



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 2GQK / pdb_00002gqk
Title : Solution structure of Human Ni(II)-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

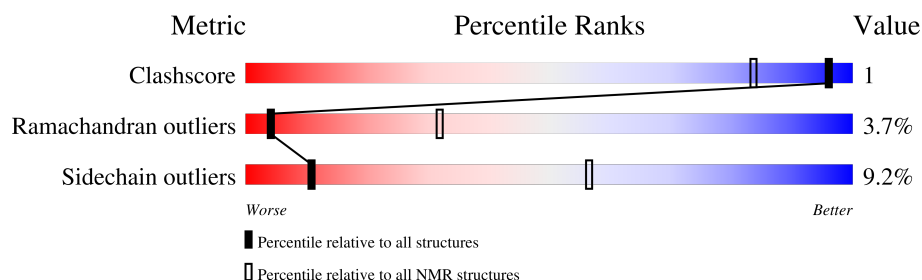
1 Overall quality at a glance

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	

2 Ensemble composition and analysis

This entry contains 30 models. Model 6 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:139-A:248, A:257-A:298 (152)	1.30	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 7 clusters and 8 single-model clusters were found.

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

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 NICKEL (II) ION (CCD ID: NI) (formula: Ni).

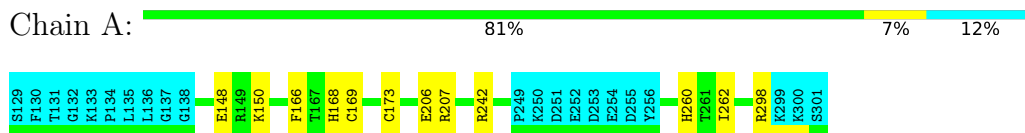
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ni
			1	1

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

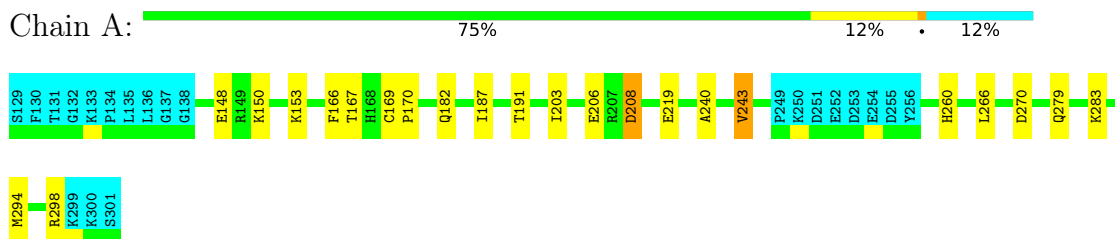


4.2 Scores per residue for each member of the ensemble

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

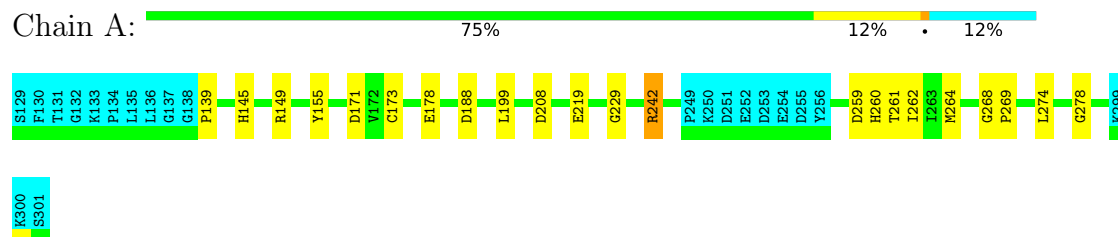
- Molecule 1: SCO1 protein homolog, mitochondrial





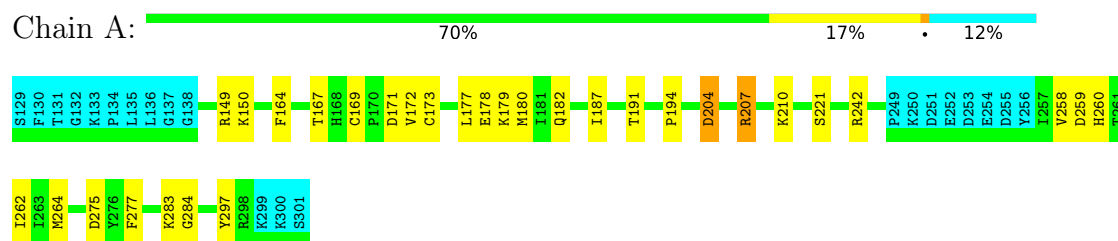
4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial



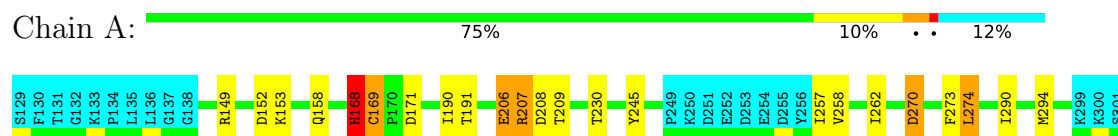
4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial



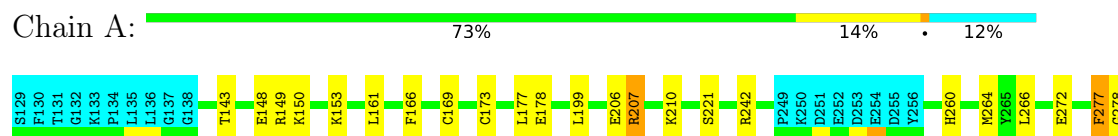
4.2.5 Score per residue for model 5

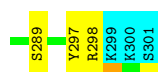
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.6 Score per residue for model 6 (medoid)

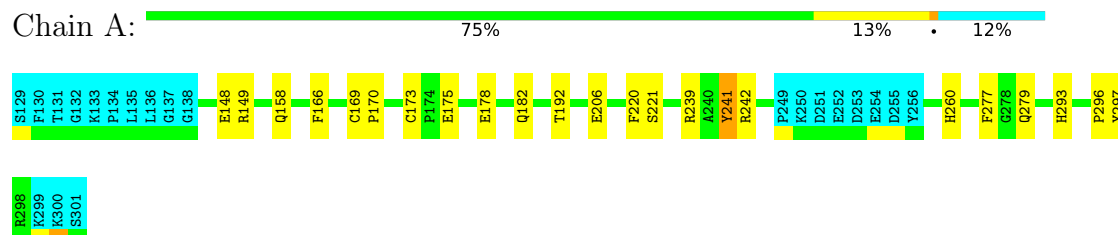
- Molecule 1: SCO1 protein homolog, mitochondrial





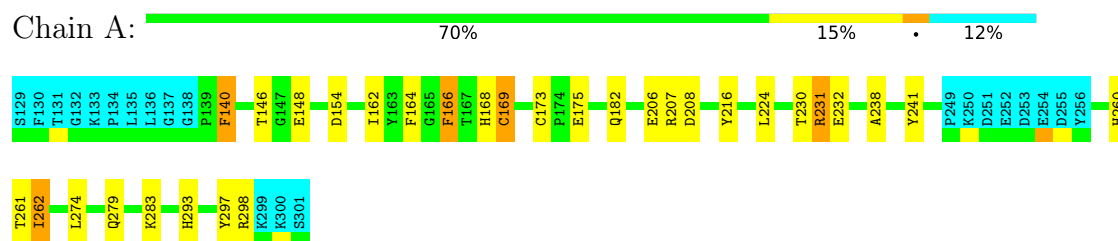
4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial



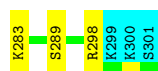
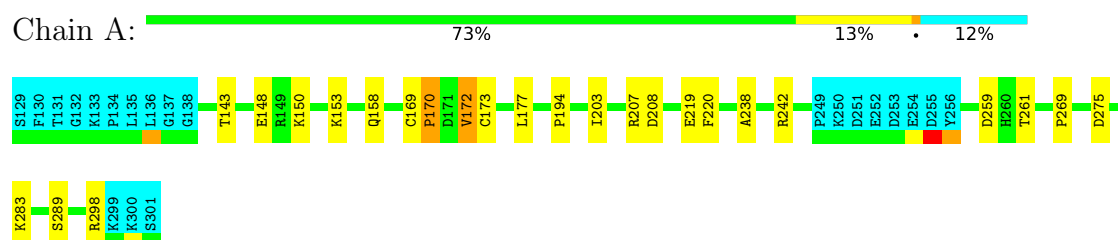
4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.9 Score per residue for model 9

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial

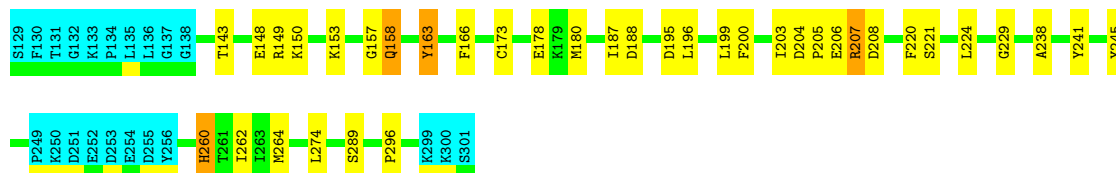




4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 66% 19% 12%



4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial

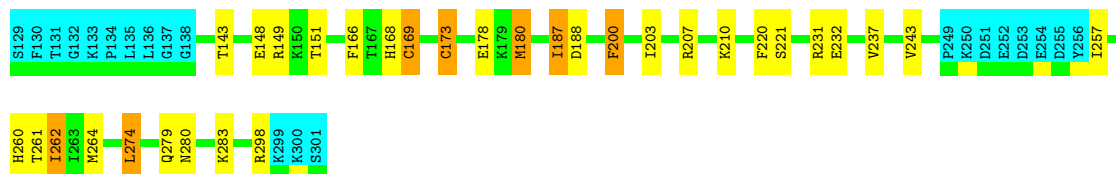
Chain A: 74% 14% 12%



4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial

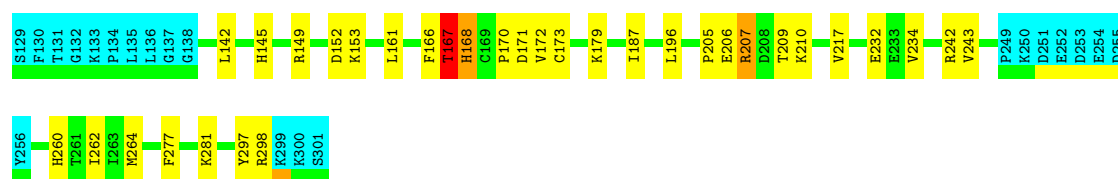
Chain A: 69% 14% 12%



4.2.14 Score per residue for model 14

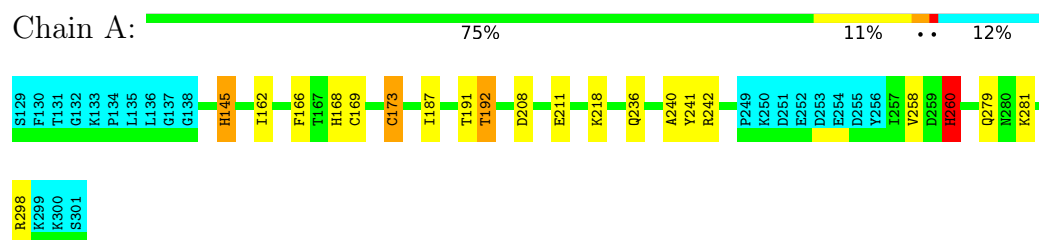
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 69% 17% 12%



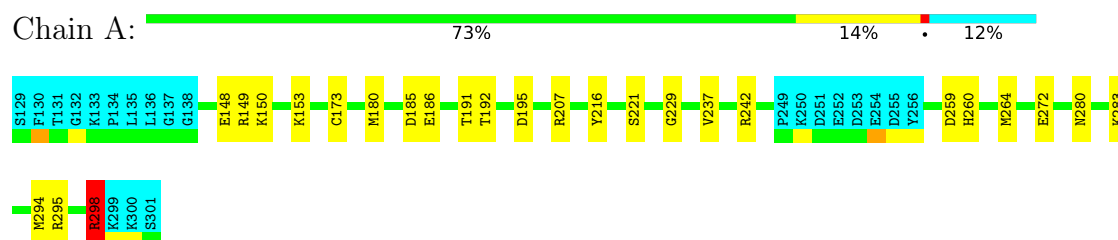
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



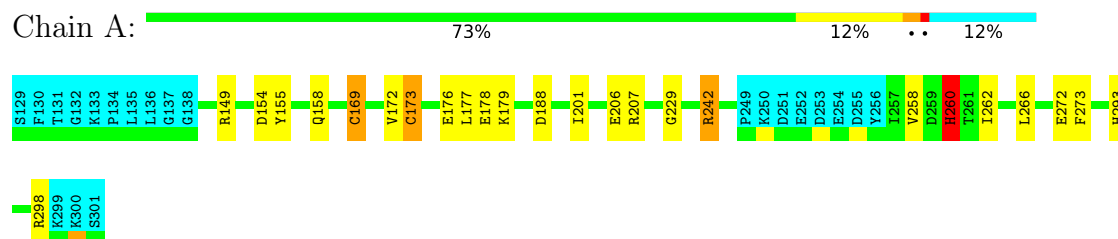
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



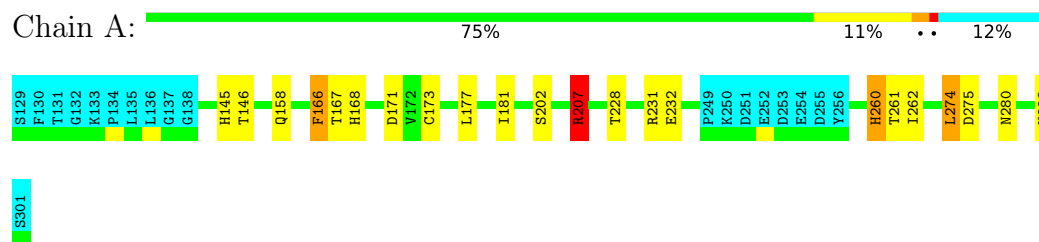
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



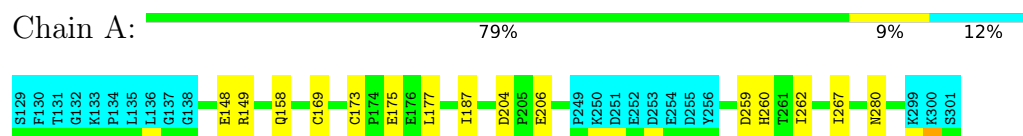
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



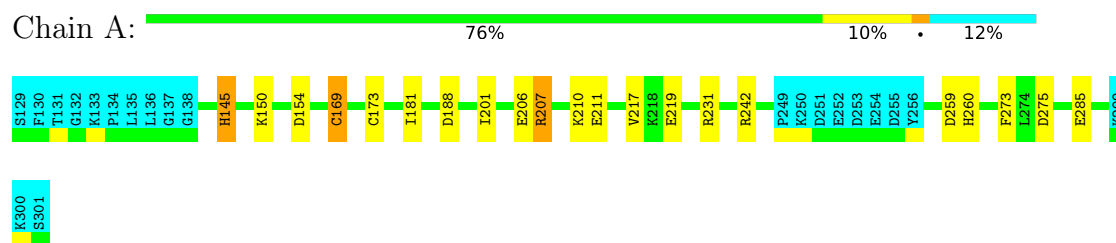
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



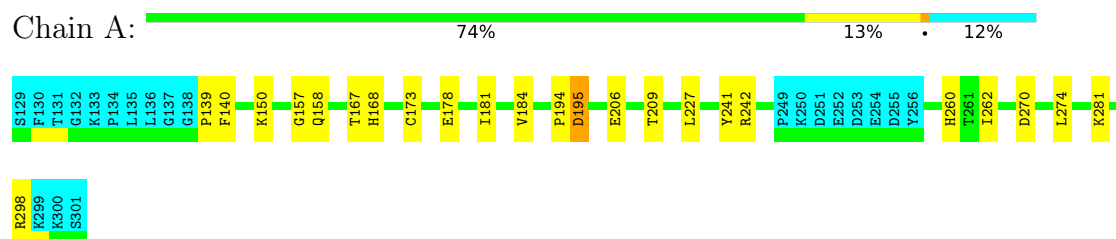
4.2.20 Score per residue for model 20

- Molecule 1: SCO1 protein homolog, mitochondrial



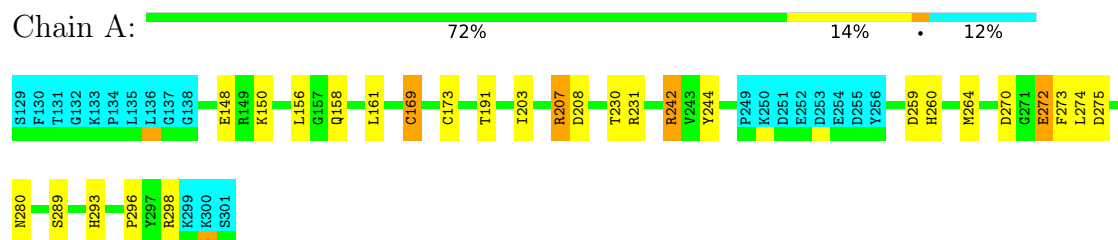
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



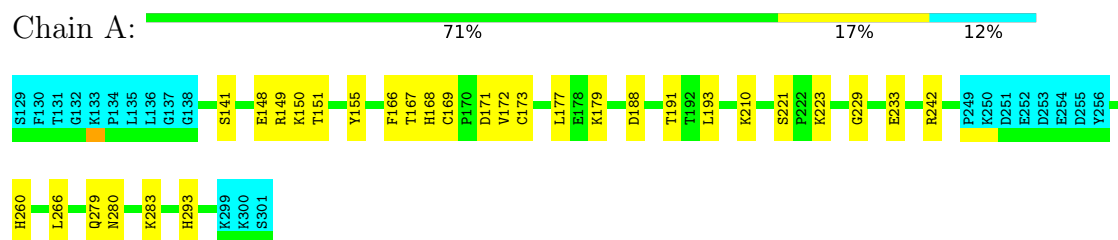
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



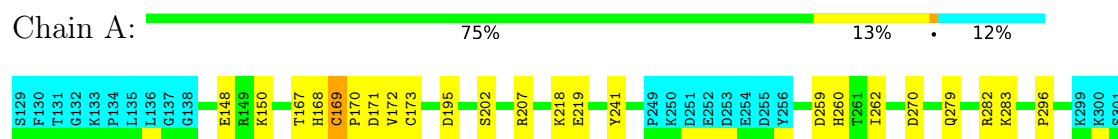
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



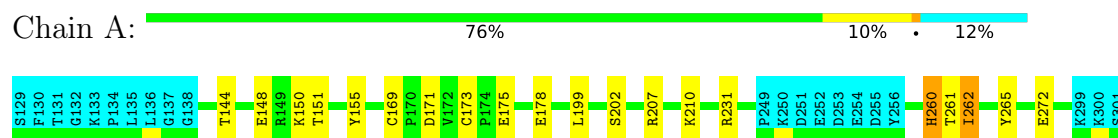
4.2.24 Score per residue for model 24

- 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

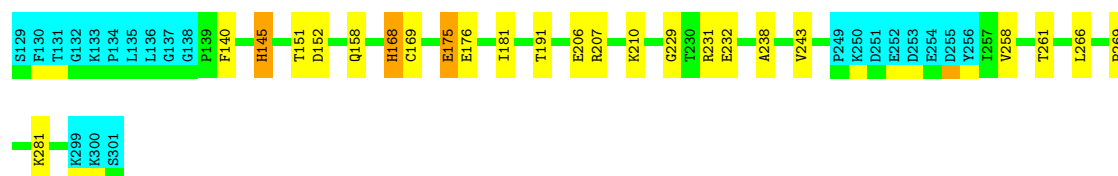
Chain A: 70% 17% 12%



4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial

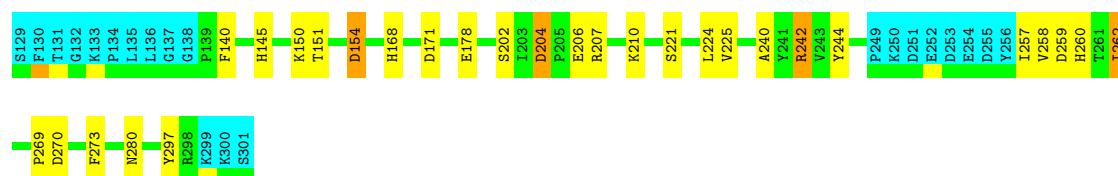
Chain A: 74% 12% 12%



4.2.29 Score per residue for model 29

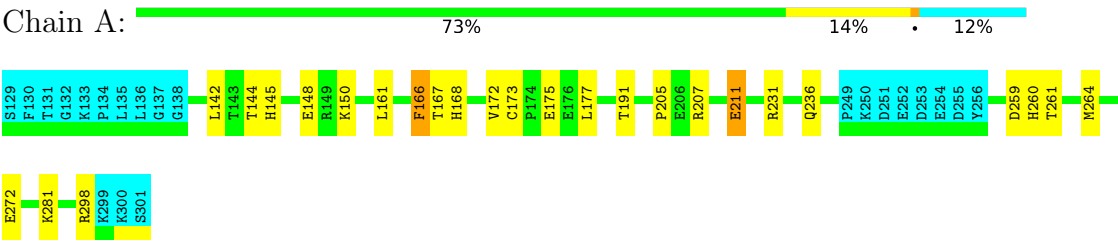
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 71% 14% 12%



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.

6 Model quality

6.1 Standard geometry

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

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	0.87±0.01	0±0/1258 (0.0± 0.0%)	1.48±0.03	7±3/1711 (0.4± 0.2%)
All	All	0.87	0/37740 (0.0%)	1.48	202/51330 (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	2.1±1.5
All	All	0	64

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	154	ASP	CA-CB-CG	10.73	123.33	112.60	29	4
1	A	282	ARG	CA-C-N	9.40	139.49	121.54	26	1
1	A	282	ARG	C-N-CA	9.40	139.49	121.54	26	1
1	A	166	PHE	CA-CB-CG	9.04	122.84	113.80	13	5
1	A	277	PHE	CA-CB-CG	8.17	121.97	113.80	6	4
1	A	169	CYS	CB-CA-C	8.07	118.57	110.33	23	8
1	A	204	ASP	CA-CB-CG	7.22	119.82	112.60	4	4
1	A	269	PRO	CA-C-N	7.13	130.55	120.28	3	4
1	A	269	PRO	C-N-CA	7.13	130.55	120.28	3	4
1	A	171	ASP	CB-CA-C	6.98	116.74	109.83	14	1
1	A	200	PHE	CA-CB-CG	6.95	120.75	113.80	11	2
1	A	236	GLN	OE1-CD-NE2	-6.79	115.81	122.60	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	273	PHE	CA-CB-CG	6.79	120.58	113.80	20	1
1	A	173	CYS	N-CA-CB	-6.67	104.05	110.39	10	3
1	A	275	ASP	CA-CB-CG	6.52	119.12	112.60	4	5
1	A	191	THR	CA-C-N	6.49	130.18	120.31	28	5
1	A	191	THR	C-N-CA	6.49	130.18	120.31	28	5
1	A	261	THR	N-CA-C	6.46	119.14	111.71	25	1
1	A	168	HIS	N-CA-CB	-6.46	101.20	110.57	15	1
1	A	140	PHE	CA-CB-CG	6.45	120.25	113.80	21	5
1	A	169	CYS	N-CA-CB	-6.37	102.22	111.20	6	3
1	A	168	HIS	CB-CG-CD2	-6.32	122.98	131.20	13	6
1	A	293	HIS	CA-CB-CG	6.31	120.11	113.80	8	3
1	A	151	THR	CA-C-N	6.31	129.56	120.79	25	1
1	A	151	THR	C-N-CA	6.31	129.56	120.79	25	1
1	A	238	ALA	CA-C-N	6.22	129.13	120.29	11	5
1	A	238	ALA	C-N-CA	6.22	129.13	120.29	11	5
1	A	152	ASP	CA-CB-CG	6.21	118.81	112.60	28	3
1	A	166	PHE	CA-C-N	6.21	129.12	120.29	6	2
1	A	166	PHE	C-N-CA	6.21	129.12	120.29	6	2
1	A	260	HIS	CA-CB-CG	6.11	119.91	113.80	29	3
1	A	241	TYR	CA-C-N	6.08	133.15	121.54	7	4
1	A	241	TYR	C-N-CA	6.08	133.15	121.54	7	4
1	A	164	PHE	CA-C-N	6.08	125.78	121.65	8	2
1	A	164	PHE	C-N-CA	6.08	125.78	121.65	8	2
1	A	210	LYS	CA-C-N	6.06	128.40	120.28	23	5
1	A	210	LYS	C-N-CA	6.06	128.40	120.28	23	5
1	A	172	VAL	CA-C-N	6.01	127.24	119.78	9	2
1	A	172	VAL	C-N-CA	6.01	127.24	119.78	9	2
1	A	187	ILE	CA-C-N	5.96	128.26	120.28	11	2
1	A	187	ILE	C-N-CA	5.96	128.26	120.28	11	2
1	A	260	HIS	CB-CG-CD2	-5.91	123.52	131.20	15	3
1	A	145	HIS	CB-CG-CD2	-5.79	123.67	131.20	15	5
1	A	272	GLU	N-CA-C	5.73	116.65	108.74	16	1
1	A	298	ARG	CA-C-N	5.72	132.47	121.54	21	1
1	A	298	ARG	C-N-CA	5.72	132.47	121.54	21	1
1	A	279	GLN	CA-C-N	5.72	132.46	121.54	26	1
1	A	279	GLN	C-N-CA	5.72	132.46	121.54	26	1
1	A	185	ASP	CA-CB-CG	5.71	118.31	112.60	2	1
1	A	262	ILE	N-CA-C	5.70	112.31	106.21	19	1
1	A	208	ASP	N-CA-C	5.67	116.03	108.38	1	1
1	A	220	PHE	CA-CB-CG	5.66	119.46	113.80	13	4
1	A	272	GLU	CA-C-N	5.63	132.30	121.54	22	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	272	GLU	C-N-CA	5.63	132.30	121.54	22	2
1	A	145	HIS	CA-C-N	5.62	128.38	120.28	26	2
1	A	145	HIS	C-N-CA	5.62	128.38	120.28	26	2
1	A	260	HIS	CA-C-N	5.59	128.33	120.28	25	1
1	A	260	HIS	C-N-CA	5.59	128.33	120.28	25	1
1	A	231	ARG	CD-NE-CZ	5.56	132.18	124.40	20	2
1	A	168	HIS	CA-CB-CG	5.54	119.34	113.80	26	3
1	A	268	GLY	CA-C-N	5.53	125.19	119.05	3	1
1	A	268	GLY	C-N-CA	5.53	125.19	119.05	3	1
1	A	297	TYR	CA-C-N	5.53	127.69	120.28	29	1
1	A	297	TYR	C-N-CA	5.53	127.69	120.28	29	1
1	A	261	THR	CA-C-N	5.53	131.91	121.97	8	1
1	A	261	THR	C-N-CA	5.53	131.91	121.97	8	1
1	A	188	ASP	CA-CB-CG	5.50	118.10	112.60	11	2
1	A	167	THR	CA-CB-CG2	5.47	119.81	110.50	10	1
1	A	206	GLU	CA-C-N	5.47	131.99	121.54	27	2
1	A	206	GLU	C-N-CA	5.47	131.99	121.54	27	2
1	A	293	HIS	CB-CG-CD2	-5.45	124.12	131.20	23	4
1	A	167	THR	CA-C-N	5.44	131.93	121.54	14	1
1	A	167	THR	C-N-CA	5.44	131.93	121.54	14	1
1	A	284	GLY	CA-C-N	5.40	127.78	120.44	4	1
1	A	284	GLY	C-N-CA	5.40	127.78	120.44	4	1
1	A	158	GLN	OE1-CD-NE2	-5.34	117.25	122.60	21	4
1	A	270	ASP	CA-CB-CG	-5.33	107.27	112.60	5	1
1	A	194	PRO	CA-C-N	5.28	128.21	120.71	9	1
1	A	194	PRO	C-N-CA	5.28	128.21	120.71	9	1
1	A	177	LEU	CA-C-N	5.25	127.26	120.44	30	1
1	A	177	LEU	C-N-CA	5.25	127.26	120.44	30	1
1	A	184	VAL	CA-C-N	5.21	127.53	120.65	21	1
1	A	184	VAL	C-N-CA	5.21	127.53	120.65	21	1
1	A	155	TYR	CA-C-N	5.19	128.22	120.90	3	1
1	A	155	TYR	C-N-CA	5.19	128.22	120.90	3	1
1	A	205	PRO	N-CA-CB	5.15	106.15	102.65	11	1
1	A	216	TYR	CA-C-N	5.05	127.02	120.70	26	1
1	A	216	TYR	C-N-CA	5.05	127.02	120.70	26	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	207	ARG	Sidechain,Peptide	8
1	A	169	CYS	Peptide	7
1	A	231	ARG	Sidechain	5
1	A	241	TYR	Sidechain	4
1	A	260	HIS	Sidechain,Peptide	4
1	A	298	ARG	Sidechain	3
1	A	170	PRO	Peptide	3
1	A	168	HIS	Sidechain,Peptide	2
1	A	153	LYS	Peptide	2
1	A	149	ARG	Sidechain	2
1	A	229	GLY	Peptide	2
1	A	295	ARG	Sidechain	2
1	A	244	TYR	Sidechain	2
1	A	203	ILE	Peptide	1
1	A	154	ASP	Peptide	1
1	A	165	GLY	Peptide	1
1	A	242	ARG	Sidechain	1
1	A	190	ILE	Peptide	1
1	A	208	ASP	Peptide	1
1	A	157	GLY	Peptide	1
1	A	167	THR	Peptide	1
1	A	228	THR	Peptide	1
1	A	139	PRO	Peptide	1
1	A	195	ASP	Peptide	1
1	A	141	SER	Peptide	1
1	A	151	THR	Peptide	1
1	A	171	ASP	Peptide	1
1	A	282	ARG	Peptide	1
1	A	258	VAL	Peptide	1
1	A	268	GLY	Peptide	1
1	A	175	GLU	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	1226	1202	1201	2±1
All	All	36810	36060	36031	64

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 1.

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	0.65	2.27	11	1
1:A:173:CYS:SG	1:A:260:HIS:CE1	0.63	2.92	23	22
1:A:180:MET:SD	1:A:264:MET:HE2	0.62	2.34	16	1
1:A:161:LEU:HD22	1:A:264:MET:HE1	0.58	1.75	26	1
1:A:161:LEU:HD12	1:A:264:MET:HE3	0.52	1.80	27	1
1:A:150:LYS:HE2	1:A:155:TYR:CE2	0.51	2.40	25	1
1:A:150:LYS:HE3	1:A:154:ASP:HB2	0.50	1.83	29	1
1:A:232:GLU:H	1:A:232:GLU:CD	0.50	2.15	14	2
1:A:171:ASP:CG	1:A:172:VAL:H	0.48	2.15	4	2
1:A:182:GLN:C	1:A:283:LYS:HE2	0.48	2.34	4	2
1:A:166:PHE:CG	1:A:167:THR:N	0.47	2.81	23	1
1:A:211:GLU:H	1:A:211:GLU:CD	0.47	2.18	30	1
1:A:290:ILE:HG22	1:A:294:MET:HE2	0.46	1.88	5	1
1:A:180:MET:SD	1:A:264:MET:HE1	0.46	2.50	27	2
1:A:180:MET:HG2	1:A:264:MET:HE2	0.46	1.87	13	1
1:A:150:LYS:HE3	1:A:154:ASP:CB	0.46	2.40	29	1
1:A:166:PHE:H	1:A:260:HIS:CD2	0.45	2.29	26	1
1:A:186:GLU:CD	1:A:283:LYS:HZ2	0.45	2.20	16	1
1:A:169:CYS:SG	1:A:260:HIS:CD2	0.45	3.10	26	3
1:A:231:ARG:HE	1:A:232:GLU:CD	0.44	2.20	8	1
1:A:180:MET:CG	1:A:264:MET:HE2	0.44	2.42	13	1
1:A:166:PHE:CZ	1:A:260:HIS:CD2	0.44	3.06	8	1
1:A:262:ILE:HD11	1:A:279:GLN:HE21	0.44	1.71	13	1
1:A:180:MET:HE1	1:A:264:MET:SD	0.44	2.53	2	1
1:A:182:GLN:CB	1:A:283:LYS:HE3	0.43	2.43	8	1
1:A:243:VAL:HG22	1:A:244:TYR:H	0.43	1.74	2	1
1:A:182:GLN:CB	1:A:283:LYS:HE2	0.43	2.44	2	1
1:A:207:ARG:HD3	1:A:207:ARG:H	0.43	1.74	14	1
1:A:172:VAL:HG23	1:A:260:HIS:CE1	0.42	2.50	30	1
1:A:232:GLU:CD	1:A:232:GLU:N	0.42	2.78	14	1
1:A:176:GLU:HA	1:A:179:LYS:HE3	0.41	1.91	17	1
1:A:161:LEU:HG	1:A:264:MET:HE1	0.41	1.91	14	1
1:A:273:PHE:CG	1:A:274:LEU:N	0.41	2.88	5	1
1:A:150:LYS:HE3	1:A:155:TYR:CD2	0.41	2.51	23	1
1:A:171:ASP:CG	1:A:172:VAL:N	0.40	2.78	4	1
1:A:206:GLU:CD	1:A:206:GLU:H	0.40	2.24	8	1
1:A:199:LEU:C	1:A:199:LEU:HD12	0.40	2.42	6	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	152/173 (88%)	128±4 (84±3%)	18±4 (12±2%)	6±2 (4±1%)	4	32
All	All	4560/5190 (88%)	3842 (84%)	550 (12%)	168 (4%)	4	32

All 47 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	242	ARG	14
1	A	262	ILE	10
1	A	279	GLN	7
1	A	168	HIS	7
1	A	207	ARG	7
1	A	206	GLU	7
1	A	298	ARG	6
1	A	221	SER	6
1	A	270	ASP	6
1	A	296	PRO	6
1	A	167	THR	5
1	A	229	GLY	5
1	A	258	VAL	5
1	A	166	PHE	5
1	A	280	ASN	5
1	A	170	PRO	4
1	A	240	ALA	4
1	A	257	ILE	4
1	A	171	ASP	4
1	A	243	VAL	3
1	A	261	THR	3
1	A	208	ASP	3
1	A	274	LEU	3
1	A	273	PHE	3
1	A	157	GLY	3
1	A	139	PRO	2
1	A	278	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	194	PRO	2
1	A	169	CYS	2
1	A	269	PRO	2
1	A	203	ILE	2
1	A	282	ARG	2
1	A	205	PRO	2
1	A	191	THR	2
1	A	148	GLU	2
1	A	272	GLU	2
1	A	209	THR	1
1	A	182	GLN	1
1	A	204	ASP	1
1	A	173	CYS	1
1	A	281	LYS	1
1	A	192	THR	1
1	A	156	LEU	1
1	A	195	ASP	1
1	A	241	TYR	1
1	A	283	LYS	1
1	A	175	GLU	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	135/153 (88%)	123±2 (91±2%)	12±2 (9±2%)	11	56
All	All	4050/4590 (88%)	3676 (91%)	374 (9%)	11	56

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	207	ARG	18
1	A	148	GLU	14
1	A	150	LYS	14
1	A	259	ASP	12
1	A	149	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	178	GLU	10
1	A	274	LEU	9
1	A	262	ILE	8
1	A	177	LEU	8
1	A	210	LYS	8
1	A	153	LYS	7
1	A	266	LEU	7
1	A	158	GLN	7
1	A	145	HIS	7
1	A	187	ILE	6
1	A	206	GLU	6
1	A	219	GLU	6
1	A	143	THR	6
1	A	175	GLU	6
1	A	242	ARG	6
1	A	224	LEU	6
1	A	298	ARG	6
1	A	167	THR	5
1	A	181	ILE	5
1	A	188	ASP	5
1	A	261	THR	5
1	A	264	MET	5
1	A	297	TYR	5
1	A	169	CYS	5
1	A	280	ASN	5
1	A	281	LYS	5
1	A	202	SER	5
1	A	191	THR	4
1	A	208	ASP	4
1	A	146	THR	4
1	A	179	LYS	4
1	A	289	SER	4
1	A	172	VAL	4
1	A	283	LYS	4
1	A	195	ASP	4
1	A	151	THR	4
1	A	294	MET	3
1	A	144	THR	3
1	A	218	LYS	3
1	A	171	ASP	3
1	A	199	LEU	3
1	A	230	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	161	LEU	3
1	A	192	THR	3
1	A	196	LEU	3
1	A	211	GLU	3
1	A	231	ARG	3
1	A	285	GLU	3
1	A	243	VAL	2
1	A	270	ASP	2
1	A	154	ASP	2
1	A	166	PHE	2
1	A	204	ASP	2
1	A	277	PHE	2
1	A	245	TYR	2
1	A	258	VAL	2
1	A	272	GLU	2
1	A	140	PHE	2
1	A	162	ILE	2
1	A	216	TYR	2
1	A	173	CYS	2
1	A	203	ILE	2
1	A	200	PHE	2
1	A	225	VAL	2
1	A	176	GLU	2
1	A	221	SER	2
1	A	232	GLU	2
1	A	237	VAL	2
1	A	142	LEU	2
1	A	209	THR	2
1	A	217	VAL	2
1	A	201	ILE	2
1	A	265	TYR	2
1	A	152	ASP	1
1	A	239	ARG	1
1	A	263	ILE	1
1	A	163	TYR	1
1	A	235	ASP	1
1	A	180	MET	1
1	A	234	VAL	1
1	A	185	ASP	1
1	A	155	TYR	1
1	A	267	ILE	1
1	A	227	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	193	LEU	1
1	A	223	LYS	1
1	A	233	GLU	1
1	A	168	HIS	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