W O R L D W I D E
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Full wwPDB NMR Structure Validation Report ⓘ

Sep 28, 2020 – 06:15 PM JST

PDB ID	:	6LUL
Title	:	NMR structure and dynamics studies of yeast respiratory super-complex factor 2 in micelles
Authors	:	Zhou, S.; Pontus, P.; Peter, B.; Maler, L.; Adelroth, P.
Deposited on	:	2020-01-29

The following versions of software and data (see references ⓘ) were used in the production of this report:

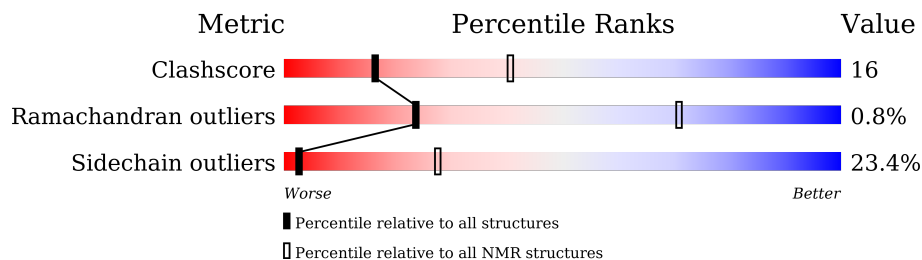|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.14.6
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 34%.

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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.8%
Sidechain outliers		23.4%

Worse　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	239	34%　20%　•　38%　6%
1	B	239	38%　18%　•　36%　6%

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)	0.37	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 (i)

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
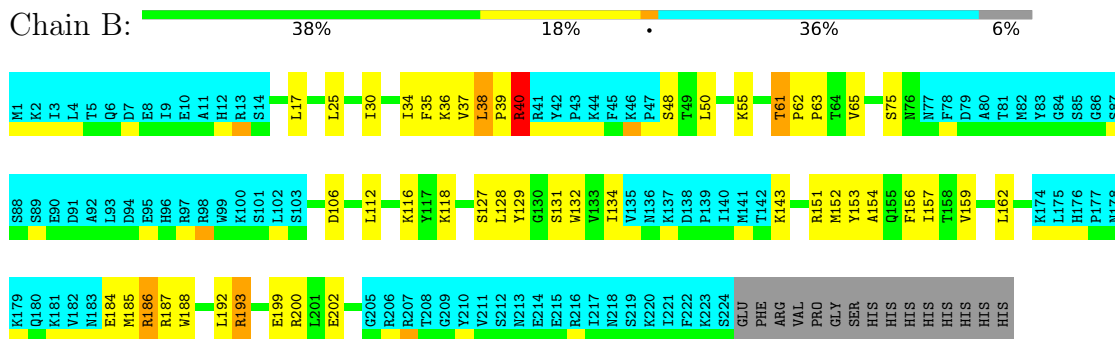
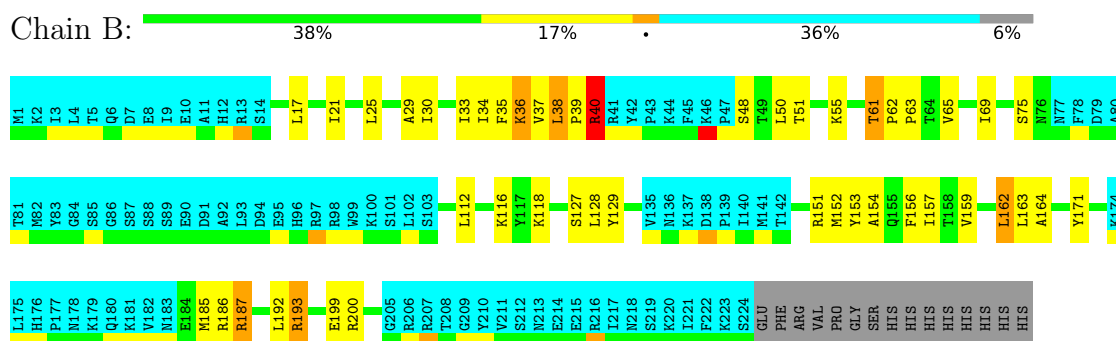• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
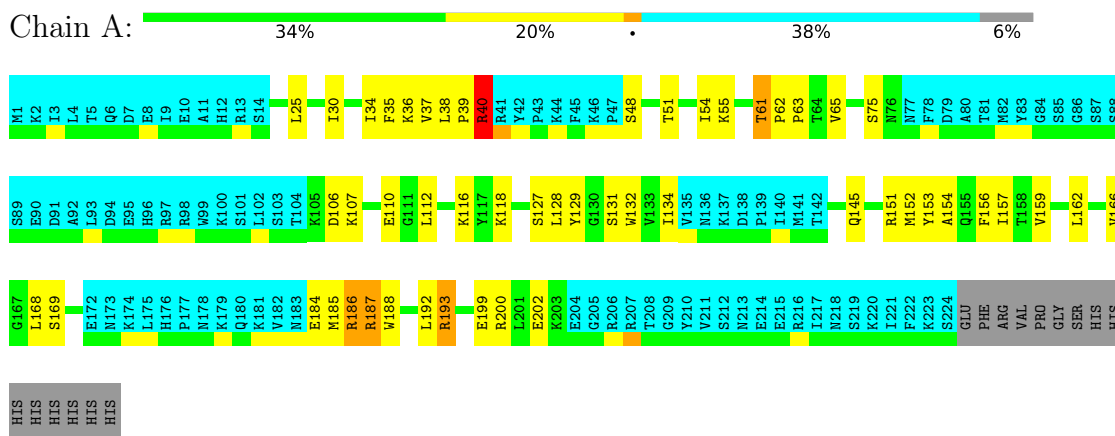
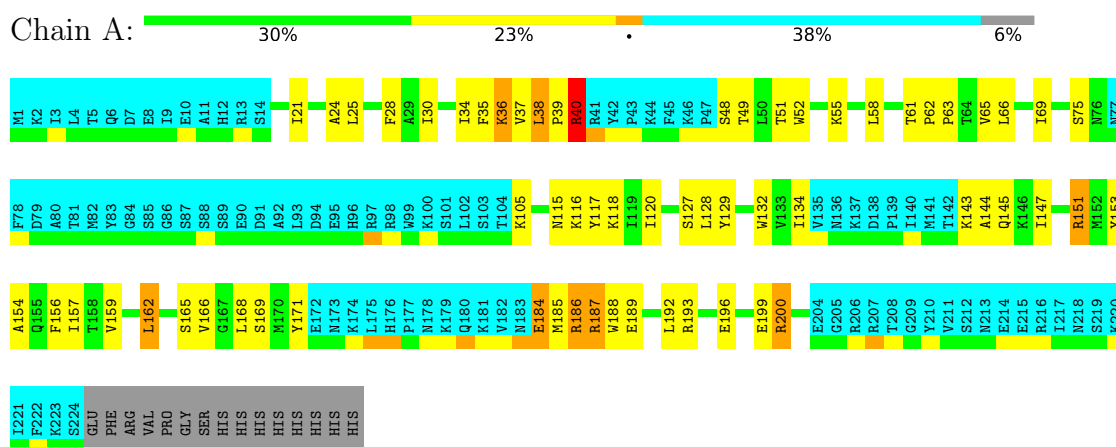## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

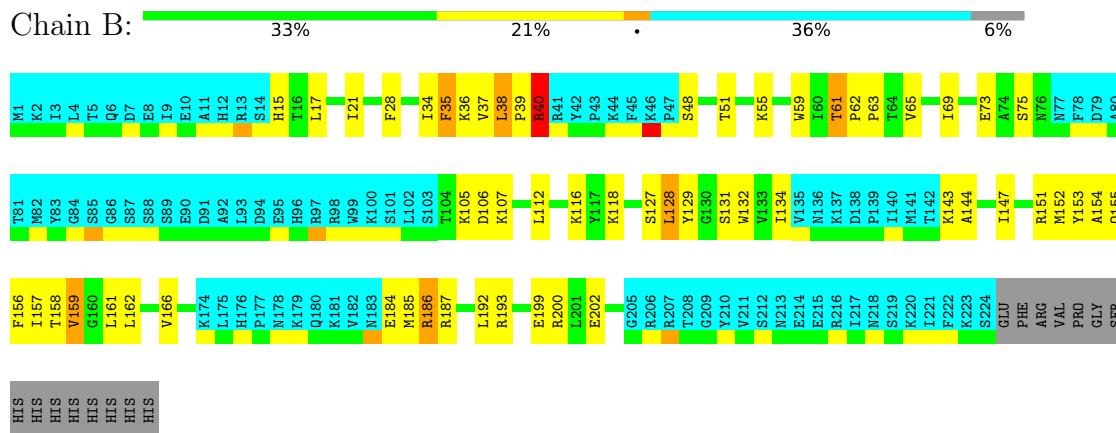• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

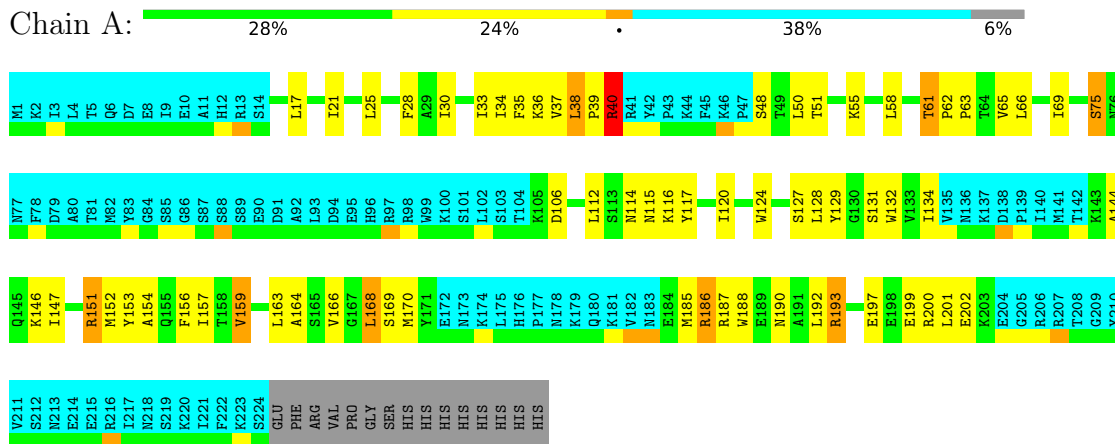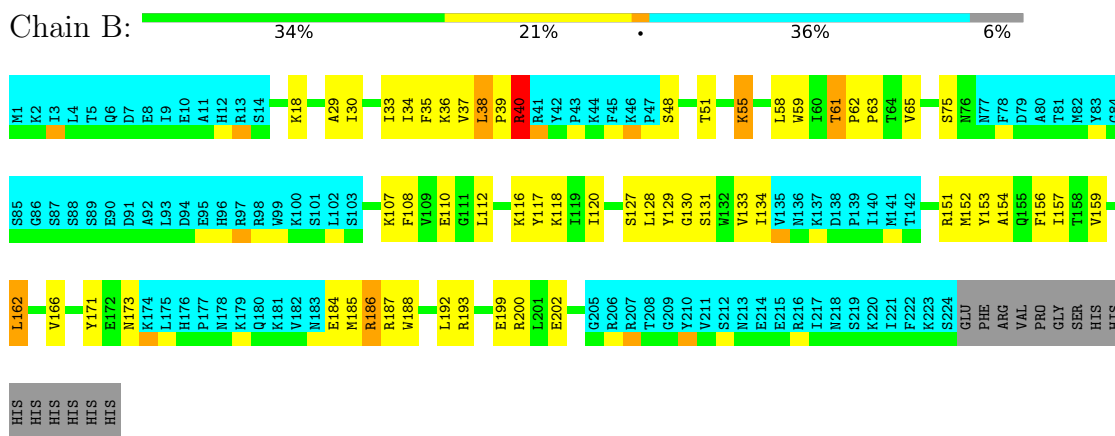• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

4.2.5 Score per residue for model 5

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

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• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
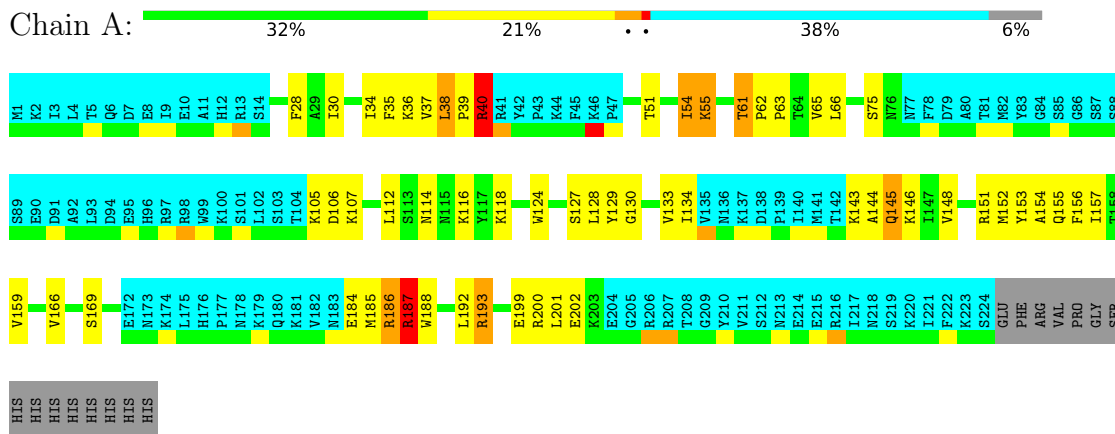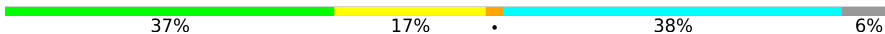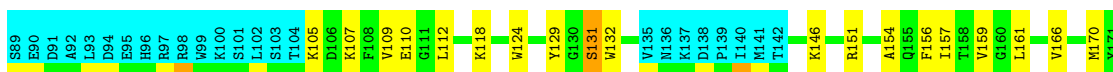
Chain A:

HIS HIS

4.2.6 Score per residue for model 6

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:

HIS HIS HIS HIS

4.2.7 Score per residue for model 7

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain B:

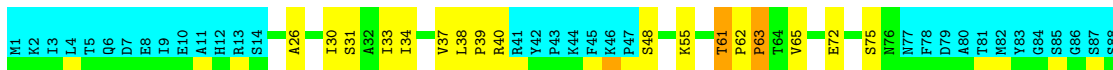• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:
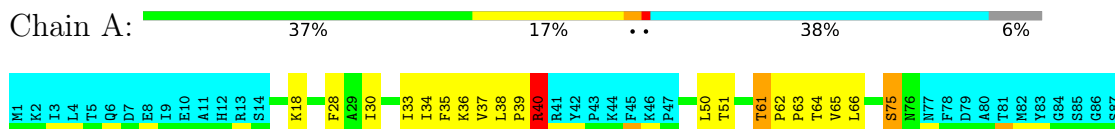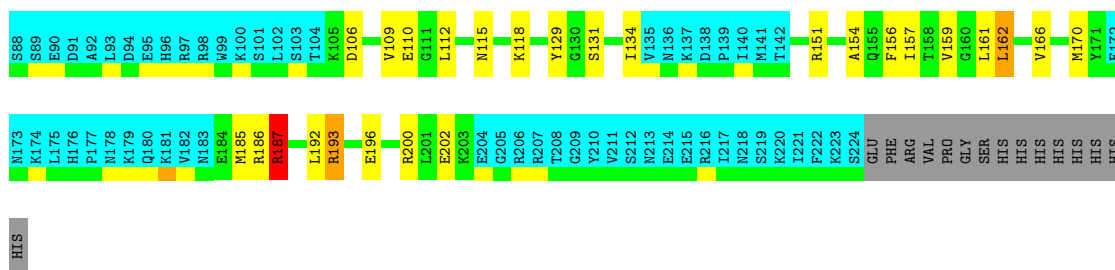
4.2.9 Score per residue for model 9

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
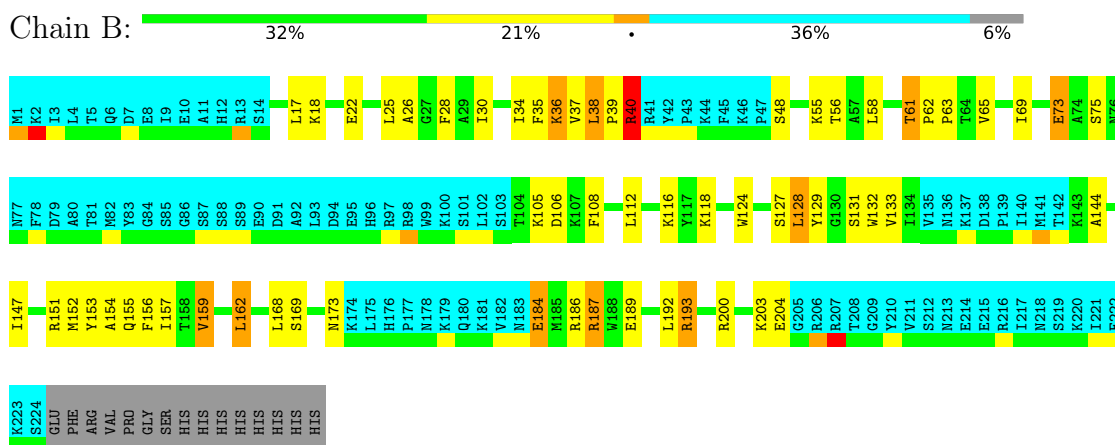
• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
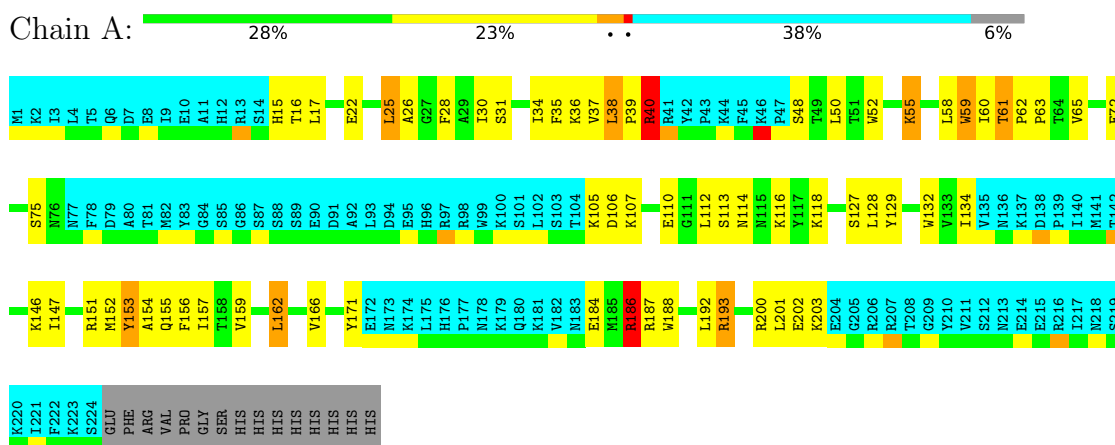
4.2.10 Score per residue for model 10

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

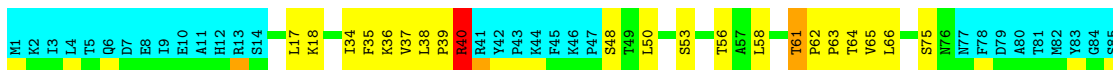• Molecule 1: Respiratory supercomplex factor 2, mitochondrial

Chain A:
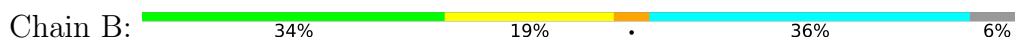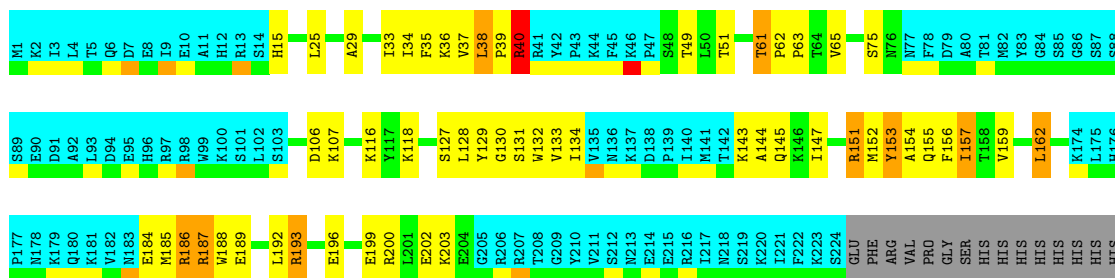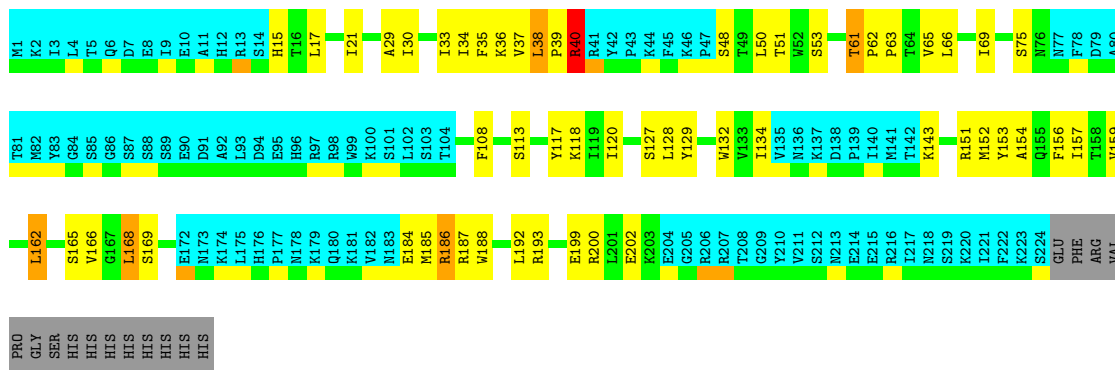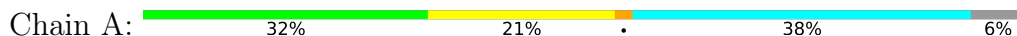
4.2.11 Score per residue for model 11

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
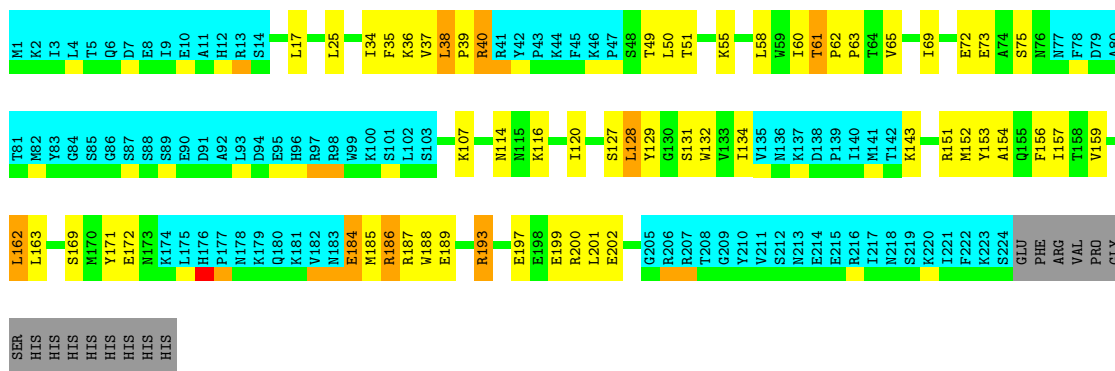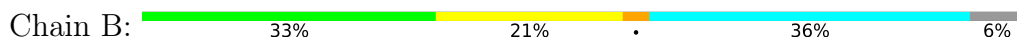
Chain B:

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
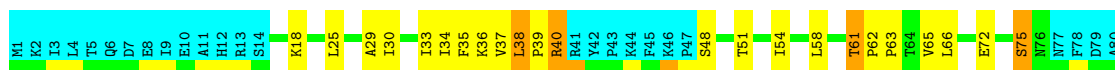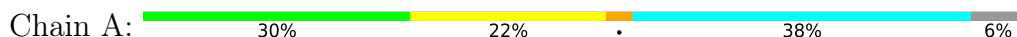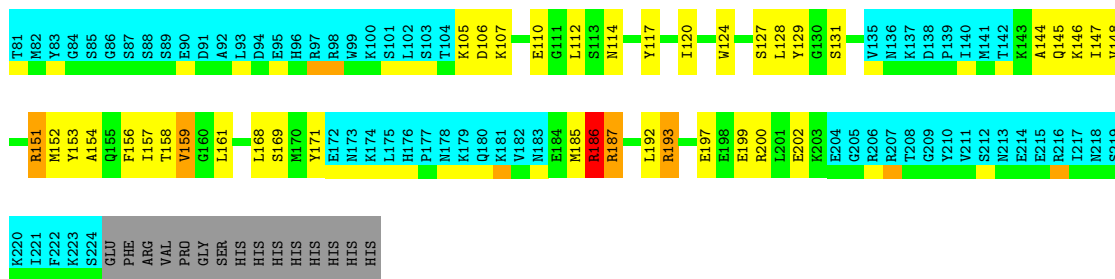
Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
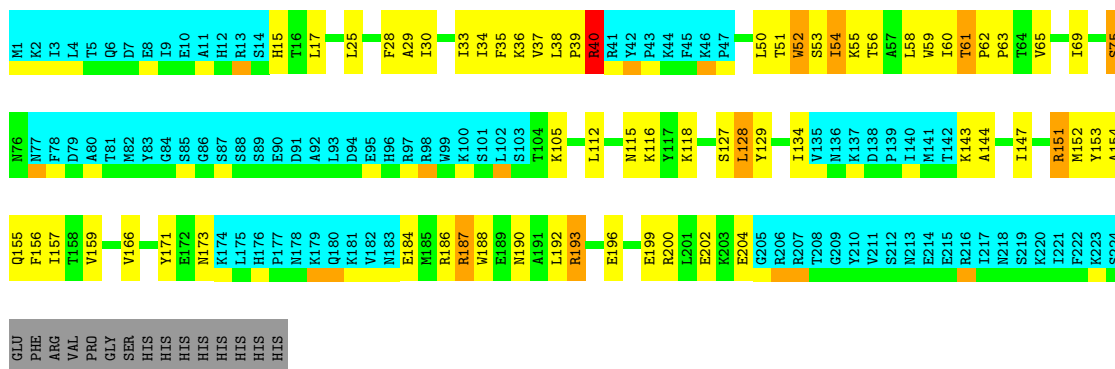
• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
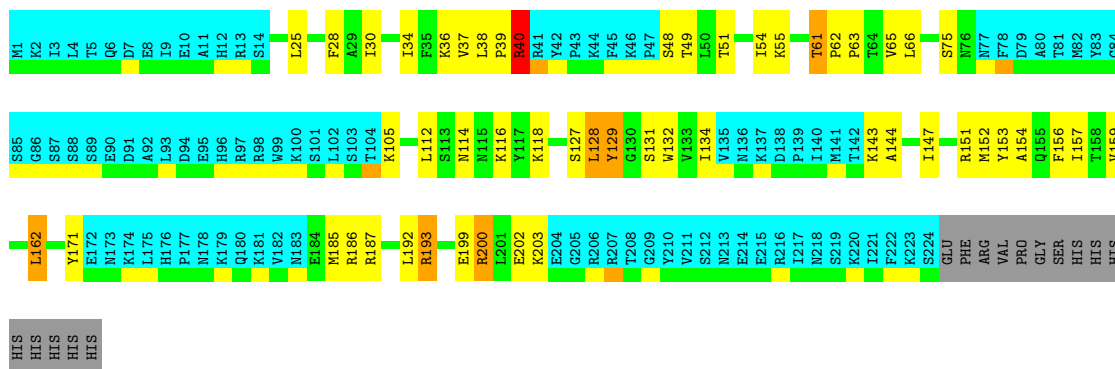
4.2.13 Score per residue for model 13

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
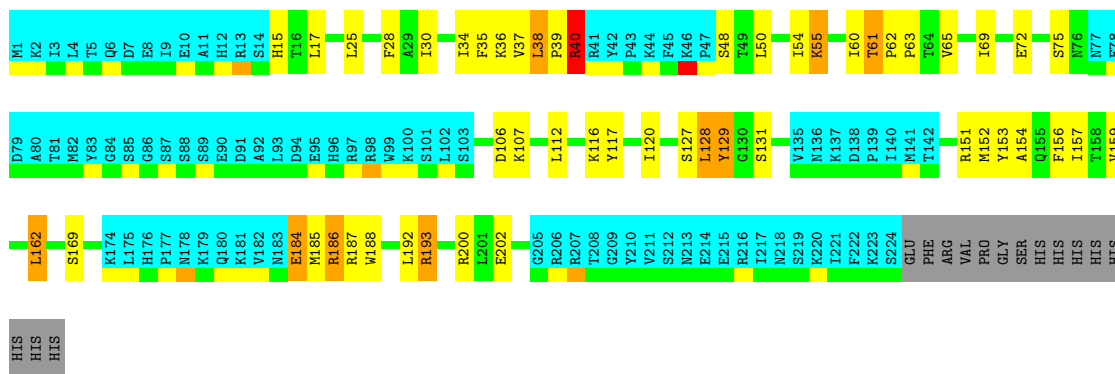
• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
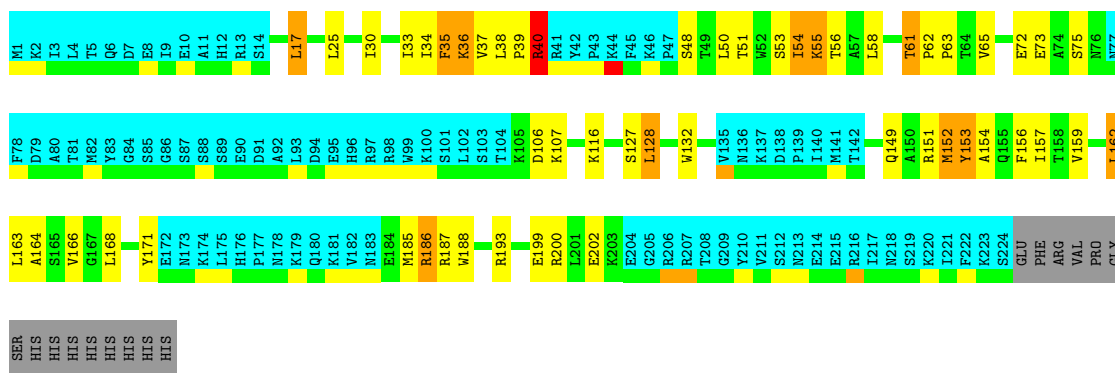
4.2.14 Score per residue for model 14

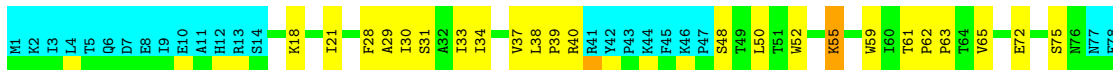• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
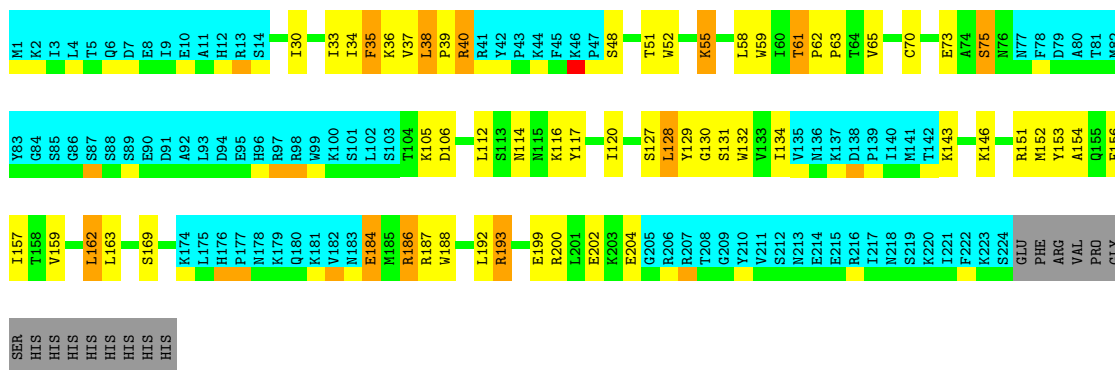
• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
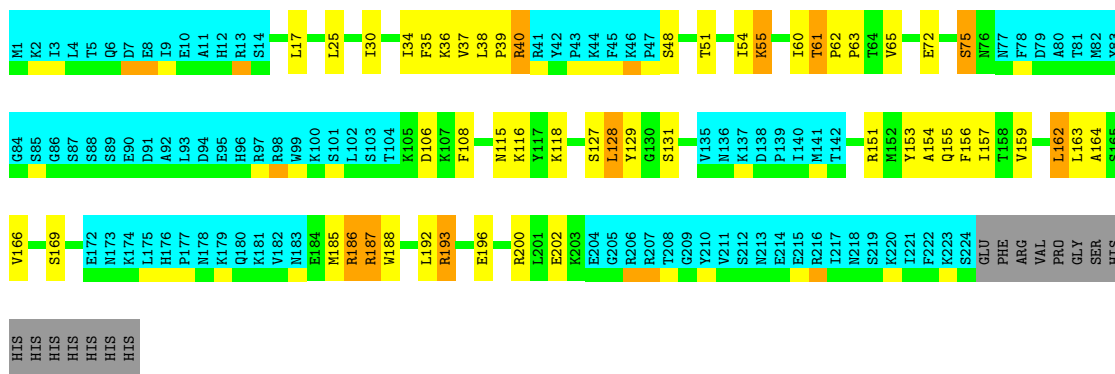
4.2.15 Score per residue for model 15

• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
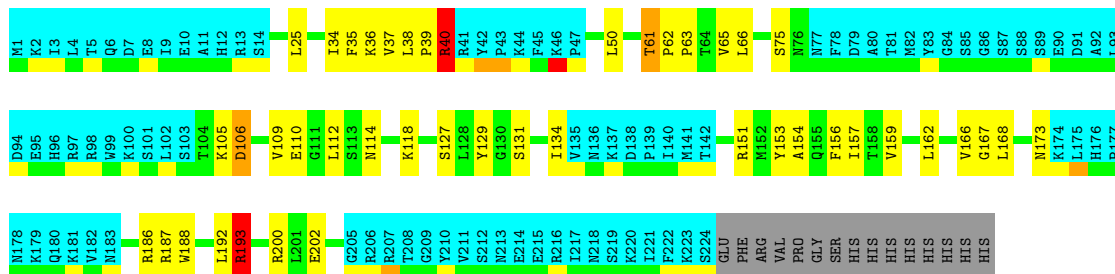
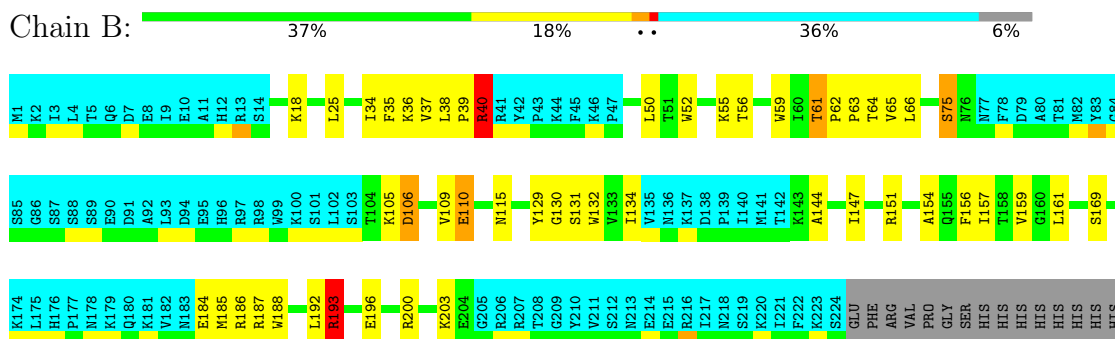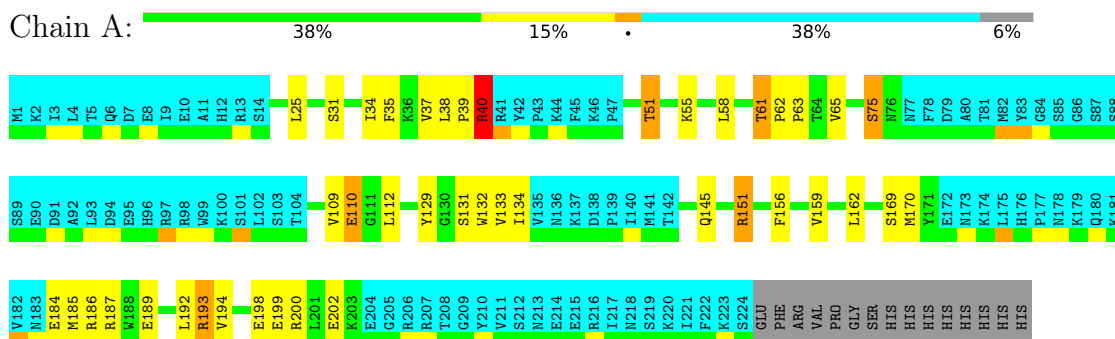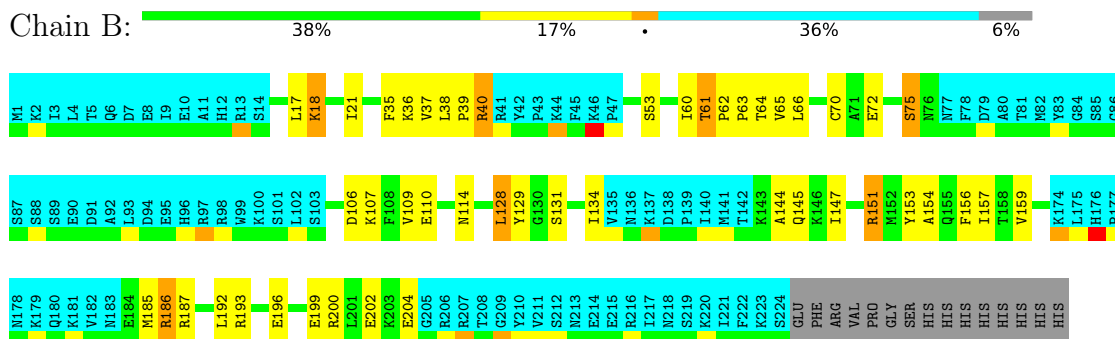• Molecule 1: Respiratory supercomplex factor 2, mitochondrial
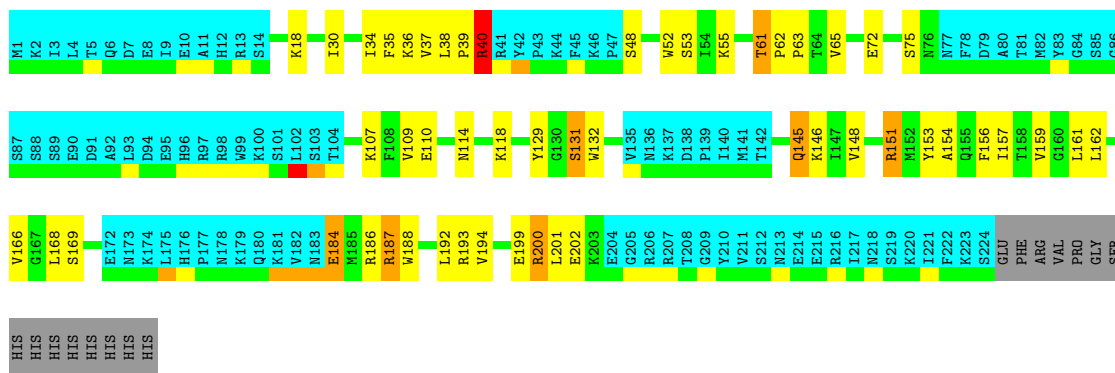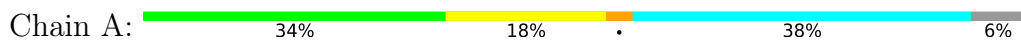
5 Refinement protocol and experimental data overview ⓘ

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)	34%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

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

There are no bond-length outliers.

There are no bond-angle outliers.

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	A	193	ARG	Sidechain	15
1	B	151	ARG	Sidechain	15
1	A	151	ARG	Sidechain	15
1	B	186	ARG	Sidechain	15
1	A	186	ARG	Sidechain	15
1	B	187	ARG	Sidechain	15
1	A	200	ARG	Sidechain	15
1	B	193	ARG	Sidechain	15
1	B	200	ARG	Sidechain	15
1	A	40	ARG	Sidechain	15
1	A	187	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	36±6
1	B	1080	1111	1111	33±6
All	All	31905	32955	32955	1023

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 16.

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: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: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:A:25:LEU:C	1:A:25:LEU:HD22	0.75	2.01	9	1
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:O	1:A:25:LEU:HD22	0.73	1.82	9	1
1:A:201:LEU:O	1:A:201:LEU:HD23	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:162:LEU:C	1:A:162:LEU:HD12	0.72	2.05	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:HG11	1:A:129:TYR:CG	0.71	2.19	7	1
1:A:61:THR:O	1:A:65:VAL:HG13	0.71	1.86	1	10
1:A:37:VAL:HG23	1:A:38:LEU:HD12	0.71	1.62	6	3
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
1:B:52:TRP:O	1:B:56:THR:HG23	0.68	1.88	12	3
1:B:201:LEU:HD13	1:B:201:LEU:O	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: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:34:ILE:HG22	1:B:129:TYR:OH	0.63	1.94	6	2
1:A:201:LEU:O	1:A:201:LEU:HD13	0.62	1.93	3	3
1:A:162:LEU:O	1:A:166:VAL:HG22	0.62	1.94	8	1
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: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:A:128:LEU:HD12	1:A:129:TYR:N	0.61	2.11	4	8
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:162:LEU:HD11	1:A:187:ARG:CG	0.60	2.25	8	1
1:B:128:LEU:HD12	1:B:129:TYR:N	0.60	2.11	1	4
1:B:37:VAL:HG21	1:B:128:LEU:HD11	0.60	1.72	1	3
1:B:17:LEU:HG	1:B:69:ILE:HG23	0.60	1.72	13	3
1:A:21:ILE:HD12	1:A:21:ILE:N	0.59	2.12	6	1
1:A:37:VAL:CG2	1:A:128:LEU:HD11	0.59	2.27	2	4
1:B:128:LEU:HD12	1:B:128:LEU:C	0.58	2.19	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:21:ILE:HD11	1:A:69:ILE:HD13	0.58	1.73	2	3
1:A:62:PRO:HG2	1:A:63:PRO:HD3	0.58	1.75	9	14
1:B:201:LEU:HD13	1:B:201:LEU:C	0.58	2.19	11	1
1:A:201:LEU:C	1:A:201:LEU:HD13	0.58	2.19	9	2
1:A:17:LEU:HD13	1:A:72:GLU:OE2	0.58	1.98	13	1
1:A:201:LEU:HD13	1:A:201:LEU:C	0.57	2.19	3	1
1:A:128:LEU:C	1:A:128:LEU:HD12	0.57	2.19	13	5
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:163:LEU:HD13	1:B:163:LEU:C	0.57	2.19	14	1
1:B:60:ILE:O	1:B:64:THR:HG23	0.57	2.00	8	1
1:B:128:LEU:C	1:B:128:LEU:HD12	0.56	2.21	4	5
1:A:62:PRO:N	1:A:63:PRO:HD2	0.56	2.14	5	15
1:A:128:LEU:HD12	1:A:128:LEU:C	0.56	2.20	3	3
1:A:30:ILE:HA	1:A:33:ILE:HD12	0.56	1.78	5	2
1:A:162:LEU:N	1:A:162:LEU:HD13	0.55	2.16	12	2
1:A:34:ILE:HG22	1:A:129:TYR:OH	0.55	2.01	8	2
1:B:128:LEU:C	1:B:128:LEU:HD22	0.55	2.21	14	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:154:ALA:HA	1:A:157:ILE:CG1	0.54	2.32	12	9
1:A:54:ILE:C	1:A:54:ILE:HD12	0.54	2.22	14	1
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:HD12	1:B:54:ILE:C	0.54	2.23	13	1
1:B:128:LEU:HD13	1:B:128:LEU:C	0.53	2.23	14	3
1:B:134:ILE:C	1:B:134:ILE:HD12	0.53	2.23	3	1
1:B:193:ARG:CZ	1:A:194:VAL:HG11	0.53	2.33	7	1
1:A:128:LEU:HD22	1:A:128:LEU:C	0.53	2.23	12	1
1:A:162:LEU:HD13	1:A:162:LEU:N	0.53	2.18	9	4
1:A:128:LEU:C	1:A:128:LEU:HD22	0.53	2.23	14	1
1:B:153:TYR:CE1	1:B:157:ILE:HG21	0.53	2.38	3	1
1:A:128:LEU:HD13	1:A:128:LEU:C	0.53	2.22	12	2
1:B:33:ILE:O	1:B:37:VAL:HG13	0.53	2.03	14	2
1:B:128:LEU:HD22	1:B:128:LEU:C	0.53	2.24	11	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: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:A:25:LEU:HD13	1:A:26:ALA:H	0.52	1.63	9	1
1:B:162:LEU:O	1:B:166:VAL:HG22	0.52	2.05	6	1
1:B:128:LEU:O	1:B:128:LEU:HD22	0.52	2.05	14	2
1:A:109:VAL:HG13	1:A:110:GLU:N	0.52	2.19	6	5
1:B:162:LEU:HD13	1:B:162:LEU:N	0.52	2.20	4	6
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: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:144:ALA:HA	1:A:147:ILE:HD13	0.51	1.81	11	1
1:B:162:LEU:N	1:B:162:LEU:HD13	0.51	2.21	3	2
1:B:62:PRO:N	1:B:63:PRO:CD	0.50	2.74	7	14
1:A:128:LEU:O	1:A:128:LEU:HD22	0.50	2.06	12	2
1:B:117:TYR:HA	1:B:120:ILE:HD12	0.50	1.83	14	4
1:A:162:LEU:C	1:A:162:LEU:CD1	0.50	2.80	4	1
1:A:54:ILE:HD13	1:A:54:ILE:C	0.50	2.26	3	2
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:B:128:LEU:HD22	1:B:128:LEU:O	0.49	2.07	2	1
1:A:61:THR:N	1:A:62:PRO:CD	0.49	2.76	6	13
1:B:54:ILE:HD13	1:B:54:ILE:C	0.49	2.27	12	1
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: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: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:61:THR:N	1:B:62:PRO:CD	0.48	2.77	7	12
1:B:36:LYS:O	1:B:40:ARG:CB	0.48	2.60	12	15
1:B:37:VAL:O	1:B:129:TYR:CE2	0.48	2.67	2	3
1:B:129:TYR:N	1:B:129:TYR:CD1	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:B:34:ILE:C	1:B:34:ILE:HD12	0.48	2.29	6	6
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: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:A:31:SER:OG	1:A:59:TRP:CH2	0.47	2.67	9	1
1:B:37:VAL:O	1:B:129:TYR:CE1	0.47	2.67	14	3
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:B:60:ILE:C	1:B:63:PRO:HD2	0.47	2.30	5	4
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:A:34:ILE:C	1:A:34:ILE:HD12	0.47	2.30	3	2
1:A:144:ALA:O	1:A:147:ILE:N	0.47	2.40	11	1
1:A:168:LEU:O	1:A:168:LEU:HD12	0.47	2.10	2	2
1:A:25:LEU:C	1:A:25:LEU:HD13	0.47	2.29	9	1
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: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:144:ALA:O	1:A:148:VAL:HG22	0.46	2.11	3	1
1:A:38:LEU:N	1:A:39:PRO:HD2	0.46	2.25	3	10
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:130:GLY:O	1:B:134:ILE:HG23	0.46	2.11	3	1
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: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:A:60:ILE:C	1:A:63:PRO:HD2	0.45	2.31	9	2
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:168:LEU:HD12	1:A:168:LEU:C	0.45	2.32	2	2
1:B:34:ILE:HD12	1:B:34:ILE:C	0.45	2.32	2	3
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:34:ILE:HD12	1:A:34:ILE:C	0.45	2.32	10	2
1:B:166:VAL:HG21	1:B:188:TRP:HZ2	0.45	1.71	3	1
1:B:55:LYS:O	1:B:59:TRP:CE3	0.45	2.70	3	2
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: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:N	1:B:188:TRP:CD1	0.44	2.84	7	4
1:A:154:ALA:O	1:A:155:GLN:C	0.44	2.55	3	3
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: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:145:GLN:O	1:B:148:VAL:HG22	0.44	2.12	5	1
1:B:58:LEU:HA	1:B:61:THR:OG1	0.44	2.12	5	1
1:B:153:TYR:CE2	1:B:157:ILE:CG2	0.44	2.99	13	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:A:29:ALA:C	1:A:33:ILE:HD12	0.43	2.34	6	1
1:A:166:VAL:HG22	1:A:184:GLU:OE2	0.43	2.14	9	1
1:B:22:GLU:O	1:B:26:ALA:HB2	0.43	2.13	9	1
1:B:30:ILE:CG2	1:B:34:ILE:CG2	0.43	2.97	14	1
1:B:37:VAL:O	1:B:129:TYR:CZ	0.42	2.72	11	2
1:A:161:LEU:N	1:A:161:LEU:CD1	0.42	2.82	15	1
1:B:29:ALA:O	1:B:33:ILE:HD12	0.42	2.13	12	4
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:B:154:ALA:O	1:B:155:GLN:C	0.42	2.58	12	2
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:A:153:TYR:CD2	1:A:157:ILE:HG21	0.42	2.50	2	1
1:B:37:VAL:HG23	1:B:38:LEU:HD12	0.42	1.89	2	1
1:B:35:PHE:O	1:B:35:PHE:CD1	0.42	2.73	10	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:61:THR:OG1	1:B:62:PRO:HD3	0.42	2.15	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:LEU:HD23	1:A:201:LEU:C	0.42	2.35	2	1
1:A:154:ALA:CA	1:A:157:ILE:HG12	0.42	2.45	3	1
1:A:37:VAL:HG21	1:A:129:TYR:CD1	0.42	2.50	7	1
1:B:35:PHE:O	1:B:39:PRO:CD	0.42	2.68	15	2
1:A:34:ILE:CD1	1:A:35:PHE:N	0.42	2.83	9	5
1:B:193:ARG:NH2	1:A:194:VAL:HG11	0.42	2.30	7	1
1:A:35:PHE:CD2	1:A:35:PHE:O	0.42	2.73	11	1
1:B:17:LEU:CD2	1:B:17:LEU:N	0.41	2.83	2	1
1:A:161:LEU:CD1	1:A:161:LEU:N	0.41	2.83	5	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:B:186:ARG:CG	1:B:187:ARG:N	0.41	2.83	10	1
1:A:24:ALA:O	1:A:28:PHE:CE2	0.41	2.74	1	1
1:A:163:LEU:HD23	1:A:163:LEU:C	0.41	2.36	2	1
1:A:37:VAL:O	1:A:129:TYR:CE2	0.41	2.73	6	3
1:A:124:TRP:O	1:A:124:TRP:CD1	0.41	2.73	3	2
1:A:52:TRP:O	1:A:55:LYS:CG	0.41	2.68	6	1
1:A:153:TYR:CZ	1:A:157:ILE:CG2	0.41	3.03	1	1
1:A:124:TRP:CZ2	1:A:157:ILE:HD12	0.41	2.50	5	1
1:A:54:ILE:CD1	1:A:54:ILE:C	0.41	2.89	3	1
1:A:30:ILE:HG22	1:A:34:ILE:HG21	0.41	1.91	13	1
1:B:35:PHE:CD1	1:B:35:PHE:O	0.41	2.73	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:A:154:ALA:O	1:A:157:ILE:CG1	0.41	2.69	3	1
1:B:62:PRO:CG	1:B:63:PRO:HD3	0.41	2.46	3	2
1:A:129:TYR:N	1:A:129:TYR:CD2	0.41	2.82	5	2
1:B:54:ILE:C	1:B:54:ILE:CD1	0.41	2.89	12	1
1:B:52:TRP:O	1:B:52:TRP:CE3	0.41	2.74	14	1
1:B:188:TRP:CD1	1:B:188:TRP:N	0.41	2.89	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
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:154:ALA:CA	1:B:157:ILE:HG12	0.40	2.46	1	1
1:A:144:ALA:O	1:A:145:GLN:C	0.40	2.59	11	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:O	1:A:52:TRP:CE3	0.40	2.75	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:54:ILE:C	1:A:54:ILE:CD1	0.40	2.89	13	1
1:A:51:THR:HA	1:A:54:ILE:CG1	0.40	2.47	14	1
1:A:124:TRP:CD1	1:A:124:TRP:O	0.40	2.74	2	1
1:B:128:LEU:CD1	1:B:128:LEU:C	0.40	2.90	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:193:ARG:NH1	1:A:194:VAL:CG1	0.40	2.84	15	1
1:B:166:VAL:HG23	1:B:167:GLY:N	0.40	2.31	15	1
1:A:124:TRP:CZ2	1:A:153:TYR:OH	0.40	2.72	3	1
1:A:117:TYR:C	1:A:117:TYR:CD2	0.40	2.95	11	1
1:A:36:LYS:HA	1:A:39:PRO:HG2	0.40	1.94	14	1
1:A:145:GLN:O	1:A:148:VAL:HG22	0.40	2.17	15	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%)	24	71
1	B	138/239 (58%)	130±2 (95±2%)	7±2 (5±2%)	1±0 (1±0%)	26	73
All	All	4080/7170 (57%)	3855 (94%)	194 (5%)	31 (1%)	24	71

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	A	75	SER	15
1	B	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±5 (76±4%)	26±5 (24±4%)	2	27
1	B	112/205 (55%)	86±5 (77±4%)	26±5 (23±4%)	3	28
All	All	3300/6150 (54%)	2527 (77%)	773 (23%)	3	27

All 143 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	192	LEU	14
1	A	202	GLU	13
1	A	192	LEU	13
1	A	61	THR	13
1	B	202	GLU	12
1	A	48	SER	12
1	A	55	LYS	12
1	B	127	SER	12
1	B	40	ARG	11
1	A	118	LYS	11
1	A	40	ARG	11
1	A	199	GLU	11
1	A	185	MET	11
1	A	169	SER	10
1	A	193	ARG	10
1	B	131	SER	10
1	B	112	LEU	10
1	B	162	LEU	10
1	B	199	GLU	10
1	A	127	SER	10
1	B	118	LYS	10
1	A	162	LEU	10
1	B	193	ARG	10
1	A	25	LEU	9
1	A	132	TRP	9
1	B	116	LYS	9
1	B	38	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	B	185	MET	9
1	B	25	LEU	9
1	A	112	LEU	8
1	B	48	SER	8
1	A	116	LYS	8
1	A	107	LYS	8
1	A	168	LEU	8
1	B	186	ARG	8
1	B	143	LYS	8
1	B	50	LEU	8
1	B	55	LYS	8
1	A	106	ASP	8
1	B	107	LYS	7
1	B	184	GLU	7
1	A	50	LEU	7
1	A	66	LEU	7
1	A	186	ARG	7
1	A	114	ASN	7
1	B	105	LYS	7
1	B	128	LEU	7
1	B	106	ASP	7
1	B	114	ASN	7
1	B	132	TRP	7
1	B	169	SER	7
1	A	131	SER	7
1	A	105	LYS	6
1	B	66	LEU	6
1	A	187	ARG	6
1	A	38	LEU	6
1	A	28	PHE	6
1	B	204	GLU	6
1	B	51	THR	6
1	B	196	GLU	5
1	A	145	GLN	5
1	A	146	LYS	5
1	B	53	SER	5
1	B	151	ARG	5
1	A	171	TYR	5
1	B	75	SER	5
1	A	115	ASN	5
1	A	170	MET	5
1	B	18	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	51	THR	5
1	A	75	SER	5
1	A	184	GLU	5
1	A	72	GLU	5
1	A	189	GLU	4
1	B	28	PHE	4
1	B	153	TYR	4
1	A	143	LYS	4
1	B	73	GLU	4
1	B	171	TYR	4
1	A	18	LYS	4
1	A	151	ARG	4
1	B	189	GLU	4
1	A	203	LYS	3
1	B	72	GLU	3
1	B	187	ARG	3
1	B	15	HIS	3
1	A	58	LEU	3
1	B	203	LYS	3
1	A	200	ARG	3
1	A	196	GLU	3
1	B	146	LYS	3
1	A	152	MET	3
1	A	113	SER	3
1	B	168	LEU	3
1	A	53	SER	3
1	A	52	TRP	3
1	A	128	LEU	3
1	A	153	TYR	3
1	A	110	GLU	3
1	A	17	LEU	3
1	A	108	PHE	3
1	A	159	VAL	3
1	A	36	LYS	3
1	B	49	THR	3
1	B	173	ASN	3
1	B	35	PHE	3
1	B	172	GLU	2
1	B	110	GLU	2
1	B	115	ASN	2
1	A	31	SER	2
1	A	59	TRP	2

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Mol	Chain	Res	Type	Models (Total)
1	B	36	LYS	2
1	B	170	MET	2
1	B	70	CYS	2
1	B	59	TRP	2
1	B	152	MET	2
1	B	145	GLN	2
1	A	49	THR	2
1	B	161	LEU	2
1	B	56	THR	2
1	B	108	PHE	2
1	A	197	GLU	2
1	B	159	VAL	2
1	B	155	GLN	2
1	A	54	ILE	2
1	A	165	SER	2
1	B	52	TRP	2
1	A	35	PHE	1
1	B	156	PHE	1
1	A	129	TYR	1
1	B	129	TYR	1
1	B	157	ILE	1
1	A	73	GLU	1
1	B	190	ASN	1
1	A	161	LEU	1
1	A	56	THR	1
1	B	58	LEU	1
1	B	54	ILE	1
1	B	17	LEU	1
1	B	165	SER	1
1	B	163	LEU	1
1	B	197	GLU	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 monosaccharides 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 34% 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 ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	219	-0.17 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_\beta$	205	0.75 ± 0.04	Should be applied
$^{13}C'$	214	-0.00 ± 0.07	None needed (< 0.5 ppm)
^{15}N	206	0.48 ± 0.16	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 34%, i.e. 1154 atoms were assigned a chemical shift out of a possible 3347. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	639/1348 (47%)	248/538 (46%)	263/544 (48%)	128/266 (48%)
Sidechain	485/1729 (28%)	263/1006 (26%)	222/652 (34%)	0/71 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/270 (11%)	30/140 (21%)	0/118 (0%)	0/12 (0%)
Overall	1154/3347 (34%)	541/1684 (32%)	485/1314 (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. 1781 atoms were assigned a chemical shift out of a possible 5646. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1038/2212 (47%)	399/882 (45%)	433/896 (48%)	206/434 (47%)
Sidechain	713/2996 (24%)	379/1762 (22%)	334/1084 (31%)	0/150 (0%)
Aromatic	30/438 (7%)	30/230 (13%)	0/188 (0%)	0/20 (0%)
Overall	1781/5646 (32%)	808/2874 (28%)	767/2168 (35%)	206/604 (34%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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.

Random coil index (RCI) for chain A: