG-CD2	-5.38	124.21	131.20	13	5
1	A	242	ARG	CA-C-N	5.36	131.62	121.97	2	1
1	A	242	ARG	C-N-CA	5.36	131.62	121.97	2	1
1	A	231	ARG	CD-NE-CZ	5.34	131.88	124.40	14	1
1	A	185	ASP	CA-CB-CG	5.32	117.92	112.60	26	3
1	A	293	HIS	CB-CG-CD2	-5.22	124.41	131.20	1	3
1	A	260	HIS	CA-C-N	5.21	131.49	121.54	14	1
1	A	260	HIS	C-N-CA	5.21	131.49	121.54	14	1
1	A	166	PHE	CA-C-N	5.18	131.43	121.54	8	2
1	A	166	PHE	C-N-CA	5.18	131.43	121.54	8	2
1	A	216	TYR	CA-C-N	5.16	127.02	120.72	13	1
1	A	216	TYR	C-N-CA	5.16	127.02	120.72	13	1
1	A	205	PRO	CA-C-N	5.16	131.39	121.54	30	1
1	A	205	PRO	C-N-CA	5.16	131.39	121.54	30	1
1	A	282	ARG	CD-NE-CZ	5.12	131.57	124.40	17	1
1	A	204	ASP	CA-C-N	5.09	126.21	119.84	21	1
1	A	204	ASP	C-N-CA	5.09	126.21	119.84	21	1
1	A	280	ASN	N-CA-C	5.08	117.48	111.33	7	1
1	A	272	GLU	N-CA-C	5.08	114.33	108.49	25	1
1	A	158	GLN	OE1-CD-NE2	-5.06	117.54	122.60	1	1
1	A	259	ASP	CA-CB-CG	5.04	117.64	112.60	7	1
1	A	203	ILE	N-CA-C	5.04	119.83	109.34	30	1
1	A	169	CYS	N-CA-C	5.04	117.45	110.20	3	1
1	A	230	THR	CA-C-N	5.03	127.28	120.38	4	1
1	A	230	THR	C-N-CA	5.03	127.28	120.38	4	1
1	A	206	GLU	CA-C-N	5.02	131.13	121.54	19	1
1	A	206	GLU	C-N-CA	5.02	131.13	121.54	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	207	ARG	Sidechain	4
1	A	269	PRO	Peptide	4
1	A	149	ARG	Sidechain	4
1	A	231	ARG	Sidechain	3
1	A	244	TYR	Sidechain	3
1	A	280	ASN	Peptide	3
1	A	163	TYR	Sidechain	3
1	A	205	PRO	Peptide	3
1	A	157	GLY	Peptide	3
1	A	259	ASP	Peptide	3
1	A	170	PRO	Peptide	2
1	A	192	THR	Peptide	2
1	A	241	TYR	Sidechain	2
1	A	278	GLY	Peptide	2
1	A	140	PHE	Peptide	2
1	A	190	ILE	Peptide	2
1	A	191	THR	Peptide	2
1	A	242	ARG	Sidechain,Peptide	2
1	A	261	THR	Peptide	2
1	A	193	LEU	Peptide	2
1	A	194	PRO	Peptide	1
1	A	243	VAL	Peptide	1
1	A	245	TYR	Sidechain	1
1	A	167	THR	Peptide	1
1	A	296	PRO	Peptide	1
1	A	195	ASP	Peptide	1
1	A	298	ARG	Peptide	1
1	A	229	GLY	Peptide	1
1	A	282	ARG	Sidechain	1
1	A	172	VAL	Peptide	1
1	A	182	GLN	Peptide	1
1	A	271	GLY	Peptide	1
1	A	279	GLN	Peptide	1
1	A	202	SER	Peptide	1
1	A	208	ASP	Peptide	1
1	A	295	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	1242	1214	1213	1±1
All	All	37290	36420	36390	26

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:163:TYR:CG	1:A:180:MET:HE1	0.51	2.40	3	3
1:A:184:VAL:HG23	1:A:196:LEU:H	0.50	1.66	21	1
1:A:175:GLU:CD	1:A:179:LYS:HZ2	0.48	2.17	25	1
1:A:182:GLN:C	1:A:283:LYS:HE3	0.47	2.35	12	1
1:A:169:CYS:HB3	1:A:171:ASP:H	0.46	1.70	26	1
1:A:163:TYR:CD1	1:A:180:MET:HE1	0.46	2.46	6	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:161:LEU:HB3	1:A:264:MET:HE2	0.45	1.86	3	1
1:A:232:GLU:H	1:A:232:GLU:CD	0.44	2.20	27	2
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:210:LYS:HZ3	1:A:211:GLU:CD	0.43	2.20	5	1
1:A:159:TRP:CD1	1:A:269:PRO:HD3	0.43	2.48	6	1
1:A:150:LYS:HE2	1:A:155:TYR:CE2	0.43	2.48	14	1
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:159:TRP:CZ2	1:A:294:MET:HE2	0.42	2.50	2	2
1:A:190:ILE:O	1:A:191:THR:HG23	0.42	2.14	16	1
1:A:161:LEU:CD1	1:A:264:MET:HE2	0.42	2.44	21	1
1:A:211:GLU:H	1:A:211:GLU:CD	0.41	2.24	10	1
1:A:165:GLY:HA3	1:A:173:CYS:SG	0.40	2.56	9	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	154/173 (89%)	129±4 (83±2%)	18±4 (11±2%)	8±3 (5±2%)	3	23
All	All	4620/5190 (89%)	3857 (83%)	529 (11%)	234 (5%)	3	23

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	194	PRO	5
1	A	204	ASP	5
1	A	171	ASP	5
1	A	203	ILE	4
1	A	167	THR	4
1	A	263	ILE	4
1	A	283	LYS	4
1	A	298	ARG	3
1	A	172	VAL	3
1	A	244	TYR	3
1	A	282	ARG	3
1	A	273	PHE	3
1	A	242	ARG	2
1	A	223	LYS	2
1	A	147	GLY	2
1	A	281	LYS	2
1	A	158	GLN	2
1	A	256	TYR	2
1	A	261	THR	2
1	A	272	GLU	2
1	A	243	VAL	1
1	A	155	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	220	PHE	1
1	A	208	ASP	1
1	A	258	VAL	1
1	A	271	GLY	1
1	A	209	THR	1
1	A	159	TRP	1
1	A	257	ILE	1
1	A	196	LEU	1
1	A	277	PHE	1
1	A	278	GLY	1
1	A	240	ALA	1
1	A	157	GLY	1
1	A	146	THR	1
1	A	174	PRO	1
1	A	193	LEU	1
1	A	228	THR	1
1	A	152	ASP	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%)	8	52
All	All	4080/4590 (89%)	3642 (89%)	438 (11%)	8	52

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	150	LYS	15
1	A	218	LYS	14
1	A	148	GLU	14
1	A	207	ARG	13
1	A	153	LYS	13
1	A	178	GLU	12
1	A	262	ILE	12
1	A	156	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	177	LEU	10
1	A	185	ASP	9
1	A	260	HIS	9
1	A	274	LEU	9
1	A	211	GLU	7
1	A	231	ARG	7
1	A	259	ASP	7
1	A	257	ILE	7
1	A	166	PHE	7
1	A	149	ARG	7
1	A	283	LYS	7
1	A	282	ARG	6
1	A	145	HIS	6
1	A	277	PHE	6
1	A	191	THR	6
1	A	179	LYS	6
1	A	210	LYS	6
1	A	281	LYS	6
1	A	192	THR	6
1	A	161	LEU	5
1	A	187	ILE	5
1	A	294	MET	5
1	A	224	LEU	5
1	A	193	LEU	5
1	A	176	GLU	5
1	A	266	LEU	5
1	A	242	ARG	5
1	A	280	ASN	5
1	A	146	THR	5
1	A	173	CYS	5
1	A	219	GLU	5
1	A	169	CYS	5
1	A	217	VAL	4
1	A	270	ASP	4
1	A	202	SER	4
1	A	160	LEU	4
1	A	158	GLN	4
1	A	175	GLU	4
1	A	234	VAL	4
1	A	144	THR	3
1	A	209	THR	3
1	A	295	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	152	ASP	3
1	A	233	GLU	3
1	A	196	LEU	3
1	A	181	ILE	3
1	A	228	THR	3
1	A	258	VAL	3
1	A	239	ARG	3
1	A	285	GLU	3
1	A	256	TYR	3
1	A	172	VAL	3
1	A	272	GLU	3
1	A	236	GLN	3
1	A	279	GLN	2
1	A	297	TYR	2
1	A	298	ARG	2
1	A	167	THR	2
1	A	195	ASP	2
1	A	223	LYS	2
1	A	230	THR	2
1	A	232	GLU	2
1	A	245	TYR	2
1	A	261	THR	2
1	A	208	ASP	2
1	A	213	ILE	2
1	A	197	THR	2
1	A	264	MET	2
1	A	154	ASP	2
1	A	168	HIS	2
1	A	151	THR	2
1	A	184	VAL	2
1	A	204	ASP	2
1	A	227	LEU	2
1	A	289	SER	2
1	A	273	PHE	2
1	A	143	THR	1
1	A	183	VAL	1
1	A	246	SER	1
1	A	267	ILE	1
1	A	237	VAL	1
1	A	180	MET	1
1	A	221	SER	1
1	A	141	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	216	TYR	1
1	A	203	ILE	1
1	A	206	GLU	1
1	A	171	ASP	1
1	A	244	TYR	1
1	A	243	VAL	1
1	A	220	PHE	1
1	A	182	GLN	1
1	A	188	ASP	1
1	A	189	SER	1
1	A	235	ASP	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