



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 5UGK / pdb_00005ugk
BMRB ID : 30227
Title : Zinc-Binding Structure of a Catalytic Amyloid from Solid-State NMR Spectroscopy
Authors : Lee, M.; Wang, T.; Makhlynets, O.V.; Wu, Y.; Polizzi, N.; Wu, H.; Gosavi, P.M.; Korendovych, I.V.; DeGrado, W.F.; Hong, M.
Deposited on : 2017-01-09

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

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 3%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:1-A:7, C:1-C:7, E:1-E:7, G:1-G:7, I:1-I:7, K:1-K:7, O:1-O:7, Q:1-Q:7, S:1-S:7, U:1-U:7, W:1-W:7, Y:1-Y:7 (84)	0.39	10

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1524 atoms, of which 780 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ILE-HIS-VAL-HIS-LEU-GLN-ILE.

Mol	Chain	Residues	Atoms					Trace
1	A	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	C	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	E	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	G	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	I	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	K	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	O	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	Q	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	S	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	U	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	W	7	Total	C	H	N	O	0
			126	40	65	12	9	
1	Y	7	Total	C	H	N	O	0
			126	40	65	12	9	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	C	1	Total	Zn
			1	1
2	E	1	Total	Zn
			1	1
2	G	1	Total	Zn
			1	1

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Mol	Chain	Residues	Atoms	
2	I	1	Total 1	Zn 1
2	K	1	Total 1	Zn 1
2	O	1	Total 1	Zn 1
2	Q	1	Total 1	Zn 1
2	S	1	Total 1	Zn 1
2	U	1	Total 1	Zn 1
2	W	1	Total 1	Zn 1
2	Y	1	Total 1	Zn 1

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: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

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: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

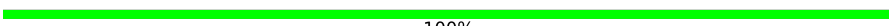
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

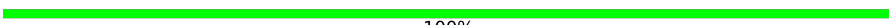
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

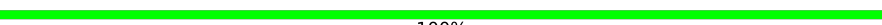
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.9 Score per residue for model 9

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.11 Score per residue for model 11

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

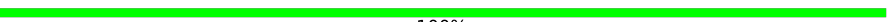
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

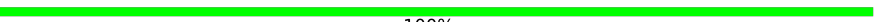
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

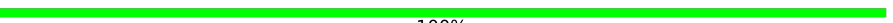
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.12 Score per residue for model 12

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.14 Score per residue for model 14

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.15 Score per residue for model 15

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.16 Score per residue for model 16

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.17 Score per residue for model 17

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.18 Score per residue for model 18

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

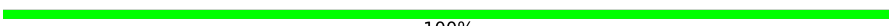
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

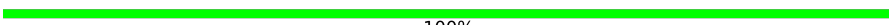
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

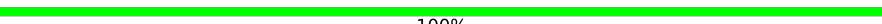
There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.19 Score per residue for model 19

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

4.2.20 Score per residue for model 20

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain K:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain O:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Q:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain S:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain U:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain W:  100%

There are no outlier residues in this chain.

- Molecule 1: ILE-HIS-VAL-HIS-LEU-GLN-ILE

Chain Y:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

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
CYANA	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	44
Number of shifts mapped to atoms	44
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *catfib.str*

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	44
Number of shifts mapped to atoms	44
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

No chemical shift referencing corrections were calculated (not enough data).

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 3%, i.e. 42 atoms were assigned a chemical shift out of a possible 1359. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	17/420 (4%)	0/168 (0%)	12/168 (7%)	5/84 (6%)
Sidechain	17/780 (2%)	0/528 (0%)	17/240 (7%)	0/12 (0%)
Aromatic	8/159 (5%)	0/96 (0%)	4/48 (8%)	4/15 (27%)
Overall	42/1359 (3%)	0/792 (0%)	33/456 (7%)	9/111 (8%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 3%, i.e. 42 atoms were assigned a chemical shift out of a possible 1359. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	17/420 (4%)	0/168 (0%)	12/168 (7%)	5/84 (6%)
Sidechain	17/780 (2%)	0/528 (0%)	17/240 (7%)	0/12 (0%)
Aromatic	8/159 (5%)	0/96 (0%)	4/48 (8%)	4/15 (27%)
Overall	42/1359 (3%)	0/792 (0%)	33/456 (7%)	9/111 (8%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

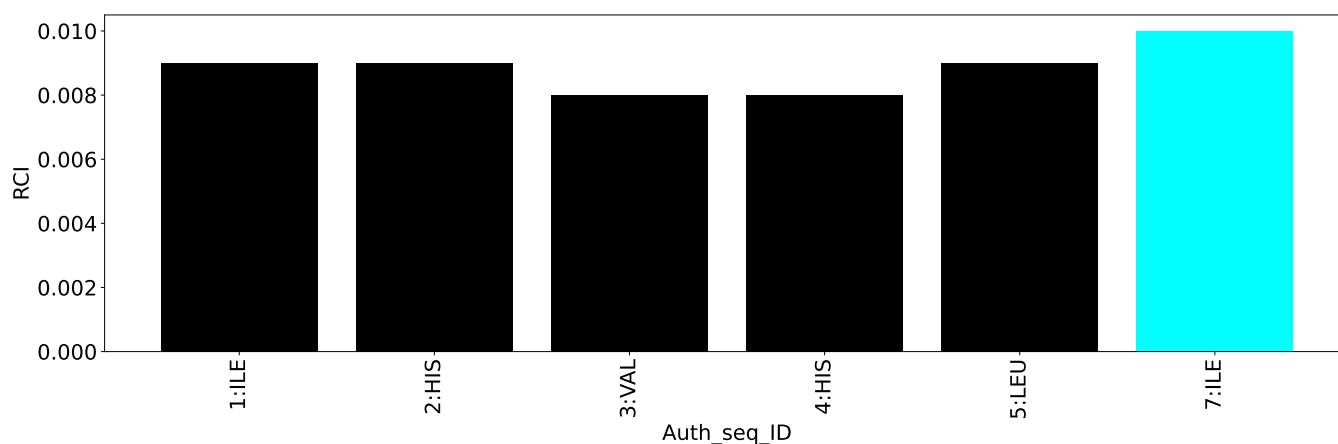
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	40
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	40
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.4
Number of long range restraints per residue ¹	0.0

¹Long 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)	0.7	0.2
0.2-0.5 (Medium)	0.3	0.35
>0.5 (Large)	16.9	7.27

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

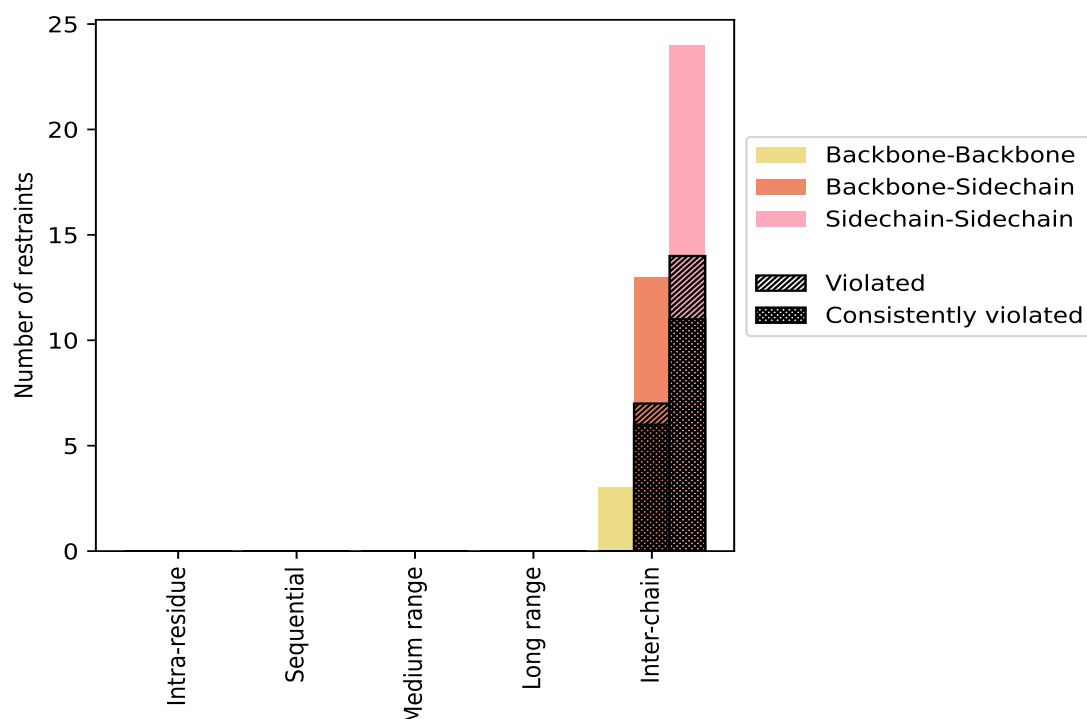
9.1 Summary of distance violations ⓘ

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
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
Inter-chain	40	100.0	21	52.5	52.5	17	42.5	42.5
Backbone-Backbone	3	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	32.5	7	53.8	17.5	6	46.2	15.0
Sidechain-Sidechain	24	60.0	14	58.3	35.0	11	45.8	27.5
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	40	100.0	21	52.5	52.5	17	42.5	42.5
Backbone-Backbone	3	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	32.5	7	53.8	17.5	6	46.2	15.0
Sidechain-Sidechain	24	60.0	14	58.3	35.0	11	45.8	27.5

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	18	18	3.65	6.4	1.56	3.8
2	0	0	0	0	18	18	3.63	6.72	1.62	3.47
3	0	0	0	0	18	18	3.38	6.59	1.64	3.46
4	0	0	0	0	17	17	3.56	6.1	1.04	3.67
5	0	0	0	0	19	19	3.36	6.21	1.71	3.58
6	0	0	0	0	18	18	3.5	6.56	1.71	3.62
7	0	0	0	0	18	18	3.59	6.07	1.49	3.82
8	0	0	0	0	18	18	3.42	6.36	1.67	3.42
9	0	0	0	0	19	19	3.37	6.62	1.84	3.6
10	0	0	0	0	18	18	3.72	7.27	1.77	3.82

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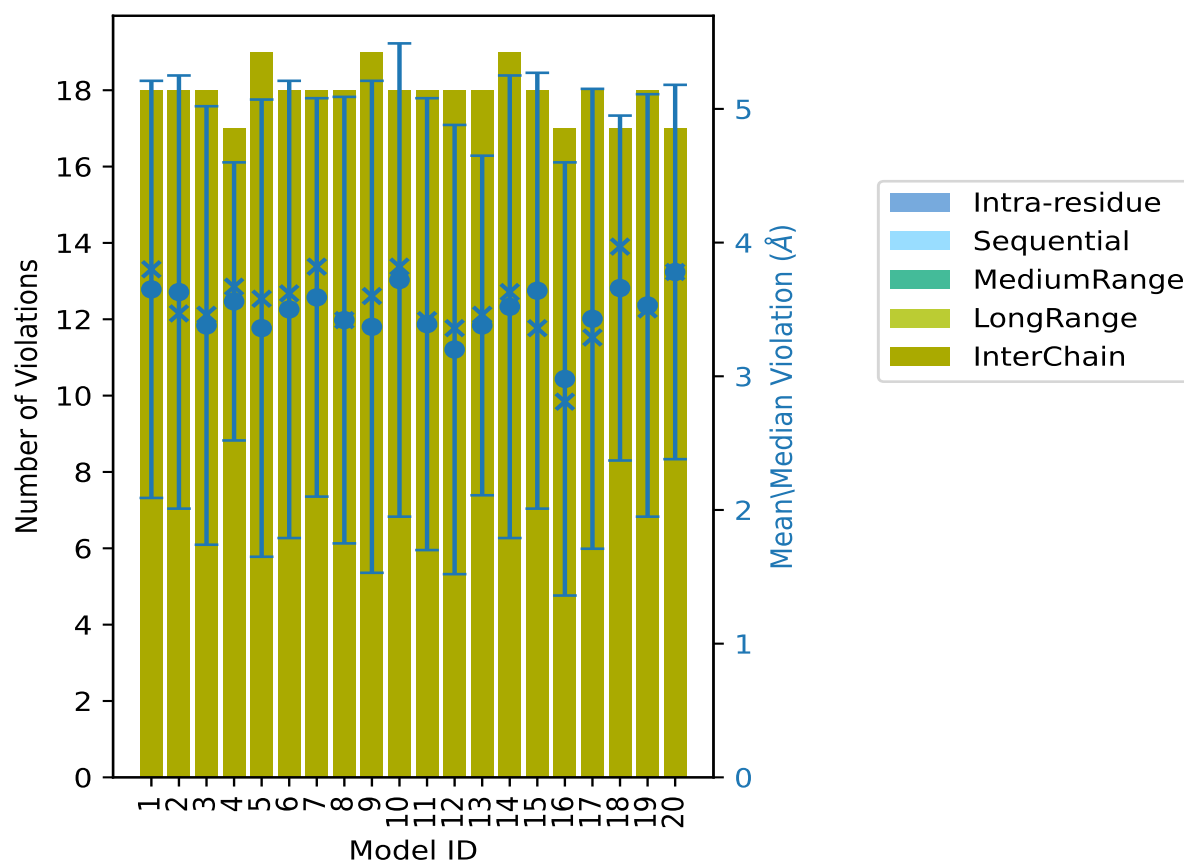
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	18	18	3.39	6.57	1.69	3.42
12	0	0	0	0	18	18	3.2	6.06	1.68	3.36
13	0	0	0	0	18	18	3.38	5.86	1.27	3.46
14	0	0	0	0	19	19	3.52	6.36	1.73	3.63
15	0	0	0	0	18	18	3.64	6.5	1.63	3.36
16	0	0	0	0	17	17	2.98	6.15	1.62	2.81
17	0	0	0	0	18	18	3.43	6.45	1.72	3.29
18	0	0	0	0	17	17	3.66	6.59	1.29	3.97
19	0	0	0	0	18	18	3.53	6.85	1.58	3.5
20	0	0	0	0	17	17	3.78	6.32	1.4	3.78

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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

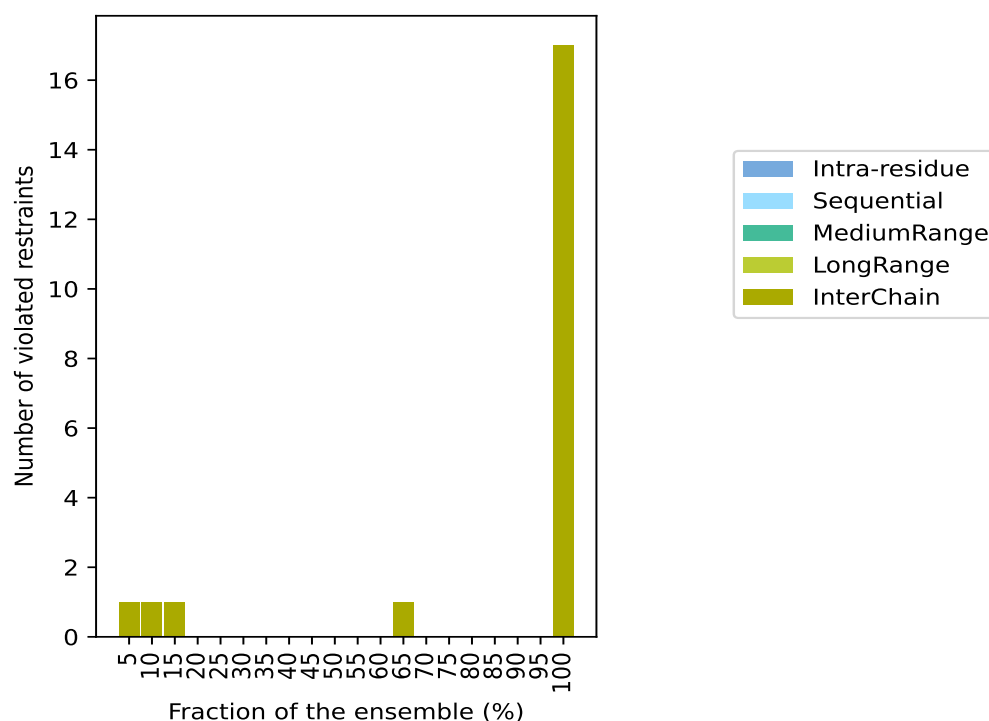
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 19(IR:0, SQ:0, MR:0, LR:0, IC:19) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	1	1	1	5.0
0	0	0	0	1	1	2	10.0
0	0	0	0	1	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	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	1	1	13	65.0
0	0	0	0	0	0	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	17	17	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

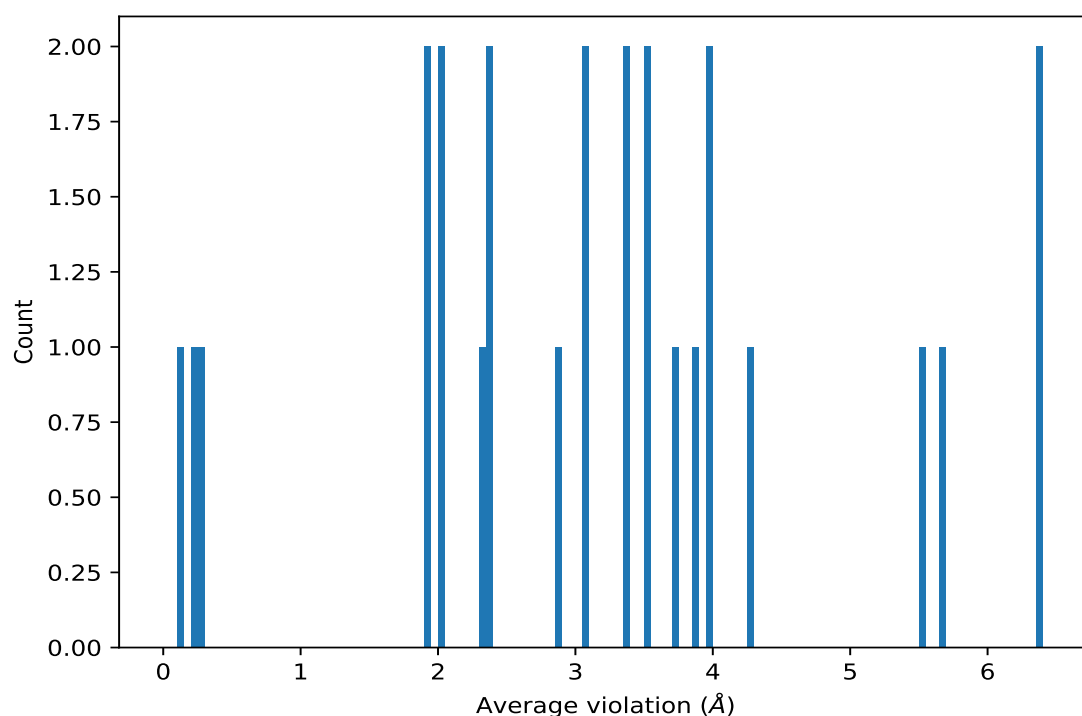
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	20	6.36	0.35	6.36
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	20	6.36	0.35	6.36
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	20	5.67	0.98	6.08
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	20	5.54	1.09	6.05
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	20	4.25	0.85	4.61
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	20	3.96	0.29	3.96
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	20	3.95	0.39	3.9
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	20	3.86	0.29	3.88
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	20	3.71	0.33	3.6
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	20	3.52	0.32	3.54
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	20	3.5	0.87	3.92
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	20	3.37	0.45	3.43
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	20	3.37	0.45	3.43
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	20	3.08	0.79	3.09
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	20	3.08	0.79	3.09
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	20	2.87	0.86	2.73

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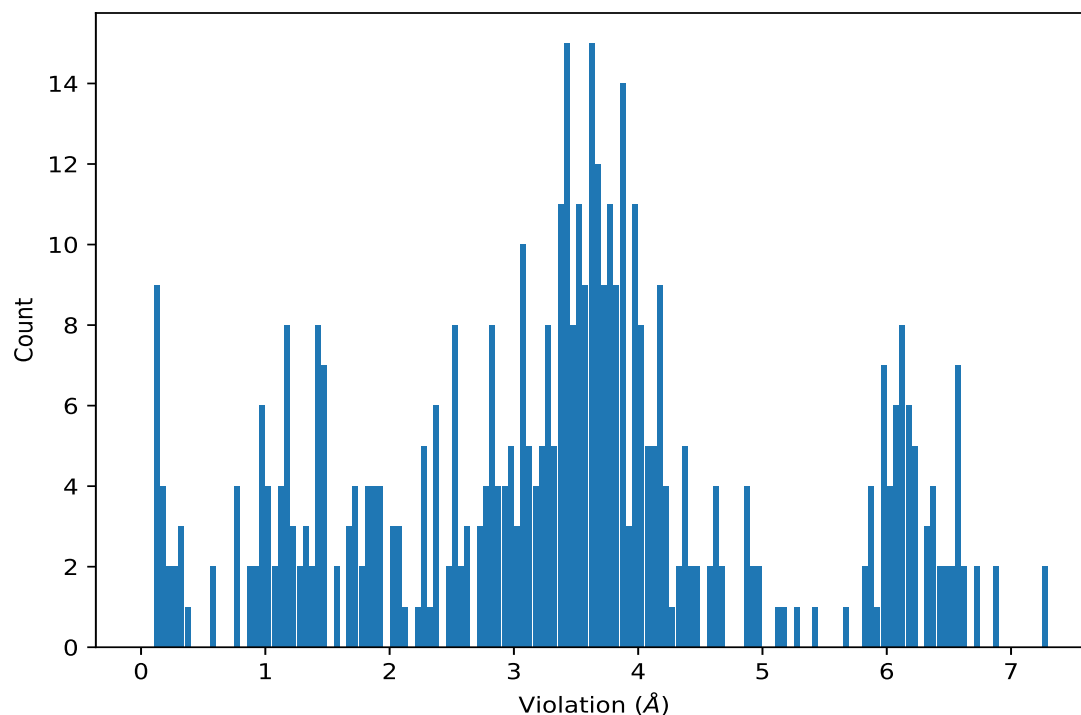
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	20	2.38	0.94	2.54
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	20	2.38	0.94	2.54
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	20	2.34	0.78	2.18
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	20	2.04	1.27	1.39
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	20	2.04	1.27	1.39
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	20	1.94	1.13	1.46
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	20	1.94	1.13	1.46
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	13	0.21	0.08	0.19
(1,38)	1:5:K:LEU:CB	1:7:I:ILE:C	3	0.15	0.04	0.13
(1,37)	1:5:K:LEU:CB	1:7:I:ILE:CG2	2	0.29	0.02	0.29

¹Number of violated models, ²Standard 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

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)
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	10	7.27
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	10	7.27
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	19	6.85
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	19	6.85
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	2	6.72
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	2	6.72
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	9	6.62
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	9	6.62
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	3	6.59
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	3	6.59
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	18	6.59
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	18	6.59
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	11	6.57
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	6	6.56
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	6	6.56
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	15	6.5
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	15	6.5
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	17	6.45
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	17	6.45
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	1	6.4
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	9	6.4
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	8	6.36
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	8	6.36
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	14	6.36
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	14	6.36
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	14	6.32
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	20	6.32
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	9	6.3
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	15	6.24
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	5	6.21
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	1	6.2
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	1	6.2
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	11	6.2
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	1	6.18
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	6	6.16
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	10	6.16
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	16	6.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	16	6.15
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	14	6.15
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	8	6.14
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	17	6.12
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	10	6.11
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	15	6.11
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	4	6.1
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	4	6.1
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	2	6.1
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	17	6.1
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	20	6.09
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	20	6.09
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	7	6.07
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	7	6.07
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	6	6.06
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	12	6.06
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	20	6.04
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	12	6.02
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	19	6.01
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	5	6.01
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	11	5.99
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	11	5.99
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	5	5.97
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	5	5.97
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	2	5.97
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	19	5.96
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	8	5.95
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	3	5.93
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	12	5.89
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	12	5.89
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG1	13	5.86
(1,17)	1:7:K:ILE:CB	1:3:I:VAL:CG2	13	5.86
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	3	5.82
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	16	5.82
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	16	5.65
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	13	5.42
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	14	5.26
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	15	5.18
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	2	5.14
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	7	4.99
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	17	4.96
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	7	4.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	18	4.9
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	10	4.89
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	7	4.87
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	7	4.87
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	9	4.86
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	4	4.68
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	13	4.65
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	8	4.64
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	3	4.61
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	12	4.61
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	10	4.6
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	7	4.58
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	14	4.56
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	7	4.48
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	7	4.48
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	15	4.43
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	18	4.41
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	6	4.39
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	4	4.38
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	18	4.38
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	8	4.37
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	11	4.35
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	2	4.34
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	2	4.32
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	7	4.26
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	18	4.24
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	4	4.24
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	9	4.22
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	17	4.21
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	3	4.19
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	1	4.19
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	7	4.19
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	17	4.18
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	18	4.17
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	18	4.17
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	6	4.16
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	15	4.16
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	13	4.15
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	18	4.14
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	10	4.12
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	5	4.11
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	8	4.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	20	4.1
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	19	4.09
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	12	4.09
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	9	4.07
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	10	4.06
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	10	4.06
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	14	4.03
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	5	4.03
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	6	4.02
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	18	4.02
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	9	4.0
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	20	4.0
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	1	4.0
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	1	4.0
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	14	3.98
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	8	3.97
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	18	3.97
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	18	3.97
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	4	3.97
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	5	3.96
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	5	3.96
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	10	3.96
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	10	3.96
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	3	3.95
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	11	3.95
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	5	3.92
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	15	3.92
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	20	3.9
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	8	3.89
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	19	3.89
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	1	3.88
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	2	3.88
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	3	3.87
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	1	3.87
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	7	3.87
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	4	3.86
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	4	3.86
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	20	3.86
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	20	3.86
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	13	3.86
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	1	3.85
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	1	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	10	3.83
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	10	3.83
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	20	3.82
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	1	3.82
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	10	3.82
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	6	3.81
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	6	3.81
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	13	3.8
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	5	3.8
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	11	3.79
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	7	3.78
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	4	3.78
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	1	3.78
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	20	3.78
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	20	3.78
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	16	3.77
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	17	3.77
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	16	3.76
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	14	3.75
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	14	3.75
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	20	3.74
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	10	3.74
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	9	3.74
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	4	3.72
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	18	3.71
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	7	3.71
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	5	3.71
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	5	3.71
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	12	3.7
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	6	3.68
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	20	3.68
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	20	3.68
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	4	3.67
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	4	3.67
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	19	3.67
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	2	3.66
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	11	3.66
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	14	3.66
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	11	3.65
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	6	3.65
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	18	3.65
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	12	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	19	3.64
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	1	3.64
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	1	3.64
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	9	3.64
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	10	3.63
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	14	3.63
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	18	3.62
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	7	3.62
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	15	3.61
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	18	3.61
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	18	3.61
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	19	3.61
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	9	3.6
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	9	3.6
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	6	3.59
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	6	3.59
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	5	3.58
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	13	3.58
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	13	3.58
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	17	3.56
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	5	3.56
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	5	3.56
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	10	3.55
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	5	3.54
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	13	3.54
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	20	3.54
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	12	3.52
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	3	3.52
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	1	3.52
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	2	3.52
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	16	3.5
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	12	3.5
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	1	3.5
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	19	3.5
(1,16)	1:7:K:ILE:CB	1:3:I:VAL:CB	13	3.49
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	6	3.49
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	6	3.49
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	19	3.49
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	19	3.49
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	3	3.49
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	8	3.46
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	16	3.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	11	3.44
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	11	3.44
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	19	3.44
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	19	3.44
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	4	3.44
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	4	3.44
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	13	3.43
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	13	3.43
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	3	3.43
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	5	3.43
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	2	3.42
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	2	3.42
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	4	3.42
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	11	3.41
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	20	3.4
(1,14)	1:5:K:LEU:CB	1:1:I:ILE:CG2	8	3.39
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	11	3.39
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	11	3.39
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	4	3.38
(1,13)	1:5:K:LEU:CB	1:1:I:ILE:CD1	13	3.36
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	15	3.36
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	15	3.36
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	15	3.35
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	15	3.35
(1,12)	1:5:K:LEU:CA	1:1:I:ILE:CG2	2	3.35
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	9	3.35
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	7	3.34
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	7	3.34
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	4	3.33
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	17	3.32
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	17	3.32
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	14	3.28
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	14	3.28
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	13	3.27
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	13	3.27
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	14	3.26
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	17	3.26
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	16	3.25
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	19	3.25
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	11	3.24
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	12	3.23
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	2	3.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	2	3.21
(1,1)	1:1:K:ILE:CB	1:5:I:LEU:CA	15	3.21
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	20	3.19
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	1	3.17
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	19	3.17
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	19	3.17
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	7	3.14
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	15	3.13
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	15	3.13
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	8	3.12
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	8	3.12
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	5	3.08
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	17	3.07
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	17	3.07
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	14	3.07
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	14	3.07
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	15	3.07
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	15	3.05
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	15	3.05
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	6	3.05
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	6	3.05
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	19	3.03
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	2	3.02
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	2	3.02
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	9	2.99
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	9	2.99
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	3	2.96
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	3	2.96
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	15	2.95
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	19	2.92
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	6	2.91
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	6	2.91
(1,11)	1:5:K:LEU:CA	1:1:I:ILE:CD1	13	2.9
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	11	2.88
(1,2)	1:1:K:ILE:CB	1:5:I:LEU:CB	17	2.86
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	3	2.85
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	3	2.85
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	13	2.83
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	13	2.83
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	17	2.82
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	17	2.82
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	12	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	12	2.81
(1,5)	1:3:K:VAL:CB	1:7:I:ILE:CG2	16	2.81
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	13	2.8
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	4	2.79
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	9	2.76
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	9	2.76
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	14	2.76
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	14	2.74
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	14	2.74
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	10	2.7
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	1	2.63
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	2	2.62
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	2	2.62
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	20	2.58
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	2	2.56
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	8	2.54
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	8	2.54
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	3	2.53
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	3	2.53
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	12	2.53
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	12	2.53
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	4	2.51
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	11	2.5
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	8	2.46
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	8	2.46
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	15	2.39
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	7	2.38
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	17	2.37
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	17	2.37
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	8	2.37
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	14	2.36
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	17	2.34
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	13	2.29
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	9	2.29
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	9	2.29
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	5	2.28
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	18	2.27
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	9	2.21
(1,10)	1:3:K:VAL:C	1:7:I:ILE:CG2	16	2.1
(1,8)	1:3:K:VAL:CG1	1:7:I:ILE:C	16	2.08
(1,8)	1:3:K:VAL:CG2	1:7:I:ILE:C	16	2.08
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	10	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	2	2.02
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	12	2.01
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	12	2.01
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	3	1.94
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	3	1.94
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	12	1.92
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	17	1.9
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	4	1.88
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	4	1.88
(1,6)	1:3:K:VAL:CG1	1:7:I:ILE:CD1	16	1.86
(1,6)	1:3:K:VAL:CG2	1:7:I:ILE:CD1	16	1.86
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	3	1.82
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	18	1.81
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	3	1.8
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	3	1.8
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	16	1.77
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	8	1.76
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	19	1.73
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	19	1.73
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	9	1.7
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	12	1.7
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	8	1.68
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	8	1.68
(1,4)	1:3:K:VAL:CB	1:7:I:ILE:CD1	6	1.67
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	1	1.57
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	1	1.57
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	11	1.47
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	11	1.47
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	16	1.47
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	20	1.46
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	20	1.46
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	1	1.45
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	1	1.45
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	18	1.4
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	18	1.4
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	4	1.4
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	4	1.4
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	10	1.4
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	10	1.4
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	16	1.4
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	16	1.4
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	13	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	13	1.38
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	3	1.34
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	11	1.31
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	11	1.31
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	18	1.28
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	18	1.28
(1,9)	1:3:K:VAL:C	1:7:I:ILE:CD1	6	1.24
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	7	1.22
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	7	1.22
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	14	1.18
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	14	1.18
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	8	1.18
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	8	1.18
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	12	1.16
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	12	1.16
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	5	1.15
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	5	1.15
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	5	1.13
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	5	1.13
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	2	1.12
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	2	1.12
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	7	1.07
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	7	1.07
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	11	1.02
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	11	1.02
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	19	1.01
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	19	1.01
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	16	0.97
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	16	0.97
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	12	0.96
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	12	0.96
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	9	0.96
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	9	0.96
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	10	0.92
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	10	0.92
(1,7)	1:3:K:VAL:CG1	1:7:I:ILE:CG2	16	0.89
(1,7)	1:3:K:VAL:CG2	1:7:I:ILE:CG2	16	0.89
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	6	0.79
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	6	0.79
(1,15)	1:5:K:LEU:CD1	1:1:I:ILE:CG2	20	0.77
(1,15)	1:5:K:LEU:CD2	1:1:I:ILE:CG2	20	0.77
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	15	0.58
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	15	0.35
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	2	0.33
(1,37)	1:5:K:LEU:CB	1:7:I:ILE:CG2	14	0.31
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	17	0.31
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	14	0.27
(1,37)	1:5:K:LEU:CB	1:7:I:ILE:CG2	13	0.26
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	19	0.24
(1,38)	1:5:K:LEU:CB	1:7:I:ILE:C	5	0.2
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	9	0.19
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	12	0.19
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	8	0.18
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	10	0.18
(1,39)	1:5:K:LEU:CG	1:3:I:VAL:CB	9	0.14
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	3	0.14
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	5	0.14
(1,38)	1:5:K:LEU:CB	1:7:I:ILE:C	11	0.13
(1,38)	1:5:K:LEU:CB	1:7:I:ILE:C	7	0.12
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	1	0.12
(1,21)	1:3:K:VAL:CB	1:1:I:ILE:CD1	6	0.12
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD1	17	0.12
(1,3)	1:1:K:ILE:CB	1:5:I:LEU:CD2	17	0.12

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found