



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 01:06 AM EST

PDB ID : 2N5N  
BMRB ID : 18906  
Title : Structure of an N-terminal domain of CHD4  
Authors : Silva, A.P.G.; Mackay, J.P.  
Deposited on : 2015-07-22

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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

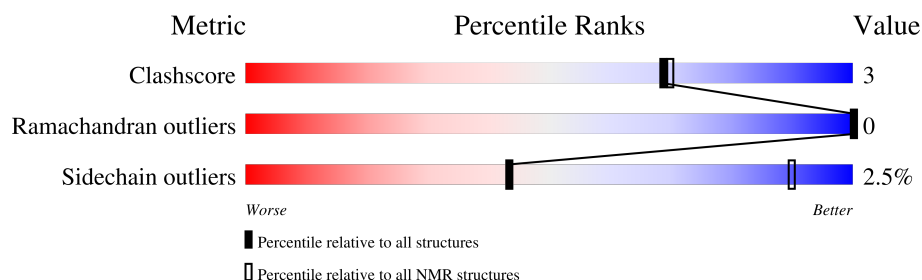
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	86	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:150-A:216 (67)	0.52	17

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 11, 12, 14, 15, 17, 18, 19, 20
2	6, 7, 16
3	2, 5, 13
4	1, 8
5	9, 10

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1334 atoms, of which 662 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chromodomain-helicase-DNA-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	86	Total	C	H	N	O	S	0
			1334	426	662	113	129	4	

There are 5 discrepancies between the modelled and reference sequences:

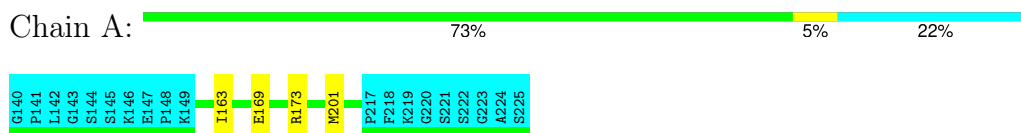
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	GLY	-	expression tag	UNP Q14839
A	141	PRO	-	expression tag	UNP Q14839
A	142	LEU	-	expression tag	UNP Q14839
A	143	GLY	-	expression tag	UNP Q14839
A	144	SER	-	expression tag	UNP Q14839

## 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: Chromodomain-helicase-DNA-binding protein 4

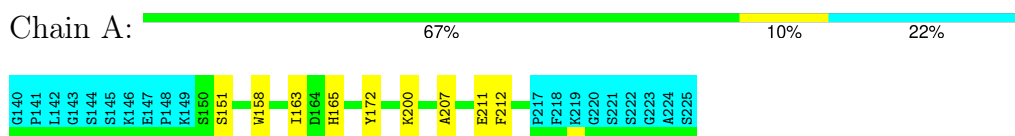


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

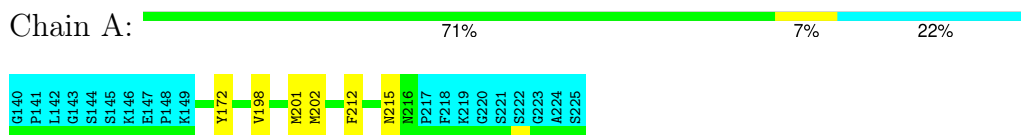
#### 4.2.1 Score per residue for model 1

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



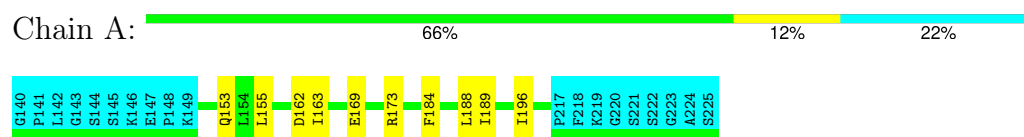
#### 4.2.2 Score per residue for model 2

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



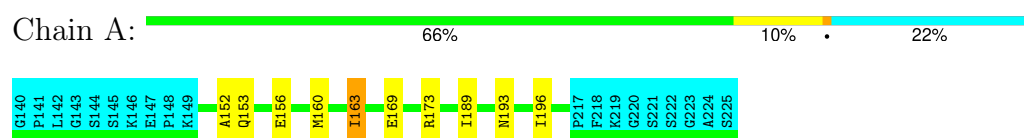
### 4.2.3 Score per residue for model 3

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



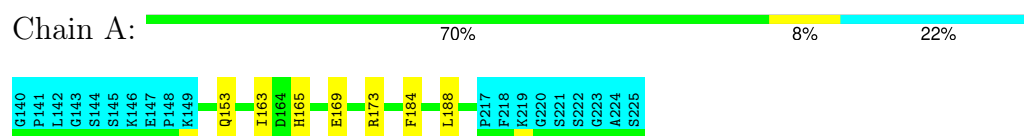
### 4.2.4 Score per residue for model 4

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



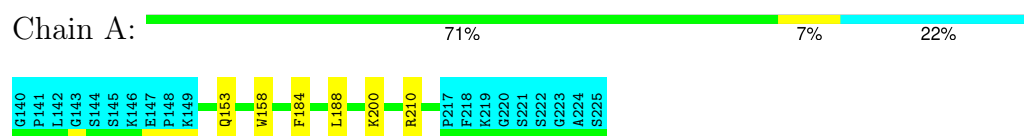
### 4.2.5 Score per residue for model 5

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



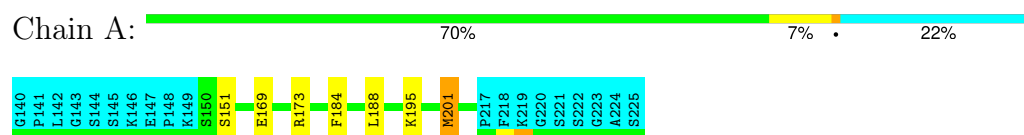
### 4.2.6 Score per residue for model 6

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



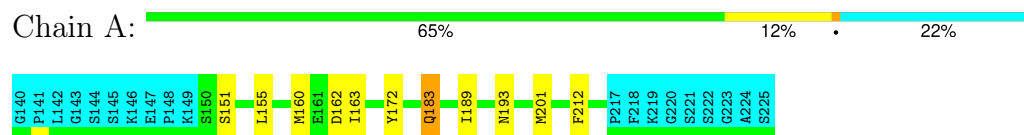
### 4.2.7 Score per residue for model 7

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



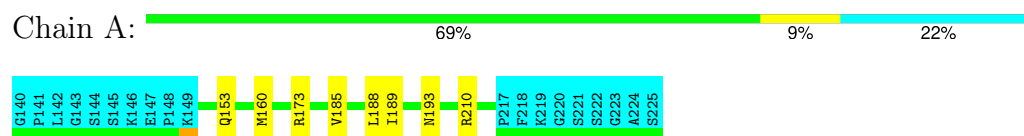
### 4.2.8 Score per residue for model 8

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



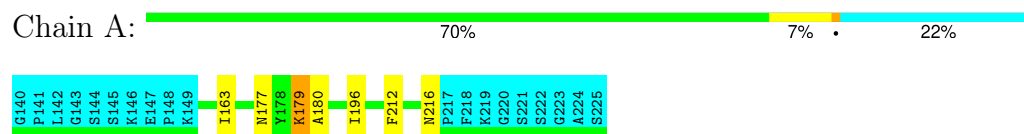
### 4.2.9 Score per residue for model 9

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



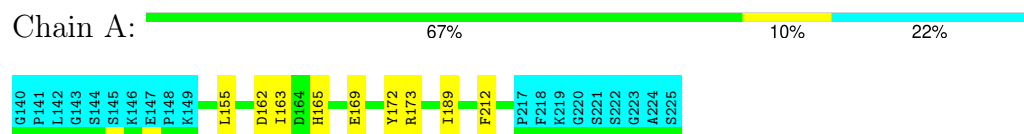
### 4.2.10 Score per residue for model 10

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



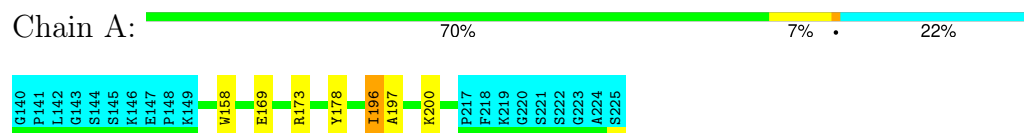
### 4.2.11 Score per residue for model 11

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



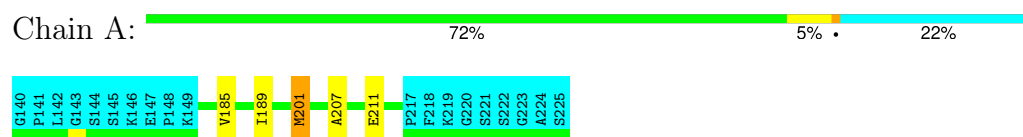
### 4.2.12 Score per residue for model 12

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



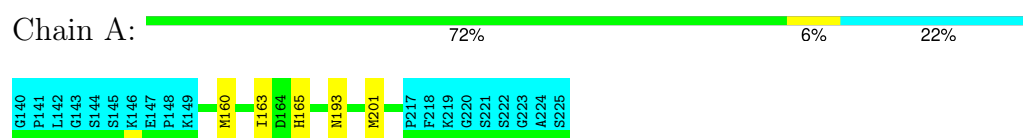
### 4.2.13 Score per residue for model 13

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



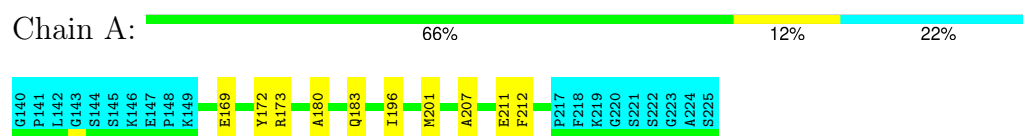
### 4.2.14 Score per residue for model 14

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



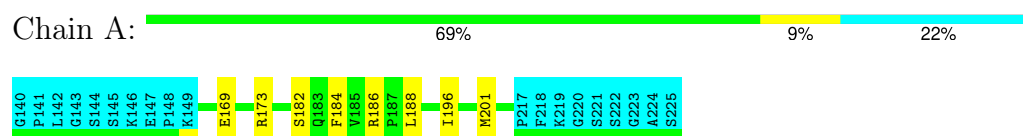
### 4.2.15 Score per residue for model 15

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



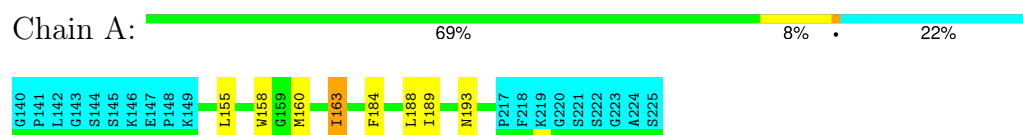
### 4.2.16 Score per residue for model 16

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



### 4.2.17 Score per residue for model 17 (medoid)

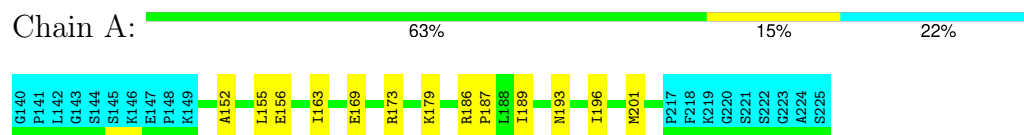
- Molecule 1: Chromodomain-helicase-DNA-binding protein 4





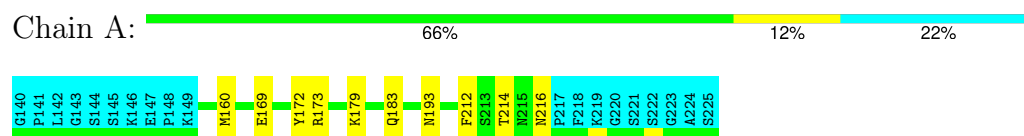
### 4.2.18 Score per residue for model 18

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



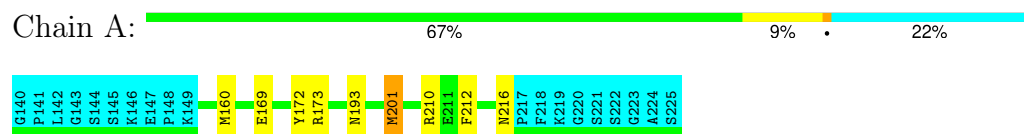
### 4.2.19 Score per residue for model 19

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



### 4.2.20 Score per residue for model 20

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 100 calculated structures, 20 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	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	930
Number of shifts mapped to atoms	930
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

## 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	0.1±0.4
All	All	0	2

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	A	173	ARG	Sidechain	1
1	A	210	ARG	Sidechain	1

### 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	544	532	532	4±1
All	All	10880	10640	10640	75

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:PHE:O	1:A:216:ASN:HB2	0.63	1.93	10	2
1:A:163:ILE:HD11	1:A:189:ILE:HA	0.56	1.76	8	5
1:A:160:MET:HB3	1:A:193:ASN:OD1	0.55	2.01	14	7
1:A:169:GLU:O	1:A:173:ARG:HG3	0.54	2.01	19	11
1:A:163:ILE:CG2	1:A:165:HIS:HB3	0.51	2.35	14	2
1:A:155:LEU:HD23	1:A:162:ASP:HA	0.50	1.83	11	3
1:A:172:TYR:HA	1:A:212:PHE:CZ	0.49	2.43	11	7
1:A:158:TRP:CZ2	1:A:200:LYS:HD2	0.48	2.43	12	2
1:A:177:ASN:OD1	1:A:179:LYS:HG3	0.48	2.08	10	1
1:A:155:LEU:HD21	1:A:193:ASN:ND2	0.48	2.23	18	1
1:A:207:ALA:O	1:A:211:GLU:HG2	0.46	2.10	1	3
1:A:210:ARG:HA	1:A:210:ARG:NE	0.46	2.25	6	2
1:A:185:VAL:O	1:A:189:ILE:HG13	0.45	2.11	9	2
1:A:198:VAL:O	1:A:202:MET:HG3	0.45	2.10	2	1
1:A:163:ILE:HG22	1:A:165:HIS:HB3	0.45	1.87	5	2
1:A:179:LYS:HD2	1:A:180:ALA:N	0.45	2.27	10	1
1:A:155:LEU:HA	1:A:158:TRP:CE3	0.44	2.48	17	1
1:A:152:ALA:O	1:A:156:GLU:HB2	0.44	2.12	4	2
1:A:184:PHE:O	1:A:188:LEU:HD23	0.44	2.12	6	4
1:A:163:ILE:CD1	1:A:189:ILE:HA	0.43	2.43	3	2
1:A:201:MET:HA	1:A:201:MET:HE3	0.43	1.91	13	3
1:A:186:ARG:HB3	1:A:187:PRO:HD3	0.43	1.91	18	1
1:A:158:TRP:CE2	1:A:200:LYS:HD2	0.42	2.49	1	1
1:A:163:ILE:HD12	1:A:163:ILE:H	0.42	1.75	4	1
1:A:183:GLN:HE21	1:A:183:GLN:HA	0.42	1.75	8	1
1:A:184:PHE:O	1:A:188:LEU:HD13	0.42	2.14	7	2
1:A:182:SER:O	1:A:186:ARG:HB3	0.41	2.15	16	1
1:A:179:LYS:O	1:A:183:GLN:HG2	0.41	2.15	19	1
1:A:163:ILE:HD12	1:A:163:ILE:N	0.41	2.30	5	1
1:A:196:ILE:HD13	1:A:197:ALA:N	0.40	2.31	12	1
1:A:180:ALA:HA	1:A:183:GLN:NE2	0.40	2.31	15	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	67/86 (78%)	66±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	1340/1720 (78%)	1315 (98%)	25 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	59/73 (81%)	58±1 (97±2%)	2±1 (3±2%)	43	90
All	All	1180/1460 (81%)	1150 (97%)	30 (3%)	43	90

All 10 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	201	MET	9
1	A	196	ILE	7
1	A	151	SER	3
1	A	163	ILE	3
1	A	153	GLN	2
1	A	179	LYS	2
1	A	215	ASN	1
1	A	195	LYS	1
1	A	183	GLN	1
1	A	188	LEU	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 86% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	930
Number of shifts mapped to atoms	930
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	$-0.21 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	76	$-0.06 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	65	$0.13 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	67	$0.16 \pm 0.27$	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 86%, i.e. 799 atoms were assigned a chemical shift out of a possible 929. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	320/333 (96%)	131/134 (98%)	127/134 (95%)	62/65 (95%)
Sidechain	442/507 (87%)	301/329 (91%)	136/158 (86%)	5/20 (25%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	37/89 (42%)	35/44 (80%)	0/42 (0%)	2/3 (67%)
Overall	799/929 (86%)	467/507 (92%)	263/334 (79%)	69/88 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 930 atoms were assigned a chemical shift out of a possible 1140. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	357/426 (84%)	147/173 (85%)	143/172 (83%)	67/81 (83%)
Sidechain	531/615 (86%)	363/399 (91%)	163/193 (84%)	5/23 (22%)
Aromatic	42/99 (42%)	40/49 (82%)	0/47 (0%)	2/3 (67%)
Overall	930/1140 (82%)	550/621 (89%)	306/412 (74%)	74/107 (69%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

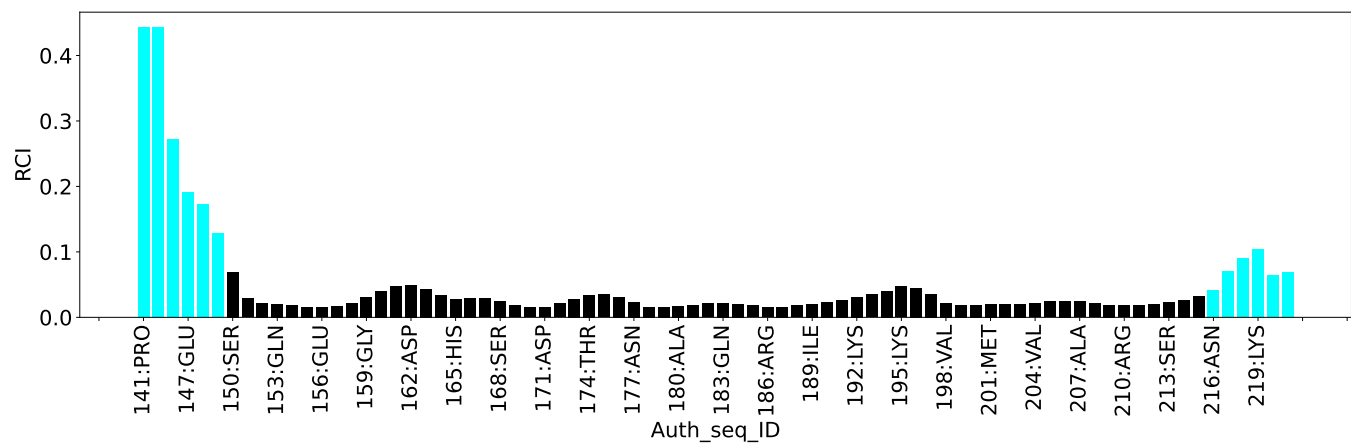
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	200	LYS	HD3	0.32	0.54 – 2.65	-6.1
1	A	200	LYS	HG3	-0.20	0.04 – 2.67	-5.9

#### 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:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1257
Intra-residue ( $ i-j =0$ )	340
Sequential ( $ i-j =1$ )	299
Medium range ( $ i-j >1$ and $ i-j <5$ )	290
Long range ( $ i-j \geq 5$ )	328
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.6
Number of long range restraints per residue <sup>1</sup>	3.8

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.0	0.18
0.2-0.5 (Medium)	0.1	0.22
>0.5 (Large)	None	None

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis

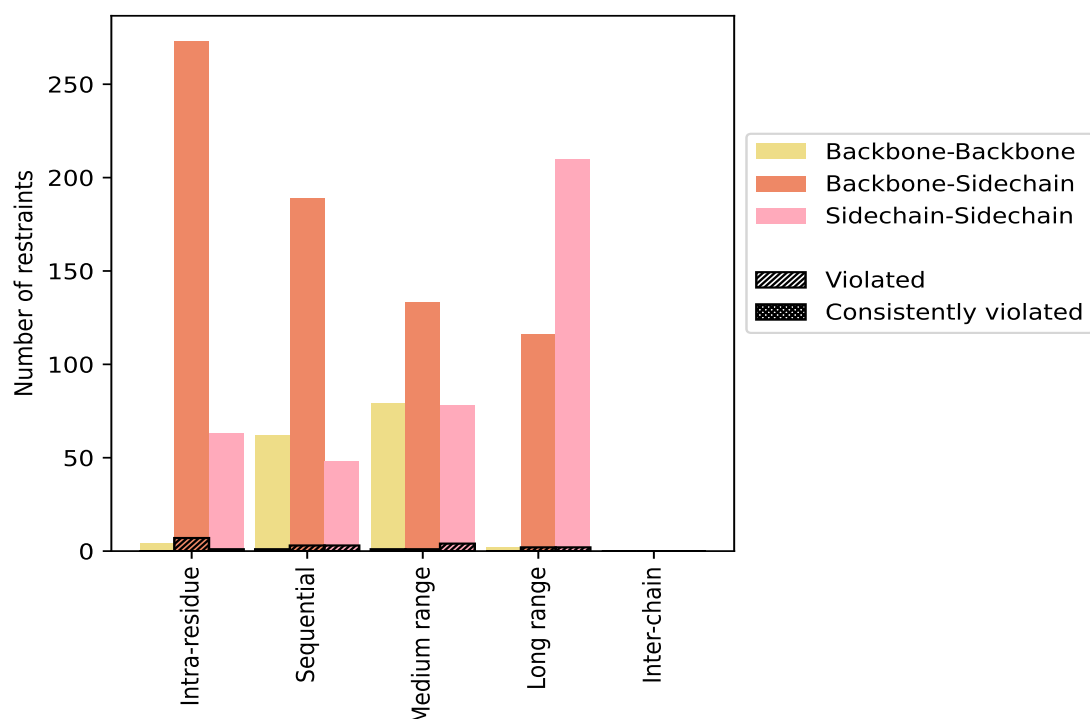
### 9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>340</b>	<b>27.0</b>	<b>8</b>	<b>2.4</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	273	21.7	7	2.6	0.6	0	0.0	0.0
Sidechain-Sidechain	63	5.0	1	1.6	0.1	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>299</b>	<b>23.8</b>	<b>7</b>	<b>2.3</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	62	4.9	1	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	189	15.0	3	1.6	0.2	0	0.0	0.0
Sidechain-Sidechain	48	3.8	3	6.2	0.2	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>290</b>	<b>23.1</b>	<b>6</b>	<b>2.1</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	79	6.3	1	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	133	10.6	1	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	78	6.2	4	5.1	0.3	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>328</b>	<b>26.1</b>	<b>4</b>	<b>1.2</b>	<b>0.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	9.2	2	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	210	16.7	2	1.0	0.2	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1257</b>	<b>100.0</b>	<b>25</b>	<b>2.0</b>	<b>2.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	147	11.7	2	1.4	0.2	0	0.0	0.0
Backbone-Sidechain	711	56.6	13	1.8	1.0	0	0.0	0.0
Sidechain-Sidechain	399	31.7	10	2.5	0.8	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	1	1	1	0	0	3	0.13	0.17	0.03	0.11
2	1	0	2	0	0	3	0.12	0.15	0.02	0.1
3	1	0	0	1	0	2	0.14	0.18	0.04	0.14
4	2	0	2	0	0	4	0.12	0.17	0.03	0.11
5	1	1	0	0	0	2	0.12	0.12	0.0	0.12
6	1	0	0	0	0	1	0.18	0.18	0.0	0.18
7	0	1	0	0	0	1	0.11	0.11	0.0	0.11
8	2	0	0	1	0	3	0.15	0.17	0.03	0.16
9	1	0	2	1	0	4	0.12	0.17	0.03	0.11
10	1	0	0	1	0	2	0.14	0.18	0.03	0.14

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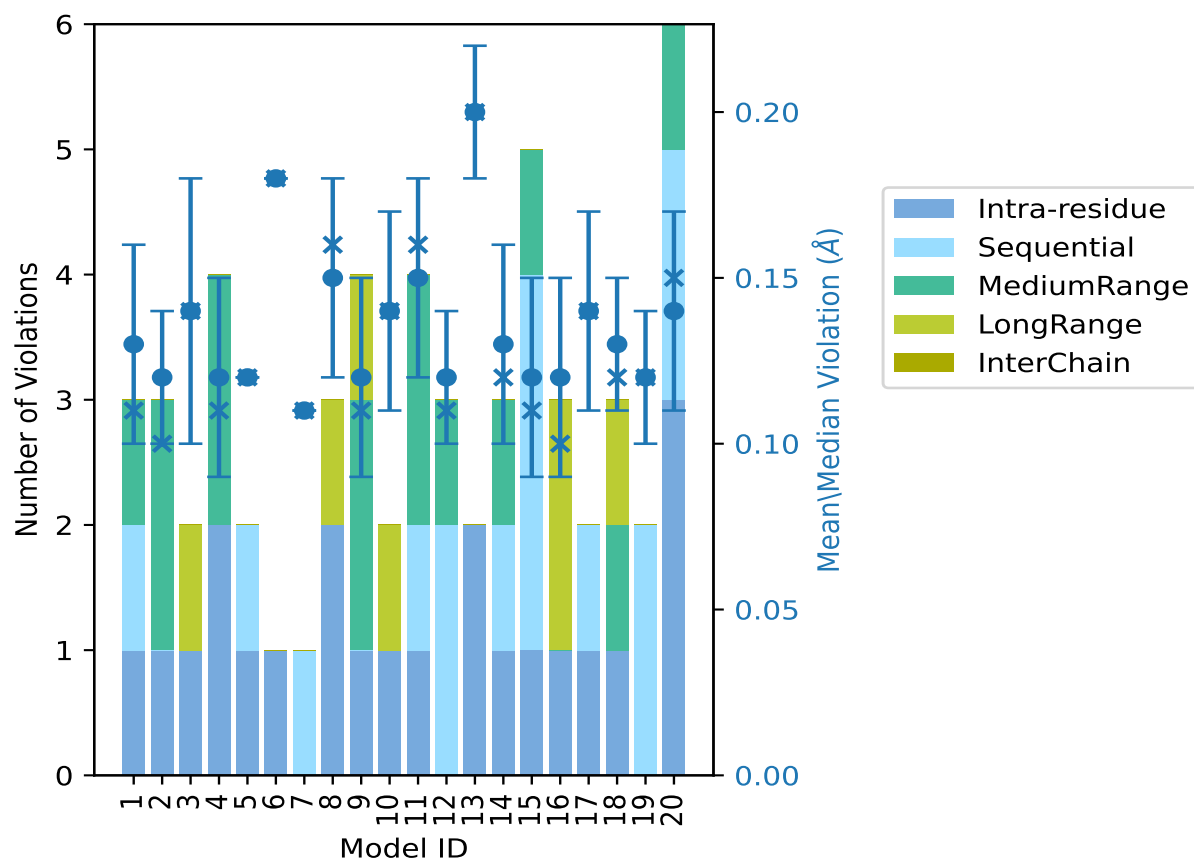
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	1	1	2	0	0	4	0.15	0.17	0.03	0.16
12	0	2	1	0	0	3	0.12	0.14	0.02	0.11
13	2	0	0	0	0	2	0.2	0.22	0.02	0.2
14	1	1	1	0	0	3	0.13	0.17	0.03	0.12
15	1	3	1	0	0	5	0.12	0.17	0.03	0.11
16	1	0	0	2	0	3	0.12	0.17	0.03	0.1
17	1	1	0	0	0	2	0.14	0.18	0.03	0.14
18	1	0	1	1	0	3	0.13	0.16	0.02	0.12
19	0	2	0	0	0	2	0.12	0.15	0.02	0.12
20	3	2	1	0	0	6	0.14	0.18	0.03	0.15

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble

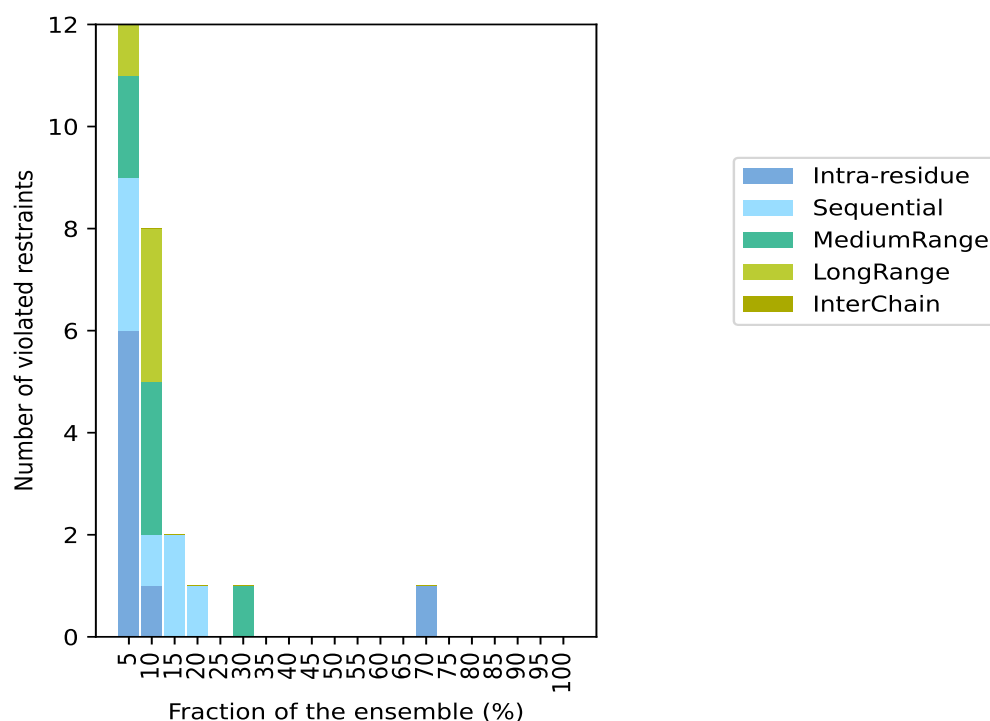
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1232(IR:332, SQ:292, MR:284, LR:324, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
6	3	2	1	0	12	1	5.0
1	1	3	3	0	8	2	10.0
0	2	0	0	0	2	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
1	0	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)

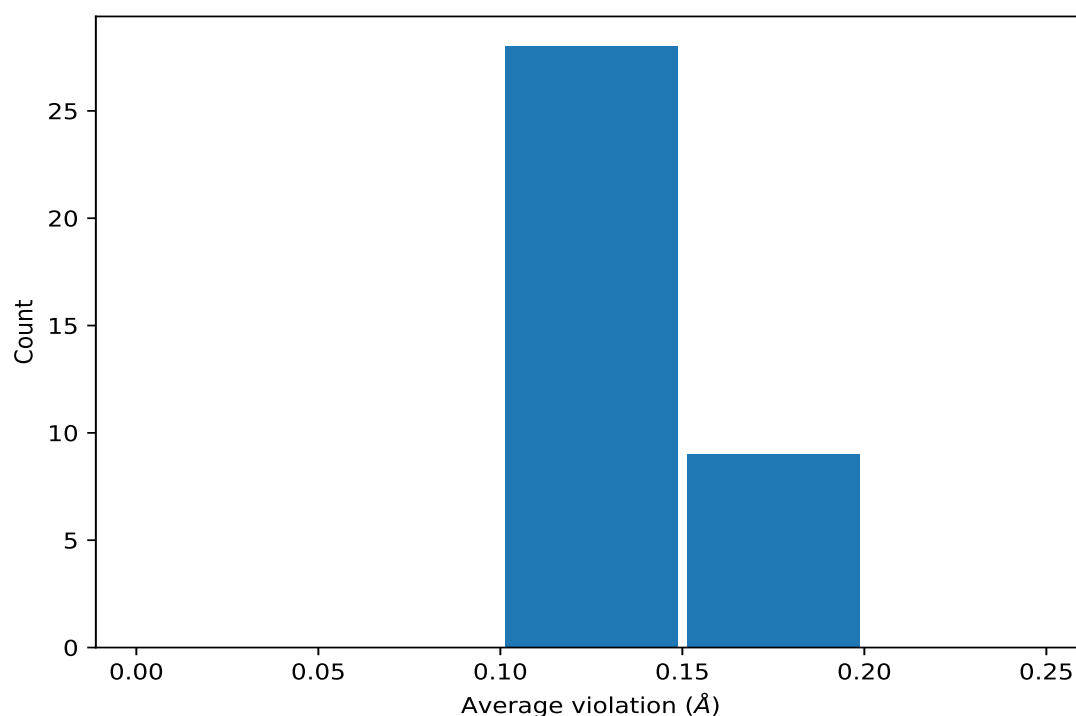


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble





#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	14	0.17	0.01	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	14	0.17	0.01	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	14	0.17	0.01	0.17
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	6	0.12	0.02	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD2	4	0.11	0.0	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD3	4	0.11	0.0	0.11
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD2	3	0.16	0.01	0.15
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD3	3	0.16	0.01	0.15
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD2	3	0.16	0.01	0.15
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD3	3	0.16	0.01	0.15
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD2	3	0.13	0.02	0.12
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD3	3	0.13	0.02	0.12
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG2	2	0.16	0.01	0.16
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG3	2	0.16	0.01	0.16
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB2	2	0.15	0.03	0.15
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB3	2	0.15	0.03	0.15

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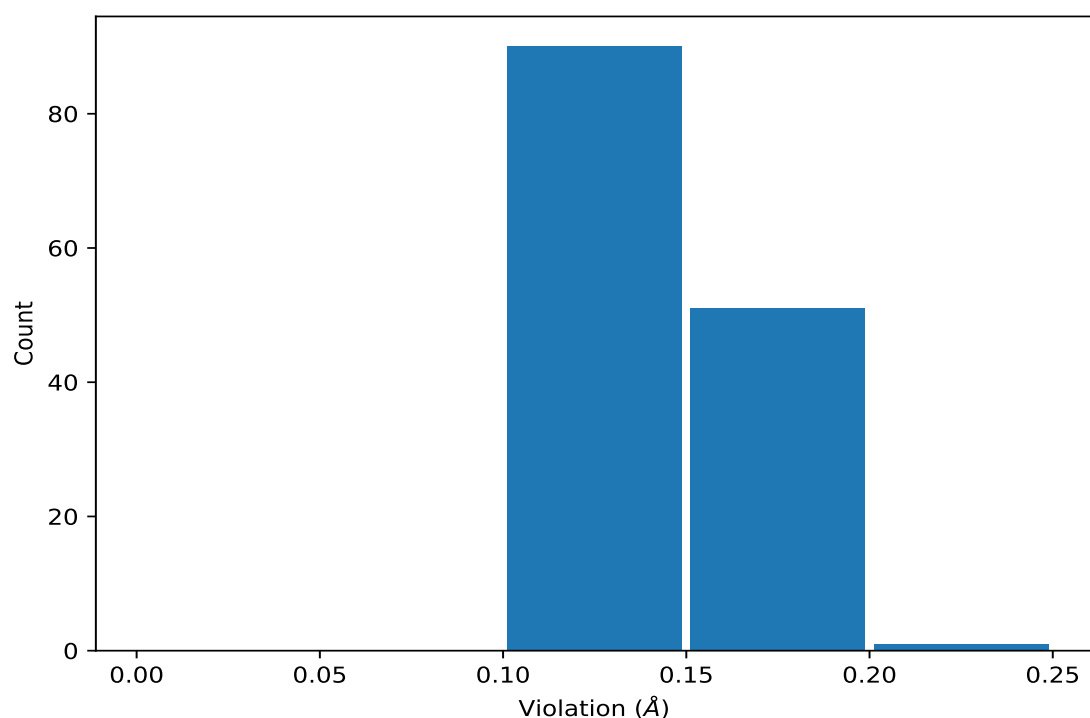
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE1	2	0.11	0.0	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE2	2	0.11	0.0	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE3	2	0.11	0.0	0.11
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG2	2	0.11	0.0	0.11
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG3	2	0.11	0.0	0.11
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG2	2	0.11	0.0	0.11
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD11	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD12	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD13	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD21	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD22	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,851)	1:155:A:LEU:HD23	1:162:A:ASP:HB3	2	0.11	0.0	0.11
(1,903)	1:186:A:ARG:HA	1:205:A:LEU:HG	2	0.11	0.0	0.11
(1,856)	1:196:A:ILE:HG21	1:197:A:ALA:HA	2	0.1	0.0	0.1
(1,856)	1:196:A:ILE:HG22	1:197:A:ALA:HA	2	0.1	0.0	0.1
(1,856)	1:196:A:ILE:HG23	1:197:A:ALA:HA	2	0.1	0.0	0.1
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG12	2	0.1	0.0	0.1
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG13	2	0.1	0.0	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG12	2	0.1	0.0	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG13	2	0.1	0.0	0.1

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:156:A:GLU:H	1:156:A:GLU:HB3	13	0.22
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	3	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	3	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	3	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	6	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	6	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	6	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	10	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	10	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	10	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	17	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	17	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	17	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	20	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	20	0.18
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB2	11	0.17
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB3	11	0.17
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD2	15	0.17
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD3	15	0.17
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD2	15	0.17
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD3	15	0.17
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG2	8	0.17
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG3	8	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	1	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	1	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	1	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	4	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	4	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	4	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	9	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	9	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	9	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	11	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	11	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	11	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	13	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	13	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	13	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	14	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	14	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	14	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	16	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	16	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	16	0.17
(1,343)	1:210:A:ARG:H	1:210:A:ARG:HB3	20	0.17
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	8	0.16
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	8	0.16
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	8	0.16
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD11	18	0.16
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD12	18	0.16
(1,567)	1:205:A:LEU:HA	1:205:A:LEU:HD13	18	0.16
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD2	11	0.15
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD3	11	0.15
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD2	11	0.15
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD3	11	0.15
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD2	20	0.15
(1,956)	1:147:A:GLU:HG2	1:148:A:PRO:HD3	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD2	20	0.15
(1,956)	1:147:A:GLU:HG3	1:148:A:PRO:HD3	20	0.15
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG2	20	0.15
(1,876)	1:153:A:GLN:HA	1:153:A:GLN:HG3	20	0.15
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD2	19	0.15
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD3	19	0.15
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	2	0.15
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	12	0.14
(1,564)	1:163:A:ILE:HA	1:163:A:ILE:HD11	15	0.13
(1,564)	1:163:A:ILE:HA	1:163:A:ILE:HD12	15	0.13
(1,564)	1:163:A:ILE:HA	1:163:A:ILE:HD13	15	0.13
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB2	14	0.12
(1,1049)	1:163:A:ILE:HB	1:165:A:HIS:HB3	14	0.12
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD2	5	0.12
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD3	5	0.12
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD2	20	0.12
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD3	20	0.12
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	18	0.12
(1,951)	1:186:A:ARG:HB2	1:186:A:ARG:HD2	5	0.11
(1,951)	1:186:A:ARG:HB2	1:186:A:ARG:HD3	5	0.11
(1,903)	1:186:A:ARG:HA	1:205:A:LEU:HG	9	0.11
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD2	12	0.11
(1,857)	1:186:A:ARG:HG3	1:187:A:PRO:HD3	12	0.11
(1,851)	1:155:A:LEU:HD11	1:162:A:ASP:HB3	8	0.11
(1,851)	1:155:A:LEU:HD12	1:162:A:ASP:HB3	8	0.11
(1,851)	1:155:A:LEU:HD13	1:162:A:ASP:HB3	8	0.11
(1,851)	1:155:A:LEU:HD21	1:162:A:ASP:HB3	8	0.11
(1,851)	1:155:A:LEU:HD22	1:162:A:ASP:HB3	8	0.11
(1,851)	1:155:A:LEU:HD23	1:162:A:ASP:HB3	8	0.11
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG2	1	0.11
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG3	1	0.11
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG2	1	0.11
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG3	1	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD2	7	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD3	7	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD2	15	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD3	15	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD2	17	0.11
(1,829)	1:186:A:ARG:HB2	1:187:A:PRO:HD3	17	0.11
(1,818)	1:149:A:LYS:HA	1:149:A:LYS:HG2	4	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE1	10	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE2	10	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE3	10	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE1	18	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE2	18	0.11
(1,753)	1:193:A:ASN:HD22	1:201:A:MET:HE3	18	0.11
(1,466)	1:190:A:ALA:HA	1:193:A:ASN:HD22	9	0.11
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG12	9	0.1
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG13	9	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG12	9	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG13	9	0.1
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG12	11	0.1
(1,1177)	1:193:A:ASN:HB2	1:196:A:ILE:HG13	11	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG12	11	0.1
(1,1177)	1:193:A:ASN:HB3	1:196:A:ILE:HG13	11	0.1
(1,903)	1:186:A:ARG:HA	1:205:A:LEU:HG	16	0.1
(1,856)	1:196:A:ILE:HG21	1:197:A:ALA:HA	12	0.1
(1,856)	1:196:A:ILE:HG22	1:197:A:ALA:HA	12	0.1
(1,856)	1:196:A:ILE:HG23	1:197:A:ALA:HA	12	0.1
(1,856)	1:196:A:ILE:HG21	1:197:A:ALA:HA	15	0.1
(1,856)	1:196:A:ILE:HG22	1:197:A:ALA:HA	15	0.1
(1,856)	1:196:A:ILE:HG23	1:197:A:ALA:HA	15	0.1
(1,851)	1:155:A:LEU:HD11	1:162:A:ASP:HB3	3	0.1
(1,851)	1:155:A:LEU:HD12	1:162:A:ASP:HB3	3	0.1
(1,851)	1:155:A:LEU:HD13	1:162:A:ASP:HB3	3	0.1
(1,851)	1:155:A:LEU:HD21	1:162:A:ASP:HB3	3	0.1
(1,851)	1:155:A:LEU:HD22	1:162:A:ASP:HB3	3	0.1
(1,851)	1:155:A:LEU:HD23	1:162:A:ASP:HB3	3	0.1
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG2	4	0.1
(1,836)	1:149:A:LYS:HD2	1:153:A:GLN:HG3	4	0.1
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG2	4	0.1
(1,836)	1:149:A:LYS:HD3	1:153:A:GLN:HG3	4	0.1
(1,750)	1:217:A:PRO:HB3	1:218:A:PHE:H	14	0.1
(1,698)	1:208:A:LYS:HB2	1:209:A:TRP:H	1	0.1
(1,618)	1:185:A:VAL:HG11	1:188:A:LEU:HB2	2	0.1
(1,618)	1:185:A:VAL:HG12	1:188:A:LEU:HB2	2	0.1
(1,618)	1:185:A:VAL:HG13	1:188:A:LEU:HB2	2	0.1
(1,528)	1:169:A:GLU:HG2	1:218:A:PHE:H	16	0.1
(1,528)	1:169:A:GLU:HG3	1:218:A:PHE:H	16	0.1
(1,521)	1:175:A:LEU:HA	1:176:A:THR:H	19	0.1
(1,306)	1:188:A:LEU:H	1:188:A:LEU:HG	2	0.1
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	4	0.1
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	15	0.1
(1,161)	1:166:A:VAL:HA	1:168:A:SER:H	20	0.1

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found