



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:00 pm GMT

PDB ID : 2GT5
Title : Solution structure of apo Human Sco1
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Deposited on : 2006-04-27

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

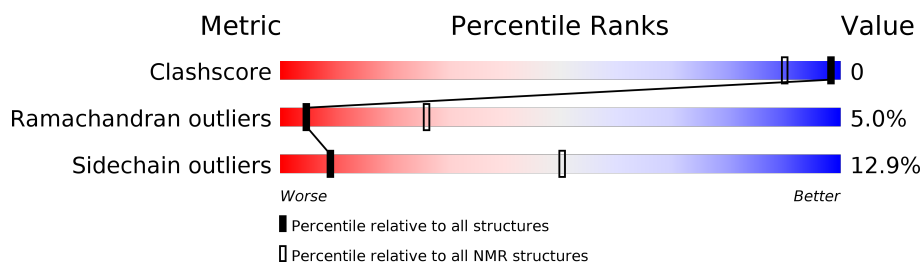
1 Overall quality at a glance

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	

2 Ensemble composition and analysis

This entry contains 30 models. Model 20 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:167, A:173-A:245, A:263-A:301 (142)	1.05	20

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2751 atoms, of which 1362 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
			2751	890	1362	224	270	5	

There are 3 discrepancies between the modelled and reference sequences:

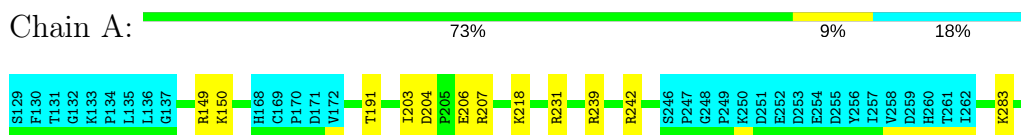
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	CLONING ARTIFACT	UNP O75880
A	130	PHE	-	CLONING ARTIFACT	UNP O75880
A	131	THR	-	CLONING ARTIFACT	UNP O75880

4 Residue-property plots

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

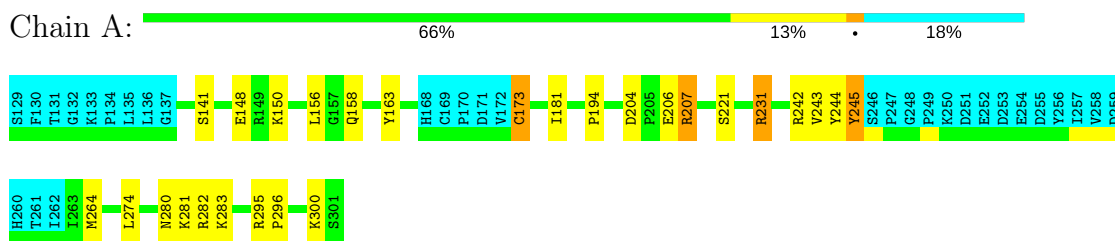


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

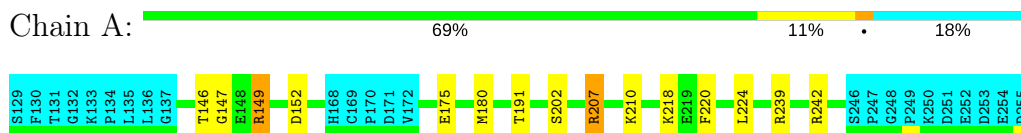
4.2.1 Score per residue for model 1

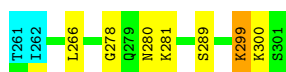
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.2 Score per residue for model 2

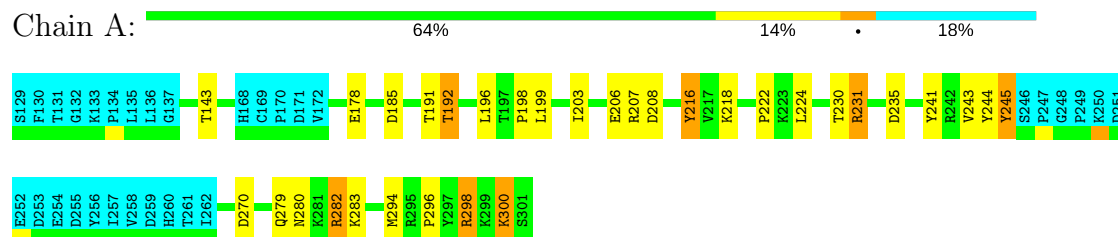
- Molecule 1: SCO1 protein homolog, mitochondrial





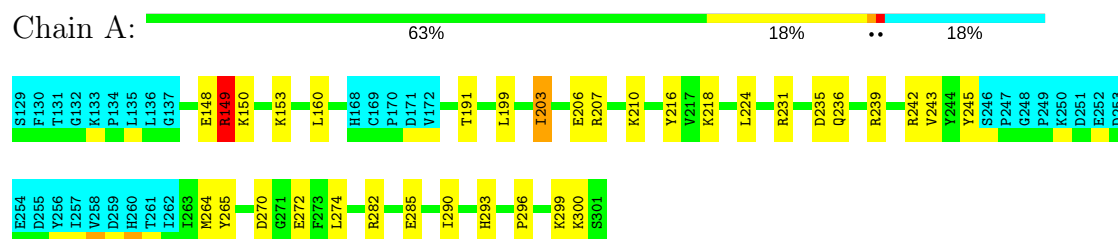
4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial



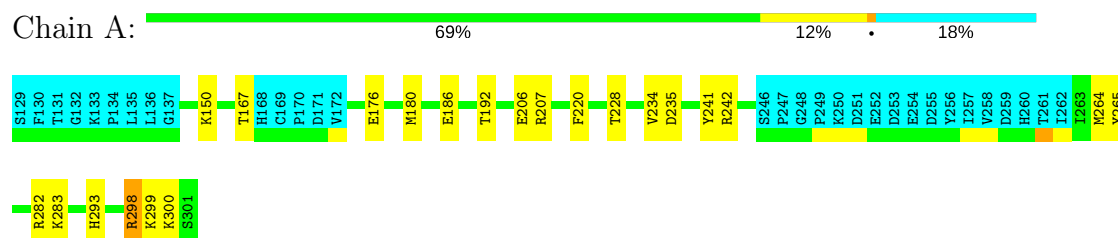
4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.5 Score per residue for model 5

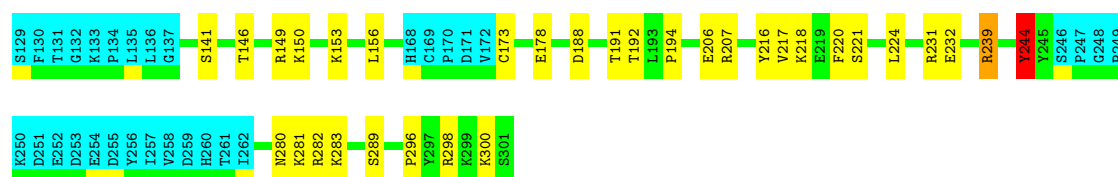
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.6 Score per residue for model 6

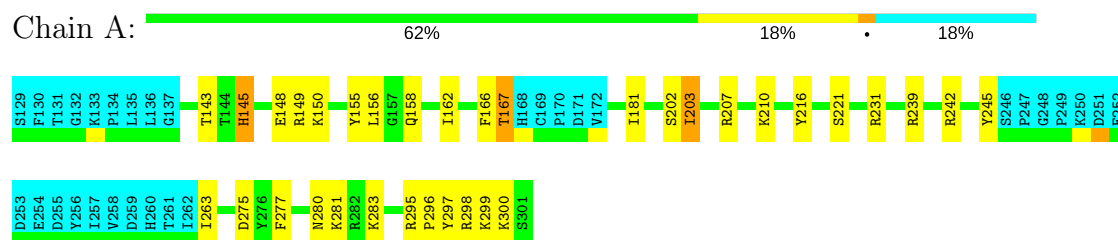
- Molecule 1: SCO1 protein homolog, mitochondrial





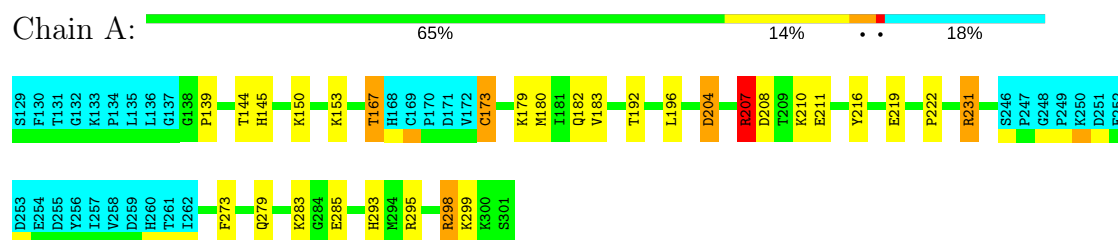
4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial



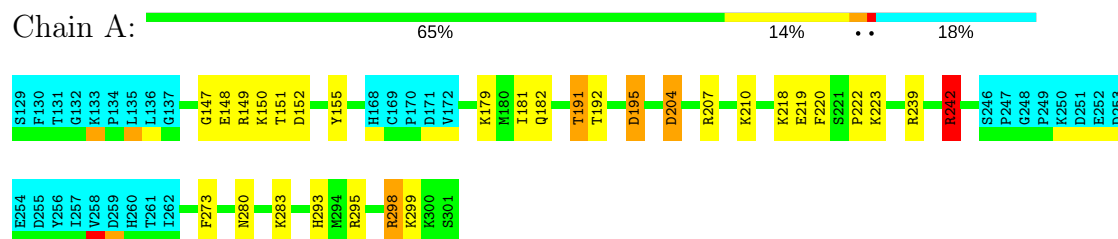
4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial



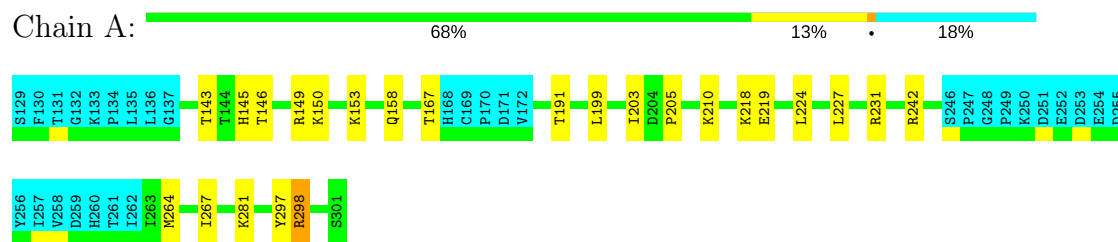
4.2.9 Score per residue for model 9

- Molecule 1: SCO1 protein homolog, mitochondrial



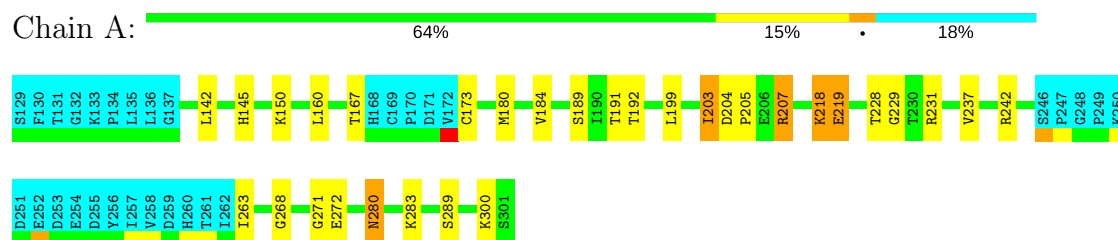
4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial



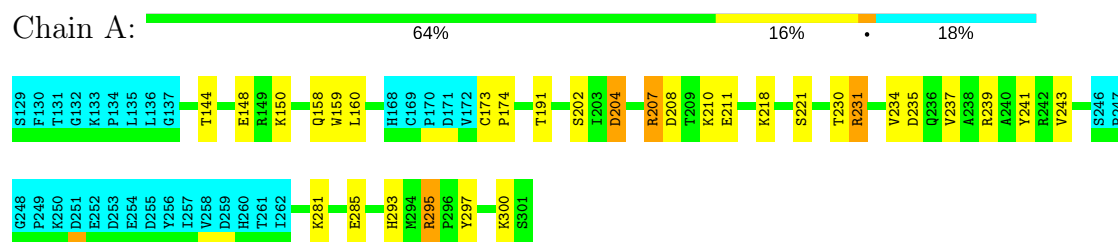
4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



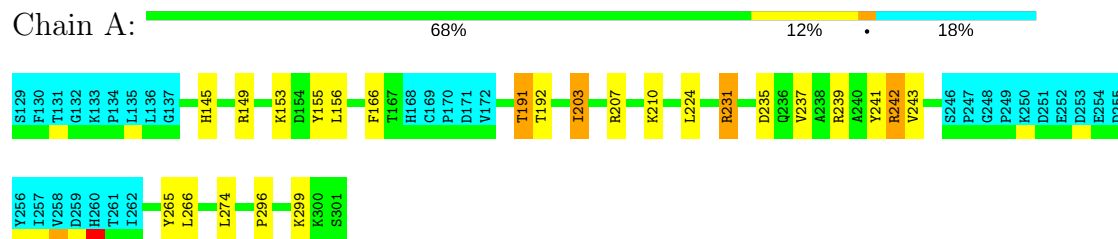
4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



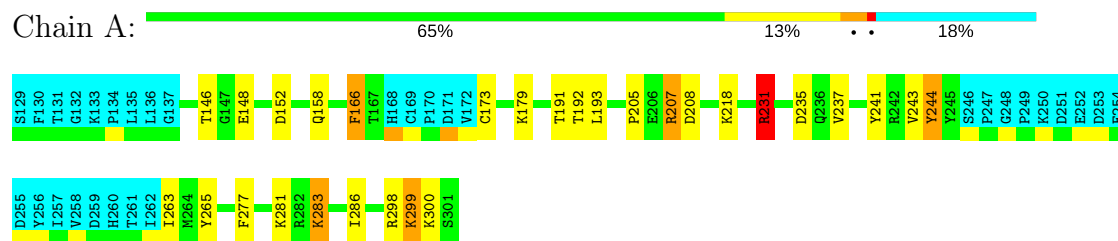
4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial



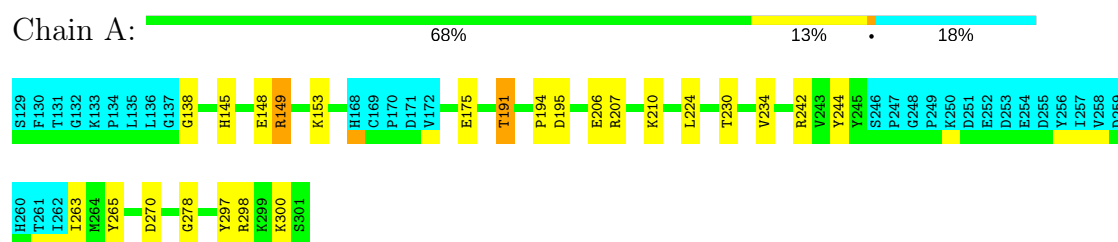
4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



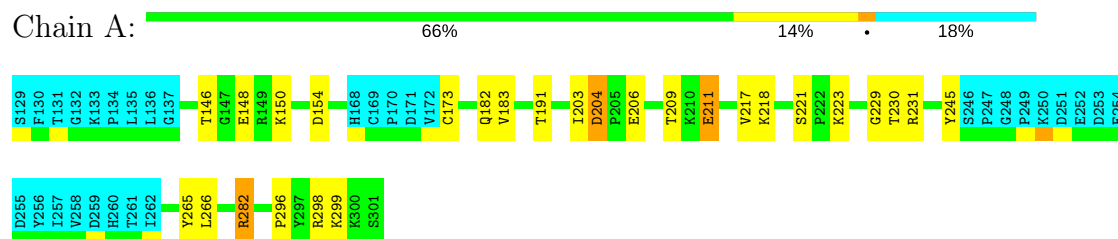
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



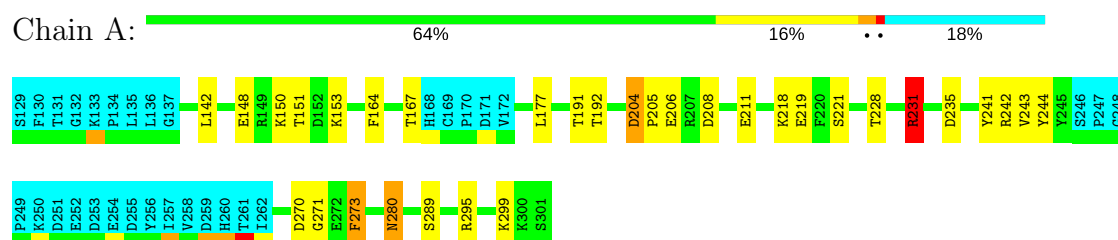
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



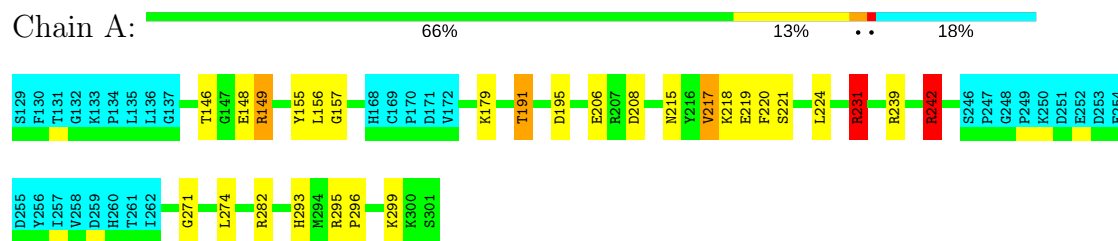
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



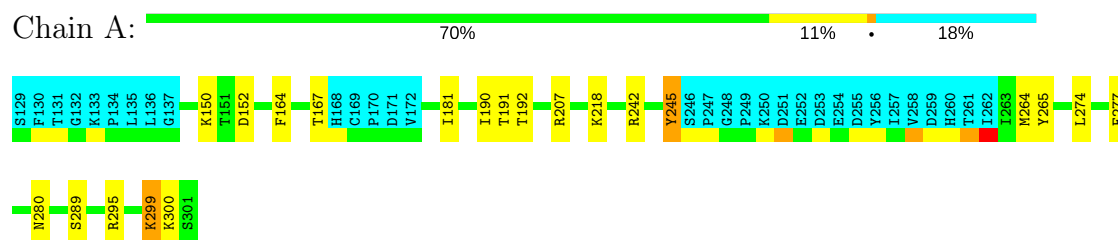
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



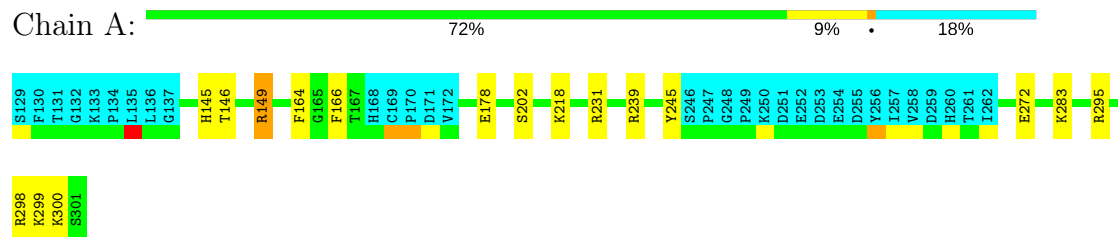
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



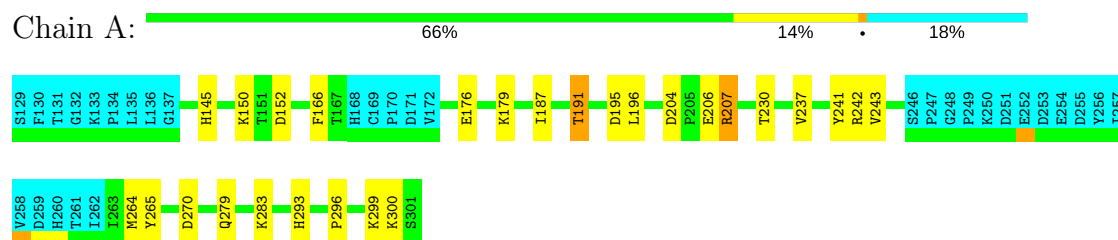
4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: SCO1 protein homolog, mitochondrial



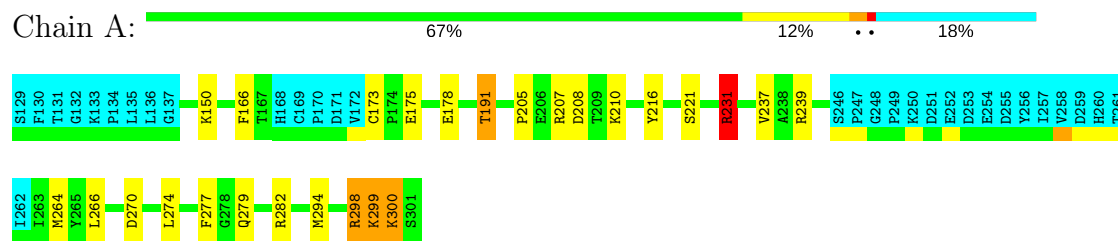
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



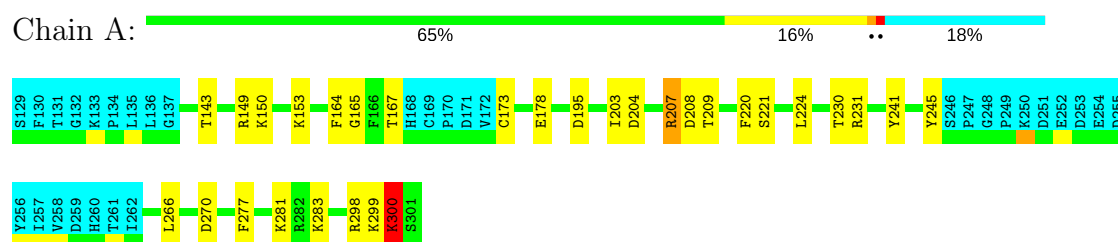
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



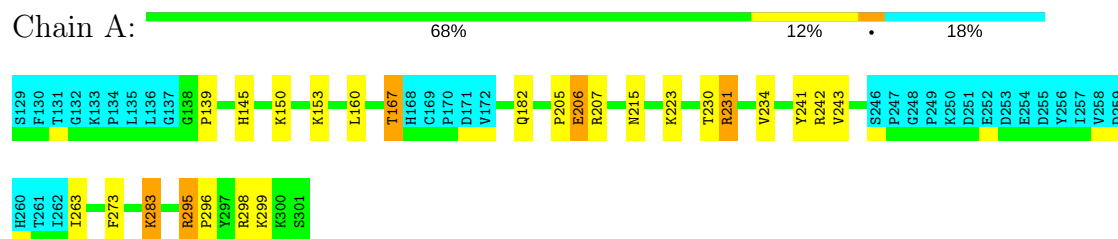
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



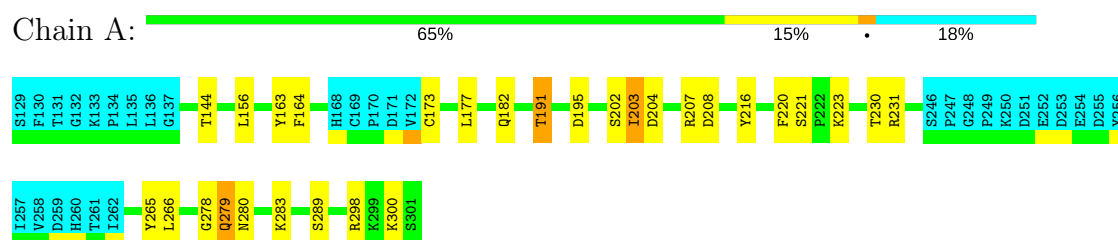
4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



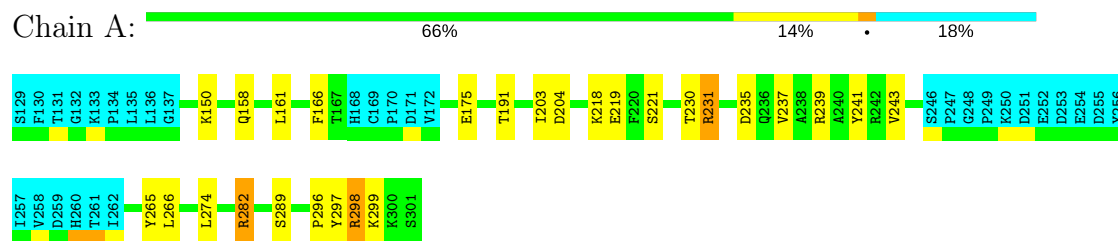
4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



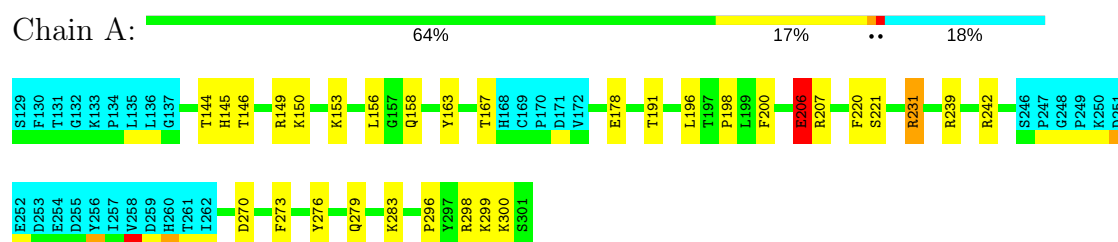
4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



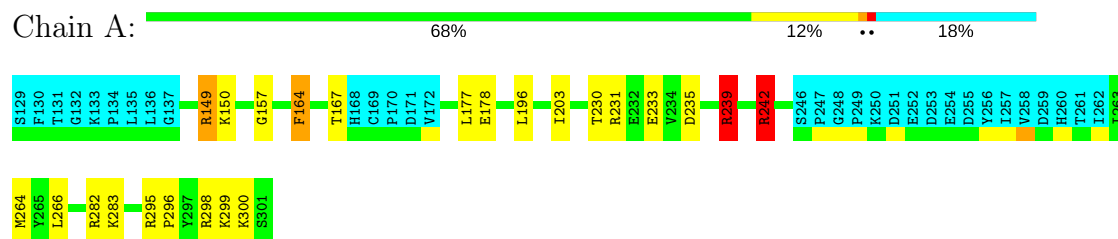
4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



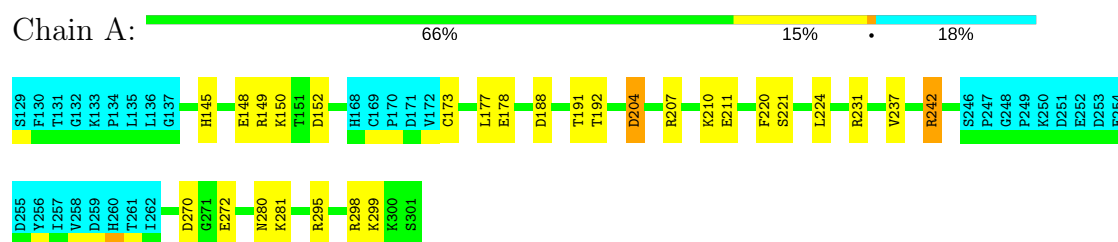
4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial



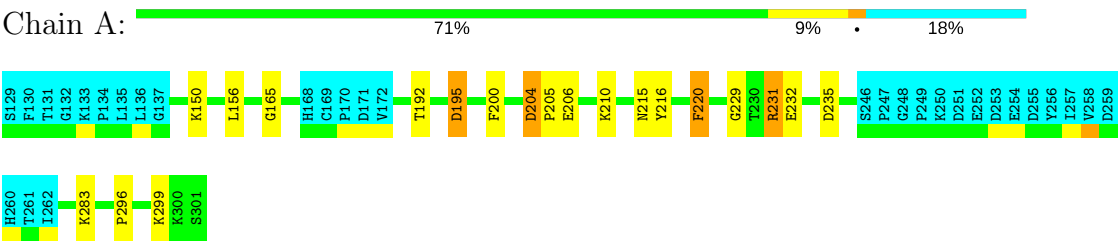
4.2.29 Score per residue for model 29

- 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/1179 (0.0±0.0%)	1.13±0.04	4±2/1594 (0.3±0.1%)
All	All	0.73	0/35370 (0.0%)	1.13	121/47820 (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	3.7±1.7
All	All	0	112

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	298	ARG	NE-CZ-NH1	12.74	126.67	120.30	22	12
1	A	207	ARG	NE-CZ-NH1	12.15	126.37	120.30	21	10
1	A	242	ARG	NE-CZ-NH1	10.77	125.68	120.30	28	10
1	A	231	ARG	NE-CZ-NH1	9.72	125.16	120.30	27	22
1	A	231	ARG	NE-CZ-NH2	-9.25	115.67	120.30	4	8
1	A	149	ARG	NE-CZ-NH1	8.39	124.49	120.30	2	8
1	A	149	ARG	NE-CZ-NH2	8.30	124.45	120.30	23	3
1	A	282	ARG	NE-CZ-NH1	7.20	123.90	120.30	22	6
1	A	166	PHE	CB-CG-CD2	-7.05	115.86	120.80	14	1
1	A	207	ARG	NE-CZ-NH2	-6.86	116.87	120.30	4	3
1	A	239	ARG	NE-CZ-NH2	6.82	123.71	120.30	28	4
1	A	207	ARG	CD-NE-CZ	6.60	132.84	123.60	21	1
1	A	239	ARG	NE-CZ-NH1	6.52	123.56	120.30	4	8
1	A	298	ARG	CD-NE-CZ	6.48	132.68	123.60	22	1
1	A	231	ARG	CD-NE-CZ	6.48	132.68	123.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	244	TYR	CB-CG-CD2	-6.42	117.14	121.00	6	1
1	A	242	ARG	CD-NE-CZ	6.32	132.45	123.60	28	1
1	A	282	ARG	NE-CZ-NH2	-6.13	117.23	120.30	3	1
1	A	295	ARG	NE-CZ-NH1	6.09	123.35	120.30	12	5
1	A	166	PHE	CB-CG-CD1	6.06	125.04	120.80	14	1
1	A	216	TYR	CB-CG-CD2	-5.87	117.48	121.00	3	1
1	A	149	ARG	CD-NE-CZ	5.57	131.40	123.60	2	1
1	A	155	TYR	CB-CG-CD2	-5.55	117.67	121.00	18	1
1	A	298	ARG	NE-CZ-NH2	-5.46	117.57	120.30	22	2
1	A	242	ARG	NE-CZ-NH2	-5.46	117.57	120.30	4	1
1	A	166	PHE	CA-CB-CG	5.45	126.97	113.90	14	1
1	A	280	ASN	C-N-CA	5.32	135.01	121.70	2	1
1	A	282	ARG	CD-NE-CZ	5.29	131.01	123.60	3	1
1	A	242	ARG	CA-CB-CG	5.27	125.00	113.40	28	1
1	A	191	THR	CA-CB-CG2	5.17	119.64	112.40	21	1
1	A	278	GLY	C-N-CA	5.16	134.59	121.70	25	1
1	A	245	TYR	CB-CG-CD2	-5.04	117.98	121.00	1	1
1	A	164	PHE	CB-CG-CD2	-5.03	117.28	120.80	28	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	204	ASP	Peptide	10
1	A	207	ARG	Sidechain,Peptide	6
1	A	220	PHE	Peptide,Sidechain	6
1	A	300	LYS	Peptide	5
1	A	206	GLU	Peptide	5
1	A	231	ARG	Sidechain	4
1	A	239	ARG	Sidechain,Peptide	4
1	A	298	ARG	Sidechain,Peptide	4
1	A	203	ILE	Peptide	4
1	A	167	THR	Peptide	4
1	A	229	GLY	Peptide	3
1	A	164	PHE	Peptide,Sidechain	3
1	A	245	TYR	Peptide	3
1	A	242	ARG	Peptide,Sidechain	3
1	A	195	ASP	Peptide	3
1	A	202	SER	Peptide	2
1	A	157	GLY	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	165	GLY	Peptide	2
1	A	149	ARG	Peptide,Sidechain	2
1	A	163	TYR	Sidechain	2
1	A	191	THR	Peptide	2
1	A	278	GLY	Peptide	2
1	A	139	PRO	Peptide	2
1	A	299	LYS	Peptide	2
1	A	166	PHE	Peptide	2
1	A	208	ASP	Peptide	2
1	A	216	TYR	Sidechain	1
1	A	295	ARG	Sidechain	1
1	A	205	PRO	Peptide	1
1	A	297	TYR	Sidechain	1
1	A	243	VAL	Peptide	1
1	A	277	PHE	Peptide	1
1	A	282	ARG	Peptide	1
1	A	265	TYR	Sidechain	1
1	A	146	THR	Peptide	1
1	A	217	VAL	Peptide	1
1	A	194	PRO	Peptide	1
1	A	182	GLN	Peptide	1
1	A	158	GLN	Peptide	1
1	A	275	ASP	Peptide	1
1	A	235	ASP	Peptide	1
1	A	241	TYR	Sidechain	1
1	A	271	GLY	Peptide	1
1	A	222	PRO	Peptide	1
1	A	244	TYR	Peptide	1
1	A	228	THR	Peptide	1
1	A	280	ASN	Peptide	1
1	A	151	THR	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	1152	1141	1141	1±1
All	All	34560	34230	34230	19

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:196:LEU:H	1:A:196:LEU:HD23	0.48	1.67	21	1
1:A:231:ARG:H	1:A:231:ARG:CD	0.48	2.20	14	1
1:A:149:ARG:HH12	1:A:233:GLU:CD	0.47	2.12	28	1
1:A:180:MET:O	1:A:183:VAL:HG22	0.47	2.09	8	1
1:A:159:TRP:CZ3	1:A:293:HIS:CE1	0.45	3.04	12	1
1:A:200:PHE:CE2	1:A:216:TYR:CE1	0.45	3.04	30	1
1:A:195:ASP:CG	1:A:223:LYS:HZ2	0.44	2.15	9	1
1:A:143:THR:HG23	1:A:210:LYS:HE2	0.43	1.90	7	1
1:A:277:PHE:CE1	1:A:281:LYS:HE3	0.43	2.48	7	1
1:A:196:LEU:HD23	1:A:196:LEU:H	0.43	1.73	8	1
1:A:146:THR:HG23	1:A:147:GLY:H	0.43	1.74	2	1
1:A:210:LYS:HE3	1:A:211:GLU:OE2	0.42	2.15	12	1
1:A:218:LYS:HZ2	1:A:219:GLU:CD	0.42	2.18	11	1
1:A:181:ILE:HD12	1:A:222:PRO:CG	0.42	2.44	9	1
1:A:203:ILE:HD13	1:A:203:ILE:H	0.42	1.75	13	1
1:A:277:PHE:CZ	1:A:286:ILE:HG23	0.42	2.49	14	1
1:A:182:GLN:CB	1:A:283:LYS:HE3	0.41	2.46	24	1
1:A:143:THR:HB	1:A:210:LYS:HE2	0.40	1.92	10	1
1:A:211:GLU:CD	1:A:211:GLU:H	0.40	2.20	16	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	141/173 (82%)	115±4 (82±3%)	19±3 (13±2%)	7±3 (5±2%)	5	26
All	All	4230/5190 (82%)	3454 (82%)	566 (13%)	210 (5%)	5	26

All 54 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	21
1	A	296	PRO	14
1	A	221	SER	12
1	A	192	THR	11
1	A	243	VAL	9
1	A	173	CYS	9
1	A	207	ARG	8
1	A	241	TYR	8
1	A	205	PRO	6
1	A	299	LYS	6
1	A	204	ASP	6
1	A	242	ARG	5
1	A	206	GLU	5
1	A	281	LYS	5
1	A	270	ASP	4
1	A	283	LYS	4
1	A	203	ILE	4
1	A	231	ARG	4
1	A	245	TYR	4
1	A	167	THR	4
1	A	145	HIS	3
1	A	156	LEU	3
1	A	195	ASP	3
1	A	282	ARG	3
1	A	273	PHE	3
1	A	280	ASN	3
1	A	300	LYS	3
1	A	198	PRO	2
1	A	208	ASP	2
1	A	217	VAL	2
1	A	271	GLY	2
1	A	244	TYR	2
1	A	158	GLN	2
1	A	152	ASP	2
1	A	220	PHE	2
1	A	272	GLU	2
1	A	279	GLN	2
1	A	219	GLU	2
1	A	194	PRO	2
1	A	263	ILE	2
1	A	138	GLY	1
1	A	268	GLY	1
1	A	147	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	264	MET	1
1	A	237	VAL	1
1	A	190	ILE	1
1	A	166	PHE	1
1	A	224	LEU	1
1	A	146	THR	1
1	A	228	THR	1
1	A	174	PRO	1
1	A	274	LEU	1
1	A	222	PRO	1
1	A	298	ARG	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/153 (82%)	109±3 (87±3%)	16±3 (13±3%)	9	50
All	All	3750/4590 (82%)	3268 (87%)	482 (13%)	9	50

All 104 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	22
1	A	299	LYS	18
1	A	218	LYS	15
1	A	300	LYS	15
1	A	283	LYS	14
1	A	148	GLU	11
1	A	230	THR	10
1	A	153	LYS	10
1	A	231	ARG	10
1	A	235	ASP	9
1	A	265	TYR	9
1	A	145	HIS	9
1	A	224	LEU	9
1	A	298	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	210	LYS	9
1	A	280	ASN	8
1	A	295	ARG	8
1	A	266	LEU	8
1	A	178	GLU	8
1	A	289	SER	7
1	A	237	VAL	7
1	A	264	MET	7
1	A	203	ILE	7
1	A	149	ARG	7
1	A	207	ARG	7
1	A	242	ARG	7
1	A	274	LEU	6
1	A	293	HIS	6
1	A	206	GLU	6
1	A	216	TYR	6
1	A	167	THR	6
1	A	244	TYR	5
1	A	146	THR	5
1	A	279	GLN	5
1	A	156	LEU	5
1	A	208	ASP	5
1	A	179	LYS	5
1	A	270	ASP	5
1	A	219	GLU	5
1	A	234	VAL	4
1	A	199	LEU	4
1	A	173	CYS	4
1	A	152	ASP	4
1	A	297	TYR	4
1	A	160	LEU	4
1	A	175	GLU	4
1	A	177	LEU	4
1	A	166	PHE	4
1	A	191	THR	4
1	A	211	GLU	4
1	A	158	GLN	4
1	A	144	THR	4
1	A	204	ASP	4
1	A	181	ILE	3
1	A	285	GLU	3
1	A	220	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	202	SER	3
1	A	215	ASN	3
1	A	223	LYS	3
1	A	182	GLN	3
1	A	282	ARG	3
1	A	196	LEU	3
1	A	273	PHE	3
1	A	245	TYR	3
1	A	164	PHE	3
1	A	180	MET	3
1	A	155	TYR	3
1	A	281	LYS	3
1	A	263	ILE	3
1	A	195	ASP	2
1	A	209	THR	2
1	A	176	GLU	2
1	A	294	MET	2
1	A	143	THR	2
1	A	277	PHE	2
1	A	192	THR	2
1	A	188	ASP	2
1	A	272	GLU	2
1	A	142	LEU	2
1	A	232	GLU	2
1	A	239	ARG	2
1	A	141	SER	2
1	A	290	ILE	1
1	A	193	LEU	1
1	A	162	ILE	1
1	A	163	TYR	1
1	A	161	LEU	1
1	A	228	THR	1
1	A	185	ASP	1
1	A	267	ILE	1
1	A	200	PHE	1
1	A	227	LEU	1
1	A	186	GLU	1
1	A	236	GLN	1
1	A	187	ILE	1
1	A	217	VAL	1
1	A	221	SER	1
1	A	241	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	184	VAL	1
1	A	189	SER	1
1	A	151	THR	1
1	A	154	ASP	1
1	A	276	TYR	1
1	A	183	VAL	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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