



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:42 PM UTC

PDB ID : 6LUL / pdb_00006lul
BMRB ID : 36312
Title : NMR structure and dynamics studies of yeast respiratory super-complex factor 2 in micelles
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Deposited on : 2020-01-29

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

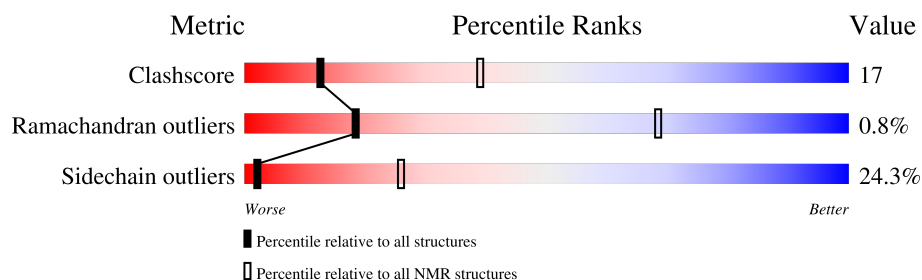
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

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	239	
1	B	239	

2 Ensemble composition and analysis

This entry contains 15 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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	B:15-B:40, B:48-B:76, B:104-B:134, B:143-B:173, B:184-B:204, A:15-A:40, A:48-A:76, A:105-A:134, A:143-A:171, A:184-A:203 (272)	0.65	2

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 2 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 9, 10, 11, 13
2	12, 14
Single-model clusters	5; 6; 7; 8; 15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7192 atoms, of which 3626 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Respiratory supercomplex factor 2, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
1	B	224	Total	C	H	N	O	S	0
			3596	1134	1813	313	329	7	
1	A	224	Total	C	H	N	O	S	0
			3596	1134	1813	313	329	7	

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLU	-	expression tag	UNP P53721
A	226	PHE	-	expression tag	UNP P53721
A	227	ARG	-	expression tag	UNP P53721
A	228	VAL	-	expression tag	UNP P53721
A	229	PRO	-	expression tag	UNP P53721
A	230	GLY	-	expression tag	UNP P53721
A	231	SER	-	expression tag	UNP P53721
A	232	HIS	-	expression tag	UNP P53721
A	233	HIS	-	expression tag	UNP P53721
A	234	HIS	-	expression tag	UNP P53721
A	235	HIS	-	expression tag	UNP P53721
A	236	HIS	-	expression tag	UNP P53721
A	237	HIS	-	expression tag	UNP P53721
A	238	HIS	-	expression tag	UNP P53721
A	239	HIS	-	expression tag	UNP P53721
B	225	GLU	-	expression tag	UNP P53721
B	226	PHE	-	expression tag	UNP P53721
B	227	ARG	-	expression tag	UNP P53721
B	228	VAL	-	expression tag	UNP P53721
B	229	PRO	-	expression tag	UNP P53721
B	230	GLY	-	expression tag	UNP P53721
B	231	SER	-	expression tag	UNP P53721
B	232	HIS	-	expression tag	UNP P53721
B	233	HIS	-	expression tag	UNP P53721
B	234	HIS	-	expression tag	UNP P53721
B	235	HIS	-	expression tag	UNP P53721
B	236	HIS	-	expression tag	UNP P53721
B	237	HIS	-	expression tag	UNP P53721
B	238	HIS	-	expression tag	UNP P53721

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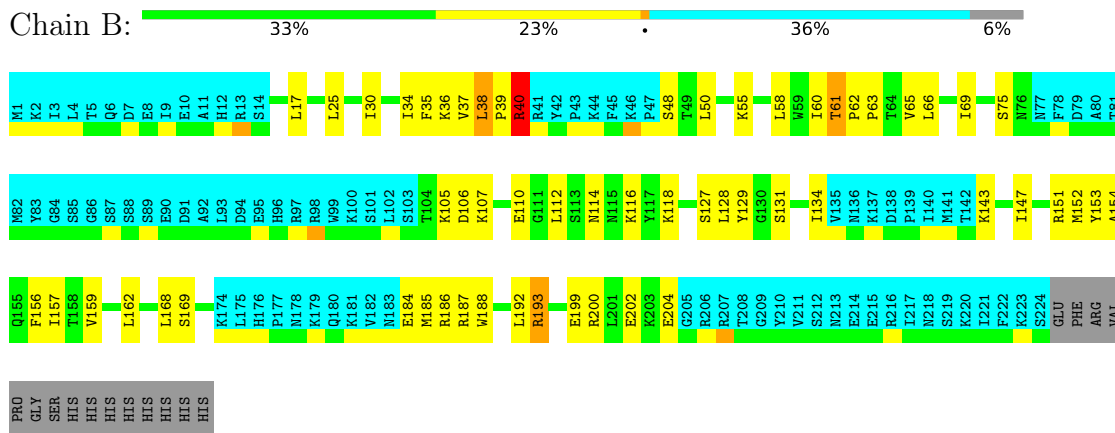
Chain	Residue	Modelled	Actual	Comment	Reference
B	239	HIS	-	expression tag	UNP P53721

4 Residue-property plots

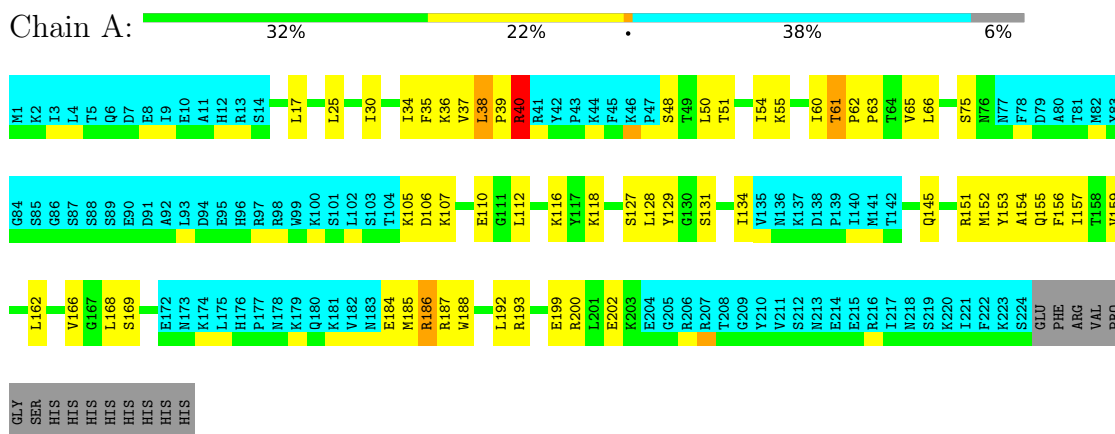
4.1 Average score per residue in the NMR ensemble

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: Respiratory supercomplex factor 2, mitochondrial



- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

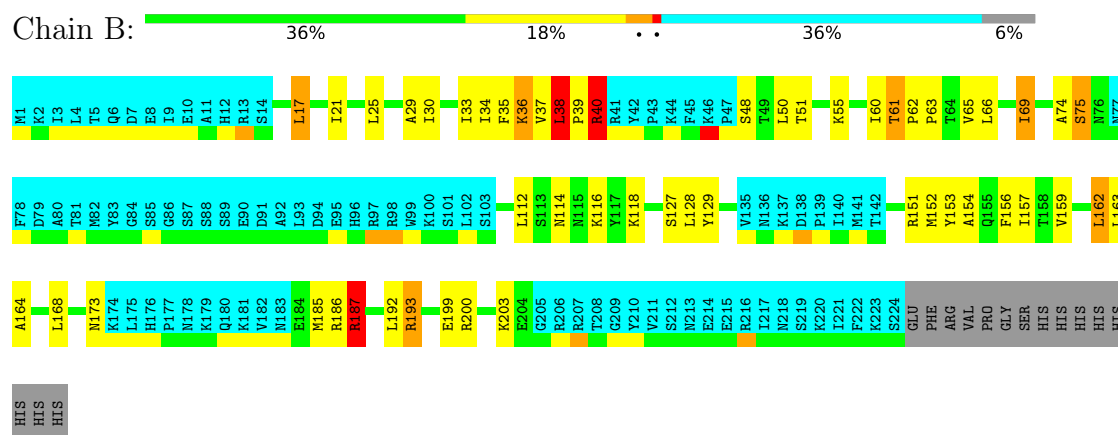


4.2 Scores per residue for each member of the ensemble

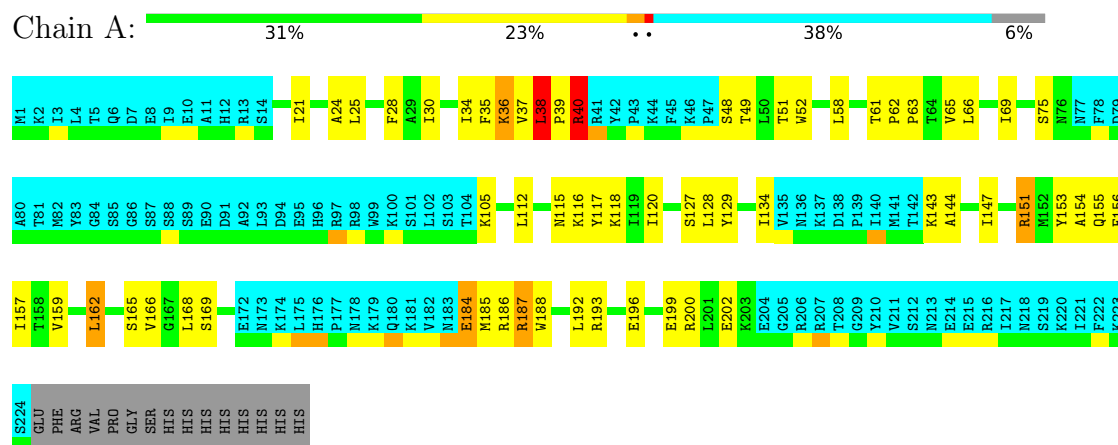
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

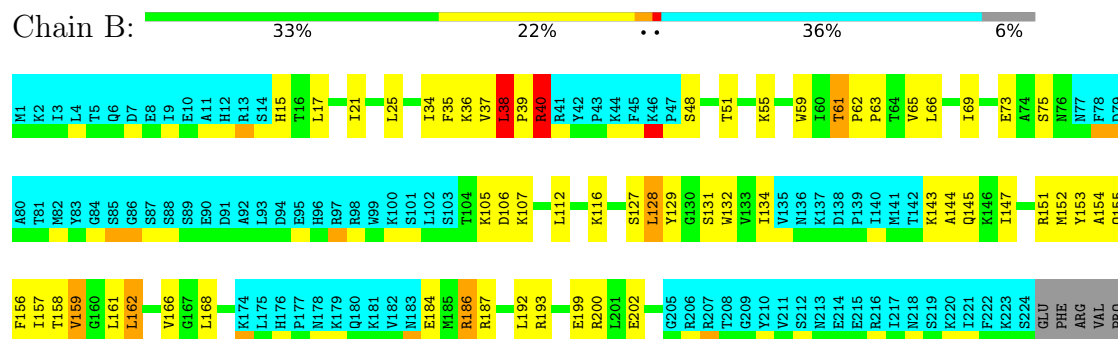


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



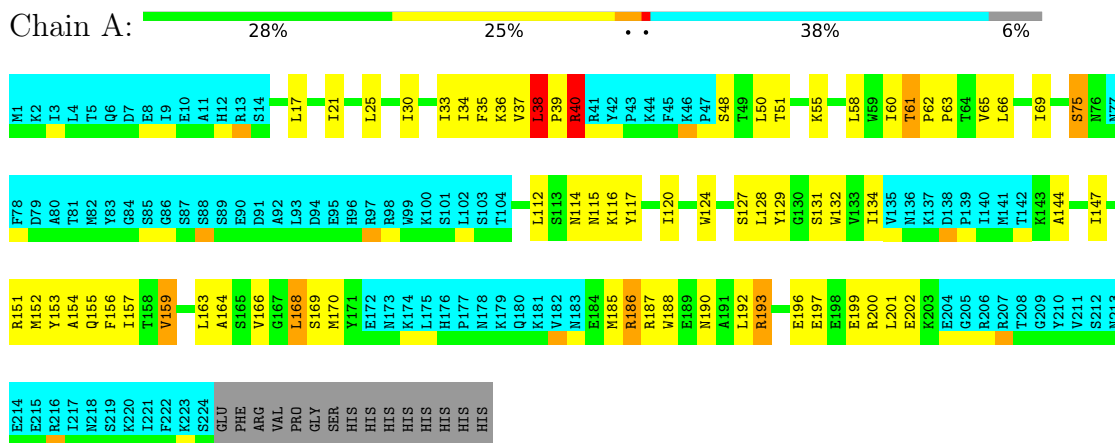
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



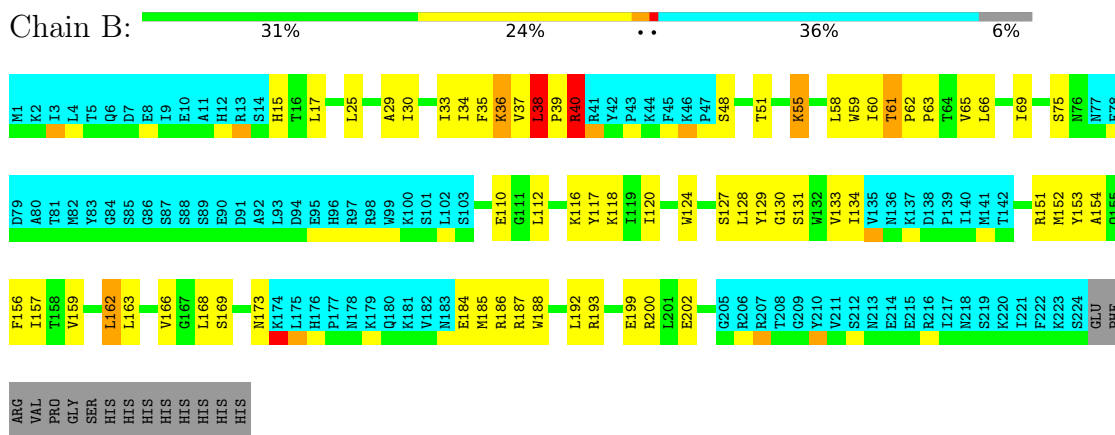
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

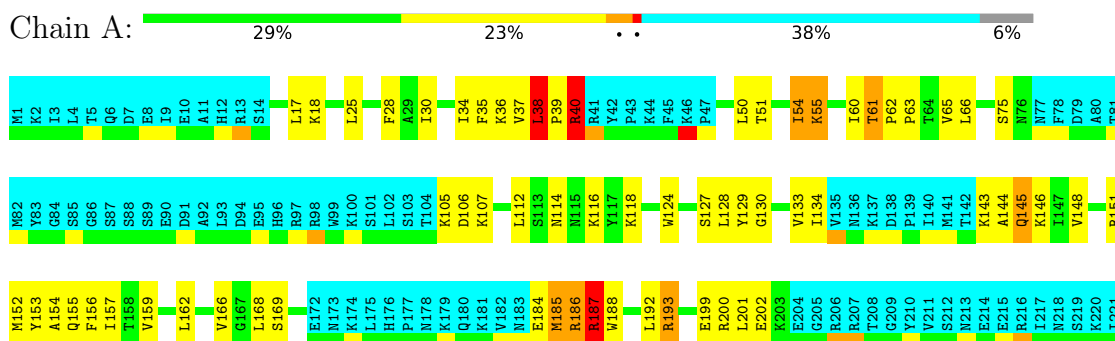


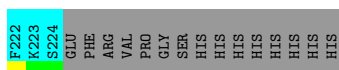
4.2.3 Score per residue for model 3

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



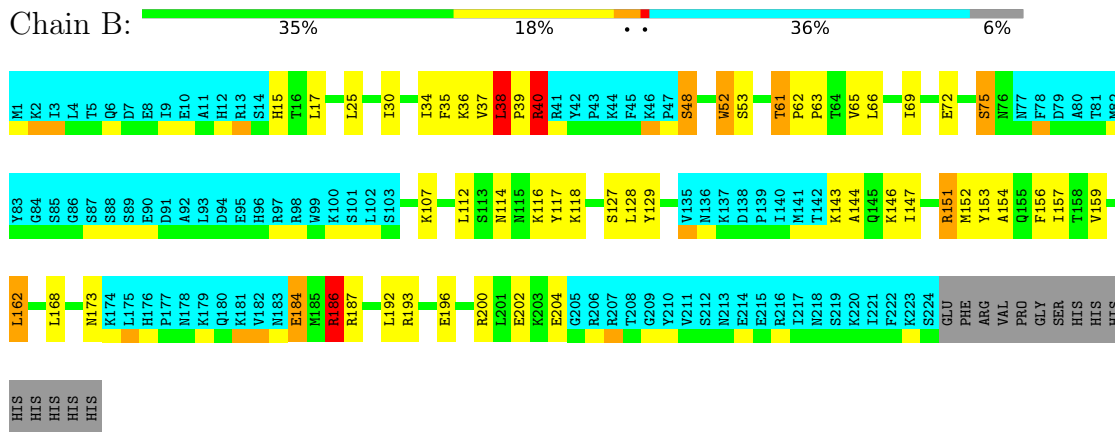
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



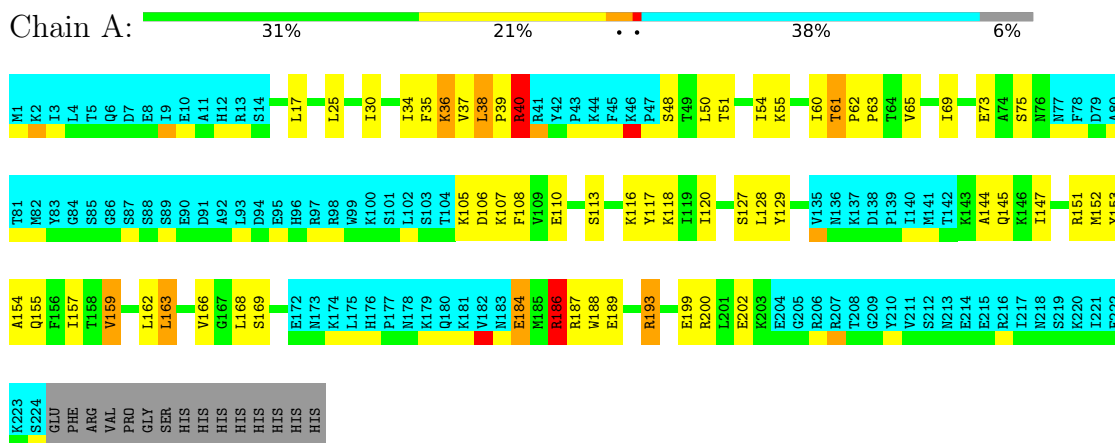


4.2.4 Score per residue for model 4

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

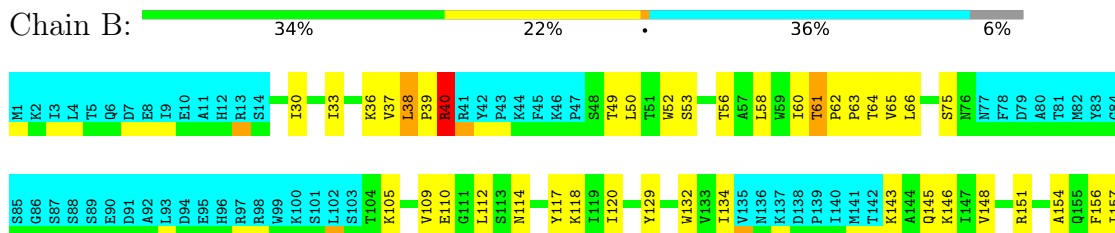


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

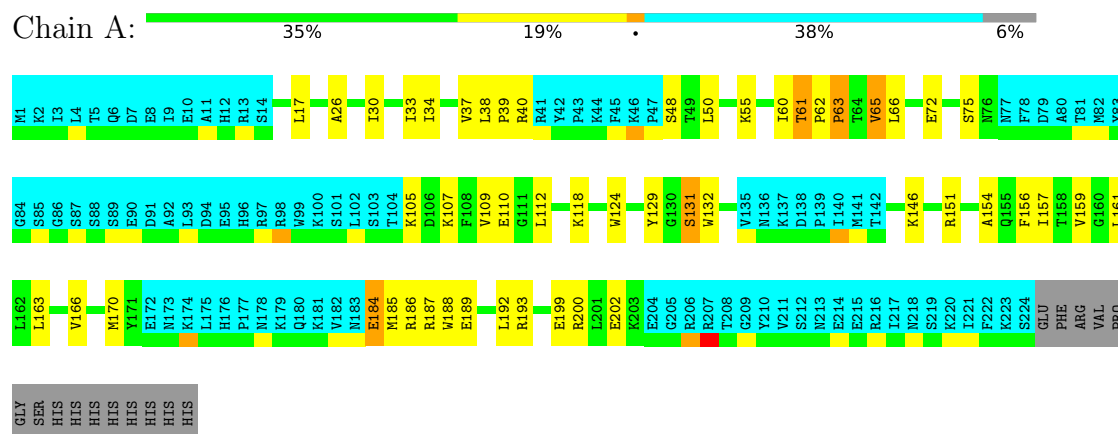


4.2.5 Score per residue for model 5

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

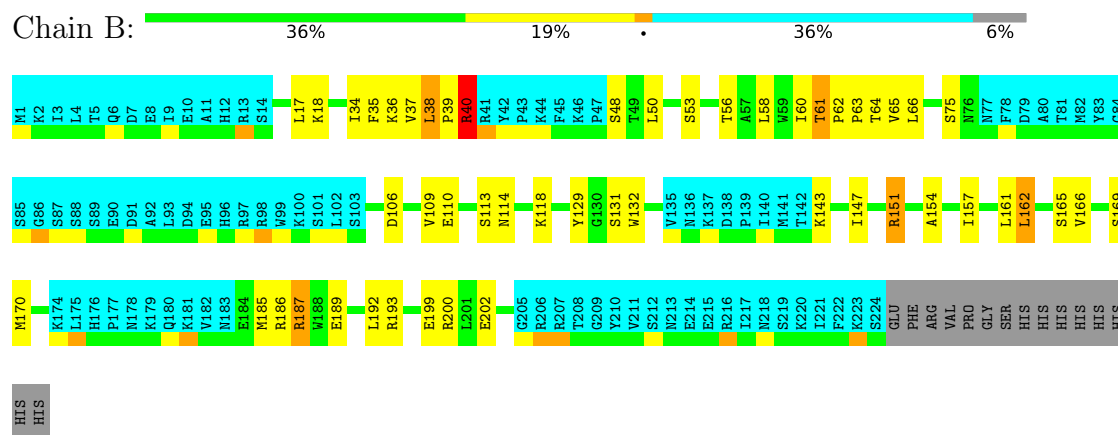


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

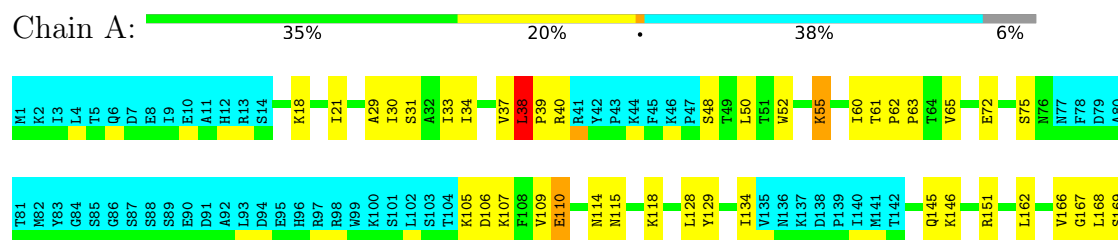


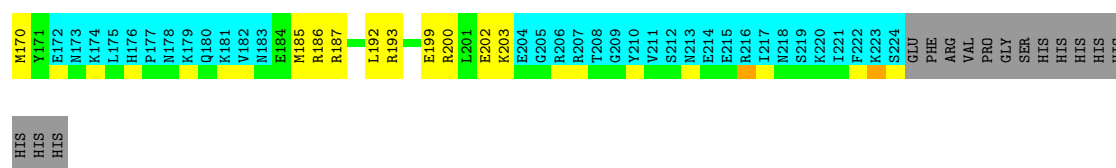
4.2.6 Score per residue for model 6

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



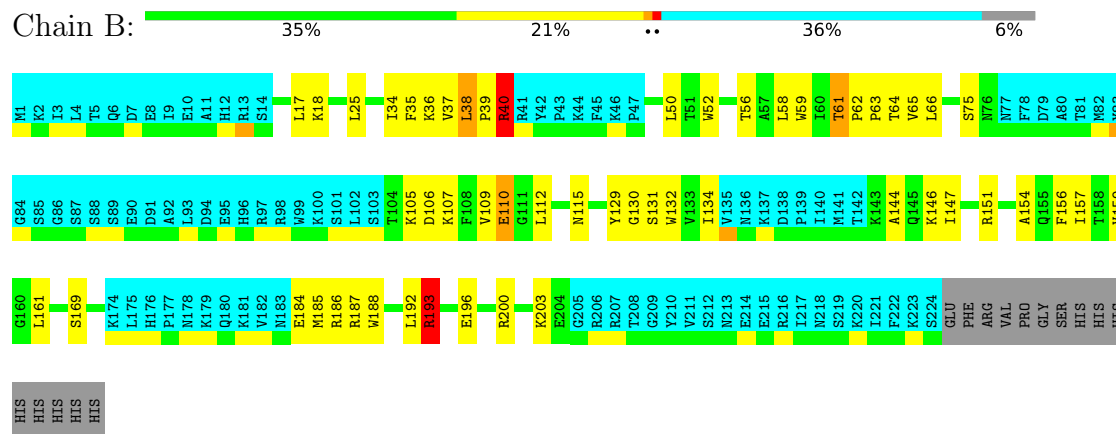
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



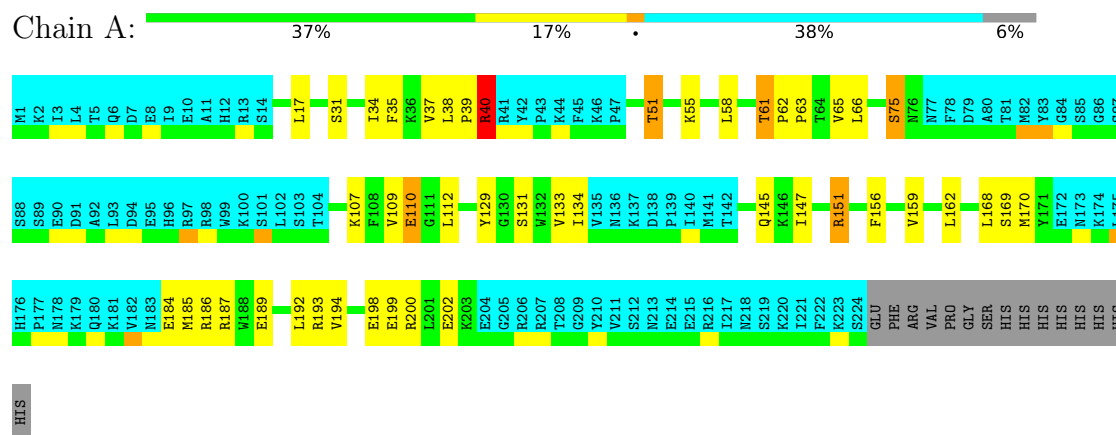


4.2.7 Score per residue for model 7

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

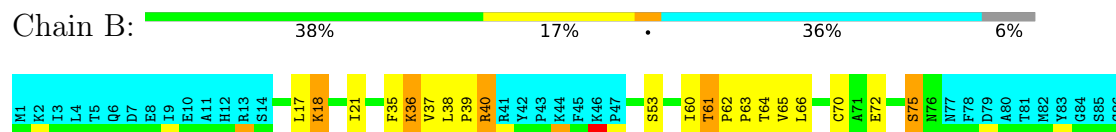


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

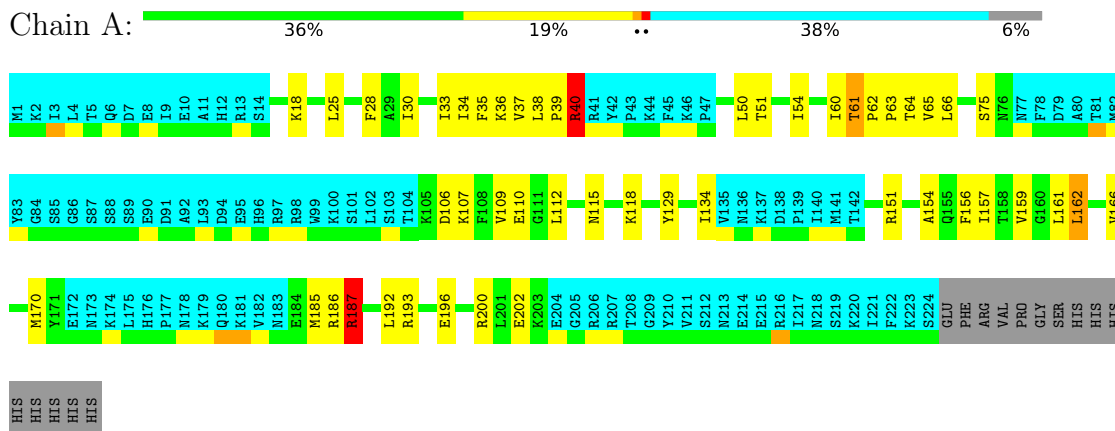


4.2.8 Score per residue for model 8

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

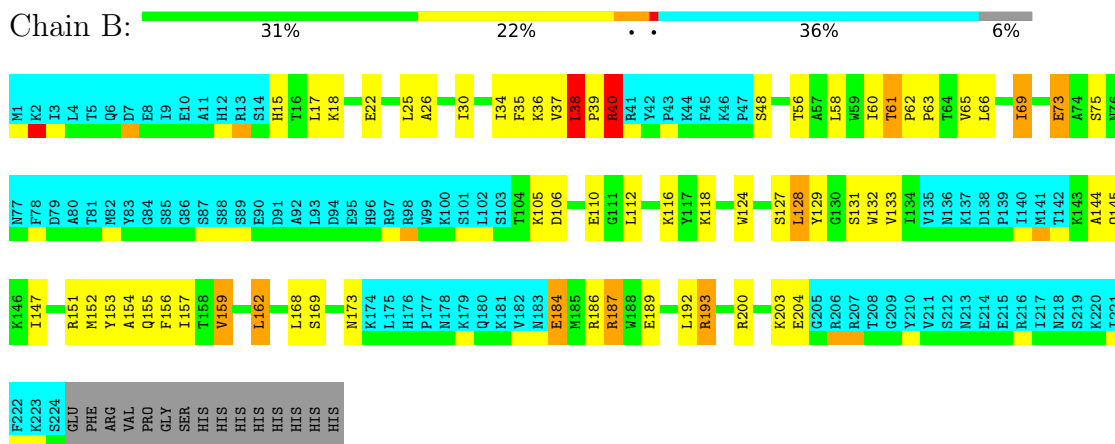


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

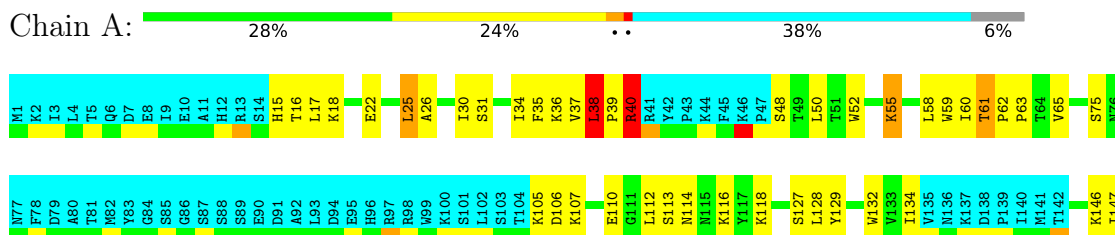


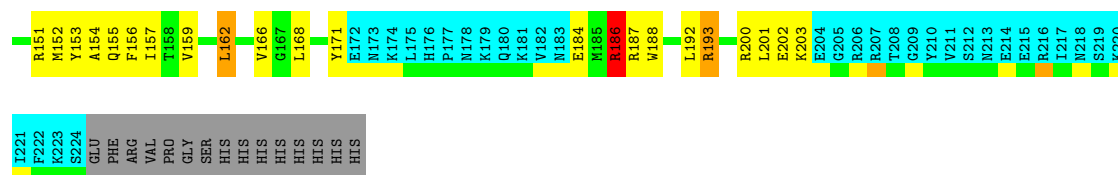
4.2.9 Score per residue for model 9

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



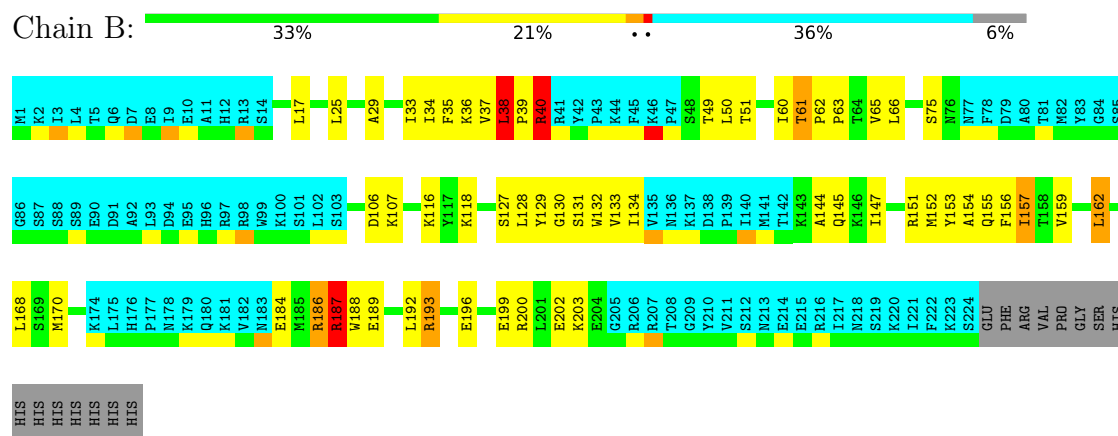
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



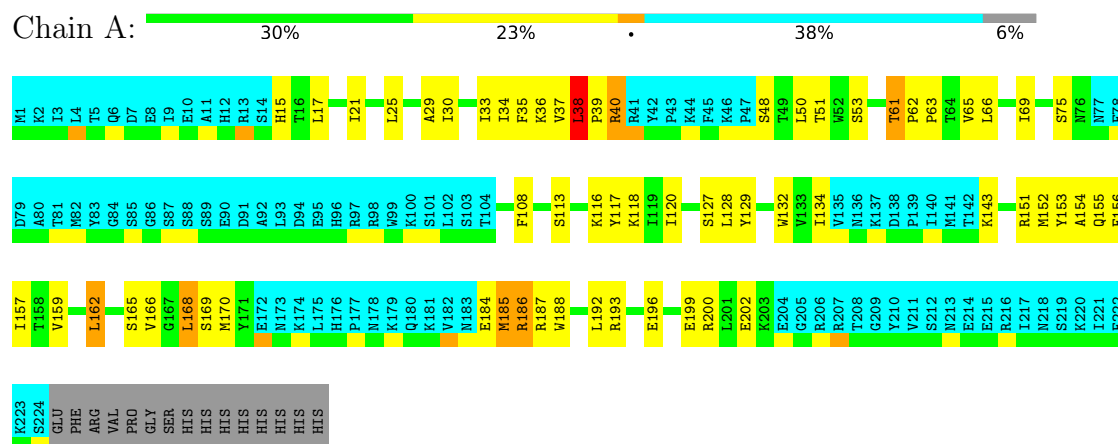


4.2.10 Score per residue for model 10

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

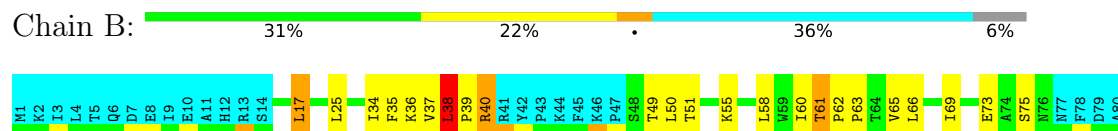


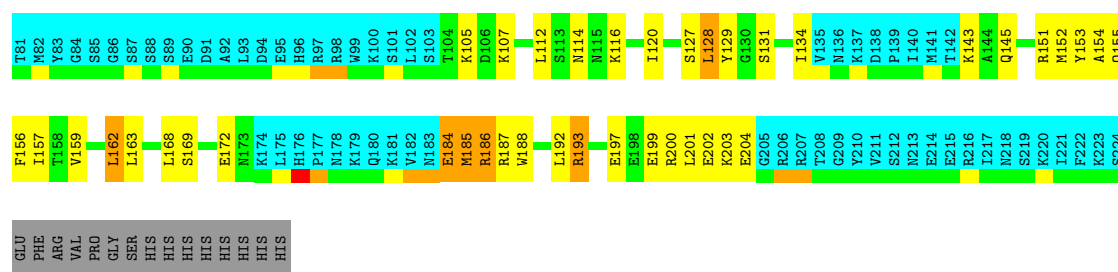
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



4.2.11 Score per residue for model 11

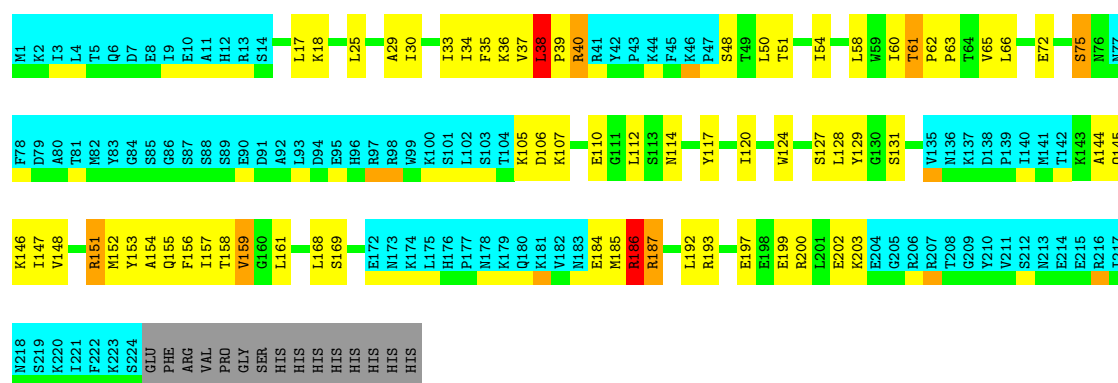
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial





• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

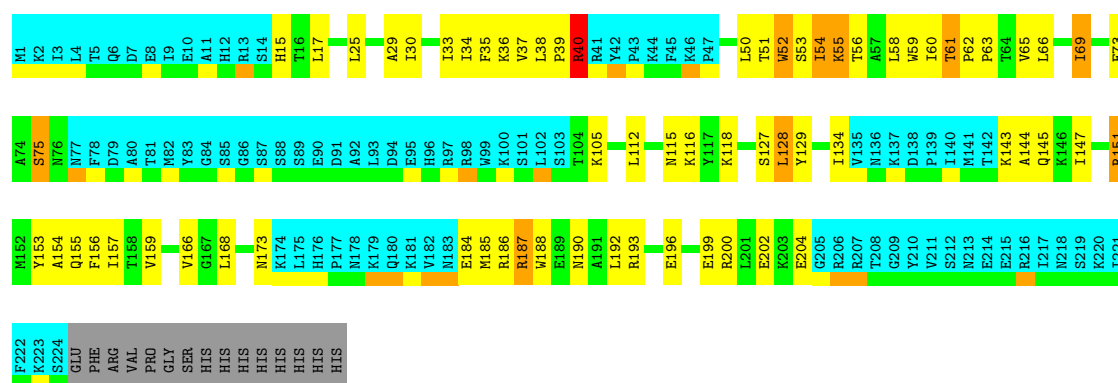
Chain A: 28% 25% 38% 6%



4.2.12 Score per residue for model 12

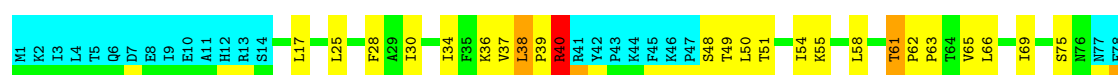
• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

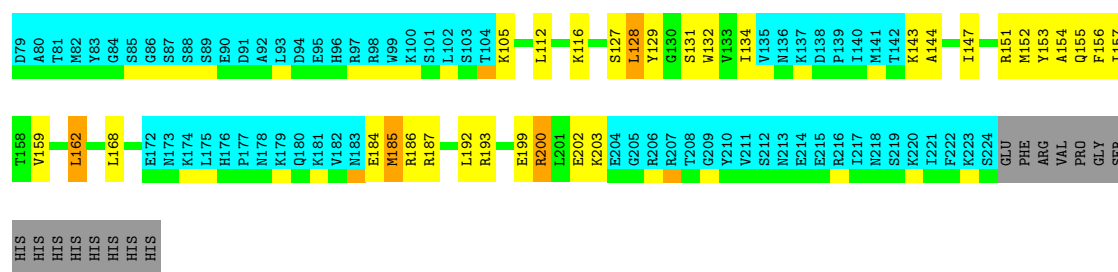
Chain B: 30% 24% 36% 6%



• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

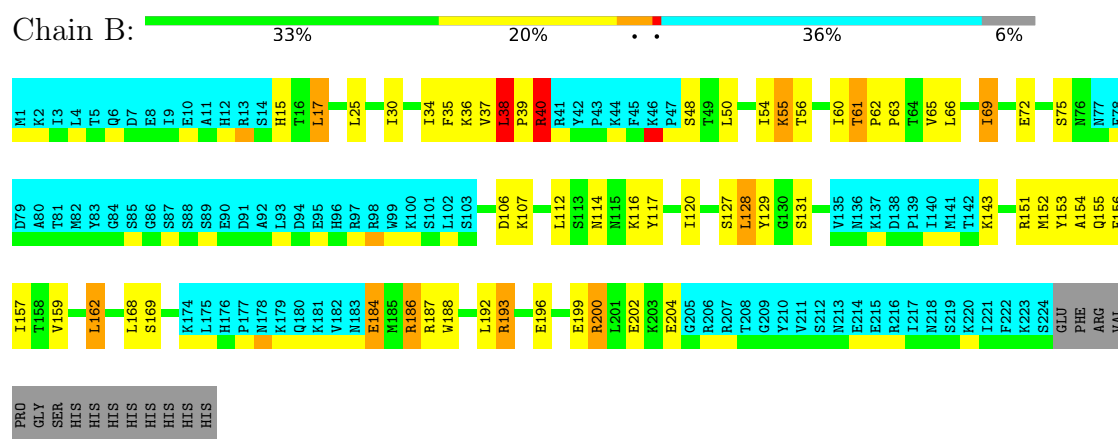
Chain A: 33% 21% 38% 6%



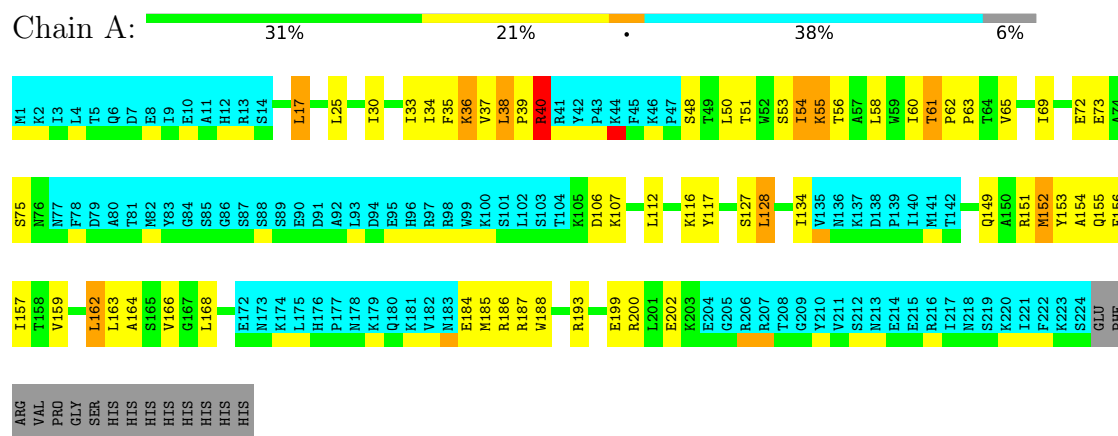


4.2.13 Score per residue for model 13

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

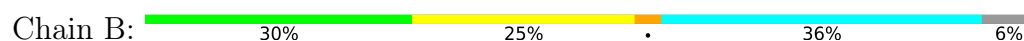


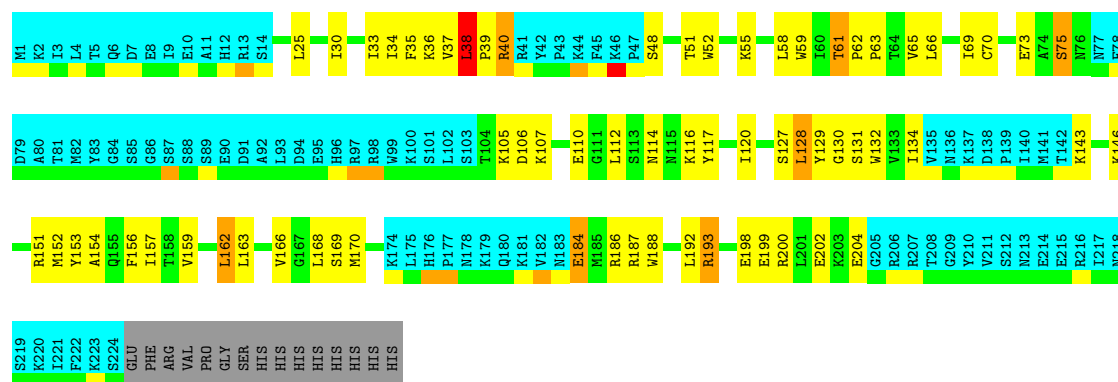
- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



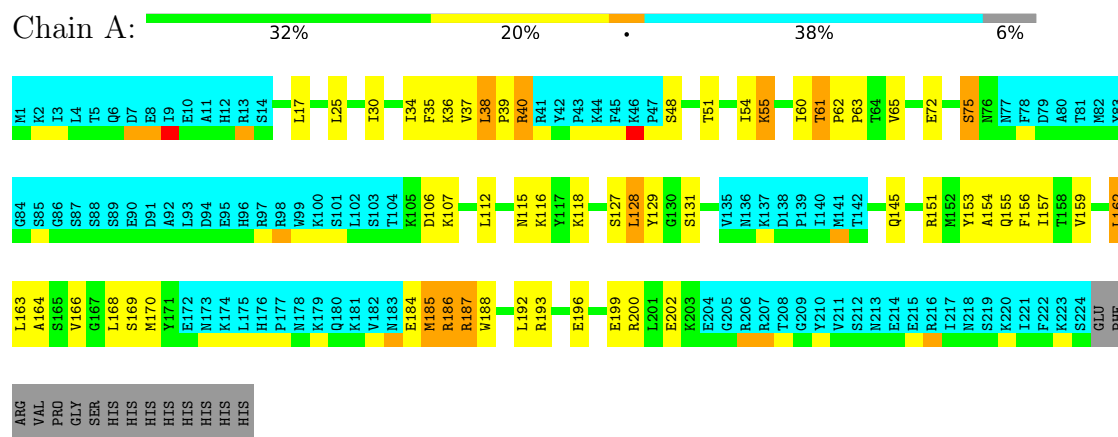
4.2.14 Score per residue for model 14

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



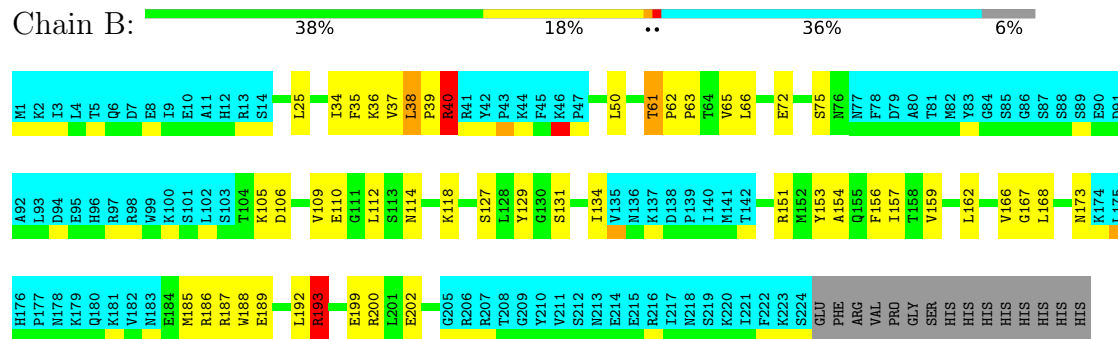


- Molecule 1: Respiratory supercomplex factor 2, mitochondrial

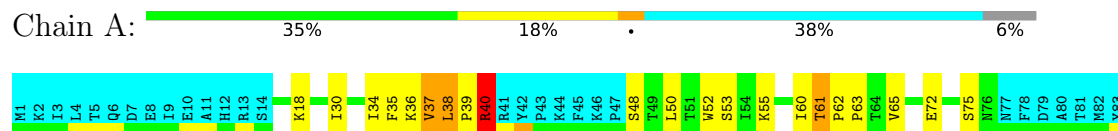


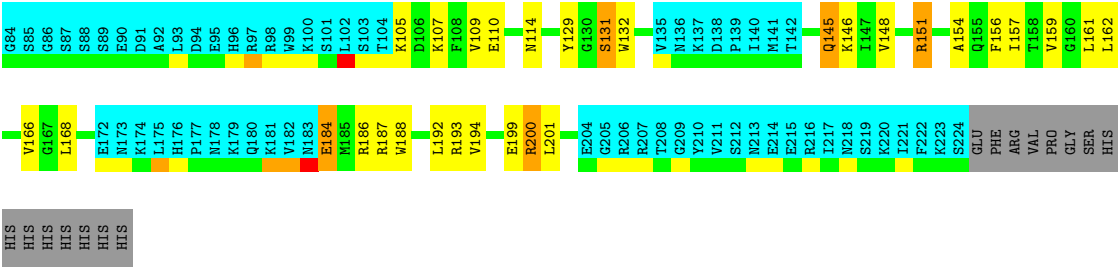
4.2.15 Score per residue for model 15

- Molecule 1: Respiratory supercomplex factor 2, mitochondrial



- Molecule 1: Respiratory supercomplex factor 2, mitochondrial





5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	structure calculation	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1996
Number of shifts mapped to atoms	1996
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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	1.51±0.01	0±0/1069 (0.0± 0.0%)	1.43±0.01	1±1/1449 (0.1± 0.0%)
1	B	1.51±0.01	0±0/1102 (0.0± 0.0%)	1.44±0.01	2±1/1494 (0.1± 0.1%)
All	All	1.51	2/32565 (0.0%)	1.43	40/44145 (0.1%)

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	6.0±0.0
1	B	0.0±0.0	6.0±0.0
All	All	0	180

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	38	LEU	N-CA	5.02	1.50	1.46	15	1
1	A	38	LEU	N-CA	5.01	1.50	1.46	6	1

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	38	LEU	N-CA-CB	-7.14	103.61	110.39	13	11
1	B	38	LEU	N-CA-CB	-7.01	103.73	110.39	13	12
1	B	69	ILE	N-CA-CB	-5.46	104.49	110.65	12	6
1	A	69	ILE	N-CA-CB	-5.43	104.51	110.65	12	2
1	B	162	LEU	N-CA-CB	-5.20	102.47	110.01	2	1
1	A	147	ILE	N-CA-CB	-5.11	104.87	110.65	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	187	ARG	N-CA-CB	-5.11	102.67	110.33	10	2
1	B	134	ILE	N-CA-CB	-5.04	105.12	110.62	5	1
1	A	134	ILE	N-CA-CB	-5.03	105.33	110.62	13	1
1	B	147	ILE	N-CA-CB	-5.03	105.14	110.62	6	1
1	A	37	VAL	N-CA-CB	-5.00	104.96	110.51	15	1
1	A	162	LEU	N-CA-CB	-5.00	102.52	110.22	3	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	B	40	ARG	Sidechain	15
1	B	151	ARG	Sidechain	15
1	B	186	ARG	Sidechain	15
1	B	187	ARG	Sidechain	15
1	B	193	ARG	Sidechain	15
1	B	200	ARG	Sidechain	15
1	A	40	ARG	Sidechain	15
1	A	151	ARG	Sidechain	15
1	A	186	ARG	Sidechain	15
1	A	187	ARG	Sidechain	15
1	A	193	ARG	Sidechain	15
1	A	200	ARG	Sidechain	15

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	1047	1086	1086	38±7
1	B	1080	1111	1111	34±6
All	All	31905	32955	32955	1088

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 17.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:VAL:HG11	1:B:129:TYR:CD1	0.92	1.99	15	2
1:A:37:VAL:HG11	1:A:129:TYR:CD1	0.91	2.00	15	1
1:A:37:VAL:HG11	1:A:129:TYR:CD2	0.89	2.02	8	1
1:A:25:LEU:HD13	1:A:26:ALA:N	0.88	1.83	9	1
1:B:128:LEU:HD13	1:B:129:TYR:N	0.85	1.87	14	3
1:A:37:VAL:HG21	1:A:129:TYR:CE2	0.85	2.07	5	3
1:A:62:PRO:O	1:A:65:VAL:HG22	0.84	1.73	9	14
1:B:37:VAL:HG21	1:B:129:TYR:CE2	0.83	2.08	5	3
1:A:154:ALA:O	1:A:157:ILE:HG22	0.83	1.73	15	3
1:A:166:VAL:HG21	1:A:188:TRP:CZ2	0.83	2.09	9	7
1:A:128:LEU:HD13	1:A:129:TYR:N	0.81	1.90	12	2
1:A:62:PRO:O	1:A:65:VAL:HG12	0.81	1.75	8	1
1:B:62:PRO:O	1:B:65:VAL:HG22	0.81	1.76	13	11
1:B:62:PRO:O	1:B:65:VAL:HG12	0.81	1.76	6	4
1:A:166:VAL:HG11	1:A:188:TRP:CZ2	0.81	2.11	5	2
1:A:156:PHE:O	1:A:159:VAL:HG12	0.80	1.76	15	13
1:B:156:PHE:O	1:B:159:VAL:HG12	0.80	1.75	1	14
1:B:154:ALA:O	1:B:157:ILE:HG22	0.80	1.76	7	5
1:A:25:LEU:C	1:A:25:LEU:HD22	0.79	2.01	9	1
1:A:37:VAL:HG21	1:A:128:LEU:HD11	0.78	1.55	2	8
1:B:37:VAL:HG11	1:B:129:TYR:CD2	0.78	2.14	7	2
1:A:162:LEU:C	1:A:162:LEU:HD12	0.76	2.05	4	1
1:B:34:ILE:O	1:B:37:VAL:HG22	0.76	1.80	12	10
1:B:61:THR:O	1:B:64:THR:HG22	0.76	1.79	7	3
1:A:34:ILE:O	1:A:37:VAL:HG22	0.76	1.80	12	12
1:B:54:ILE:HD12	1:B:55:LYS:N	0.75	1.96	13	1
1:B:153:TYR:O	1:B:157:ILE:HG23	0.75	1.82	10	4
1:B:61:THR:O	1:B:65:VAL:HG13	0.74	1.83	15	11
1:A:54:ILE:HD12	1:A:55:LYS:N	0.74	1.97	14	1
1:A:25:LEU:HD22	1:A:25:LEU:O	0.73	1.82	9	1
1:A:201:LEU:HD23	1:A:201:LEU:O	0.73	1.84	2	1
1:B:54:ILE:HD13	1:B:55:LYS:N	0.72	1.98	12	1
1:A:33:ILE:O	1:A:37:VAL:HG13	0.72	1.84	13	2
1:A:37:VAL:HG11	1:A:129:TYR:CG	0.71	2.19	7	1
1:A:37:VAL:HG23	1:A:38:LEU:HD12	0.71	1.62	6	3
1:A:61:THR:O	1:A:65:VAL:HG13	0.71	1.86	1	10
1:A:54:ILE:HD13	1:A:55:LYS:N	0.70	2.00	13	2
1:B:37:VAL:HG21	1:B:129:TYR:CZ	0.70	2.20	5	4
1:A:37:VAL:HG11	1:A:129:TYR:HB3	0.70	1.64	7	1
1:A:144:ALA:HA	1:A:147:ILE:HD12	0.70	1.63	12	4
1:B:153:TYR:CE2	1:B:157:ILE:HG21	0.69	2.22	13	4
1:A:117:TYR:HA	1:A:120:ILE:HD12	0.69	1.65	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:52:TRP:O	1:B:56:THR:HG23	0.68	1.88	12	3
1:B:201:LEU:O	1:B:201:LEU:HD13	0.68	1.87	11	1
1:A:34:ILE:HD12	1:A:35:PHE:N	0.68	2.03	4	11
1:A:166:VAL:HG21	1:A:188:TRP:CE2	0.68	2.23	9	2
1:B:185:MET:HE3	1:B:189:GLU:OE1	0.67	1.89	15	2
1:A:61:THR:O	1:A:64:THR:HG22	0.67	1.89	8	1
1:B:162:LEU:HD11	1:B:187:ARG:HD3	0.66	1.67	6	1
1:A:30:ILE:O	1:A:34:ILE:HG23	0.66	1.90	9	12
1:B:30:ILE:HA	1:B:33:ILE:HD12	0.66	1.68	5	1
1:B:166:VAL:HG21	1:B:188:TRP:CZ2	0.65	2.26	12	2
1:A:144:ALA:O	1:A:147:ILE:HG12	0.65	1.90	11	1
1:B:34:ILE:HD12	1:B:35:PHE:N	0.65	2.06	3	12
1:A:37:VAL:HG11	1:A:129:TYR:CB	0.64	2.23	7	1
1:A:166:VAL:HG22	1:A:184:GLU:HG2	0.63	1.70	15	1
1:B:128:LEU:C	1:B:128:LEU:HD12	0.63	2.19	3	7
1:B:34:ILE:HG22	1:B:129:TYR:OH	0.63	1.94	6	2
1:B:201:LEU:HD13	1:B:201:LEU:C	0.63	2.19	11	1
1:A:201:LEU:O	1:A:201:LEU:HD13	0.62	1.93	3	1
1:A:201:LEU:C	1:A:201:LEU:HD13	0.62	2.19	9	2
1:A:201:LEU:HD13	1:A:201:LEU:C	0.62	2.19	3	1
1:A:162:LEU:O	1:A:166:VAL:HG22	0.62	1.94	8	1
1:A:128:LEU:C	1:A:128:LEU:HD12	0.62	2.19	13	6
1:A:153:TYR:CE2	1:A:157:ILE:HG21	0.62	2.30	1	3
1:A:162:LEU:HD12	1:A:163:LEU:N	0.62	2.09	4	1
1:B:163:LEU:C	1:B:163:LEU:HD13	0.62	2.19	14	1
1:A:201:LEU:HD13	1:A:201:LEU:O	0.61	1.94	9	2
1:B:18:LYS:O	1:B:21:ILE:HG22	0.61	1.96	8	1
1:B:37:VAL:HG13	1:B:129:TYR:CD2	0.61	2.30	8	1
1:B:116:LYS:O	1:B:120:ILE:HD12	0.61	1.96	11	1
1:B:17:LEU:HD11	1:B:69:ILE:HA	0.61	1.71	9	5
1:B:30:ILE:O	1:B:34:ILE:HG23	0.61	1.96	4	6
1:A:37:VAL:HG21	1:A:128:LEU:CD1	0.61	2.26	6	2
1:A:128:LEU:HD12	1:A:129:TYR:N	0.61	2.11	4	8
1:A:162:LEU:HD11	1:A:187:ARG:CG	0.60	2.25	8	1
1:B:37:VAL:HG21	1:B:128:LEU:HD11	0.60	1.72	1	3
1:B:128:LEU:HD12	1:B:129:TYR:N	0.60	2.11	1	4
1:B:17:LEU:HG	1:B:69:ILE:HG23	0.60	1.72	13	3
1:A:128:LEU:HD12	1:A:128:LEU:C	0.59	2.21	11	2
1:B:128:LEU:C	1:B:128:LEU:HD22	0.59	2.21	14	3
1:A:54:ILE:HD12	1:A:54:ILE:C	0.59	2.22	14	1
1:A:21:ILE:HD12	1:A:21:ILE:N	0.59	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:CG2	1:A:128:LEU:HD11	0.59	2.27	2	4
1:A:21:ILE:HD11	1:A:69:ILE:HD13	0.58	1.73	2	3
1:B:128:LEU:HD13	1:B:128:LEU:C	0.58	2.23	14	3
1:B:134:ILE:HD12	1:B:134:ILE:C	0.58	2.23	3	1
1:B:54:ILE:HD12	1:B:54:ILE:C	0.58	2.23	13	1
1:A:62:PRO:HG2	1:A:63:PRO:HD3	0.58	1.75	9	14
1:A:128:LEU:C	1:A:128:LEU:HD22	0.58	2.23	12	2
1:B:128:LEU:HD12	1:B:128:LEU:C	0.58	2.23	1	1
1:A:128:LEU:HD13	1:A:128:LEU:C	0.58	2.22	12	2
1:A:17:LEU:HD13	1:A:72:GLU:OE2	0.58	1.98	13	1
1:A:153:TYR:CD1	1:A:157:ILE:HG23	0.57	2.34	13	2
1:B:62:PRO:HG2	1:B:63:PRO:HD3	0.57	1.76	9	14
1:B:60:ILE:O	1:B:64:THR:HG23	0.57	2.00	8	1
1:A:62:PRO:N	1:A:63:PRO:HD2	0.56	2.14	5	15
1:A:30:ILE:HA	1:A:33:ILE:HD12	0.56	1.78	5	2
1:A:184:GLU:HB2	1:A:185:MET:HE3	0.56	1.76	14	2
1:A:162:LEU:HD13	1:A:162:LEU:N	0.55	2.16	12	6
1:A:34:ILE:HG22	1:A:129:TYR:OH	0.55	2.01	8	2
1:A:30:ILE:HG22	1:A:34:ILE:CG2	0.55	2.32	12	2
1:A:17:LEU:HD12	1:A:69:ILE:CG1	0.55	2.32	2	1
1:B:62:PRO:N	1:B:63:PRO:HD2	0.55	2.17	5	15
1:A:166:VAL:HG21	1:A:188:TRP:HE1	0.55	1.62	15	2
1:B:154:ALA:HA	1:B:157:ILE:CG1	0.55	2.32	13	8
1:A:184:GLU:CB	1:A:185:MET:HE3	0.55	2.32	12	1
1:A:54:ILE:HD13	1:A:54:ILE:C	0.54	2.26	3	2
1:A:154:ALA:HA	1:A:157:ILE:CG1	0.54	2.32	12	9
1:B:144:ALA:HA	1:B:147:ILE:HD12	0.54	1.78	7	7
1:A:35:PHE:CZ	1:A:51:THR:HG23	0.54	2.36	13	1
1:A:62:PRO:N	1:A:63:PRO:CD	0.54	2.71	6	15
1:B:130:GLY:O	1:B:134:ILE:HD12	0.54	2.02	14	2
1:A:153:TYR:O	1:A:157:ILE:HG23	0.54	2.02	2	2
1:B:54:ILE:HD13	1:B:54:ILE:C	0.54	2.27	12	1
1:B:193:ARG:CZ	1:A:194:VAL:HG11	0.53	2.33	7	1
1:B:153:TYR:CE1	1:B:157:ILE:HG21	0.53	2.38	3	1
1:B:33:ILE:O	1:B:37:VAL:HG13	0.53	2.03	14	2
1:B:162:LEU:O	1:B:166:VAL:HG23	0.52	2.04	2	1
1:B:109:VAL:HG13	1:B:110:GLU:N	0.52	2.19	8	5
1:B:21:ILE:HD11	1:B:69:ILE:HD13	0.52	1.79	2	2
1:B:34:ILE:HD12	1:B:34:ILE:C	0.52	2.29	6	11
1:A:25:LEU:HD13	1:A:26:ALA:H	0.52	1.63	9	1
1:A:162:LEU:C	1:A:162:LEU:CD1	0.52	2.80	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:162:LEU:O	1:B:166:VAL:HG22	0.52	2.05	6	1
1:B:128:LEU:HD22	1:B:128:LEU:O	0.52	2.05	14	3
1:B:60:ILE:C	1:B:63:PRO:HD2	0.52	2.30	5	9
1:B:162:LEU:HD13	1:B:162:LEU:N	0.52	2.20	4	7
1:A:34:ILE:HD12	1:A:34:ILE:C	0.52	2.30	3	7
1:A:37:VAL:CG2	1:A:38:LEU:HD12	0.52	2.34	6	1
1:B:128:LEU:HG	1:B:129:TYR:N	0.52	2.20	9	4
1:A:61:THR:N	1:A:62:PRO:HD2	0.52	2.20	6	14
1:A:154:ALA:HA	1:A:157:ILE:HG12	0.52	1.82	3	9
1:B:61:THR:N	1:B:62:PRO:HD2	0.51	2.20	7	14
1:A:166:VAL:HG13	1:A:184:GLU:OE2	0.51	2.05	3	1
1:A:25:LEU:HD13	1:A:25:LEU:C	0.51	2.29	9	1
1:B:37:VAL:HG11	1:B:129:TYR:CE2	0.51	2.39	5	2
1:A:37:VAL:HG21	1:A:129:TYR:CZ	0.51	2.39	5	3
1:A:109:VAL:HG13	1:A:110:GLU:N	0.51	2.19	6	5
1:A:144:ALA:HA	1:A:147:ILE:HD13	0.51	1.81	11	1
1:B:62:PRO:N	1:B:63:PRO:CD	0.50	2.74	7	14
1:A:128:LEU:HD22	1:A:128:LEU:O	0.50	2.06	12	2
1:B:117:TYR:HA	1:B:120:ILE:HD12	0.50	1.83	14	4
1:A:60:ILE:C	1:A:63:PRO:HD2	0.50	2.31	9	11
1:A:35:PHE:CE1	1:A:51:THR:HG23	0.50	2.41	11	1
1:B:62:PRO:CD	1:B:63:PRO:HD2	0.50	2.37	5	9
1:A:38:LEU:HB2	1:A:39:PRO:HD3	0.50	1.84	12	8
1:A:168:LEU:C	1:A:168:LEU:HD12	0.49	2.32	2	1
1:A:34:ILE:C	1:A:34:ILE:HD12	0.49	2.31	8	2
1:A:61:THR:N	1:A:62:PRO:CD	0.49	2.76	6	13
1:B:37:VAL:HG13	1:B:129:TYR:CG	0.49	2.43	8	1
1:B:37:VAL:HG21	1:B:129:TYR:CD2	0.49	2.42	15	1
1:B:163:LEU:HD23	1:B:164:ALA:N	0.49	2.22	1	1
1:A:154:ALA:O	1:A:155:GLN:C	0.49	2.55	3	10
1:A:35:PHE:CD2	1:A:51:THR:HG21	0.49	2.43	8	1
1:A:55:LYS:O	1:A:59:TRP:CE3	0.49	2.65	9	1
1:B:37:VAL:HG23	1:B:38:LEU:N	0.49	2.23	12	10
1:A:153:TYR:CE1	1:A:157:ILE:HG21	0.49	2.42	14	1
1:B:38:LEU:CB	1:B:39:PRO:CD	0.49	2.90	9	11
1:B:154:ALA:HA	1:B:157:ILE:HG12	0.48	1.84	1	9
1:A:62:PRO:CD	1:A:63:PRO:HD2	0.48	2.38	5	5
1:A:37:VAL:HG23	1:A:38:LEU:N	0.48	2.23	9	12
1:B:36:LYS:O	1:B:40:ARG:CB	0.48	2.60	12	15
1:B:61:THR:N	1:B:62:PRO:CD	0.48	2.77	7	12
1:A:38:LEU:CB	1:A:39:PRO:CD	0.48	2.91	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:VAL:O	1:B:129:TYR:CE2	0.48	2.67	2	3
1:B:129:TYR:CD1	1:B:129:TYR:N	0.48	2.80	6	2
1:B:69:ILE:HG22	1:B:73:GLU:OE2	0.48	2.08	9	1
1:A:36:LYS:O	1:A:40:ARG:CB	0.48	2.61	10	12
1:A:17:LEU:HD22	1:A:72:GLU:OE1	0.48	2.09	13	1
1:A:163:LEU:HD23	1:A:164:ALA:N	0.48	2.24	13	3
1:A:159:VAL:HG23	1:A:162:LEU:HD21	0.48	1.85	4	1
1:A:168:LEU:HD12	1:A:168:LEU:C	0.48	2.34	10	1
1:A:37:VAL:O	1:A:129:TYR:CZ	0.48	2.67	14	1
1:A:62:PRO:O	1:A:65:VAL:CG2	0.47	2.61	15	4
1:B:37:VAL:O	1:B:129:TYR:CE1	0.47	2.67	14	3
1:A:31:SER:OG	1:A:59:TRP:CH2	0.47	2.67	9	1
1:A:29:ALA:C	1:A:33:ILE:HD12	0.47	2.34	6	1
1:A:35:PHE:CD2	1:A:51:THR:CG2	0.47	2.97	7	1
1:A:22:GLU:O	1:A:25:LEU:CD1	0.47	2.62	9	1
1:A:153:TYR:CD2	1:A:157:ILE:HD13	0.47	2.45	1	1
1:A:62:PRO:CD	1:A:63:PRO:CD	0.47	2.93	5	12
1:B:21:ILE:CD1	1:B:69:ILE:HD13	0.47	2.40	2	1
1:A:153:TYR:CZ	1:A:157:ILE:HG21	0.47	2.44	1	1
1:B:154:ALA:O	1:B:155:GLN:C	0.47	2.58	12	4
1:A:144:ALA:O	1:A:147:ILE:N	0.47	2.40	11	1
1:A:168:LEU:HD12	1:A:168:LEU:O	0.47	2.10	2	2
1:B:38:LEU:HB2	1:B:39:PRO:HD3	0.47	1.87	12	1
1:A:166:VAL:HG22	1:A:184:GLU:CG	0.47	2.38	15	1
1:A:201:LEU:HD23	1:A:201:LEU:C	0.46	2.35	2	1
1:B:131:SER:O	1:B:134:ILE:HD11	0.46	2.10	3	1
1:B:166:VAL:HG13	1:B:184:GLU:HG2	0.46	1.86	3	1
1:A:35:PHE:O	1:A:39:PRO:CD	0.46	2.63	7	3
1:B:37:VAL:CG2	1:B:128:LEU:HD11	0.46	2.41	1	1
1:A:38:LEU:N	1:A:39:PRO:HD2	0.46	2.25	3	10
1:A:144:ALA:O	1:A:148:VAL:HG22	0.46	2.11	3	1
1:A:163:LEU:C	1:A:163:LEU:HD23	0.46	2.36	2	2
1:A:152:MET:CG	1:A:153:TYR:N	0.46	2.78	11	5
1:A:37:VAL:HG23	1:A:38:LEU:H	0.46	1.71	3	3
1:A:35:PHE:CE1	1:A:51:THR:CG2	0.46	2.99	11	1
1:B:152:MET:CG	1:B:153:TYR:N	0.46	2.78	2	8
1:A:133:VAL:HG23	1:A:134:ILE:N	0.46	2.25	7	1
1:B:37:VAL:HG23	1:B:38:LEU:H	0.46	1.71	12	3
1:A:62:PRO:CG	1:A:63:PRO:HD3	0.46	2.39	1	8
1:A:186:ARG:O	1:A:190:ASN:HB2	0.46	2.11	2	1
1:B:130:GLY:O	1:B:134:ILE:HG23	0.46	2.11	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ILE:C	1:A:54:ILE:CD1	0.46	2.89	3	3
1:B:58:LEU:O	1:B:62:PRO:CD	0.46	2.64	6	5
1:A:131:SER:HA	1:A:134:ILE:HD12	0.46	1.87	2	1
1:B:54:ILE:C	1:B:54:ILE:CD1	0.45	2.89	12	1
1:A:128:LEU:CD1	1:A:129:TYR:N	0.45	2.80	11	5
1:A:36:LYS:O	1:A:40:ARG:HB3	0.45	2.12	8	6
1:B:35:PHE:CE1	1:B:51:THR:HG23	0.45	2.46	12	1
1:B:128:LEU:C	1:B:128:LEU:CD1	0.45	2.90	3	4
1:A:147:ILE:CG1	1:A:148:VAL:N	0.45	2.79	11	1
1:B:62:PRO:CD	1:B:63:PRO:CD	0.45	2.94	5	14
1:A:17:LEU:HD12	1:A:69:ILE:HG12	0.45	1.87	2	1
1:A:38:LEU:HB2	1:A:39:PRO:CD	0.45	2.41	13	5
1:B:130:GLY:O	1:B:134:ILE:HG22	0.45	2.11	7	1
1:A:144:ALA:O	1:A:145:GLN:C	0.45	2.59	11	1
1:A:153:TYR:HD1	1:A:157:ILE:HG23	0.45	1.69	13	2
1:A:26:ALA:O	1:A:30:ILE:HD12	0.45	2.11	5	1
1:A:106:ASP:O	1:A:109:VAL:HG12	0.45	2.12	8	2
1:A:117:TYR:CD2	1:A:117:TYR:C	0.45	2.95	11	2
1:B:55:LYS:O	1:B:59:TRP:CE3	0.45	2.70	3	2
1:B:166:VAL:HG21	1:B:188:TRP:HZ2	0.45	1.71	3	1
1:B:17:LEU:HD21	1:B:73:GLU:OE2	0.45	2.12	9	1
1:A:130:GLY:O	1:A:134:ILE:HG23	0.45	2.11	3	1
1:B:38:LEU:N	1:B:39:PRO:HD2	0.45	2.28	11	6
1:A:128:LEU:C	1:A:128:LEU:CD1	0.45	2.89	13	3
1:A:153:TYR:CE1	1:A:157:ILE:CG2	0.45	2.99	4	1
1:B:38:LEU:HD12	1:B:38:LEU:N	0.45	2.27	5	1
1:A:21:ILE:N	1:A:21:ILE:CD1	0.45	2.79	6	1
1:A:21:ILE:CD1	1:A:69:ILE:HD13	0.44	2.42	2	2
1:B:188:TRP:CD1	1:B:188:TRP:N	0.44	2.84	7	2
1:B:162:LEU:N	1:B:162:LEU:HD13	0.44	2.28	10	1
1:A:17:LEU:HD13	1:A:72:GLU:CD	0.44	2.37	13	1
1:B:163:LEU:C	1:B:163:LEU:HD23	0.44	2.37	3	1
1:B:153:TYR:O	1:B:157:ILE:HG12	0.44	2.12	4	1
1:A:166:VAL:HG21	1:A:188:TRP:HZ2	0.44	1.70	10	3
1:B:158:THR:HA	1:B:161:LEU:HD12	0.44	1.90	2	1
1:A:25:LEU:C	1:A:25:LEU:CD2	0.44	2.75	9	1
1:A:51:THR:HA	1:A:54:ILE:CD1	0.44	2.43	12	2
1:B:36:LYS:O	1:B:40:ARG:N	0.44	2.51	2	2
1:B:58:LEU:HA	1:B:61:THR:OG1	0.44	2.12	5	1
1:B:145:GLN:O	1:B:148:VAL:HG22	0.44	2.12	5	1
1:B:153:TYR:CE2	1:B:157:ILE:CG2	0.44	2.99	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:GLN:HG3	1:A:146:LYS:N	0.43	2.28	3	1
1:B:36:LYS:O	1:B:40:ARG:HB3	0.43	2.13	1	5
1:B:128:LEU:CD1	1:B:129:TYR:N	0.43	2.81	10	5
1:B:35:PHE:O	1:B:39:PRO:CG	0.43	2.66	8	5
1:A:185:MET:O	1:A:186:ARG:C	0.43	2.61	3	1
1:A:201:LEU:C	1:A:201:LEU:CD1	0.43	2.90	3	3
1:B:38:LEU:HB2	1:B:39:PRO:CD	0.43	2.43	12	4
1:B:161:LEU:N	1:B:161:LEU:CD1	0.43	2.82	7	1
1:B:109:VAL:CG1	1:B:110:GLU:N	0.43	2.82	8	4
1:B:129:TYR:O	1:B:133:VAL:HG23	0.43	2.13	9	1
1:A:29:ALA:O	1:A:33:ILE:HD12	0.43	2.14	10	2
1:A:162:LEU:N	1:A:162:LEU:CD1	0.43	2.82	12	1
1:A:153:TYR:CD1	1:A:157:ILE:CG2	0.43	3.02	13	1
1:A:166:VAL:HG23	1:A:167:GLY:N	0.43	2.29	6	1
1:B:34:ILE:CD1	1:B:35:PHE:N	0.43	2.80	12	6
1:A:61:THR:OG1	1:A:62:PRO:HD3	0.43	2.14	8	2
1:B:124:TRP:CD1	1:B:124:TRP:O	0.43	2.72	9	1
1:A:163:LEU:HD23	1:A:163:LEU:C	0.43	2.38	13	1
1:B:55:LYS:O	1:B:59:TRP:CD1	0.43	2.72	14	1
1:B:48:SER:O	1:B:52:TRP:CD1	0.43	2.72	4	1
1:B:58:LEU:O	1:B:62:PRO:HD3	0.43	2.13	5	1
1:B:153:TYR:CZ	1:B:157:ILE:CG2	0.43	3.01	12	1
1:B:163:LEU:C	1:B:163:LEU:CD1	0.43	2.91	14	1
1:B:22:GLU:O	1:B:26:ALA:HB2	0.43	2.13	9	1
1:A:166:VAL:HG22	1:A:184:GLU:OE2	0.43	2.14	9	1
1:B:30:ILE:CG2	1:B:34:ILE:CG2	0.43	2.97	14	1
1:A:161:LEU:CD1	1:A:161:LEU:N	0.42	2.82	15	2
1:B:37:VAL:O	1:B:129:TYR:CZ	0.42	2.72	11	2
1:B:29:ALA:O	1:B:33:ILE:HD12	0.42	2.13	12	4
1:B:117:TYR:CD2	1:B:117:TYR:C	0.42	2.97	3	3
1:A:186:ARG:CG	1:A:187:ARG:N	0.42	2.82	3	1
1:B:184:GLU:O	1:B:188:TRP:CG	0.42	2.73	11	2
1:A:61:THR:O	1:A:65:VAL:CG1	0.42	2.66	5	1
1:A:15:HIS:CD2	1:A:15:HIS:N	0.42	2.88	9	1
1:A:158:THR:HA	1:A:161:LEU:HD12	0.42	1.90	11	1
1:A:31:SER:HB2	1:A:58:LEU:HD21	0.42	1.90	7	1
1:A:17:LEU:HD21	1:A:72:GLU:HB3	0.42	1.91	14	1
1:A:51:THR:HA	1:A:54:ILE:HD12	0.42	1.91	11	1
1:A:129:TYR:CD1	1:A:129:TYR:N	0.42	2.84	15	1
1:B:35:PHE:CD1	1:B:35:PHE:O	0.42	2.73	10	2
1:B:37:VAL:HG23	1:B:38:LEU:HD12	0.42	1.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:TYR:CD2	1:A:157:ILE:HG21	0.42	2.50	2	1
1:A:37:VAL:HG21	1:A:128:LEU:HD21	0.42	1.90	13	1
1:B:37:VAL:CG1	1:B:129:TYR:CD2	0.42	3.01	8	3
1:B:106:ASP:O	1:B:109:VAL:HG12	0.42	2.15	6	4
1:A:37:VAL:O	1:A:129:TYR:CE1	0.42	2.73	1	2
1:A:109:VAL:CG1	1:A:110:GLU:N	0.42	2.82	15	4
1:B:188:TRP:N	1:B:188:TRP:CD1	0.42	2.87	10	3
1:B:61:THR:OG1	1:B:62:PRO:HD3	0.42	2.15	13	6
1:A:154:ALA:CA	1:A:157:ILE:HG12	0.42	2.45	3	1
1:B:35:PHE:O	1:B:39:PRO:CD	0.42	2.68	15	2
1:A:37:VAL:HG21	1:A:129:TYR:CD1	0.42	2.50	7	1
1:A:185:MET:HE2	1:A:185:MET:H	0.42	1.74	10	1
1:A:34:ILE:CD1	1:A:35:PHE:N	0.42	2.83	9	5
1:A:52:TRP:CD1	1:A:52:TRP:C	0.42	2.98	6	1
1:B:193:ARG:NH2	1:A:194:VAL:HG11	0.42	2.30	7	1
1:A:35:PHE:O	1:A:35:PHE:CD2	0.42	2.73	11	1
1:B:17:LEU:N	1:B:17:LEU:CD2	0.41	2.83	2	1
1:A:153:TYR:CD1	1:A:157:ILE:HG21	0.41	2.50	4	1
1:A:38:LEU:HD11	1:A:129:TYR:CE2	0.41	2.50	7	1
1:A:24:ALA:O	1:A:28:PHE:CE2	0.41	2.74	1	1
1:A:37:VAL:O	1:A:129:TYR:CE2	0.41	2.73	6	3
1:A:124:TRP:CD1	1:A:124:TRP:O	0.41	2.73	3	2
1:A:52:TRP:O	1:A:55:LYS:CG	0.41	2.68	6	1
1:B:166:VAL:HG13	1:B:184:GLU:CD	0.41	2.40	14	1
1:A:153:TYR:CZ	1:A:157:ILE:CG2	0.41	3.03	1	1
1:A:35:PHE:C	1:A:35:PHE:CD2	0.41	2.98	2	1
1:A:124:TRP:CZ2	1:A:157:ILE:HD12	0.41	2.50	5	1
1:A:30:ILE:HG22	1:A:34:ILE:HG21	0.41	1.91	13	1
1:B:74:ALA:O	1:B:75:SER:C	0.41	2.63	1	1
1:B:109:VAL:O	1:B:113:SER:HB3	0.41	2.15	6	1
1:A:151:ARG:NH2	1:A:198:GLU:CG	0.41	2.84	7	1
1:A:58:LEU:O	1:A:62:PRO:CD	0.41	2.69	11	2
1:A:35:PHE:O	1:A:39:PRO:CG	0.41	2.68	2	2
1:B:62:PRO:CG	1:B:63:PRO:HD3	0.41	2.46	3	2
1:A:154:ALA:O	1:A:157:ILE:CG1	0.41	2.69	3	1
1:A:129:TYR:N	1:A:129:TYR:CD2	0.41	2.82	5	1
1:A:129:TYR:CD2	1:A:129:TYR:N	0.41	2.84	8	1
1:B:186:ARG:CG	1:B:187:ARG:N	0.41	2.83	10	1
1:B:52:TRP:O	1:B:52:TRP:CE3	0.41	2.74	14	1
1:B:153:TYR:CD2	1:B:157:ILE:HG21	0.41	2.50	2	1
1:A:69:ILE:HG22	1:A:73:GLU:OE1	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:SER:O	1:A:35:PHE:CD1	0.41	2.74	7	1
1:B:17:LEU:HD13	1:B:72:GLU:OE1	0.41	2.15	8	1
1:B:201:LEU:C	1:B:201:LEU:CD1	0.41	2.90	11	1
1:B:154:ALA:CA	1:B:157:ILE:HG12	0.40	2.46	1	1
1:A:145:GLN:HG2	1:A:146:LYS:N	0.40	2.30	11	1
1:B:184:GLU:O	1:B:188:TRP:CD1	0.40	2.74	14	1
1:A:52:TRP:CE3	1:A:52:TRP:O	0.40	2.75	1	1
1:A:17:LEU:HD11	1:A:69:ILE:HA	0.40	1.92	10	1
1:A:51:THR:HA	1:A:54:ILE:CG2	0.40	2.47	13	1
1:A:51:THR:HA	1:A:54:ILE:CG1	0.40	2.47	14	1
1:A:124:TRP:O	1:A:124:TRP:CD1	0.40	2.74	2	1
1:B:124:TRP:CD2	1:B:124:TRP:C	0.40	2.99	3	1
1:A:37:VAL:O	1:A:40:ARG:HG3	0.40	2.17	7	1
1:A:34:ILE:CG2	1:A:129:TYR:OH	0.40	2.69	8	1
1:A:144:ALA:O	1:A:147:ILE:CG1	0.40	2.65	11	1
1:B:166:VAL:HG23	1:B:167:GLY:N	0.40	2.31	15	1
1:B:193:ARG:NH1	1:A:194:VAL:CG1	0.40	2.84	15	1
1:A:36:LYS:HA	1:A:39:PRO:HG2	0.40	1.94	14	1
1:A:153:TYR:O	1:A:154:ALA:C	0.40	2.65	14	1
1:A:145:GLN:O	1:A:148:VAL:HG22	0.40	2.17	15	1
1:B:29:ALA:C	1:B:33:ILE:HD12	0.40	2.42	1	1
1:A:149:GLN:O	1:A:152:MET:CG	0.40	2.70	13	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	134/239 (56%)	127±2 (94±1%)	6±2 (5±1%)	1±0 (1±0%)	18	68
1	B	138/239 (58%)	130±2 (95±2%)	7±2 (5±2%)	1±0 (1±0%)	20	70
All	All	4080/7170 (57%)	3855 (94%)	194 (5%)	31 (1%)	18	68

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	75	SER	15
1	A	75	SER	15
1	A	63	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	108/205 (53%)	82±3 (76±3%)	26±3 (24±3%)	2	26
1	B	112/205 (55%)	85±5 (76±4%)	27±5 (24±4%)	2	25
All	All	3300/6150 (54%)	2499 (76%)	801 (24%)	2	26

All 137 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	B	61	THR	15
1	B	66	LEU	15
1	B	192	LEU	15
1	A	202	GLU	14
1	A	168	LEU	13
1	A	192	LEU	13
1	A	199	GLU	13
1	A	61	THR	13
1	B	25	LEU	12
1	B	40	ARG	12
1	B	112	LEU	12
1	B	168	LEU	12
1	B	199	GLU	12
1	A	48	SER	12
1	A	185	MET	12
1	B	202	GLU	12
1	A	50	LEU	12
1	B	127	SER	11
1	A	25	LEU	11
1	A	112	LEU	11
1	A	55	LYS	11
1	A	107	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	B	162	LEU	10
1	A	40	ARG	10
1	A	127	SER	10
1	A	162	LEU	10
1	B	131	SER	10
1	B	38	LEU	9
1	B	50	LEU	9
1	B	114	ASN	9
1	B	116	LYS	9
1	B	118	LYS	9
1	B	193	ARG	9
1	A	66	LEU	9
1	A	105	LYS	9
1	A	116	LYS	9
1	A	118	LYS	9
1	A	169	SER	9
1	B	48	SER	8
1	A	38	LEU	8
1	B	105	LYS	8
1	B	107	LYS	8
1	B	143	LYS	8
1	B	169	SER	8
1	A	17	LEU	8
1	B	204	GLU	8
1	B	17	LEU	7
1	B	128	LEU	7
1	A	170	MET	7
1	B	184	GLU	7
1	B	51	THR	6
1	B	55	LYS	6
1	B	185	MET	6
1	B	145	GLN	6
1	A	114	ASN	6
1	A	132	TRP	6
1	A	18	LYS	6
1	A	106	ASP	6
1	B	196	GLU	6
1	A	131	SER	6
1	B	203	LYS	5
1	A	51	THR	5
1	A	115	ASN	5
1	A	184	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	187	ARG	5
1	A	196	GLU	5
1	B	15	HIS	5
1	B	73	GLU	5
1	B	106	ASP	5
1	B	132	TRP	5
1	B	186	ARG	5
1	A	145	GLN	5
1	B	53	SER	5
1	A	186	ARG	5
1	B	173	ASN	4
1	A	143	LYS	4
1	A	58	LEU	4
1	A	75	SER	4
1	A	193	ARG	4
1	B	110	GLU	4
1	B	75	SER	4
1	B	146	LYS	4
1	B	151	ARG	4
1	A	110	GLU	4
1	A	72	GLU	4
1	A	146	LYS	4
1	B	18	LYS	4
1	A	203	LYS	4
1	B	36	LYS	3
1	B	187	ARG	3
1	A	36	LYS	3
1	A	151	ARG	3
1	A	152	MET	3
1	A	159	VAL	3
1	A	28	PHE	3
1	A	54	ILE	3
1	B	72	GLU	3
1	A	113	SER	3
1	A	189	GLU	3
1	B	49	THR	3
1	B	189	GLU	3
1	B	56	THR	3
1	B	170	MET	3
1	B	115	ASN	3
1	A	53	SER	3
1	A	128	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	49	THR	2
1	A	165	SER	2
1	B	59	TRP	2
1	B	155	GLN	2
1	B	159	VAL	2
1	A	197	GLU	2
1	B	58	LEU	2
1	B	52	TRP	2
1	A	108	PHE	2
1	B	161	LEU	2
1	B	172	GLU	2
1	B	198	GLU	2
1	B	70	CYS	2
1	A	52	TRP	2
1	A	200	ARG	2
1	A	163	LEU	1
1	A	65	VAL	1
1	B	165	SER	1
1	A	31	SER	1
1	A	161	LEU	1
1	A	171	TYR	1
1	B	157	ILE	1
1	B	163	LEU	1
1	B	197	GLU	1
1	B	54	ILE	1
1	B	190	ASN	1
1	B	152	MET	1
1	B	200	ARG	1
1	A	56	THR	1
1	A	73	GLU	1
1	B	153	TYR	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 [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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 32% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1996
Number of shifts mapped to atoms	1996
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	219	-0.18 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	205	0.75 ± 0.06	Should be checked
$^{13}\text{C}'$	214	-0.00 ± 0.11	None needed (< 0.5 ppm)
^{15}N	206	0.49 ± 0.11	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 35%, i.e. 1333 atoms were assigned a chemical shift out of a possible 3771. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	647/1366 (47%)	256/556 (46%)	263/544 (48%)	128/266 (48%)
Sidechain	656/2119 (31%)	426/1396 (31%)	230/652 (35%)	0/71 (0%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	30/286 (10%)	30/140 (21%)	0/134 (0%)	0/12 (0%)
Overall	1333/3771 (35%)	712/2092 (34%)	493/1330 (37%)	128/349 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 1993 atoms were assigned a chemical shift out of a possible 6228. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1050/2238 (47%)	411/908 (45%)	433/896 (48%)	206/434 (47%)
Sidechain	913/3524 (26%)	568/2290 (25%)	345/1084 (32%)	0/150 (0%)
Aromatic	30/466 (6%)	30/230 (13%)	0/216 (0%)	0/20 (0%)
Overall	1993/6228 (32%)	1009/3428 (29%)	778/2196 (35%)	206/604 (34%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

