



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 21, 2020 – 02:16 PM JST

PDB ID : 7CLV  
Title : Solution structure of mitochondrial Tim23 channel in complex with a signaling peptide  
Authors : Zhou, S.; Ruan, M.S.; Li, Y.Y.; Yang, J.; Richter, C.; Schwalbe, H.; Shen, B.; Wang, J.F.  
Deposited on : 2020-07-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

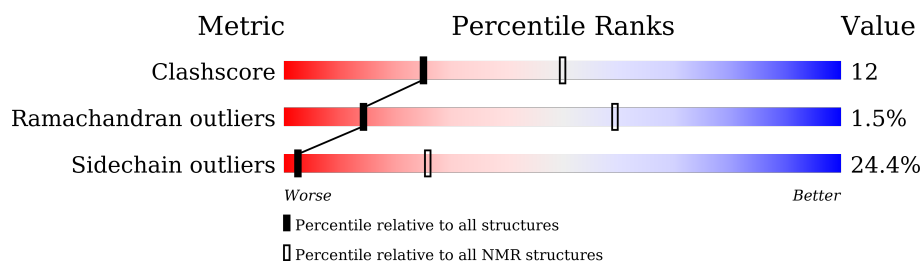
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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	222	
1	B	222	
2	C	25	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 5 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	A:64-A:75, A:91-A:124, A:151-A:216, B:64-B:79, B:91-B:122, B:150-B:216 (227)	0.78	5

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 6, 8, 9, 11, 12, 13, 14, 15
2	3, 4, 7, 10

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6985 atoms, of which 3514 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TIM23 isoform 1.

Mol	Chain	Residues	Atoms						Trace
1	A	222	Total	C	H	N	O	S	0
			3274	1026	1643	281	315	9	
1	B	222	Total	C	H	N	O	S	0
			3274	1026	1643	281	315	9	

- Molecule 2 is a protein called COX4 isoform 1.

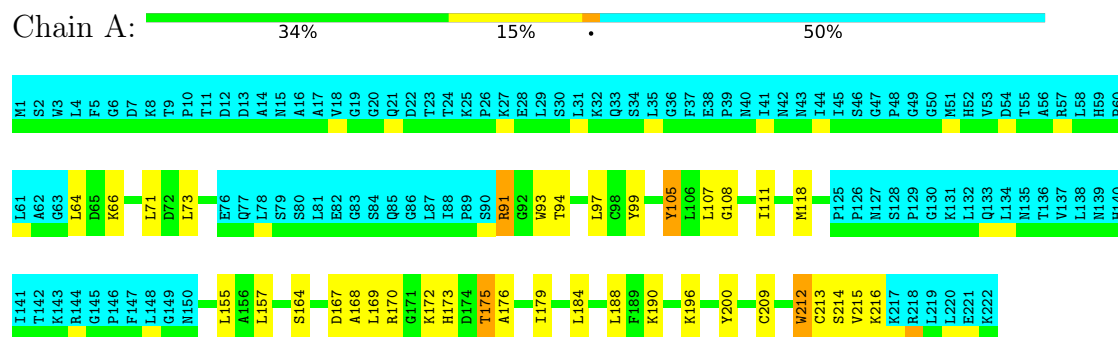
Mol	Chain	Residues	Atoms						Trace
2	C	25	Total	C	H	N	O	S	0
			437	134	228	39	34	2	

## 4 Residue-property plots

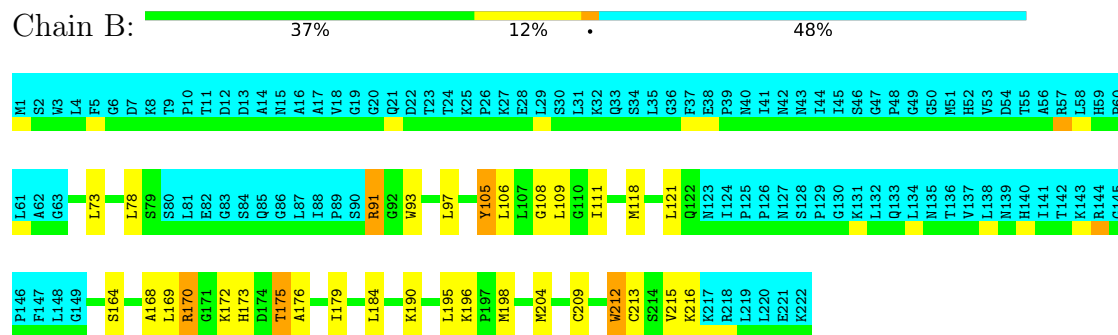
### 4.1 Average score per residue in the NMR ensemble

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.

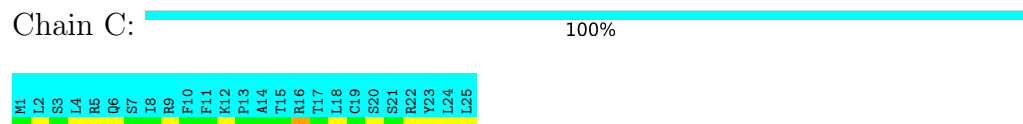
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1



- Molecule 2: COX4 isoform 1

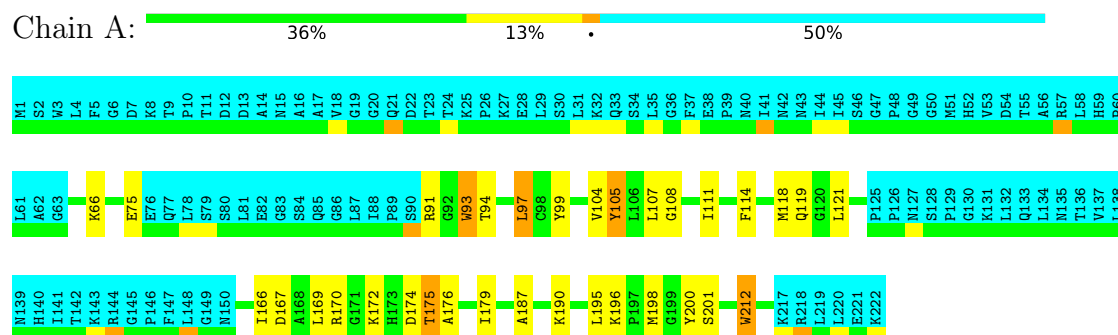


### 4.2 Scores per residue for each member of the ensemble

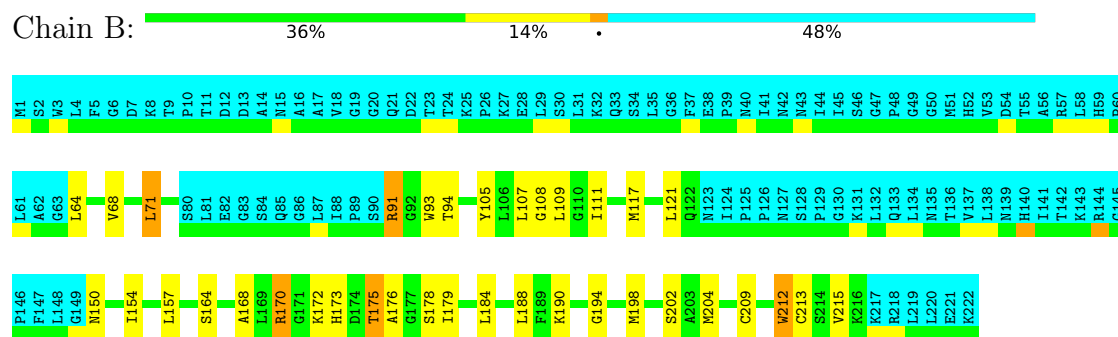
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

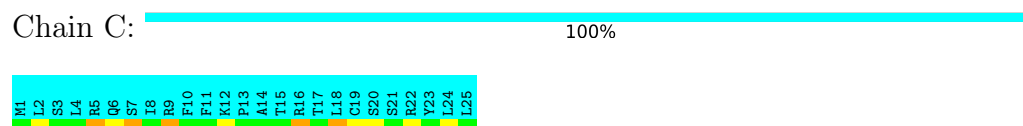
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1

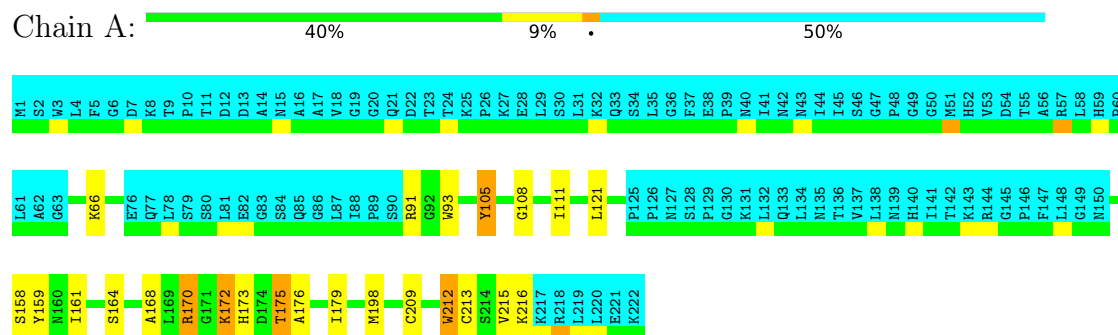


- Molecule 2: COX4 isoform 1

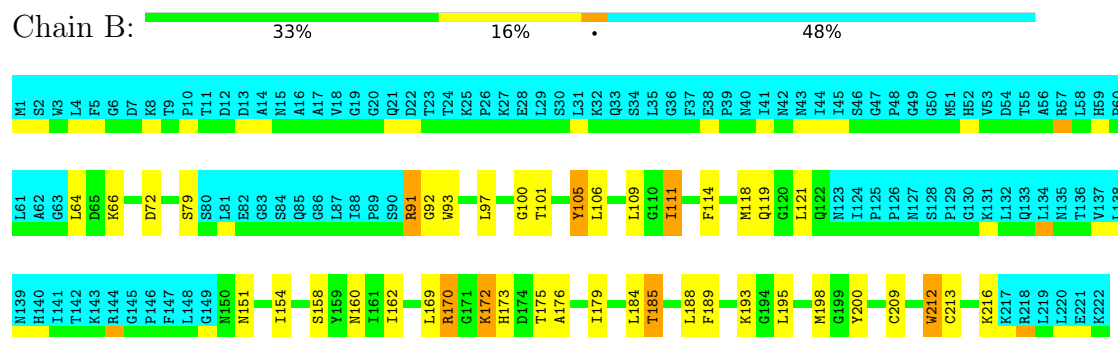


### 4.2.2 Score per residue for model 2

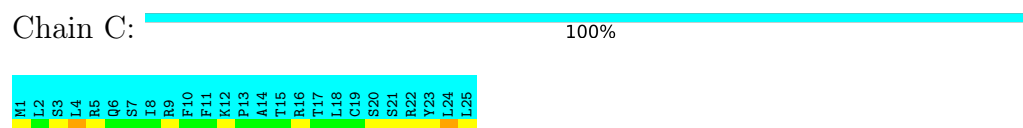
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1



- Molecule 2: COX4 isoform 1



#### 4.2.3 Score per residue for model 3

- Molecule 1: TIM23 isoform 1

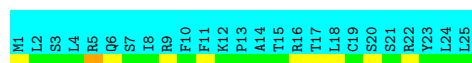


- Molecule 1: TIM23 isoform 1



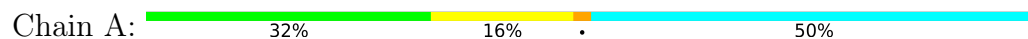
- Molecule 2: COX4 isoform 1



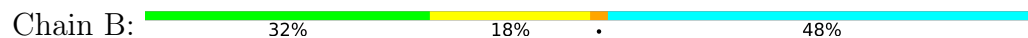


#### 4.2.4 Score per residue for model 4

- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1

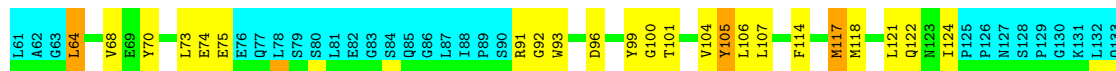
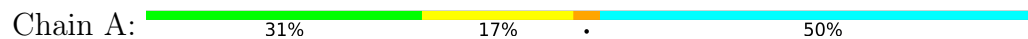


- Molecule 2: COX4 isoform 1

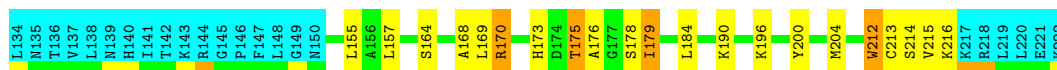


#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: TIM23 isoform 1

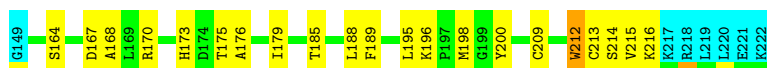






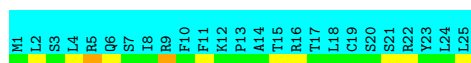
• Molecule 1: TIM23 isoform 1

Chain B: 37% 12% • 48%



• Molecule 2: COX4 isoform 1

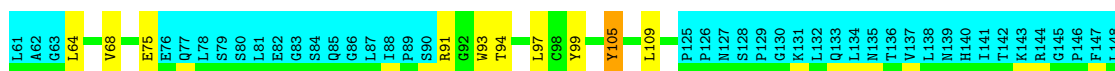
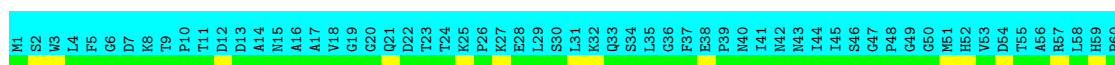
Chain C: 100%



#### 4.2.6 Score per residue for model 6

• Molecule 1: TIM23 isoform 1

Chain A: 34% 14% • 50%



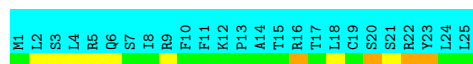
• Molecule 1: TIM23 isoform 1

Chain B: 36% 13% • 48%




• Molecule 2: COX4 isoform 1

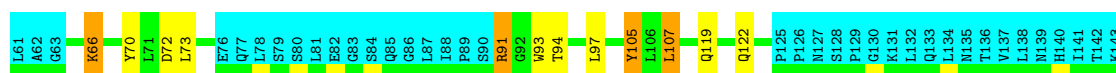
Chain C:  100%




#### 4.2.7 Score per residue for model 7

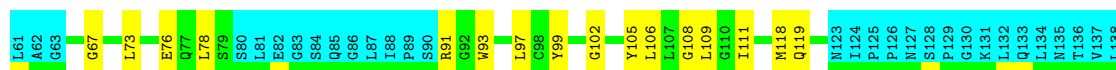
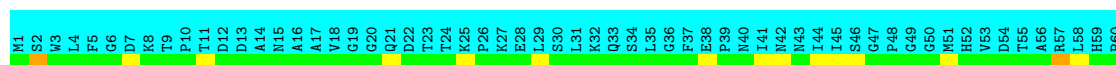
- Molecule 1: TIM23 isoform 1

Chain A:  34% 13% 50%



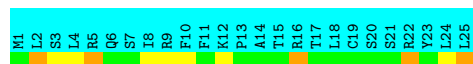
- Molecule 1: TIM23 isoform 1

Chain B:  33% 17% 48%




- Molecule 2: COX4 isoform 1

Chain C:  100%

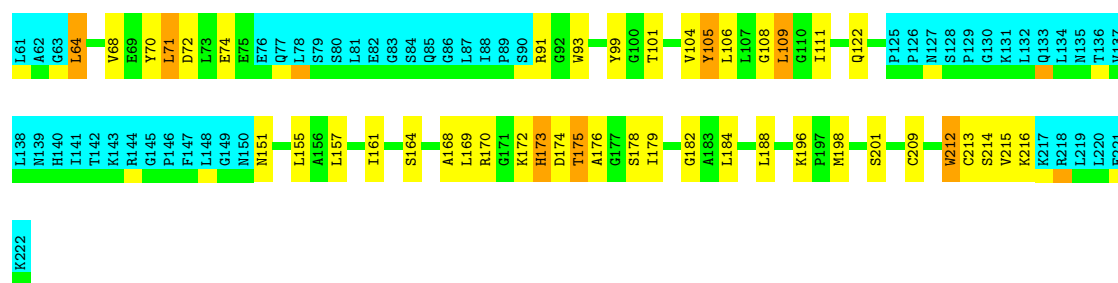


#### 4.2.8 Score per residue for model 8

- Molecule 1: TIM23 isoform 1

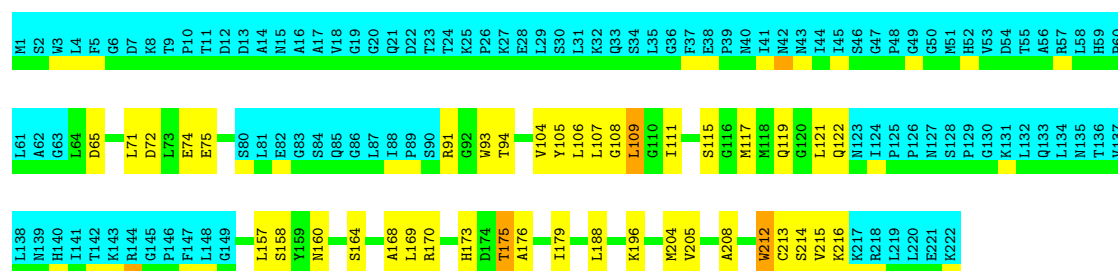
Chain A:  31% 17% 50%





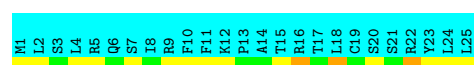
- Molecule 1: TIM23 isoform 1

Chain B: 33% 17% 48%



- Molecule 2: COX4 isoform 1

Chain C: 100%



#### 4.2.9 Score per residue for model 9

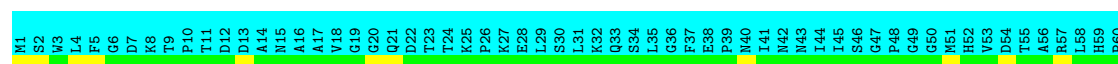
- Molecule 1: TIM23 isoform 1

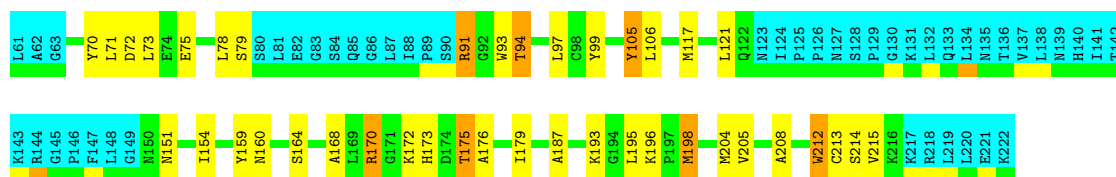
Chain A: 32% 15% 50%



- Molecule 1: TIM23 isoform 1

Chain B: 34% 15% 48%






- Molecule 2: COX4 isoform 1

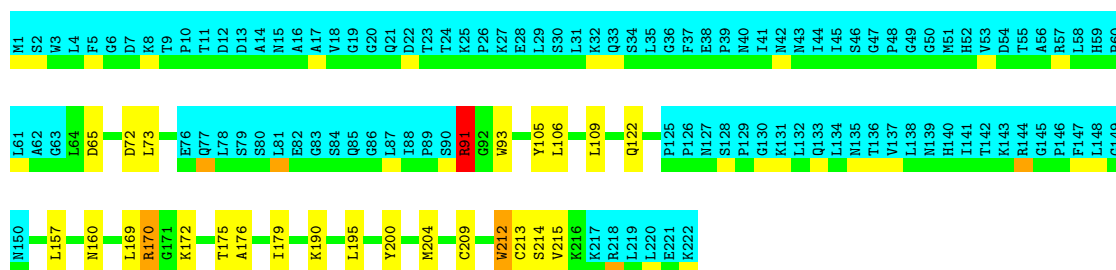
Chain C:  100%




#### 4.2.10 Score per residue for model 10

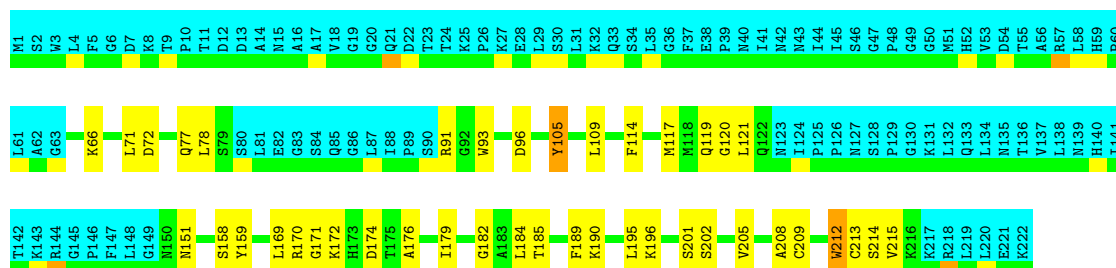
- Molecule 1: TIM23 isoform 1

Chain A:  39% 10% 50%



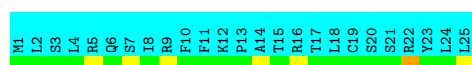
- Molecule 1: TIM23 isoform 1

Chain B:  33% 18% 48%



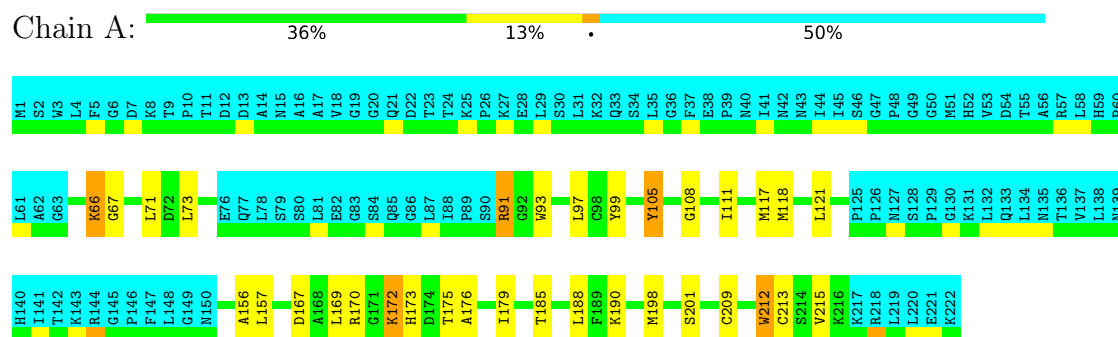
- Molecule 2: COX4 isoform 1

Chain C:  100%



### 4.2.11 Score per residue for model 11

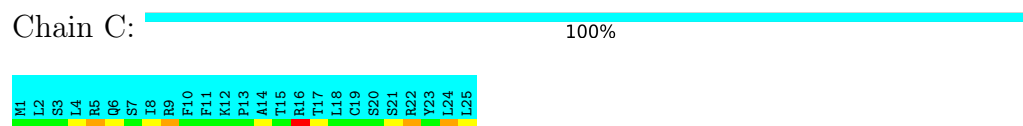
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1

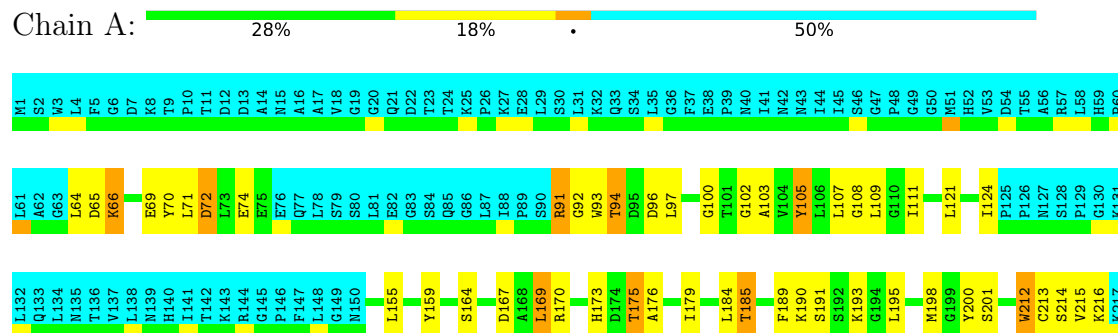


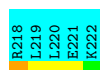
- Molecule 2: COX4 isoform 1



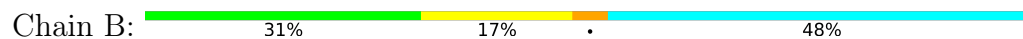
### 4.2.12 Score per residue for model 12

- Molecule 1: TIM23 isoform 1





• Molecule 1: TIM23 isoform 1

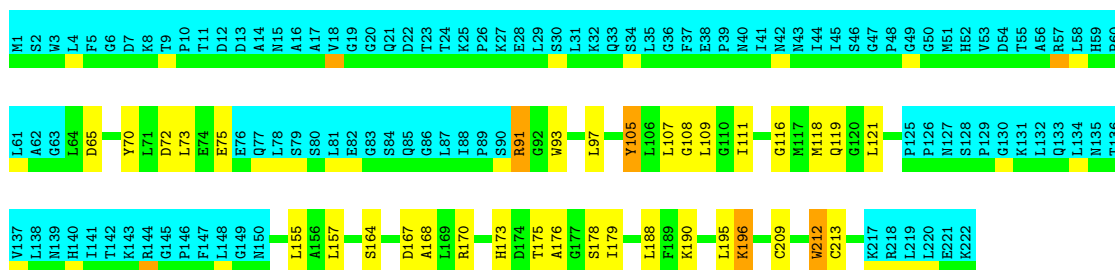
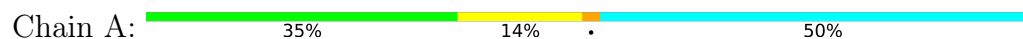


• Molecule 2: COX4 isoform 1

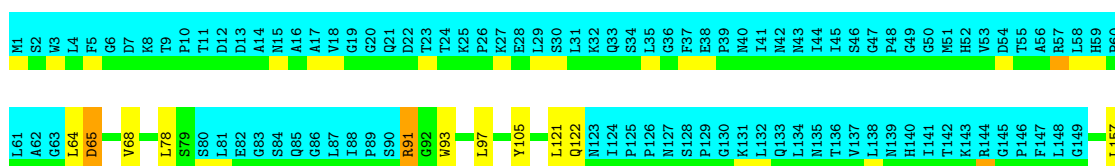
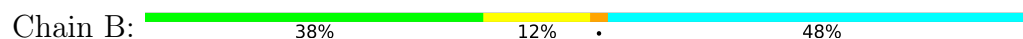


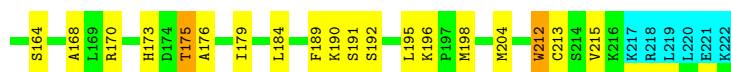
#### 4.2.13 Score per residue for model 13

• Molecule 1: TIM23 isoform 1



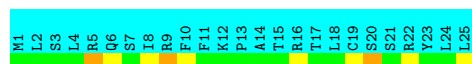
• Molecule 1: TIM23 isoform 1





- Molecule 2: COX4 isoform 1

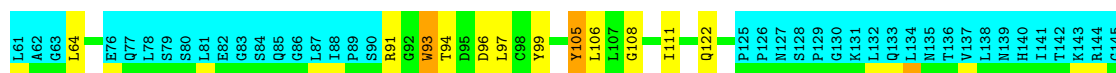
Chain C: 100%



#### 4.2.14 Score per residue for model 14

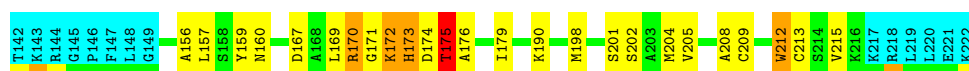
- Molecule 1: TIM23 isoform 1

Chain A: 32% 16% 50%



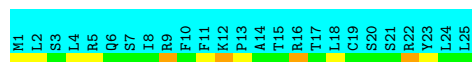
- Molecule 1: TIM23 isoform 1

Chain B: 33% 15% 48%



- Molecule 2: COX4 isoform 1

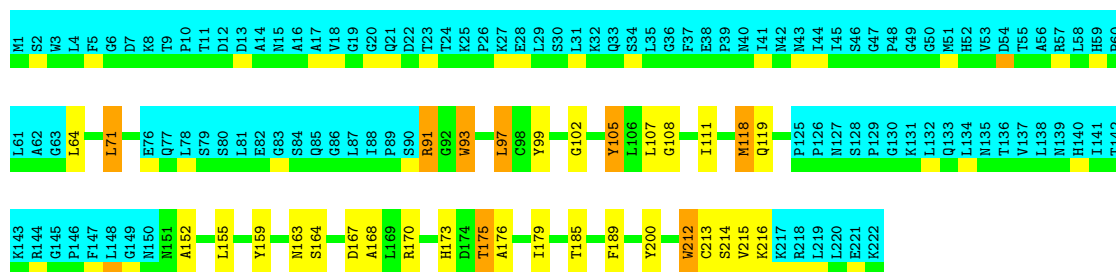
Chain C: 100%



#### 4.2.15 Score per residue for model 15

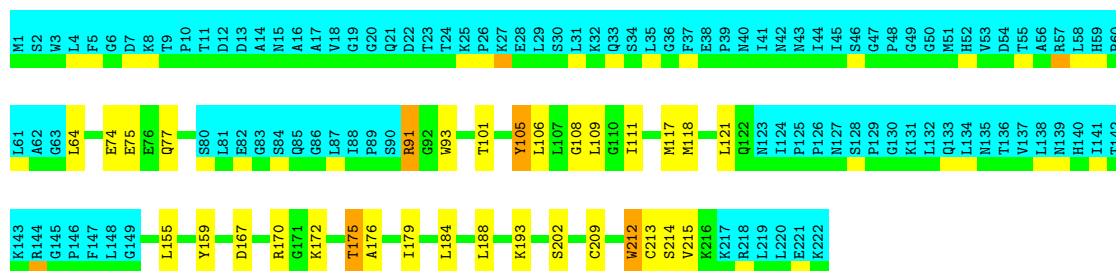
- Molecule 1: TIM23 isoform 1

Chain A: 36% 11% 50%



• Molecule 1: TIM23 isoform 1

Chain B: 37% 13% 48%



• Molecule 2: COX4 isoform 1

Chain C: 100%





## 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
X-PLOR NIH	structure calculation	
X-PLOR NIH	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	1891
Number of shifts mapped to atoms	1891
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%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	1.9±0.2
1	B	0.0±0.0	2.0±0.0
All	All	0	59

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	91	ARG	Sidechain	15
1	B	170	ARG	Sidechain	15
1	A	170	ARG	Sidechain	15
1	A	91	ARG	Sidechain	14

### 6.2 Too-close contacts [i](#)

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	807	809	809	22±5
1	B	831	828	828	21±5
2	C	0	0	0	0±0
All	All	24570	24555	24555	570

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:THR:HG21	1:A:212:TRP:CD1	0.86	2.05	14	2
1:A:175:THR:HG23	1:B:105:TYR:CZ	0.85	2.07	2	9
1:A:105:TYR:CZ	1:B:175:THR:HG23	0.81	2.10	13	9
1:A:173:HIS:O	1:A:215:VAL:HG22	0.81	1.74	7	1
1:A:176:ALA:HB1	1:A:179:ILE:CG1	0.79	2.08	1	1
1:B:185:THR:HG22	1:B:189:PHE:CE2	0.77	2.14	2	2
1:A:176:ALA:CB	1:A:179:ILE:HD12	0.76	2.09	9	3
1:A:175:THR:HG23	1:B:105:TYR:OH	0.76	1.80	15	11
1:B:176:ALA:CB	1:B:179:ILE:HD12	0.76	2.11	8	1
1:B:173:HIS:O	1:B:215:VAL:HG22	0.75	1.81	4	2
1:A:179:ILE:CG1	1:B:109:LEU:HD23	0.75	2.12	8	1
1:A:212:TRP:O	1:A:215:VAL:HG23	0.75	1.82	7	1
1:B:212:TRP:O	1:B:215:VAL:HG23	0.74	1.82	4	3
1:A:93:TRP:CD1	1:A:105:TYR:OH	0.74	2.41	14	15
1:A:175:THR:HG21	1:A:212:TRP:CE2	0.74	2.18	8	2
1:A:185:THR:HG22	1:A:189:PHE:CE2	0.73	2.17	12	1
1:B:93:TRP:CD1	1:B:105:TYR:OH	0.73	2.42	1	15
1:A:179:ILE:HG13	1:B:109:LEU:HD23	0.73	1.59	8	1
1:A:105:TYR:OH	1:B:175:THR:HG23	0.73	1.84	8	12
1:B:176:ALA:O	1:B:179:ILE:HG22	0.73	1.84	3	5
1:B:176:ALA:HB1	1:B:179:ILE:CG1	0.72	2.14	5	7
1:A:173:HIS:CD2	1:A:175:THR:HG23	0.72	2.19	6	1
1:A:176:ALA:O	1:A:179:ILE:HG22	0.71	1.86	8	6
1:B:176:ALA:HB1	1:B:179:ILE:HG12	0.70	1.63	5	6
1:B:108:GLY:HA2	1:B:111:ILE:HD12	0.69	1.64	4	6
1:B:118:MET:SD	1:B:156:ALA:HB2	0.69	2.27	14	1
1:A:176:ALA:HB1	1:A:179:ILE:HG12	0.67	1.66	1	1
1:A:212:TRP:HA	1:A:212:TRP:CE3	0.67	2.25	6	7
1:A:109:LEU:HD12	1:B:179:ILE:HD12	0.66	1.67	13	1
1:A:64:LEU:O	1:A:68:VAL:HG23	0.66	1.91	8	4
1:A:97:LEU:O	1:A:97:LEU:HD23	0.66	1.89	7	1
1:A:108:GLY:HA2	1:A:111:ILE:HD12	0.66	1.66	14	7
1:A:175:THR:HG21	1:A:212:TRP:NE1	0.66	2.06	8	2
1:B:174:ASP:O	1:B:175:THR:HG23	0.66	1.90	14	1
1:A:179:ILE:HG23	1:B:109:LEU:HD13	0.65	1.69	10	1
1:A:175:THR:HG21	1:A:212:TRP:CG	0.65	2.27	14	2
1:B:185:THR:HG22	1:B:189:PHE:CZ	0.64	2.28	2	1
1:A:185:THR:HG22	1:A:189:PHE:CE1	0.63	2.29	15	1
1:B:163:ASN:OD1	1:B:166:ILE:HD13	0.62	1.95	4	1
1:A:109:LEU:O	1:A:109:LEU:HD23	0.62	1.95	12	1
1:A:64:LEU:HD12	1:B:66:LYS:HD3	0.62	1.70	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:HIS:CD2	1:A:212:TRP:CD2	0.62	2.88	4	1
1:A:165:THR:O	1:A:169:LEU:HD12	0.61	1.95	4	1
1:A:175:THR:HG22	1:A:176:ALA:N	0.61	2.11	1	12
1:B:157:LEU:O	1:B:157:LEU:HD23	0.61	1.96	8	1
1:A:179:ILE:O	1:A:179:ILE:HD13	0.60	1.96	5	1
1:A:169:LEU:HD12	1:A:169:LEU:O	0.60	1.95	11	1
1:B:212:TRP:CE3	1:B:212:TRP:HA	0.60	2.31	14	8
1:A:212:TRP:CE3	1:A:212:TRP:HA	0.60	2.32	9	8
1:A:164:SER:O	1:A:168:ALA:HB2	0.60	1.97	6	10
1:B:169:LEU:HD23	1:B:169:LEU:O	0.59	1.97	3	2
1:B:212:TRP:HA	1:B:212:TRP:CE3	0.59	2.31	4	7
1:B:118:MET:CE	1:B:156:ALA:HB2	0.59	2.27	6	1
1:B:175:THR:HG22	1:B:176:ALA:N	0.58	2.13	6	13
1:B:150:ASN:O	1:B:154:ILE:HG22	0.58	1.98	1	1
1:B:108:GLY:O	1:B:111:ILE:HG22	0.58	1.99	6	5
1:A:69:GLU:OE1	1:A:73:LEU:HD22	0.58	1.99	3	1
1:B:151:ASN:O	1:B:154:ILE:HG22	0.58	1.99	2	1
1:B:118:MET:HE2	1:B:156:ALA:HB2	0.58	1.76	6	1
1:B:111:ILE:O	1:B:111:ILE:HG22	0.57	1.99	2	1
1:B:164:SER:O	1:B:168:ALA:HB2	0.57	1.99	7	8
1:A:70:TYR:CE2	1:B:71:LEU:HD13	0.57	2.34	8	1
1:A:103:ALA:HB1	1:A:107:LEU:HD13	0.57	1.77	12	1
1:B:176:ALA:HB1	1:B:179:ILE:HG13	0.57	1.77	14	1
1:B:93:TRP:CD1	1:B:93:TRP:N	0.56	2.74	14	5
1:A:107:LEU:HD11	1:A:166:ILE:HG21	0.56	1.78	4	1
1:A:107:LEU:HD13	1:A:107:LEU:O	0.56	2.01	7	1
1:A:94:THR:O	1:A:94:THR:HG22	0.55	2.01	3	1
1:B:68:VAL:HA	1:B:71:LEU:HD12	0.55	1.78	1	1
1:A:109:LEU:HD12	1:B:179:ILE:CD1	0.55	2.32	13	1
1:A:173:HIS:CD2	1:A:212:TRP:CE2	0.55	2.95	4	1
1:A:176:ALA:HB1	1:A:179:ILE:HD13	0.55	1.78	7	2
1:B:97:LEU:O	1:B:97:LEU:HD23	0.54	2.03	6	1
1:B:187:ALA:HB3	1:B:198:MET:CE	0.54	2.33	9	1
1:B:173:HIS:CG	1:B:212:TRP:CZ3	0.54	2.96	9	4
1:A:97:LEU:O	1:A:97:LEU:HD13	0.53	2.03	3	1
1:A:175:THR:HG21	1:A:212:TRP:CD2	0.53	2.38	8	2
1:B:173:HIS:CG	1:B:212:TRP:CH2	0.53	2.97	4	2
1:B:151:ASN:HA	1:B:154:ILE:HD12	0.53	1.81	4	2
1:A:117:MET:CE	1:A:121:LEU:HD13	0.53	2.34	5	1
1:A:97:LEU:HD12	1:A:102:GLY:HA3	0.53	1.79	15	1
1:B:176:ALA:HB1	1:B:179:ILE:HD13	0.52	1.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:173:HIS:CB	1:B:212:TRP:CZ3	0.52	2.92	2	9
1:A:166:ILE:HA	1:A:169:LEU:HD12	0.52	1.82	1	1
1:A:205:VAL:O	1:A:208:ALA:HB3	0.51	2.05	7	2
1:A:173:HIS:CB	1:A:212:TRP:CZ3	0.51	2.94	13	6
1:B:121:LEU:HD23	1:B:121:LEU:O	0.51	2.05	4	1
1:A:70:TYR:HE2	1:B:71:LEU:HD13	0.51	1.65	8	1
1:A:151:ASN:O	1:A:154:ILE:HG22	0.51	2.04	7	1
1:A:71:LEU:HD13	1:B:70:TYR:CE2	0.51	2.41	11	1
1:B:174:ASP:O	1:B:176:ALA:N	0.51	2.44	11	1
1:A:175:THR:HG23	1:A:176:ALA:N	0.51	2.19	8	2
1:A:174:ASP:OD2	1:A:215:VAL:HG11	0.50	2.06	6	1
1:A:93:TRP:N	1:A:93:TRP:CD1	0.50	2.80	10	4
1:A:212:TRP:HE3	1:A:212:TRP:HA	0.50	1.64	6	3
1:B:205:VAL:O	1:B:208:ALA:HB3	0.50	2.07	14	6
1:A:174:ASP:O	1:A:176:ALA:N	0.50	2.45	1	1
1:A:213:CYS:O	1:A:215:VAL:HG12	0.50	2.06	14	8
1:A:172:LYS:HB3	1:A:212:TRP:CH2	0.50	2.40	6	1
1:B:93:TRP:N	1:B:93:TRP:CD1	0.50	2.80	15	2
1:A:100:GLY:O	1:A:101:THR:HG23	0.50	2.06	5	1
1:A:182:GLY:HA3	1:B:109:LEU:HD11	0.50	1.82	8	1
1:B:187:ALA:HB1	1:B:198:MET:SD	0.50	2.47	12	1
1:A:109:LEU:HD12	1:B:179:ILE:HG23	0.49	1.84	8	1
1:B:158:SER:O	1:B:162:ILE:HD12	0.49	2.06	6	3
1:A:173:HIS:CE1	1:A:212:TRP:O	0.49	2.66	4	1
1:B:173:HIS:O	1:B:212:TRP:O	0.49	2.30	8	1
1:A:93:TRP:CD1	1:A:93:TRP:N	0.49	2.81	7	4
1:A:71:LEU:HD23	1:A:72:ASP:OD1	0.49	2.08	12	1
1:A:173:HIS:CG	1:A:212:TRP:CZ3	0.49	3.00	7	3
1:B:169:LEU:HD12	1:B:169:LEU:O	0.49	2.07	7	1
1:A:94:THR:HG22	1:A:97:LEU:HB2	0.49	1.84	1	1
1:B:213:CYS:O	1:B:215:VAL:HG12	0.49	2.07	11	8
1:B:213:CYS:O	1:B:215:VAL:N	0.48	2.47	9	12
1:A:174:ASP:O	1:A:175:THR:O	0.48	2.30	6	1
1:A:174:ASP:O	1:A:175:THR:C	0.48	2.52	8	1
1:B:109:LEU:HD23	1:B:109:LEU:C	0.48	2.29	1	1
1:B:100:GLY:O	1:B:101:THR:HG23	0.48	2.08	2	1
1:A:71:LEU:HD23	1:B:74:GLU:OE1	0.48	2.08	15	2
1:A:107:LEU:O	1:A:107:LEU:HD23	0.48	2.08	1	1
1:A:70:TYR:CD2	1:B:71:LEU:HD12	0.48	2.43	5	1
1:A:108:GLY:O	1:A:111:ILE:HG22	0.48	2.07	15	1
1:A:74:GLU:HG2	1:B:71:LEU:HD12	0.48	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ALA:HB3	1:A:179:ILE:HD12	0.48	1.85	14	1
1:A:107:LEU:O	1:A:111:ILE:HG23	0.47	2.08	12	1
1:A:173:HIS:O	1:A:212:TRP:O	0.47	2.31	15	1
1:B:173:HIS:HB3	1:B:212:TRP:CZ3	0.47	2.44	3	3
1:A:173:HIS:CD2	1:A:212:TRP:CE3	0.47	3.02	4	1
1:A:173:HIS:CD2	1:A:175:THR:H	0.47	2.28	4	1
1:A:213:CYS:O	1:A:215:VAL:N	0.47	2.47	14	9
1:A:94:THR:HA	1:A:97:LEU:HD12	0.47	1.84	14	1
1:B:103:ALA:HB1	1:B:107:LEU:HD13	0.47	1.85	12	1
1:A:175:THR:CG2	1:A:212:TRP:CE2	0.46	2.95	8	1
1:A:185:THR:HA	1:A:188:LEU:HD12	0.46	1.88	3	1
1:A:96:ASP:OD1	1:A:104:VAL:HG21	0.46	2.10	9	1
1:A:175:THR:HG23	1:B:105:TYR:CE1	0.46	2.45	2	1
1:A:209:CYS:O	1:A:213:CYS:CB	0.46	2.63	14	10
1:A:118:MET:SD	1:A:156:ALA:HB2	0.46	2.51	9	2
1:A:169:LEU:HD23	1:A:169:LEU:O	0.46	2.11	12	1
1:B:175:THR:OG1	1:B:212:TRP:CZ2	0.45	2.64	15	5
1:B:169:LEU:O	1:B:169:LEU:HD12	0.45	2.11	2	1
1:A:173:HIS:O	1:A:212:TRP:CD2	0.45	2.69	6	1
1:B:187:ALA:HB3	1:B:198:MET:HE3	0.45	1.87	9	1
1:A:176:ALA:HB1	1:A:179:ILE:HG13	0.45	1.84	1	1
1:A:157:LEU:CD2	1:A:161:ILE:HD11	0.45	2.41	8	1
1:A:175:THR:OG1	1:A:212:TRP:CZ2	0.45	2.63	10	4
1:A:74:GLU:CG	1:B:71:LEU:HD12	0.45	2.42	8	1
1:B:173:HIS:HB3	1:B:212:TRP:CD2	0.45	2.47	14	1
1:A:174:ASP:CG	1:A:215:VAL:HG11	0.45	2.32	6	1
1:A:175:THR:HB	1:A:212:TRP:NE1	0.45	2.27	5	4
1:A:105:TYR:CE1	1:B:175:THR:HG23	0.45	2.45	13	1
1:A:124:ILE:O	1:A:124:ILE:HG23	0.45	2.12	5	2
1:A:71:LEU:HD12	1:B:70:TYR:HE1	0.44	1.73	9	1
1:B:176:ALA:CB	1:B:179:ILE:CG1	0.44	2.94	9	1
1:A:172:LYS:O	1:A:173:HIS:O	0.44	2.35	6	1
1:A:162:ILE:O	1:A:165:THR:HG22	0.44	2.13	14	1
1:B:104:VAL:HG13	1:B:105:TYR:N	0.44	2.27	8	3
1:B:108:GLY:O	1:B:111:ILE:CG2	0.44	2.66	8	4
1:A:175:THR:CG2	1:A:176:ALA:N	0.44	2.81	1	1
1:A:179:ILE:HG23	1:B:109:LEU:CD1	0.44	2.42	10	1
1:B:175:THR:HB	1:B:212:TRP:NE1	0.44	2.28	1	5
1:B:65:ASP:HA	1:B:68:VAL:HG12	0.44	1.88	13	1
1:A:212:TRP:HA	1:A:212:TRP:HE3	0.44	1.72	8	2
1:A:172:LYS:CB	1:A:212:TRP:CZ3	0.44	3.01	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:GLY:HA3	1:B:109:LEU:HD21	0.44	1.89	8	1
1:B:209:CYS:O	1:B:213:CYS:CB	0.43	2.66	12	9
1:A:174:ASP:N	1:A:174:ASP:OD2	0.43	2.50	6	1
1:B:172:LYS:O	1:B:212:TRP:CZ3	0.43	2.71	14	1
1:A:176:ALA:CB	1:A:179:ILE:CD1	0.43	2.95	10	1
1:A:94:THR:HG22	1:A:102:GLY:CA	0.43	2.43	12	1
1:B:173:HIS:CB	1:B:212:TRP:CD2	0.43	3.01	14	1
1:A:173:HIS:ND1	1:A:212:TRP:O	0.43	2.51	4	1
1:B:212:TRP:HA	1:B:212:TRP:HE3	0.43	1.71	4	2
1:A:164:SER:O	1:A:168:ALA:N	0.43	2.52	6	1
1:A:172:LYS:O	1:A:172:LYS:CD	0.43	2.67	11	1
1:A:104:VAL:HG23	1:A:105:TYR:N	0.43	2.28	5	1
1:A:173:HIS:NE2	1:A:175:THR:HG23	0.43	2.28	6	1
1:A:109:LEU:CD1	1:B:179:ILE:HG23	0.43	2.43	8	1
1:A:175:THR:CG2	1:A:212:TRP:NE1	0.43	2.80	14	2
1:A:93:TRP:CD2	1:A:93:TRP:N	0.43	2.86	14	1
1:B:157:LEU:C	1:B:157:LEU:HD23	0.42	2.33	8	1
1:A:70:TYR:CE2	1:B:71:LEU:HD12	0.42	2.48	5	1
1:A:93:TRP:NE1	1:B:174:ASP:OD1	0.42	2.51	10	1
1:B:185:THR:OG1	1:B:189:PHE:CE1	0.42	2.72	10	1
1:A:165:THR:HG23	1:A:166:ILE:N	0.42	2.29	14	1
1:A:175:THR:O	1:A:179:ILE:HG22	0.42	2.15	6	1
1:B:212:TRP:HE3	1:B:212:TRP:HA	0.42	1.73	11	1
1:B:188:LEU:HD12	1:B:198:MET:SD	0.42	2.55	1	1
1:B:172:LYS:O	1:B:172:LYS:CG	0.42	2.67	7	1
1:B:176:ALA:HB1	1:B:179:ILE:HD12	0.42	1.88	8	1
1:A:118:MET:HE3	1:A:118:MET:HA	0.42	1.91	15	1
1:B:213:CYS:C	1:B:215:VAL:N	0.42	2.72	9	6
1:A:71:LEU:HD13	1:B:70:TYR:HE2	0.42	1.74	11	1
1:A:173:HIS:CG	1:A:212:TRP:CH2	0.42	3.07	7	2
1:B:173:HIS:CE1	1:B:211:VAL:O	0.42	2.72	7	1
1:B:94:THR:HG22	1:B:97:LEU:HB2	0.42	1.91	9	1
1:A:104:VAL:HG13	1:A:105:TYR:N	0.42	2.29	8	2
1:A:179:ILE:HG23	1:A:180:GLY:N	0.42	2.30	6	1
1:A:75:GLU:HG2	1:B:78:LEU:HD12	0.42	1.91	5	1
1:A:92:GLY:O	1:A:93:TRP:CE3	0.41	2.73	5	1
1:A:157:LEU:HD12	1:A:204:MET:CE	0.41	2.45	14	1
1:A:105:TYR:OH	1:B:175:THR:HA	0.41	2.15	4	1
1:A:173:HIS:HB3	1:A:212:TRP:CZ3	0.41	2.50	11	1
1:B:69:GLU:HG2	1:B:73:LEU:HD13	0.41	1.90	12	1
1:A:187:ALA:HB1	1:A:198:MET:SD	0.41	2.55	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:LYS:HB2	1:A:212:TRP:CZ3	0.41	2.49	6	1
1:B:173:HIS:O	1:B:215:VAL:HB	0.41	2.15	8	1
1:A:188:LEU:HD11	1:A:196:LYS:HE2	0.41	1.91	13	1
1:A:175:THR:CB	1:A:212:TRP:CE2	0.41	3.03	14	1
1:A:213:CYS:C	1:A:215:VAL:N	0.41	2.74	7	6
1:B:103:ALA:O	1:B:107:LEU:CB	0.41	2.69	11	1
1:B:94:THR:HG23	1:B:94:THR:O	0.41	2.15	1	1
1:A:158:SER:HA	1:A:161:ILE:HD12	0.41	1.92	2	1
1:A:172:LYS:CG	1:A:172:LYS:O	0.41	2.69	3	1
1:A:170:ARG:HB3	1:A:173:HIS:NE2	0.41	2.31	5	1
1:A:96:ASP:OD1	1:A:173:HIS:CE1	0.41	2.74	5	1
1:B:92:GLY:O	1:B:93:TRP:CE3	0.41	2.74	2	1
1:A:173:HIS:CD2	1:A:175:THR:CG2	0.41	2.99	6	1
1:A:176:ALA:O	1:A:180:GLY:N	0.41	2.54	6	1
1:B:172:LYS:HG2	1:B:172:LYS:O	0.41	2.16	12	1
1:B:174:ASP:O	1:B:175:THR:CG2	0.41	2.66	14	1
1:B:92:GLY:O	1:B:93:TRP:CD2	0.41	2.74	2	1
1:A:175:THR:HA	1:B:105:TYR:OH	0.41	2.16	4	1
1:B:185:THR:HG22	1:B:189:PHE:CE1	0.41	2.50	5	1
1:B:99:TYR:CG	1:B:99:TYR:O	0.41	2.74	6	1
1:B:173:HIS:HB2	1:B:212:TRP:CZ3	0.41	2.51	7	1
1:A:92:GLY:C	1:A:93:TRP:CG	0.41	2.94	12	1
1:A:96:ASP:O	1:A:100:GLY:N	0.41	2.54	12	1
1:A:184:LEU:C	1:A:184:LEU:HD23	0.41	2.36	14	1
1:A:176:ALA:HB3	1:A:179:ILE:HG12	0.41	1.93	15	1
1:A:172:LYS:O	1:A:172:LYS:HG2	0.41	2.15	2	1
1:B:104:VAL:CG2	1:B:170:ARG:NE	0.41	2.84	6	1
1:B:69:GLU:CG	1:B:73:LEU:HD13	0.41	2.46	12	1
1:B:172:LYS:CG	1:B:172:LYS:O	0.40	2.68	2	1
1:A:109:LEU:HD23	1:A:109:LEU:O	0.40	2.15	6	1
1:A:179:ILE:CG2	1:A:180:GLY:N	0.40	2.85	6	1
1:A:103:ALA:O	1:A:107:LEU:CB	0.40	2.69	9	1
1:B:176:ALA:O	1:B:179:ILE:CG1	0.40	2.68	11	1
1:A:185:THR:O	1:A:189:PHE:CD2	0.40	2.73	14	1
1:B:185:THR:CG2	1:B:189:PHE:CZ	0.40	3.03	2	1
1:B:97:LEU:C	1:B:97:LEU:HD23	0.40	2.36	4	1
1:A:109:LEU:HD11	1:B:182:GLY:HA3	0.40	1.92	10	1
1:B:96:ASP:N	1:B:96:ASP:OD1	0.40	2.54	10	1
1:A:116:GLY:CA	1:B:189:PHE:CB	0.40	2.99	13	1
1:A:175:THR:OG1	1:A:212:TRP:NE1	0.40	2.54	14	1
1:A:71:LEU:HD12	1:B:70:TYR:CE1	0.40	2.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:TYR:CD2	1:B:67:GLY:O	0.40	2.74	7	1
1:B:97:LEU:HD12	1:B:102:GLY:HA2	0.40	1.93	7	1
1:A:101:THR:O	1:A:101:THR:HG22	0.40	2.17	4	1
1:B:174:ASP:HB3	1:B:215:VAL:HG11	0.40	1.93	11	1
1:A:67:GLY:O	1:B:70:TYR:CD2	0.40	2.74	11	1
1:A:94:THR:CG2	1:A:102:GLY:CA	0.40	2.99	12	1
1:A:173:HIS:O	1:A:215:VAL:HB	0.40	2.17	12	1
1:A:173:HIS:CE1	1:B:93:TRP:CZ2	0.40	3.10	8	1
1:B:109:LEU:HD13	1:B:109:LEU:C	0.40	2.37	8	1
1:A:109:LEU:C	1:A:109:LEU:HD23	0.40	2.37	9	1
1:A:65:ASP:O	1:A:68:VAL:HG22	0.40	2.17	9	1
1:A:108:GLY:O	1:A:111:ILE:CG1	0.40	2.70	12	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	112/222 (50%)	101±3 (90±2%)	10±3 (9±2%)	2±1 (1±1%)	15	61
1	B	115/222 (52%)	103±2 (89±2%)	11±2 (9±2%)	2±1 (2±1%)	14	59
2	C	0	-	-	-	-	-
All	All	3405/7035 (48%)	3049 (90%)	306 (9%)	50 (1%)	14	59

All 12 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	175	THR	12
1	A	175	THR	12
1	A	214	SER	8
1	B	214	SER	5
1	B	216	LYS	3
1	B	91	ARG	2
1	B	171	GLY	2
1	A	91	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	B	111	ILE	1
1	B	194	GLY	1
1	A	192	SER	1
1	A	173	HIS	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	81/173 (47%)	62±4 (76±5%)	19±4 (24±5%)	2	26
1	B	84/173 (49%)	63±4 (75±5%)	21±4 (25±5%)	2	25
2	C	0	-	-	-	-
All	All	2475/5550 (45%)	1871 (76%)	604 (24%)	2	26

All 122 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	212	TRP	15
1	B	212	TRP	15
1	A	105	TYR	13
1	B	172	LYS	12
1	A	172	LYS	11
1	B	78	LEU	10
1	A	99	TYR	10
1	B	184	LEU	10
1	B	105	TYR	10
1	A	196	LYS	9
1	B	121	LEU	9
1	A	200	TYR	9
1	B	106	LEU	9
1	A	190	LYS	9
1	A	216	LYS	9
1	B	190	LYS	8
1	B	198	MET	8
1	B	204	MET	8
1	A	155	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	97	LEU	8
1	A	167	ASP	8
1	B	73	LEU	8
1	B	195	LEU	8
1	B	196	LYS	8
1	A	184	LEU	8
1	A	91	ARG	8
1	B	170	ARG	7
1	B	72	ASP	7
1	B	91	ARG	7
1	A	201	SER	7
1	A	195	LEU	7
1	A	188	LEU	7
1	A	73	LEU	7
1	B	193	LYS	6
1	B	118	MET	6
1	A	66	LYS	6
1	B	188	LEU	6
1	B	117	MET	6
1	B	119	GLN	6
1	A	157	LEU	6
1	A	122	GLN	6
1	B	64	LEU	6
1	A	121	LEU	6
1	B	66	LYS	6
1	B	159	TYR	6
1	B	160	ASN	5
1	A	169	LEU	5
1	A	159	TYR	5
1	A	106	LEU	5
1	B	200	TYR	5
1	A	118	MET	5
1	A	198	MET	5
1	B	155	LEU	5
1	A	107	LEU	5
1	B	169	LEU	5
1	B	201	SER	5
1	B	157	LEU	5
1	B	167	ASP	5
1	B	107	LEU	5
1	A	72	ASP	5
1	B	109	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	64	LEU	5
1	B	216	LYS	5
1	B	99	TYR	4
1	B	71	LEU	4
1	A	65	ASP	4
1	A	164	SER	4
1	B	97	LEU	4
1	B	79	SER	4
1	A	170	ARG	4
1	B	77	GLN	4
1	B	202	SER	4
1	B	114	PHE	4
1	A	204	MET	4
1	B	75	GLU	4
1	A	93	TRP	4
1	A	75	GLU	4
1	B	163	ASN	3
1	B	178	SER	3
1	A	114	PHE	3
1	A	94	THR	3
1	A	178	SER	3
1	A	163	ASN	3
1	B	65	ASP	3
1	A	119	GLN	3
1	A	117	MET	3
1	A	71	LEU	3
1	B	191	SER	3
1	A	193	LYS	3
1	B	76	GLU	3
1	B	151	ASN	2
1	B	94	THR	2
1	B	115	SER	2
1	A	173	HIS	2
1	B	122	GLN	2
1	B	173	HIS	2
1	B	158	SER	2
1	A	192	SER	2
1	A	151	ASN	2
1	B	150	ASN	2
1	B	101	THR	2
1	A	74	GLU	2
1	A	191	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	96	ASP	2
1	A	160	ASN	2
1	A	69	GLU	2
1	B	214	SER	2
1	A	185	THR	2
1	B	96	ASP	1
1	B	185	THR	1
1	B	111	ILE	1
1	A	189	PHE	1
1	A	101	THR	1
1	A	154	ILE	1
1	A	202	SER	1
1	A	179	ILE	1
1	A	109	LEU	1
1	A	158	SER	1
1	B	192	SER	1
1	B	175	THR	1
1	A	70	TYR	1
1	B	95	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 6.7 Other polymers ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 30% 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	1891
Number of shifts mapped to atoms	1891
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
$^{13}\text{C}_\alpha$	211	$0.40 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	178	$0.72 \pm 0.04$	Should be applied
$^{13}\text{C}'$	197	$0.10 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	198	$0.70 \pm 0.18$	Should be applied

#### 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. 849 atoms were assigned a chemical shift out of a possible 2487. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	502/1131 (44%)	190/452 (42%)	209/454 (46%)	103/225 (46%)
Sidechain	324/1178 (28%)	194/682 (28%)	130/459 (28%)	0/37 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	23/178 (13%)	21/92 (23%)	0/80 (0%)	2/6 (33%)
Overall	849/2487 (34%)	405/1226 (33%)	339/993 (34%)	105/268 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 1620 atoms were assigned a chemical shift out of a possible 5399. 0 out of 79 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	983/2299 (43%)	377/915 (41%)	408/938 (43%)	198/446 (44%)
Sidechain	610/2776 (22%)	367/1628 (23%)	243/1038 (23%)	0/110 (0%)
Aromatic	27/324 (8%)	25/172 (15%)	0/138 (0%)	2/14 (14%)
Overall	1620/5399 (30%)	769/2715 (28%)	651/2114 (31%)	200/570 (35%)

#### 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.

Random coil index (RCI) for chain A:

