



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 2HRN / pdb_00002hrn
Title : Solution Structure of Cu(I) P174L-HSco1
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Deposited on : 2006-07-20

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

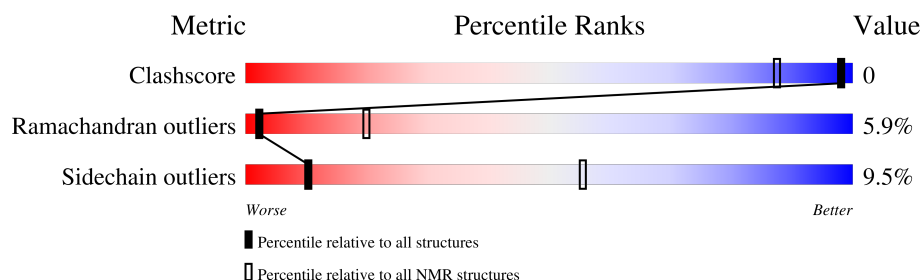
1 Overall quality at a glance

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 authors have identified model ? as representative, based on the following criterion: *minimized average structure*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:138-A:246, A:258-A:298 (150)	1.56	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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2755 atoms, of which 1364 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
			2754	891	1364	224	270	5	

There are 4 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
A	174	LEU	PRO	engineered mutation	UNP O75880

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

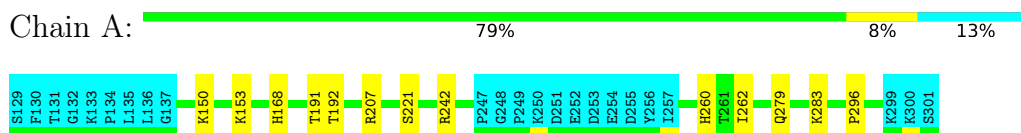
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

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

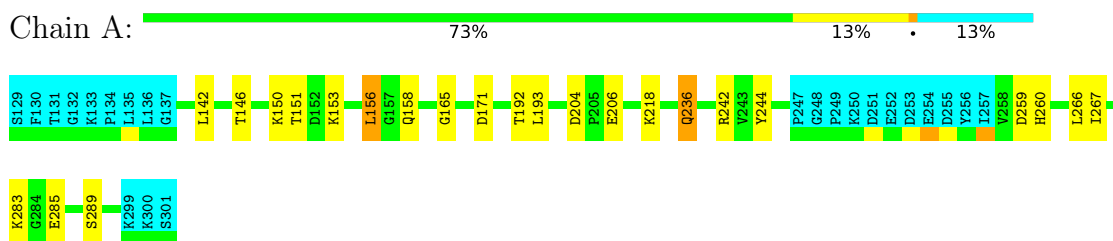


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

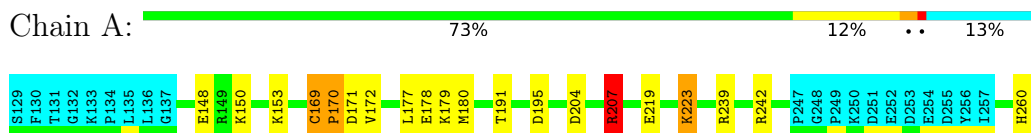
4.2.1 Score per residue for model 1

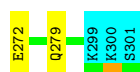
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.2 Score per residue for model 2

- Molecule 1: SCO1 protein homolog, mitochondrial

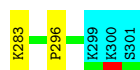
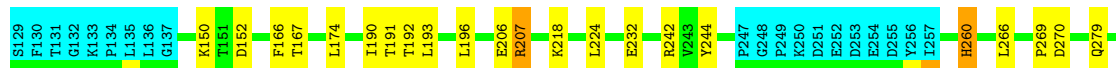




4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial

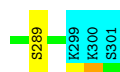
Chain A: 73% 13% • 13%



4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial

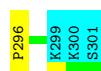
Chain A: 74% 12% • 13%



4.2.5 Score per residue for model 5

- Molecule 1: SCO1 protein homolog, mitochondrial

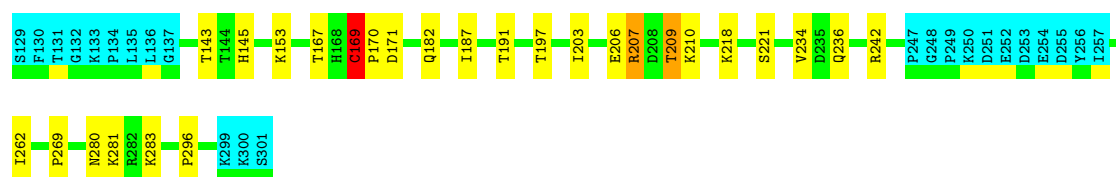
Chain A: 74% 11% • 13%



4.2.6 Score per residue for model 6 (medoid)

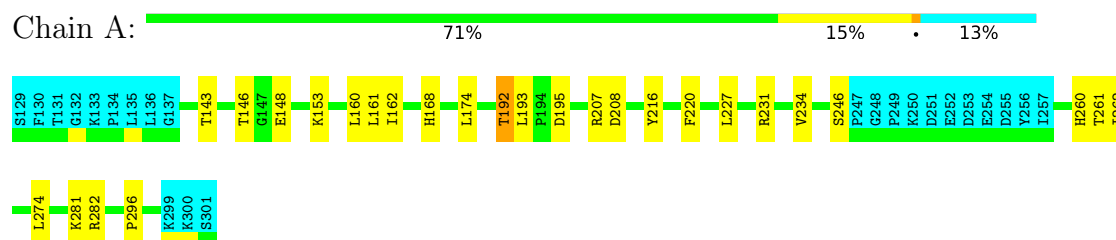
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 71% 14% • 13%



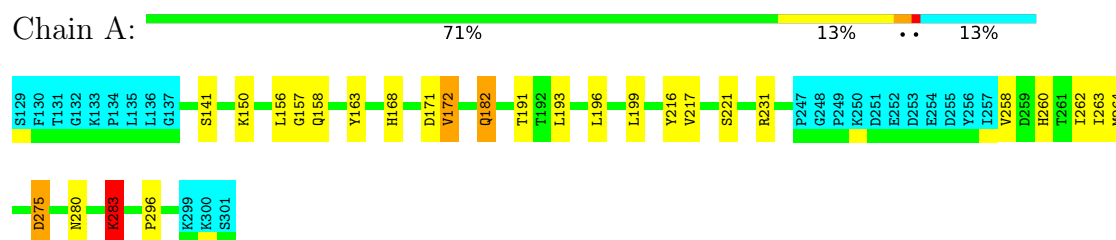
4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial



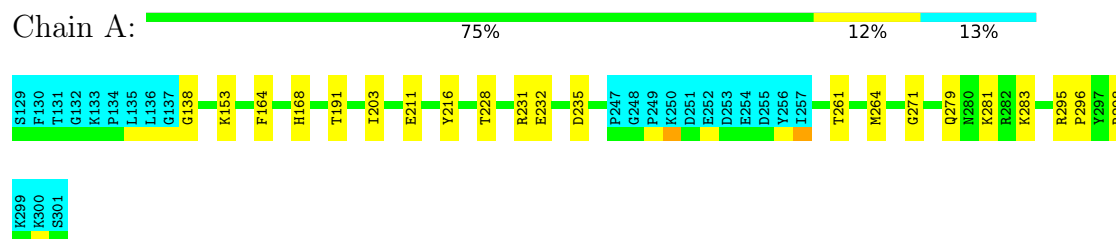
4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial



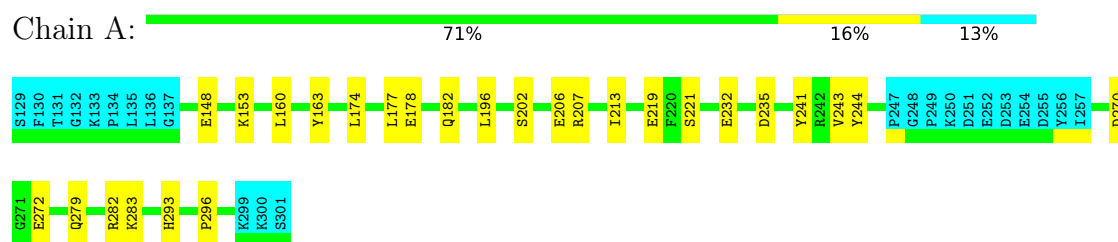
4.2.9 Score per residue for model 9

- Molecule 1: SCO1 protein homolog, mitochondrial



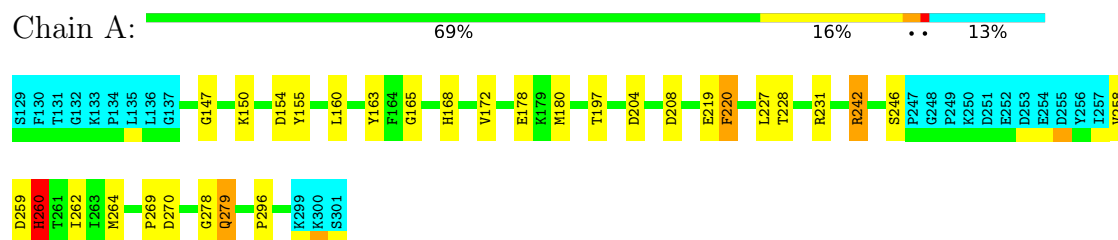
4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial



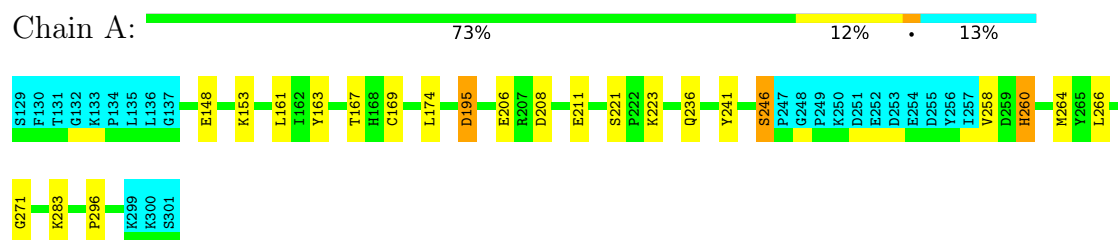
4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



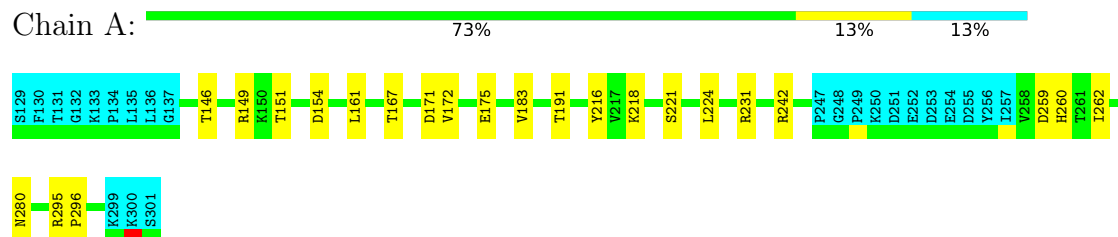
4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



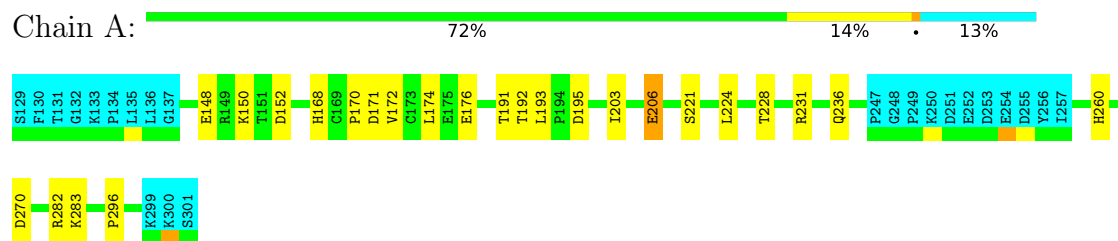
4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial



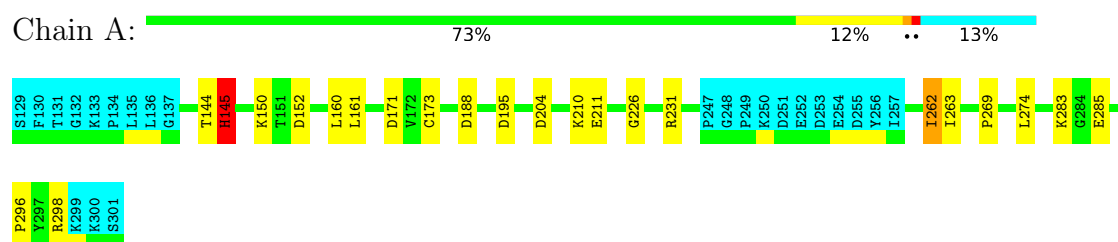
4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



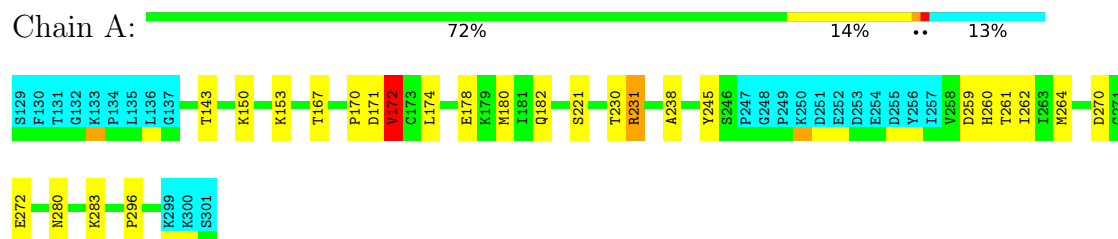
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



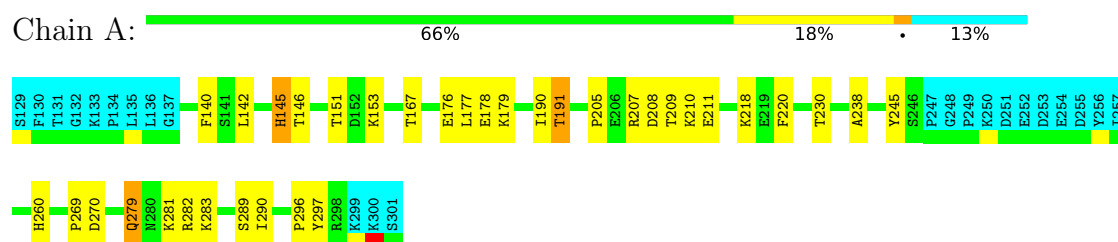
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



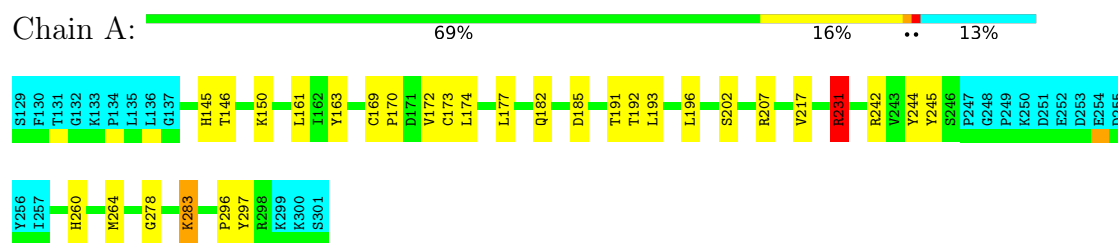
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



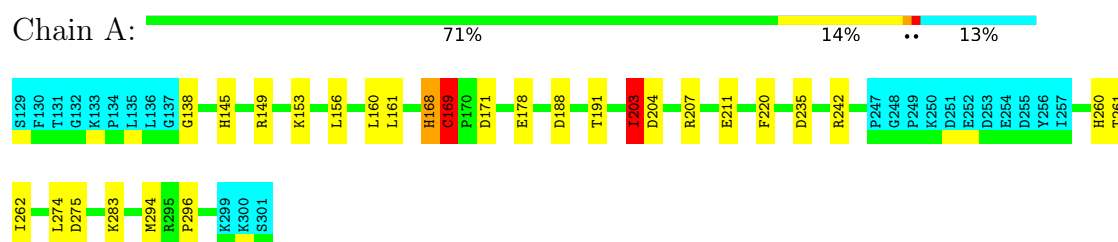
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



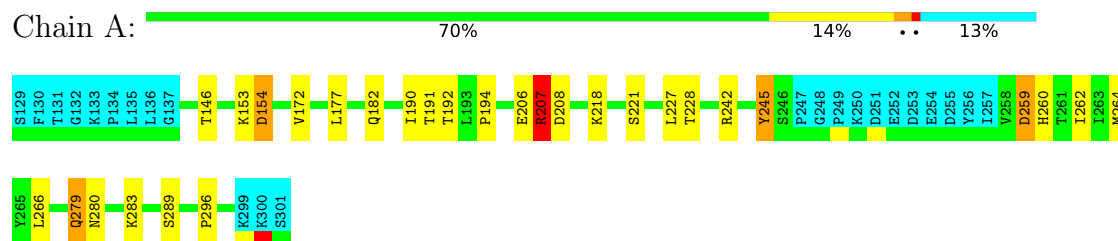
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



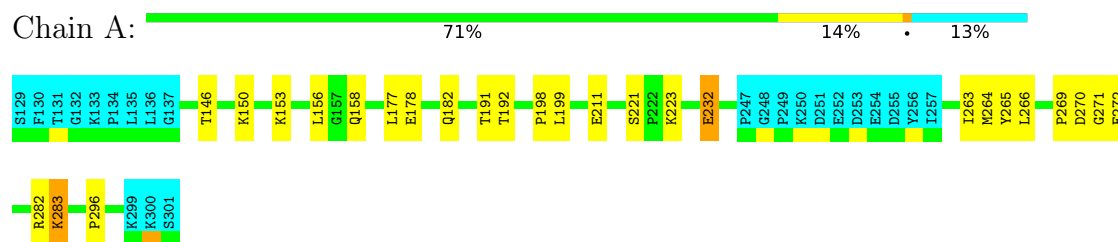
4.2.20 Score per residue for model 20

- Molecule 1: SCO1 protein homolog, mitochondrial



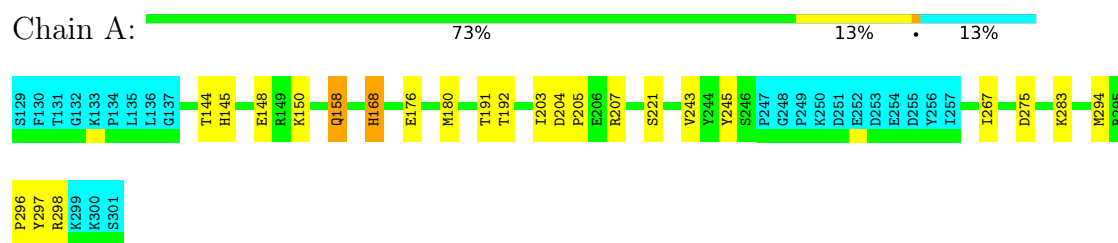
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



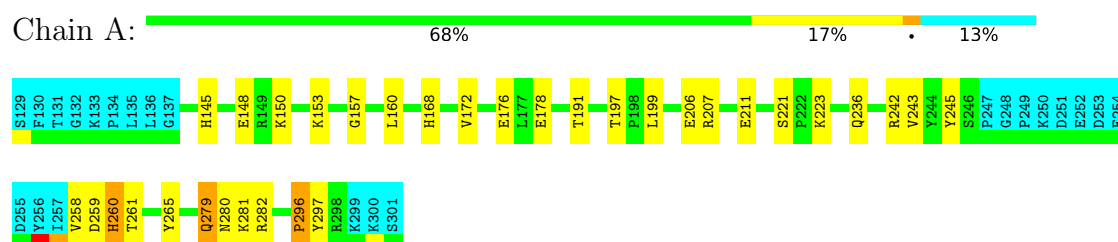
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



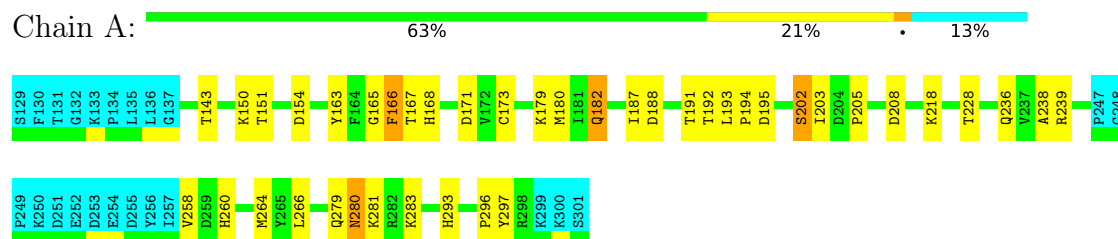
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



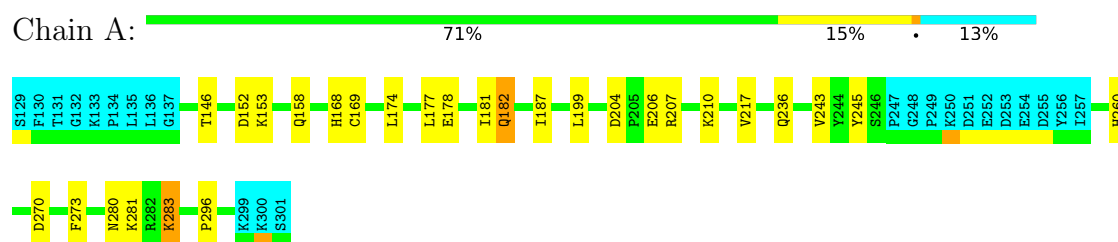
4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



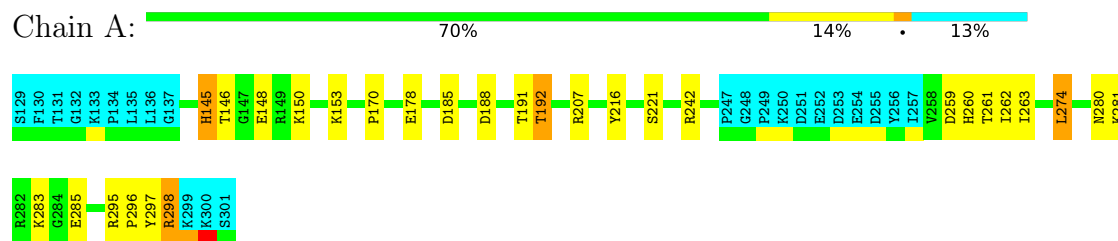
4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



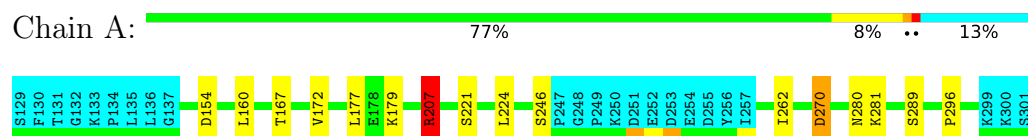
4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



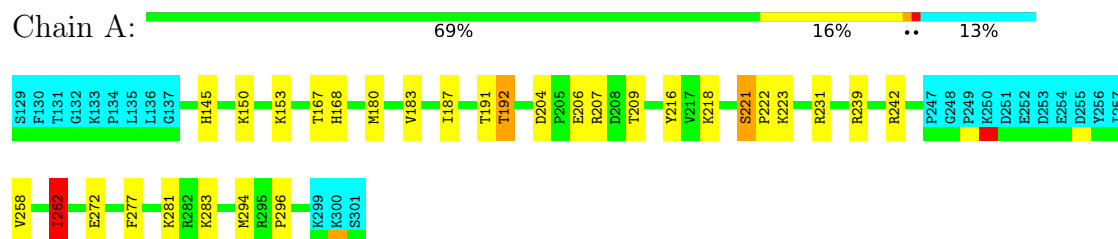
4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



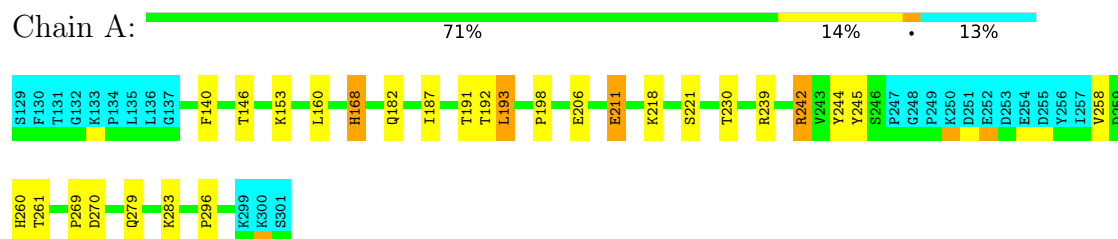
4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial



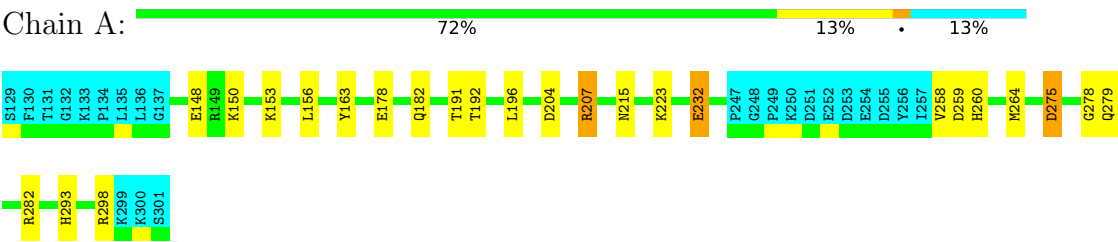
4.2.29 Score per residue for model 29

- 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.

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±0/1242 (0.0± 0.0%)	1.45±0.04	6±3/1688 (0.3± 0.1%)
All	All	0.86	0/37260 (0.0%)	1.45	176/50640 (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	2.2±1.2
All	All	0	65

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	275	ASP	CA-CB-CG	8.76	121.36	112.60	30	4
1	A	238	ALA	CA-C-N	7.44	130.86	120.29	17	3
1	A	238	ALA	C-N-CA	7.44	130.86	120.29	17	3
1	A	195	ASP	CA-CB-CG	7.39	119.99	112.60	12	1
1	A	210	LYS	CA-C-N	7.23	129.96	120.28	17	1
1	A	210	LYS	C-N-CA	7.23	129.96	120.28	17	1
1	A	154	ASP	CA-CB-CG	6.99	119.59	112.60	20	4
1	A	152	ASP	CA-CB-CG	6.98	119.58	112.60	14	2
1	A	260	HIS	CB-CG-CD2	-6.91	122.22	131.20	4	13
1	A	259	ASP	CA-CB-CG	6.78	119.38	112.60	13	2
1	A	172	VAL	CA-CB-CG2	6.78	121.92	110.40	16	1
1	A	182	GLN	OE1-CD-NE2	-6.61	115.99	122.60	10	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	171	ASP	CA-C-N	6.37	133.44	121.97	14	3
1	A	171	ASP	C-N-CA	6.37	133.44	121.97	14	3
1	A	198	PRO	N-CA-CB	6.36	106.48	102.92	29	2
1	A	145	HIS	CB-CG-CD2	-6.34	122.96	131.20	5	9
1	A	166	PHE	CA-CB-CG	6.24	120.04	113.80	24	1
1	A	259	ASP	CA-C-N	6.12	133.23	121.54	16	1
1	A	259	ASP	C-N-CA	6.12	133.23	121.54	16	1
1	A	260	HIS	CA-CB-CG	6.00	119.80	113.80	23	2
1	A	164	PHE	CA-C-N	5.95	126.28	122.18	9	1
1	A	164	PHE	C-N-CA	5.95	126.28	122.18	9	1
1	A	140	PHE	CA-CB-CG	5.94	119.74	113.80	17	1
1	A	204	ASP	CA-CB-CG	5.92	118.52	112.60	1	2
1	A	190	ILE	CA-C-N	5.88	132.78	121.54	3	2
1	A	190	ILE	C-N-CA	5.88	132.78	121.54	3	2
1	A	235	ASP	CA-CB-CG	5.81	118.41	112.60	19	2
1	A	231	ARG	CA-C-N	5.78	128.02	120.28	18	4
1	A	231	ARG	C-N-CA	5.78	128.02	120.28	18	4
1	A	271	GLY	CA-C-N	5.77	128.81	120.38	9	1
1	A	271	GLY	C-N-CA	5.77	128.81	120.38	9	1
1	A	231	ARG	CD-NE-CZ	5.74	132.44	124.40	4	3
1	A	185	ASP	CA-CB-CG	5.72	118.32	112.60	26	1
1	A	170	PRO	CA-C-N	5.72	132.46	121.54	2	2
1	A	170	PRO	C-N-CA	5.72	132.46	121.54	2	2
1	A	146	THR	CA-C-N	5.67	126.53	122.16	18	1
1	A	146	THR	C-N-CA	5.67	126.53	122.16	18	1
1	A	283	LYS	N-CA-C	5.65	119.28	112.38	21	1
1	A	221	SER	N-CA-C	5.64	116.75	109.65	28	1
1	A	258	VAL	CA-C-N	5.63	132.30	121.54	30	1
1	A	258	VAL	C-N-CA	5.63	132.30	121.54	30	1
1	A	227	LEU	CA-C-N	5.63	129.99	120.81	11	1
1	A	227	LEU	C-N-CA	5.63	129.99	120.81	11	1
1	A	293	HIS	CB-CG-CD2	-5.62	123.89	131.20	24	3
1	A	234	VAL	CA-C-N	5.62	128.26	120.29	5	1
1	A	234	VAL	C-N-CA	5.62	128.26	120.29	5	1
1	A	208	ASP	CA-CB-CG	5.58	118.18	112.60	5	1
1	A	168	HIS	CB-CG-CD2	-5.55	123.98	131.20	5	3
1	A	228	THR	CA-C-N	5.54	127.26	120.51	24	1
1	A	228	THR	C-N-CA	5.54	127.26	120.51	24	1
1	A	278	GLY	CA-C-N	5.51	132.06	121.54	30	2
1	A	278	GLY	C-N-CA	5.51	132.06	121.54	30	2
1	A	244	TYR	CA-C-N	5.49	132.02	121.54	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	244	TYR	C-N-CA	5.49	132.02	121.54	3	1
1	A	298	ARG	CA-C-N	5.48	132.00	121.54	26	1
1	A	298	ARG	C-N-CA	5.48	132.00	121.54	26	1
1	A	211	GLU	CB-CG-CD	5.46	121.88	112.60	12	1
1	A	279	GLN	OE1-CD-NE2	-5.46	117.14	122.60	11	2
1	A	236	GLN	OE1-CD-NE2	-5.39	117.21	122.60	1	2
1	A	206	GLU	CA-C-N	5.35	131.75	121.54	25	4
1	A	206	GLU	C-N-CA	5.35	131.75	121.54	25	4
1	A	187	ILE	CA-C-N	5.34	127.98	120.28	28	1
1	A	187	ILE	C-N-CA	5.34	127.98	120.28	28	1
1	A	205	PRO	N-CA-CB	5.33	105.91	102.92	22	1
1	A	188	ASP	CA-CB-CG	5.31	117.91	112.60	24	3
1	A	208	ASP	CA-C-N	5.31	128.38	120.90	7	1
1	A	208	ASP	C-N-CA	5.31	128.38	120.90	7	1
1	A	260	HIS	CA-C-N	5.31	131.68	121.54	29	1
1	A	260	HIS	C-N-CA	5.31	131.68	121.54	29	1
1	A	220	PHE	CA-CB-CG	5.30	119.10	113.80	11	1
1	A	158	GLN	OE1-CD-NE2	-5.28	117.32	122.60	25	4
1	A	202	SER	CA-C-N	5.28	131.47	121.97	24	1
1	A	202	SER	C-N-CA	5.28	131.47	121.97	24	1
1	A	279	GLN	CA-C-N	5.26	131.59	121.54	23	1
1	A	279	GLN	C-N-CA	5.26	131.59	121.54	23	1
1	A	269	PRO	CA-C-N	5.26	128.30	120.31	3	2
1	A	269	PRO	C-N-CA	5.26	128.30	120.31	3	2
1	A	179	LYS	CA-C-N	5.21	127.21	120.44	17	1
1	A	179	LYS	C-N-CA	5.21	127.21	120.44	17	1
1	A	207	ARG	CA-C-N	5.20	131.47	121.54	20	1
1	A	207	ARG	C-N-CA	5.20	131.47	121.54	20	1
1	A	207	ARG	CA-CB-CG	5.11	124.31	114.10	30	1
1	A	205	PRO	CA-C-N	5.11	127.83	120.38	17	1
1	A	205	PRO	C-N-CA	5.11	127.83	120.38	17	1
1	A	203	ILE	CA-C-N	5.08	129.26	123.21	6	1
1	A	203	ILE	C-N-CA	5.08	129.26	123.21	6	1
1	A	207	ARG	CB-CA-C	5.06	119.54	111.24	27	1
1	A	203	ILE	CB-CA-C	5.06	119.58	111.29	19	1
1	A	174	LEU	CA-C-N	5.04	127.29	120.38	3	1
1	A	174	LEU	C-N-CA	5.04	127.29	120.38	3	1
1	A	297	TYR	CA-C-N	5.04	131.16	121.54	26	2
1	A	297	TYR	C-N-CA	5.04	131.16	121.54	26	2
1	A	245	TYR	N-CA-C	5.03	117.19	110.35	17	1
1	A	262	ILE	CA-CB-CG1	5.03	118.94	110.40	28	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	169	CYS	CA-C-N	5.02	126.12	119.84	2	1
1	A	169	CYS	C-N-CA	5.02	126.12	119.84	2	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	6
1	A	269	PRO	Peptide	5
1	A	216	TYR	Sidechain	4
1	A	231	ARG	Sidechain	4
1	A	206	GLU	Peptide	3
1	A	168	HIS	Peptide	3
1	A	282	ARG	Sidechain,Peptide	3
1	A	169	CYS	Peptide	2
1	A	170	PRO	Peptide	2
1	A	241	TYR	Sidechain,Peptide	2
1	A	242	ARG	Sidechain	2
1	A	246	SER	Peptide	2
1	A	295	ARG	Sidechain	2
1	A	297	TYR	Sidechain	2
1	A	156	LEU	Peptide	1
1	A	165	GLY	Peptide	1
1	A	167	THR	Peptide	1
1	A	260	HIS	Sidechain	1
1	A	280	ASN	Peptide	1
1	A	281	LYS	Peptide	1
1	A	192	THR	Peptide	1
1	A	298	ARG	Sidechain	1
1	A	163	TYR	Sidechain	1
1	A	208	ASP	Peptide	1
1	A	271	GLY	Peptide	1
1	A	138	GLY	Peptide	1
1	A	149	ARG	Sidechain	1
1	A	194	PRO	Peptide	1
1	A	203	ILE	Peptide	1
1	A	157	GLY	Peptide	1
1	A	258	VAL	Peptide	1
1	A	296	PRO	Peptide	1
1	A	204	ASP	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	221	SER	Peptide	1
1	A	239	ARG	Sidechain	1
1	A	140	PHE	Sidechain	1
1	A	193	LEU	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	1212	1188	1187	1±1
All	All	36390	35640	35610	31

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:CD1	1:A:180:MET:HE1	0.61	2.31	24	1
1:A:203:ILE:HG23	1:A:204:ASP:H	0.54	1.63	19	1
1:A:161:LEU:CB	1:A:264:MET:HE2	0.52	2.34	18	1
1:A:211:GLU:H	1:A:211:GLU:CD	0.52	2.13	29	4
1:A:232:GLU:H	1:A:232:GLU:CD	0.51	2.14	30	3
1:A:163:TYR:HB2	1:A:264:MET:HE3	0.50	1.83	18	5
1:A:180:MET:HE2	1:A:264:MET:HE1	0.48	1.85	11	1
1:A:182:GLN:C	1:A:283:LYS:HE3	0.45	2.36	18	2
1:A:172:VAL:CG1	1:A:261:THR:HG21	0.44	2.43	16	1
1:A:180:MET:CE	1:A:264:MET:HE3	0.44	2.42	16	1
1:A:232:GLU:N	1:A:232:GLU:CD	0.44	2.76	10	1
1:A:180:MET:O	1:A:183:VAL:HG22	0.43	2.13	28	1
1:A:207:ARG:HA	1:A:207:ARG:CZ	0.43	2.44	2	1
1:A:145:HIS:CE1	1:A:226:GLY:H	0.43	2.32	15	1
1:A:182:GLN:HB3	1:A:283:LYS:HE3	0.43	1.90	25	2
1:A:165:GLY:HA2	1:A:260:HIS:CD2	0.43	2.48	11	1
1:A:264:MET:HE3	1:A:265:TYR:H	0.42	1.74	21	1
1:A:279:GLN:CD	1:A:279:GLN:H	0.41	2.24	29	1
1:A:172:VAL:HG12	1:A:261:THR:HG21	0.41	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:CYS:SG	1:A:170:PRO:HD2	0.40	2.56	6	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	150/173 (87%)	122±4 (81±3%)	19±3 (13±2%)	9±3 (6±2%)	2	20
All	All	4500/5190 (87%)	3653 (81%)	580 (13%)	267 (6%)	2	20

All 58 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	296	PRO	26
1	A	191	THR	17
1	A	192	THR	14
1	A	221	SER	13
1	A	207	ARG	12
1	A	242	ARG	11
1	A	262	ILE	10
1	A	270	ASP	9
1	A	172	VAL	8
1	A	168	HIS	8
1	A	171	ASP	7
1	A	245	TYR	7
1	A	204	ASP	6
1	A	279	GLN	6
1	A	261	THR	6
1	A	258	VAL	6
1	A	223	LYS	5
1	A	167	THR	5
1	A	243	VAL	5
1	A	260	HIS	5
1	A	208	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	280	ASN	5
1	A	244	TYR	4
1	A	283	LYS	4
1	A	272	GLU	4
1	A	263	ILE	4
1	A	193	LEU	4
1	A	170	PRO	3
1	A	195	ASP	3
1	A	281	LYS	3
1	A	145	HIS	3
1	A	246	SER	3
1	A	203	ILE	3
1	A	259	ASP	3
1	A	169	CYS	2
1	A	209	THR	2
1	A	220	PHE	2
1	A	282	ARG	2
1	A	274	LEU	2
1	A	298	ARG	2
1	A	166	PHE	1
1	A	146	THR	1
1	A	148	GLU	1
1	A	157	GLY	1
1	A	138	GLY	1
1	A	228	THR	1
1	A	147	GLY	1
1	A	206	GLU	1
1	A	231	ARG	1
1	A	278	GLY	1
1	A	156	LEU	1
1	A	271	GLY	1
1	A	165	GLY	1
1	A	194	PRO	1
1	A	205	PRO	1
1	A	152	ASP	1
1	A	273	PHE	1
1	A	222	PRO	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	133/153 (87%)	120±3 (90±2%)	13±3 (10±2%)	10	55
All	All	3990/4590 (87%)	3609 (90%)	381 (10%)	10	55

All 100 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	153	LYS	20
1	A	150	LYS	17
1	A	283	LYS	17
1	A	178	GLU	11
1	A	218	LYS	9
1	A	148	GLU	9
1	A	260	HIS	9
1	A	160	LEU	9
1	A	146	THR	8
1	A	177	LEU	8
1	A	281	LYS	8
1	A	262	ILE	7
1	A	174	LEU	7
1	A	236	GLN	6
1	A	266	LEU	6
1	A	279	GLN	6
1	A	280	ASN	6
1	A	289	SER	5
1	A	207	ARG	5
1	A	270	ASP	5
1	A	196	LEU	5
1	A	224	LEU	5
1	A	167	THR	5
1	A	169	CYS	5
1	A	161	LEU	5
1	A	211	GLU	5
1	A	151	THR	4
1	A	156	LEU	4
1	A	193	LEU	4
1	A	285	GLU	4
1	A	195	ASP	4
1	A	264	MET	4
1	A	143	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	182	GLN	4
1	A	187	ILE	4
1	A	191	THR	4
1	A	172	VAL	4
1	A	199	LEU	4
1	A	168	HIS	4
1	A	206	GLU	4
1	A	176	GLU	4
1	A	259	ASP	3
1	A	179	LYS	3
1	A	219	GLU	3
1	A	239	ARG	3
1	A	197	THR	3
1	A	210	LYS	3
1	A	274	LEU	3
1	A	158	GLN	3
1	A	216	TYR	3
1	A	217	VAL	3
1	A	232	GLU	3
1	A	202	SER	3
1	A	228	THR	3
1	A	242	ARG	3
1	A	173	CYS	3
1	A	230	THR	3
1	A	294	MET	3
1	A	142	LEU	2
1	A	267	ILE	2
1	A	180	MET	2
1	A	223	LYS	2
1	A	188	ASP	2
1	A	209	THR	2
1	A	234	VAL	2
1	A	227	LEU	2
1	A	275	ASP	2
1	A	231	ARG	2
1	A	220	PHE	2
1	A	203	ILE	2
1	A	282	ARG	2
1	A	144	THR	2
1	A	298	ARG	2
1	A	245	TYR	2
1	A	190	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	297	TYR	2
1	A	154	ASP	2
1	A	192	THR	2
1	A	162	ILE	1
1	A	141	SER	1
1	A	295	ARG	1
1	A	213	ILE	1
1	A	235	ASP	1
1	A	155	TYR	1
1	A	149	ARG	1
1	A	175	GLU	1
1	A	183	VAL	1
1	A	145	HIS	1
1	A	152	ASP	1
1	A	171	ASP	1
1	A	290	ILE	1
1	A	185	ASP	1
1	A	221	SER	1
1	A	272	GLU	1
1	A	265	TYR	1
1	A	166	PHE	1
1	A	181	ILE	1
1	A	263	ILE	1
1	A	277	PHE	1
1	A	215	ASN	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 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