



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 04:31 AM UTC

PDB ID : 2GT5 / pdb_00002gt5
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

<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

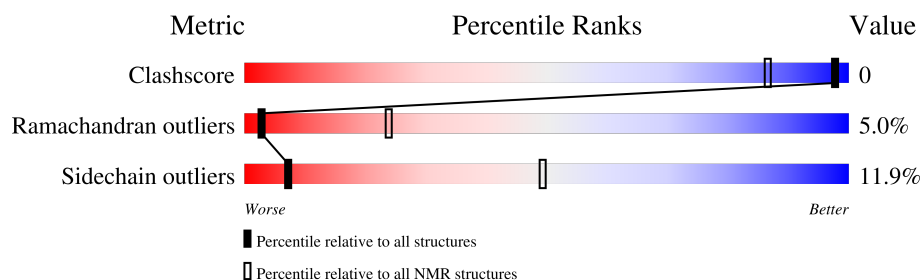
1 Overall quality at a glance

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	73% 9% 18%

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)	1.83	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 4 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	4, 11, 12, 13, 17, 19, 21, 23
3	9, 30
4	27, 28
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:

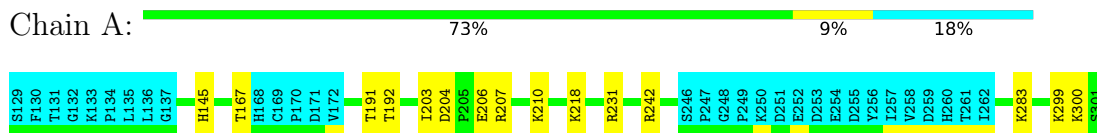
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	cloning artifact	UNP O75880
A	130	PHE	-	cloning artifact	UNP O75880
A	131	THR	-	cloning artifact	UNP O75880

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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

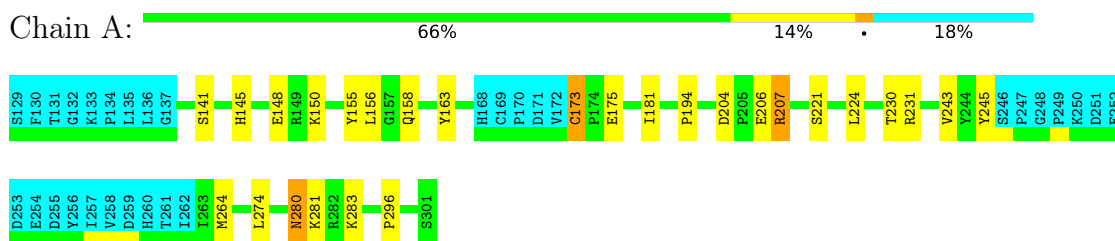


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

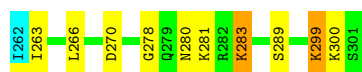
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.2 Score per residue for model 2

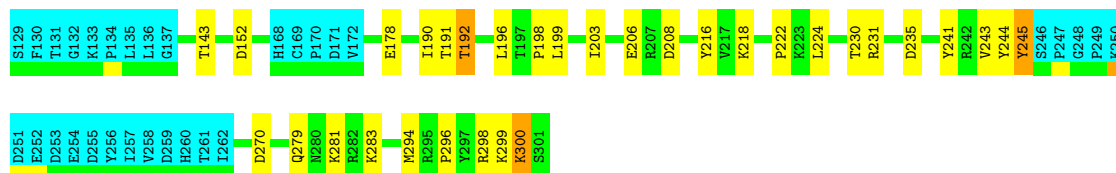
- Molecule 1: SCO1 protein homolog, mitochondrial





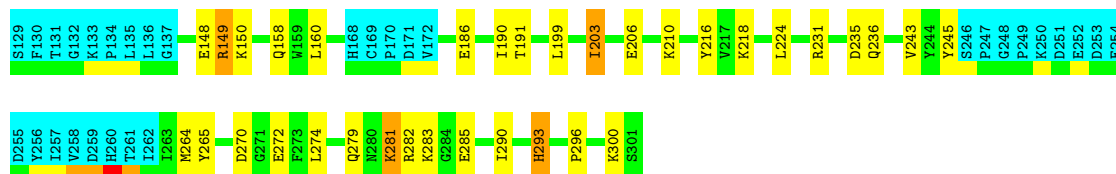
4.2.3 Score per residue for model 3

- Molecule 1: SCO1 protein homolog, mitochondrial



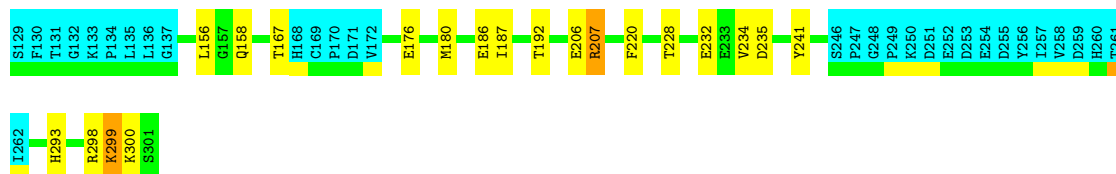
4.2.4 Score per residue for model 4

- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.5 Score per residue for model 5

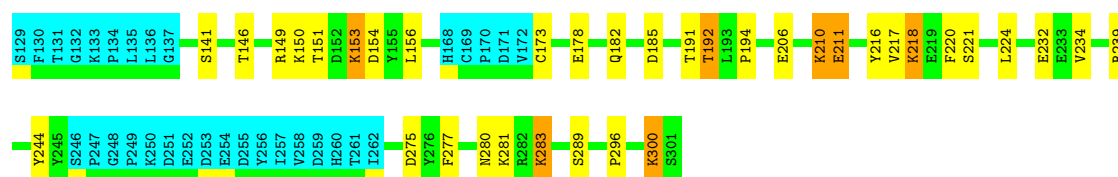
- Molecule 1: SCO1 protein homolog, mitochondrial



4.2.6 Score per residue for model 6

- Molecule 1: SCO1 protein homolog, mitochondrial

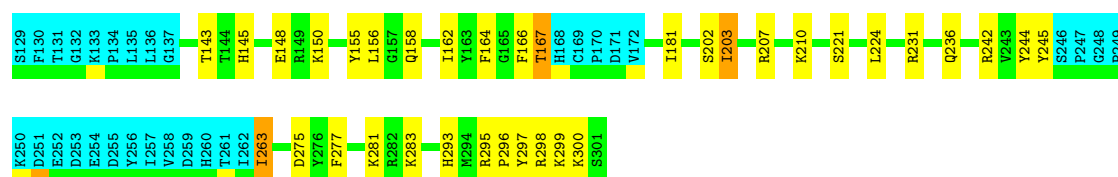




4.2.7 Score per residue for model 7

- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 62% 18% 18%



4.2.8 Score per residue for model 8

- Molecule 1: SCO1 protein homolog, mitochondrial

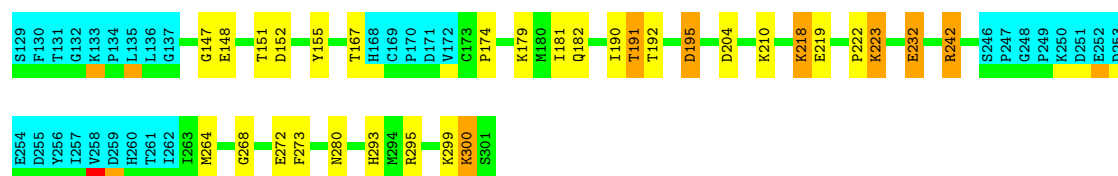
Chain A: 64% 16% 18%



4.2.9 Score per residue for model 9

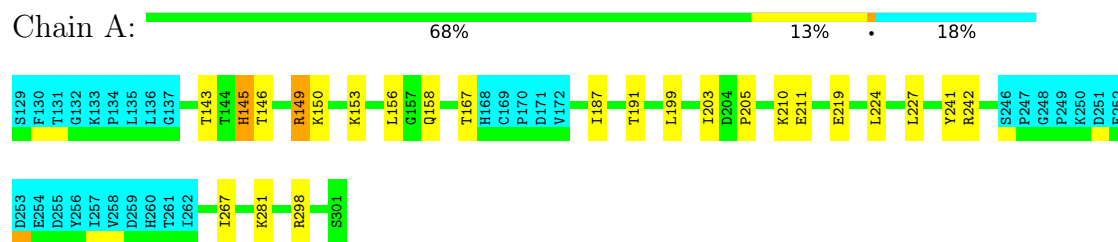
- Molecule 1: SCO1 protein homolog, mitochondrial

Chain A: 64% 14% 18%



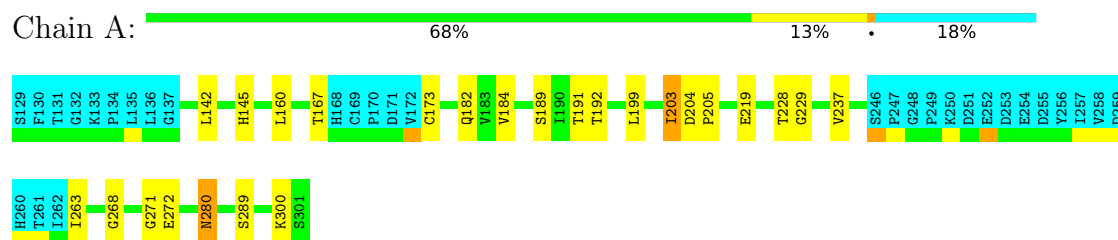
4.2.10 Score per residue for model 10

- Molecule 1: SCO1 protein homolog, mitochondrial



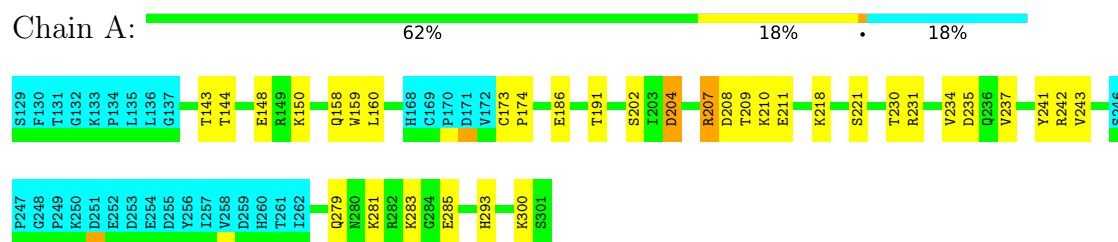
4.2.11 Score per residue for model 11

- Molecule 1: SCO1 protein homolog, mitochondrial



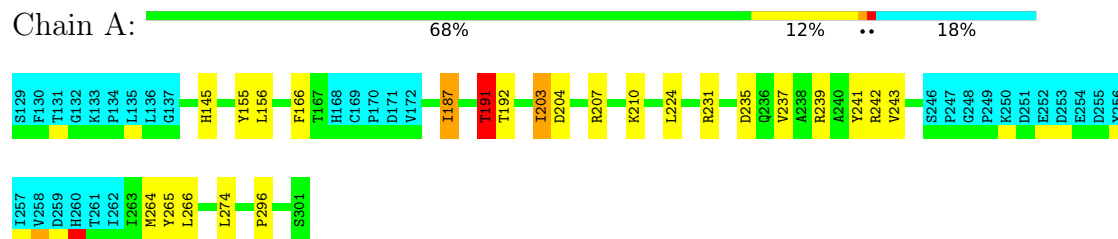
4.2.12 Score per residue for model 12

- Molecule 1: SCO1 protein homolog, mitochondrial



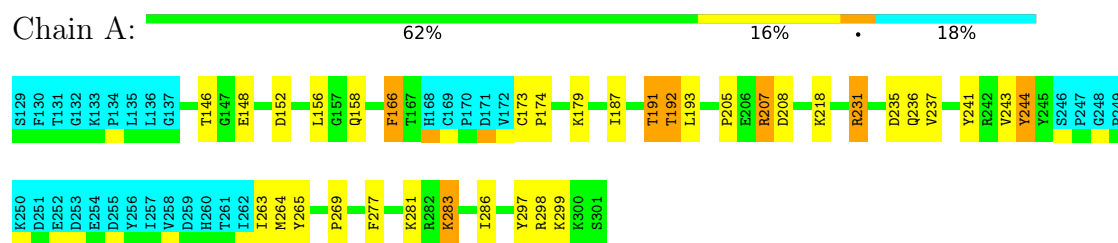
4.2.13 Score per residue for model 13

- Molecule 1: SCO1 protein homolog, mitochondrial



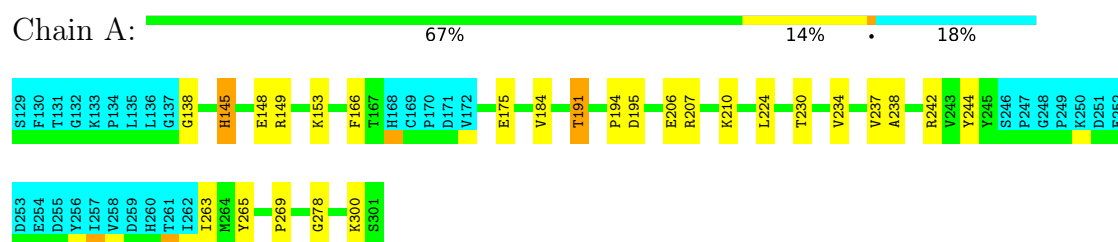
4.2.14 Score per residue for model 14

- Molecule 1: SCO1 protein homolog, mitochondrial



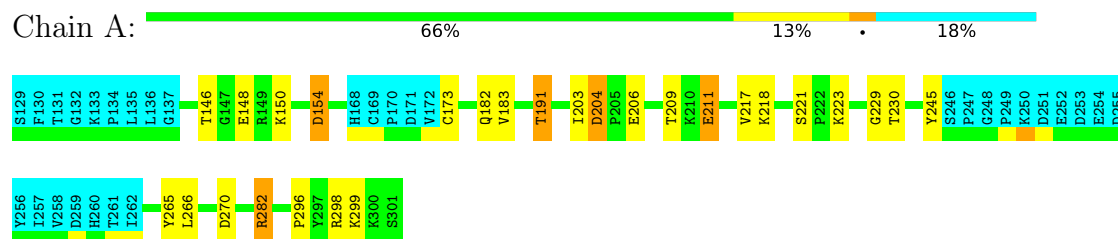
4.2.15 Score per residue for model 15

- Molecule 1: SCO1 protein homolog, mitochondrial



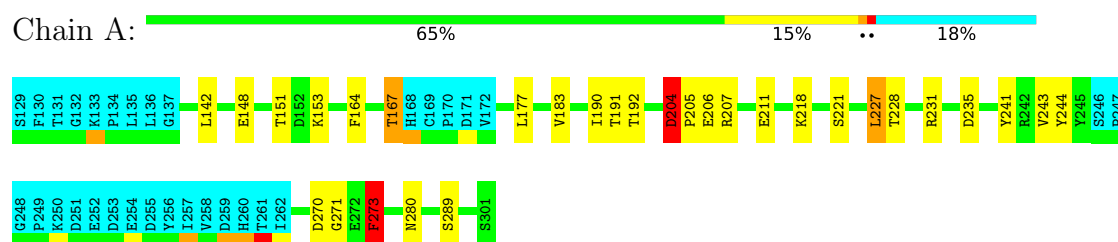
4.2.16 Score per residue for model 16

- Molecule 1: SCO1 protein homolog, mitochondrial



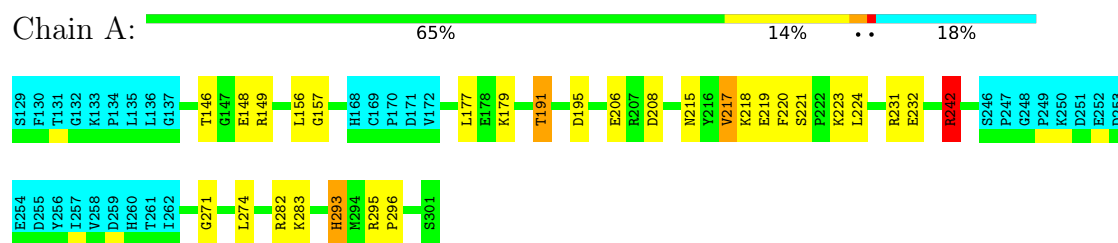
4.2.17 Score per residue for model 17

- Molecule 1: SCO1 protein homolog, mitochondrial



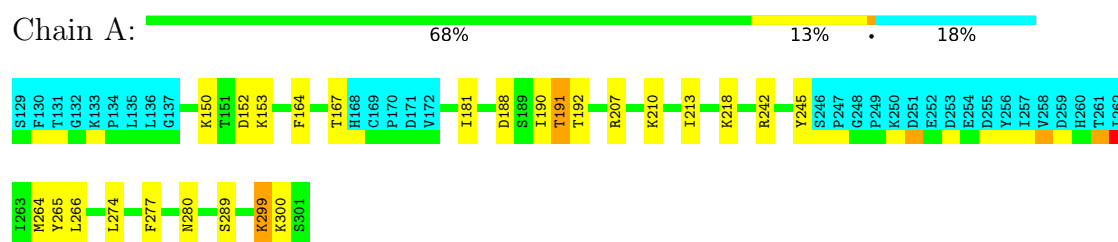
4.2.18 Score per residue for model 18

- Molecule 1: SCO1 protein homolog, mitochondrial



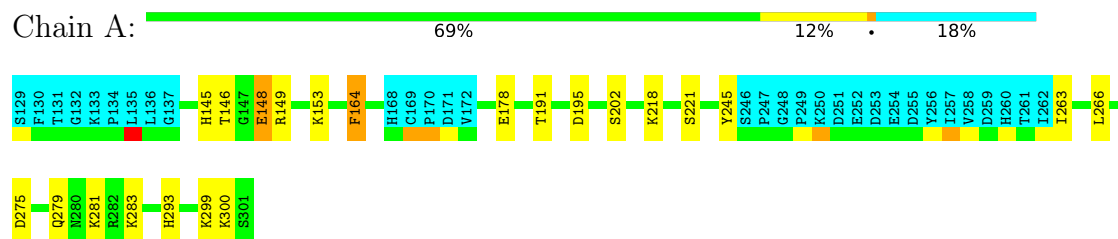
4.2.19 Score per residue for model 19

- Molecule 1: SCO1 protein homolog, mitochondrial



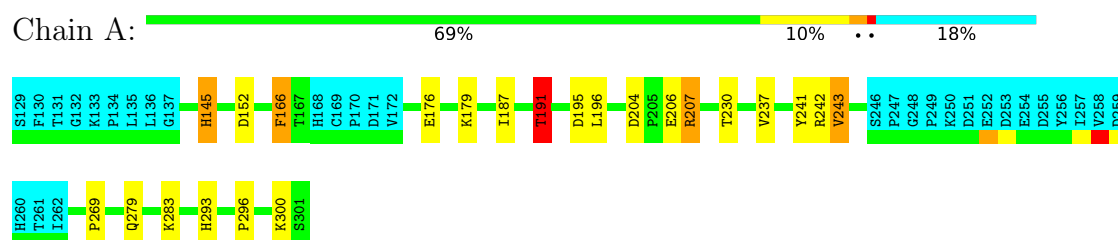
4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: SCO1 protein homolog, mitochondrial



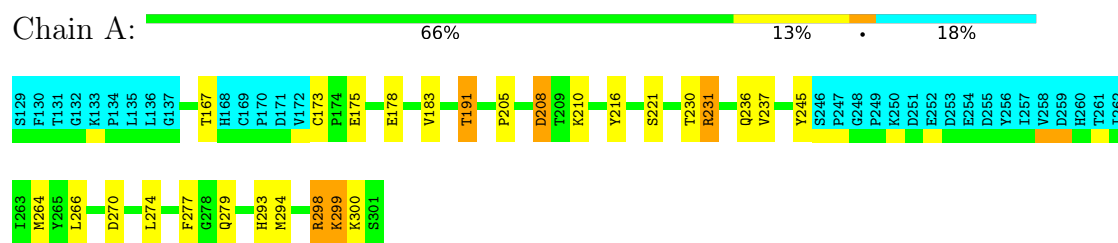
4.2.21 Score per residue for model 21

- Molecule 1: SCO1 protein homolog, mitochondrial



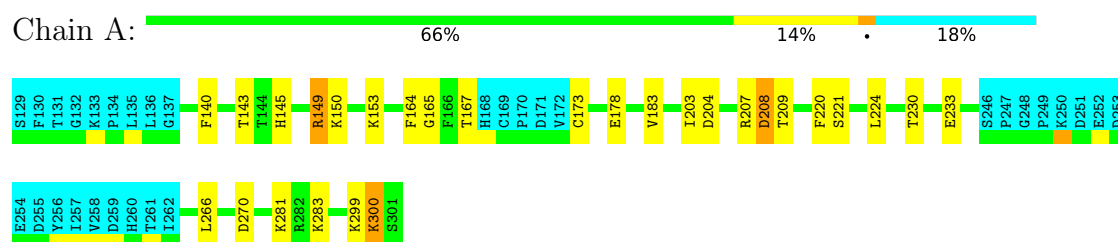
4.2.22 Score per residue for model 22

- Molecule 1: SCO1 protein homolog, mitochondrial



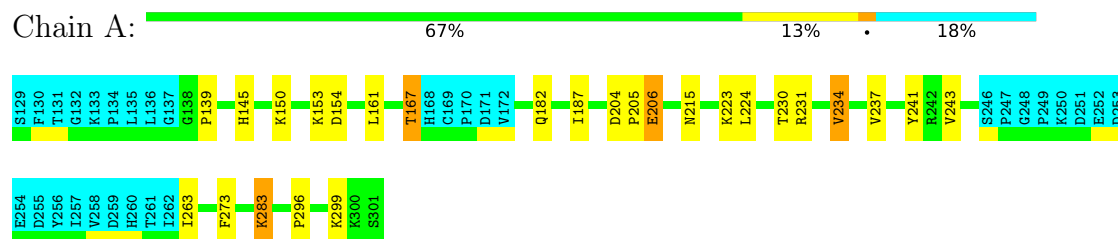
4.2.23 Score per residue for model 23

- Molecule 1: SCO1 protein homolog, mitochondrial



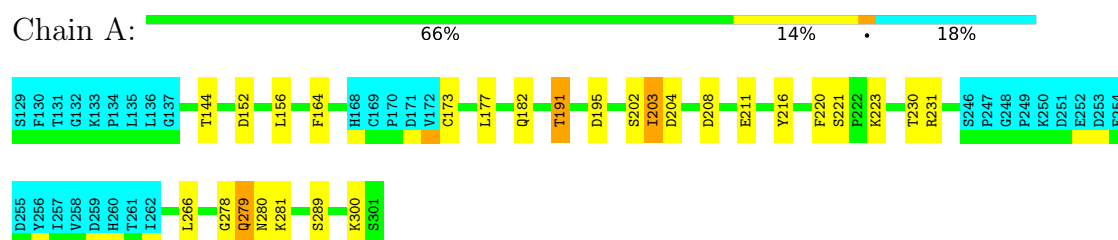
4.2.24 Score per residue for model 24

- Molecule 1: SCO1 protein homolog, mitochondrial



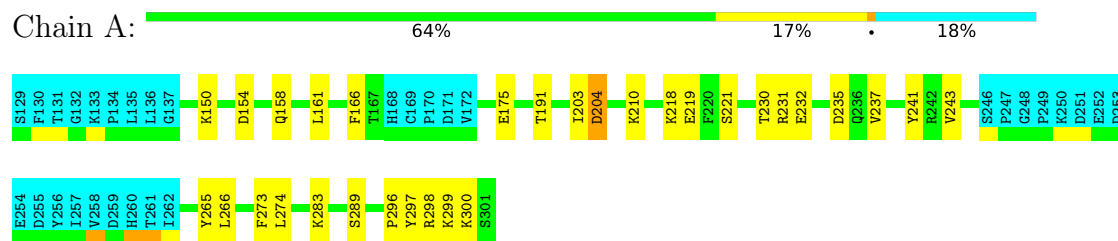
4.2.25 Score per residue for model 25

- Molecule 1: SCO1 protein homolog, mitochondrial



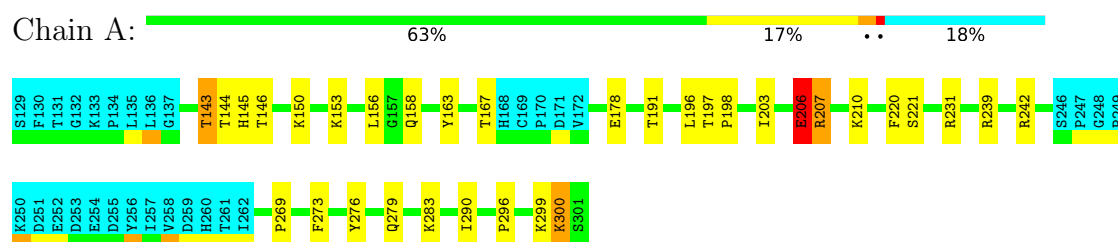
4.2.26 Score per residue for model 26

- Molecule 1: SCO1 protein homolog, mitochondrial



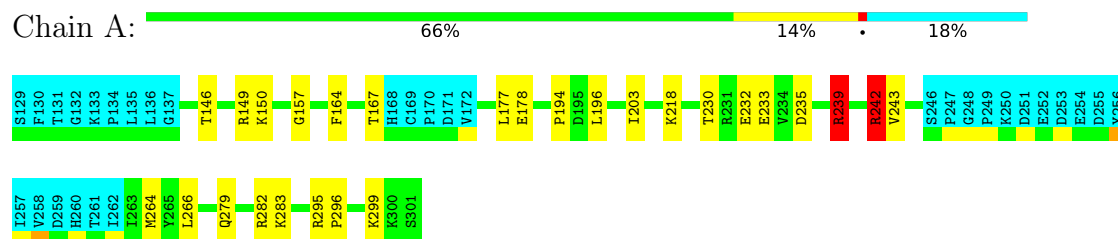
4.2.27 Score per residue for model 27

- Molecule 1: SCO1 protein homolog, mitochondrial



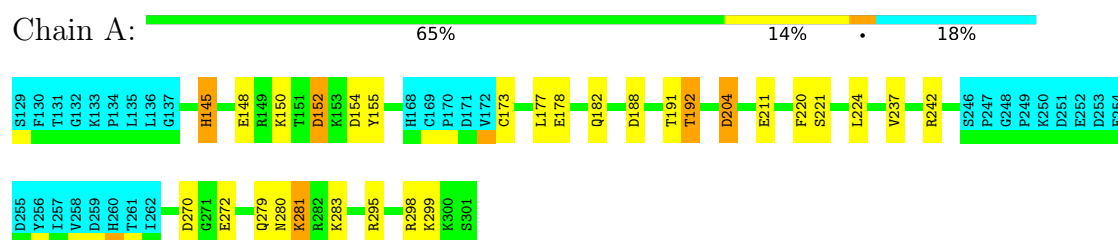
4.2.28 Score per residue for model 28

- Molecule 1: SCO1 protein homolog, mitochondrial



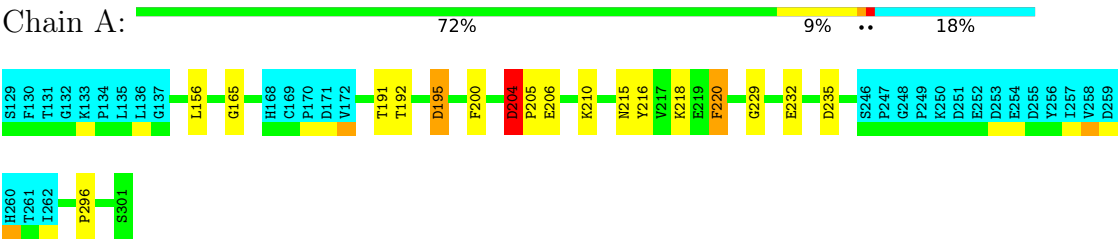
4.2.29 Score per residue for model 29

- 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.

6 Model quality

6.1 Standard geometry

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	0.85±0.02	0±0/1179 (0.0± 0.0%)	1.48±0.04	7±4/1594 (0.4± 0.2%)
All	All	0.85	0/35370 (0.0%)	1.48	205/47820 (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	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	166	PHE	CA-CB-CG	13.17	126.97	113.80	14	3
1	A	203	ILE	N-CA-C	8.14	118.07	110.42	27	1
1	A	164	PHE	CA-CB-CG	7.58	121.38	113.80	20	3
1	A	151	THR	CA-C-N	7.47	130.79	120.63	6	1
1	A	151	THR	C-N-CA	7.47	130.79	120.63	6	1
1	A	280	ASN	CA-C-N	7.05	135.01	121.54	2	2
1	A	280	ASN	C-N-CA	7.05	135.01	121.54	2	2
1	A	204	ASP	CA-CB-CG	6.89	119.49	112.60	30	2
1	A	278	GLY	CA-C-N	6.83	134.59	121.54	25	1
1	A	278	GLY	C-N-CA	6.83	134.59	121.54	25	1
1	A	204	ASP	CB-CA-C	6.81	117.11	110.71	26	1
1	A	187	ILE	N-CA-CB	-6.76	106.09	111.64	8	1
1	A	191	THR	CA-C-N	6.61	131.87	120.58	20	4
1	A	191	THR	C-N-CA	6.61	131.87	120.58	20	4
1	A	221	SER	N-CA-C	6.56	114.03	108.13	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	208	ASP	CA-CB-CG	6.35	118.95	112.60	22	1
1	A	273	PHE	CA-CB-CG	6.34	120.14	113.80	17	3
1	A	183	VAL	CA-C-N	6.33	129.00	121.84	22	1
1	A	183	VAL	C-N-CA	6.33	129.00	121.84	22	1
1	A	300	LYS	CA-C-N	6.30	133.04	121.70	26	5
1	A	300	LYS	C-N-CA	6.30	133.04	121.70	26	5
1	A	283	LYS	N-CA-C	6.29	119.80	111.75	29	2
1	A	234	VAL	CA-C-N	6.16	129.15	120.28	6	2
1	A	234	VAL	C-N-CA	6.16	129.15	120.28	6	2
1	A	277	PHE	CA-CB-CG	6.12	119.92	113.80	6	1
1	A	204	ASP	CA-C-N	6.11	126.06	119.76	26	4
1	A	204	ASP	C-N-CA	6.11	126.06	119.76	26	4
1	A	153	LYS	CA-C-N	6.11	128.47	120.28	6	1
1	A	153	LYS	C-N-CA	6.11	128.47	120.28	6	1
1	A	269	PRO	CA-C-N	6.09	129.06	120.28	21	4
1	A	269	PRO	C-N-CA	6.09	129.06	120.28	21	4
1	A	190	ILE	CA-C-N	6.06	133.11	121.54	3	4
1	A	190	ILE	C-N-CA	6.06	133.11	121.54	3	4
1	A	207	ARG	CD-NE-CZ	6.03	132.84	124.40	21	1
1	A	154	ASP	CA-CB-CG	5.98	118.58	112.60	26	5
1	A	245	TYR	CA-C-N	5.97	132.45	121.70	22	1
1	A	245	TYR	C-N-CA	5.97	132.45	121.70	22	1
1	A	145	HIS	CA-C-N	5.96	129.37	120.31	23	2
1	A	145	HIS	C-N-CA	5.96	129.37	120.31	23	2
1	A	293	HIS	CB-CG-CD2	-5.93	123.49	131.20	22	5
1	A	298	ARG	CD-NE-CZ	5.91	132.68	124.40	22	1
1	A	231	ARG	CD-NE-CZ	5.91	132.68	124.40	4	1
1	A	270	ASP	CA-C-N	5.91	125.67	121.65	2	1
1	A	270	ASP	C-N-CA	5.91	125.67	121.65	2	1
1	A	187	ILE	CB-CA-C	5.88	117.03	111.44	13	1
1	A	227	LEU	CA-C-N	5.86	132.74	121.54	17	1
1	A	227	LEU	C-N-CA	5.86	132.74	121.54	17	1
1	A	174	PRO	CA-C-N	5.85	128.92	120.79	14	3
1	A	174	PRO	C-N-CA	5.85	128.92	120.79	14	3
1	A	167	THR	CA-C-N	5.84	132.70	121.54	9	3
1	A	167	THR	C-N-CA	5.84	132.70	121.54	9	3
1	A	149	ARG	NE-CZ-NH2	5.83	124.45	119.20	23	1
1	A	281	LYS	CA-C-N	5.76	132.55	121.54	4	2
1	A	281	LYS	C-N-CA	5.76	132.55	121.54	4	2
1	A	194	PRO	CA-C-N	5.76	131.67	122.10	28	1
1	A	194	PRO	C-N-CA	5.76	131.67	122.10	28	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	155	TYR	N-CA-CB	-5.75	102.67	110.95	29	1
1	A	242	ARG	CD-NE-CZ	5.75	132.45	124.40	28	1
1	A	236	GLN	OE1-CD-NE2	-5.75	116.85	122.60	7	2
1	A	272	GLU	CA-C-N	5.72	132.47	121.54	9	1
1	A	272	GLU	C-N-CA	5.72	132.47	121.54	9	1
1	A	178	GLU	CB-CG-CD	-5.71	102.90	112.60	8	1
1	A	279	GLN	OE1-CD-NE2	-5.71	116.89	122.60	12	4
1	A	279	GLN	CB-CA-C	5.70	119.11	111.82	4	1
1	A	242	ARG	CA-C-N	5.64	132.12	121.97	21	2
1	A	242	ARG	C-N-CA	5.64	132.12	121.97	21	2
1	A	244	TYR	CA-C-N	5.63	132.30	121.54	7	1
1	A	244	TYR	C-N-CA	5.63	132.30	121.54	7	1
1	A	158	GLN	OE1-CD-NE2	-5.60	117.00	122.60	4	2
1	A	145	HIS	CB-CG-CD2	-5.60	123.92	131.20	15	4
1	A	152	ASP	N-CA-C	5.58	119.83	113.19	9	1
1	A	210	LYS	CA-C-N	5.57	127.68	120.44	26	3
1	A	210	LYS	C-N-CA	5.57	127.68	120.44	26	3
1	A	156	LEU	N-CA-CB	-5.57	102.71	110.29	14	1
1	A	182	GLN	OE1-CD-NE2	-5.57	117.03	122.60	29	2
1	A	149	ARG	CB-CA-C	5.54	119.09	110.67	10	1
1	A	275	ASP	CA-CB-CG	5.53	118.13	112.60	20	3
1	A	188	ASP	CA-C-N	5.53	129.53	120.63	19	1
1	A	188	ASP	C-N-CA	5.53	129.53	120.63	19	1
1	A	231	ARG	CA-C-N	5.49	127.91	120.44	26	1
1	A	231	ARG	C-N-CA	5.49	127.91	120.44	26	1
1	A	187	ILE	CA-C-N	5.49	127.64	120.28	10	1
1	A	187	ILE	C-N-CA	5.49	127.64	120.28	10	1
1	A	242	ARG	CA-CB-CG	5.45	125.00	114.10	28	1
1	A	208	ASP	N-CA-C	5.38	115.65	108.23	23	1
1	A	191	THR	CA-CB-CG2	5.38	119.64	110.50	21	1
1	A	203	ILE	CA-C-N	5.37	126.45	120.06	8	1
1	A	203	ILE	C-N-CA	5.37	126.45	120.06	8	1
1	A	152	ASP	CA-CB-CG	-5.35	107.25	112.60	29	2
1	A	155	TYR	CA-C-N	5.34	131.73	121.54	1	1
1	A	155	TYR	C-N-CA	5.34	131.73	121.54	1	1
1	A	185	ASP	CA-CB-CG	5.31	117.91	112.60	6	1
1	A	218	LYS	CA-C-N	5.25	131.57	121.54	9	2
1	A	218	LYS	C-N-CA	5.25	131.57	121.54	9	2
1	A	297	TYR	CA-C-N	5.23	131.53	121.54	14	1
1	A	297	TYR	C-N-CA	5.23	131.53	121.54	14	1
1	A	140	PHE	CA-CB-CG	5.23	119.03	113.80	23	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	238	ALA	CA-C-N	5.23	127.55	120.38	15	1
1	A	238	ALA	C-N-CA	5.23	127.55	120.38	15	1
1	A	270	ASP	CA-CB-CG	5.23	117.83	112.60	16	1
1	A	293	HIS	CA-CB-CG	5.17	118.97	113.80	7	1
1	A	298	ARG	NE-CZ-NH1	5.17	126.67	121.50	22	1
1	A	241	TYR	CA-C-N	5.15	131.37	121.54	10	1
1	A	241	TYR	C-N-CA	5.15	131.37	121.54	10	1
1	A	230	THR	CA-C-N	5.14	131.36	121.54	22	1
1	A	230	THR	C-N-CA	5.14	131.36	121.54	22	1
1	A	268	GLY	CA-C-N	5.12	125.81	120.12	9	1
1	A	268	GLY	C-N-CA	5.12	125.81	120.12	9	1
1	A	263	ILE	CA-CB-CG1	5.12	119.10	110.40	7	1
1	A	184	VAL	CA-C-N	5.11	127.39	120.44	15	1
1	A	184	VAL	C-N-CA	5.11	127.39	120.44	15	1
1	A	207	ARG	CA-C-N	5.10	131.28	121.54	17	1
1	A	207	ARG	C-N-CA	5.10	131.28	121.54	17	1
1	A	195	ASP	CA-CB-CG	-5.09	107.51	112.60	20	1
1	A	243	VAL	N-CA-C	5.08	117.41	111.05	28	1
1	A	277	PHE	N-CA-C	5.07	115.74	108.74	6	1
1	A	143	THR	CA-CB-CG2	5.06	119.10	110.50	27	1
1	A	148	GLU	CA-C-N	5.03	129.11	122.42	20	1
1	A	148	GLU	C-N-CA	5.03	129.11	122.42	20	1
1	A	239	ARG	NE-CZ-NH2	5.01	123.71	119.20	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	203	ILE	Peptide	4
1	A	167	THR	Peptide	4
1	A	239	ARG	Sidechain,Peptide	4
1	A	298	ARG	Sidechain,Peptide	4
1	A	245	TYR	Peptide	3
1	A	229	GLY	Peptide	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	195	ASP	Peptide	3
1	A	242	ARG	Sidechain,Peptide	3
1	A	164	PHE	Peptide,Sidechain	3
1	A	163	TYR	Sidechain	2
1	A	278	GLY	Peptide	2
1	A	149	ARG	Peptide,Sidechain	2
1	A	202	SER	Peptide	2
1	A	139	PRO	Peptide	2
1	A	191	THR	Peptide	2
1	A	166	PHE	Peptide	2
1	A	299	LYS	Peptide	2
1	A	157	GLY	Peptide	2
1	A	208	ASP	Peptide	2
1	A	165	GLY	Peptide	2
1	A	194	PRO	Peptide	1
1	A	243	VAL	Peptide	1
1	A	216	TYR	Sidechain	1
1	A	241	TYR	Sidechain	1
1	A	228	THR	Peptide	1
1	A	235	ASP	Peptide	1
1	A	275	ASP	Peptide	1
1	A	297	TYR	Sidechain	1
1	A	222	PRO	Peptide	1
1	A	151	THR	Peptide	1
1	A	182	GLN	Peptide	1
1	A	205	PRO	Peptide	1
1	A	158	GLN	Peptide	1
1	A	265	TYR	Sidechain	1
1	A	244	TYR	Peptide	1
1	A	282	ARG	Peptide	1
1	A	217	VAL	Peptide	1
1	A	271	GLY	Peptide	1
1	A	277	PHE	Peptide	1
1	A	146	THR	Peptide	1
1	A	295	ARG	Sidechain	1
1	A	280	ASN	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	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:149:ARG:HH12	1:A:233:GLU:CD	0.52	2.12	28	2
1:A:196:LEU:H	1:A:196:LEU:HD23	0.48	1.67	21	2
1:A:231:ARG:H	1:A:231:ARG:CD	0.48	2.20	14	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:211:GLU:H	1:A:211:GLU:CD	0.45	2.20	16	1
1:A:200:PHE:CE2	1:A:216:TYR:CE1	0.45	3.04	30	1
1:A:232:GLU:H	1:A:232:GLU:CD	0.44	2.20	9	3
1:A:175:GLU:CD	1:A:175:GLU:H	0.43	2.21	1	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: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:195:ASP:CG	1:A:223:LYS:HZ1	0.42	2.22	9	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:210:LYS:HZ3	1:A:211:GLU:CD	0.42	2.21	6	1
1:A:188:ASP:CG	1:A:223:LYS:HZ1	0.41	2.23	2	1
1:A:182:GLN:CB	1:A:283:LYS:HE3	0.41	2.46	24	1
1:A:182:GLN:C	1:A:283:LYS:HE3	0.41	2.41	6	1
1:A:186:GLU:CD	1:A:283:LYS:HZ2	0.41	2.24	12	2
1:A:148:GLU:CD	1:A:149:ARG:H	0.41	2.24	20	1
1:A:232:GLU:N	1:A:232:GLU:CD	0.41	2.79	18	1
1:A:143:THR:HB	1:A:210:LYS:HE2	0.40	1.92	10	1
1:A:232:GLU:CD	1:A:232:GLU:H	0.40	2.24	5	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%)	3	24
All	All	4230/5190 (82%)	3454 (82%)	566 (13%)	210 (5%)	3	24

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	173	CYS	9
1	A	243	VAL	9
1	A	207	ARG	8
1	A	241	TYR	8
1	A	204	ASP	6
1	A	299	LYS	6
1	A	205	PRO	6
1	A	206	GLU	5
1	A	281	LYS	5
1	A	242	ARG	5
1	A	245	TYR	4
1	A	231	ARG	4
1	A	270	ASP	4
1	A	167	THR	4
1	A	283	LYS	4
1	A	203	ILE	4
1	A	156	LEU	3
1	A	282	ARG	3
1	A	145	HIS	3
1	A	195	ASP	3
1	A	273	PHE	3
1	A	280	ASN	3
1	A	300	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	158	GLN	2
1	A	198	PRO	2
1	A	208	ASP	2
1	A	244	TYR	2
1	A	272	GLU	2
1	A	220	PHE	2
1	A	194	PRO	2
1	A	217	VAL	2
1	A	219	GLU	2
1	A	263	ILE	2
1	A	271	GLY	2
1	A	152	ASP	2
1	A	279	GLN	2
1	A	222	PRO	1
1	A	166	PHE	1
1	A	147	GLY	1
1	A	268	GLY	1
1	A	174	PRO	1
1	A	298	ARG	1
1	A	138	GLY	1
1	A	228	THR	1
1	A	190	ILE	1
1	A	146	THR	1
1	A	237	VAL	1
1	A	224	LEU	1
1	A	274	LEU	1
1	A	264	MET	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	125/153 (82%)	110±3 (88±3%)	15±3 (12±3%)	7	49
All	All	3750/4590 (82%)	3302 (88%)	448 (12%)	7	49

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	224	LEU	12
1	A	283	LYS	12
1	A	299	LYS	12
1	A	148	GLU	11
1	A	230	THR	11
1	A	266	LEU	10
1	A	300	LYS	10
1	A	210	LYS	9
1	A	235	ASP	9
1	A	153	LYS	9
1	A	237	VAL	9
1	A	178	GLU	8
1	A	264	MET	7
1	A	231	ARG	7
1	A	289	SER	7
1	A	281	LYS	7
1	A	203	ILE	7
1	A	156	LEU	7
1	A	211	GLU	7
1	A	145	HIS	7
1	A	191	THR	7
1	A	274	LEU	6
1	A	265	TYR	6
1	A	293	HIS	6
1	A	206	GLU	6
1	A	146	THR	6
1	A	167	THR	6
1	A	280	ASN	5
1	A	149	ARG	5
1	A	263	ILE	5
1	A	192	THR	5
1	A	298	ARG	5
1	A	187	ILE	5
1	A	207	ARG	5
1	A	242	ARG	5
1	A	179	LYS	5
1	A	223	LYS	5
1	A	177	LEU	5
1	A	173	CYS	4
1	A	152	ASP	4
1	A	175	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	202	SER	4
1	A	143	THR	4
1	A	199	LEU	4
1	A	279	GLN	4
1	A	216	TYR	4
1	A	234	VAL	4
1	A	295	ARG	4
1	A	144	THR	4
1	A	208	ASP	4
1	A	219	GLU	4
1	A	158	GLN	4
1	A	181	ILE	3
1	A	196	LEU	3
1	A	160	LEU	3
1	A	285	GLU	3
1	A	290	ILE	3
1	A	232	GLU	3
1	A	155	TYR	3
1	A	182	GLN	3
1	A	204	ASP	3
1	A	209	THR	3
1	A	244	TYR	3
1	A	183	VAL	3
1	A	215	ASN	3
1	A	141	SER	2
1	A	180	MET	2
1	A	294	MET	2
1	A	236	GLN	2
1	A	176	GLU	2
1	A	227	LEU	2
1	A	142	LEU	2
1	A	166	PHE	2
1	A	164	PHE	2
1	A	270	ASP	2
1	A	161	LEU	2
1	A	220	PHE	2
1	A	245	TYR	1
1	A	186	GLU	1
1	A	162	ILE	1
1	A	267	ILE	1
1	A	184	VAL	1
1	A	189	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	228	THR	1
1	A	193	LEU	1
1	A	154	ASP	1
1	A	217	VAL	1
1	A	282	ARG	1
1	A	151	THR	1
1	A	273	PHE	1
1	A	195	ASP	1
1	A	213	ILE	1
1	A	277	PHE	1
1	A	243	VAL	1
1	A	221	SER	1
1	A	297	TYR	1
1	A	197	THR	1
1	A	276	TYR	1
1	A	239	ARG	1
1	A	188	ASP	1
1	A	272	GLU	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](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided