Full wwPDB NMR Structure Validation Report (i)

May 29, 2024 – 04:45 PM EDT

PDB ID	:	8UTX
BMRB ID	:	31123
Title	:	Solution structure of a 12-mer peptide bearing a bicyclic Asx motif mimic (BAMM) as a synthetic N-cap
Authors	:	Mi, T.X.; Burgess, K.
Deposited on	:	2023-10-31

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

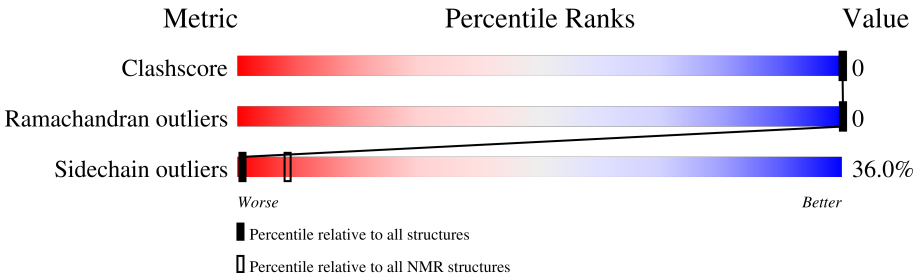
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	13	54% 8% 38%

2 Ensemble composition and analysis (i)

This entry contains 50 models. Model 21 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:333-A:340 (8)	0.10	21

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 6 clusters and 8 single-model clusters were found.

Cluster number	Models
1	13, 16, 17, 21, 24, 31, 33, 35, 38, 41, 44, 45
2	2, 5, 9, 10, 15, 18, 19, 29, 30, 40
3	1, 6, 11, 32, 37, 42, 43, 49
4	14, 20, 22, 28, 34, 39, 46, 47
5	4, 7, 23, 26
6	12, 27
Single-model clusters	3; 8; 25; 36; 48; 50

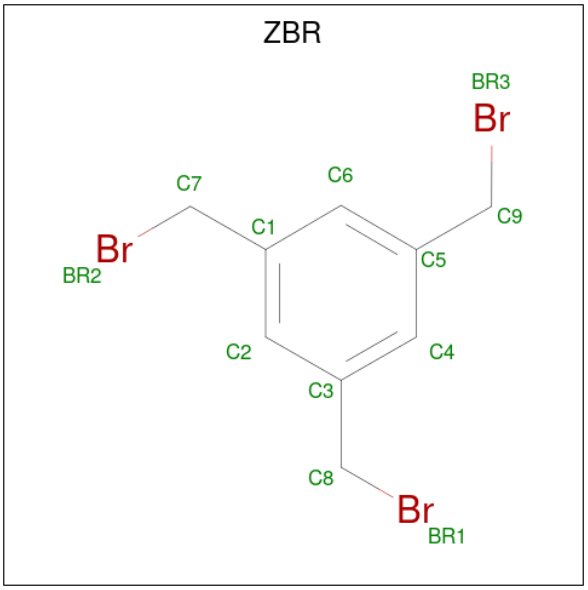
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 171 atoms, of which 82 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	13	153	48	73	15	14	3	1

- Molecule 2 is 1,3,5-tris(bromomethyl)benzene (three-letter code: ZBR) (formula: $C_9H_9Br_3$).



Mol	Chain	Residues	Atoms		
			Total	C	H
2	A	1	18	9	9

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: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

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: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.2 Score per residue for model 2

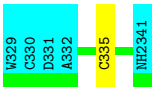
• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

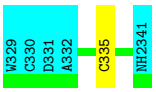
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

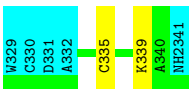
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

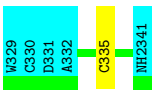
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

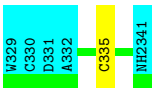
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

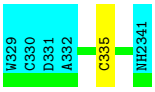
Chain A: 



4.2.8 Score per residue for model 8

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

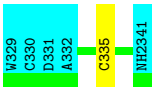
Chain A: 



4.2.9 Score per residue for model 9

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

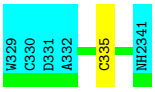
Chain A: 



4.2.10 Score per residue for model 10

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

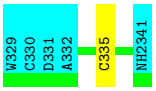
Chain A: 



4.2.11 Score per residue for model 11

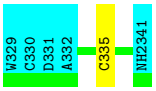
• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A: 



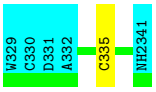
4.2.12 Score per residue for model 12

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide



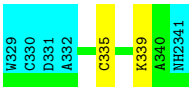
4.2.13 Score per residue for model 13

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide



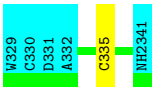
4.2.14 Score per residue for model 14

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide



4.2.15 Score per residue for model 15

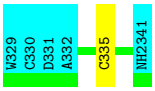
• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide



4.2.16 Score per residue for model 16

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

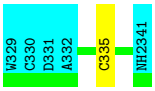
Chain A: 



4.2.17 Score per residue for model 17

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

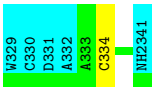
Chain A: 



4.2.18 Score per residue for model 18

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

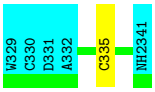
Chain A: 



4.2.19 Score per residue for model 19

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

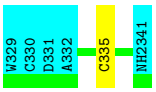
Chain A: 



4.2.20 Score per residue for model 20

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

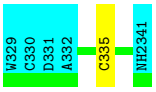
Chain A: 



4.2.21 Score per residue for model 21 (medoid)

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

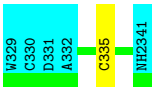
Chain A: 



4.2.22 Score per residue for model 22

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

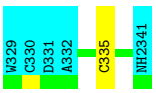
Chain A: 



4.2.23 Score per residue for model 23

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

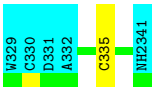
Chain A: 



4.2.24 Score per residue for model 24

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

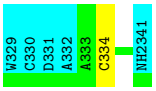
Chain A: 



4.2.25 Score per residue for model 25

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

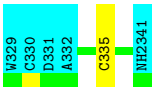
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

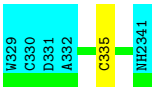
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

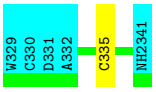
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.30 Score per residue for model 30

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.31 Score per residue for model 31

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.32 Score per residue for model 32

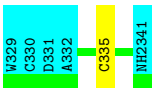
• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A:

4.2.33 Score per residue for model 33

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

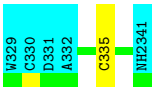
Chain A: 



4.2.34 Score per residue for model 34

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

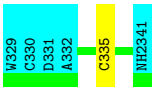
Chain A: 



4.2.35 Score per residue for model 35

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

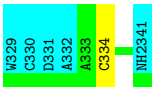
Chain A: 



4.2.36 Score per residue for model 36

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

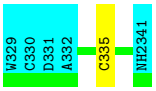
Chain A: 



4.2.37 Score per residue for model 37

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

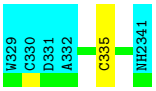
Chain A: 



4.2.38 Score per residue for model 38

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

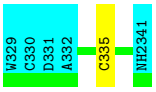
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

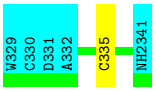
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

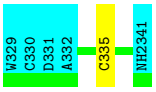
Chain A:



4.2.41 Score per residue for model 41

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

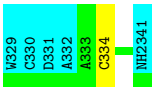
Chain A:



4.2.42 Score per residue for model 42

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

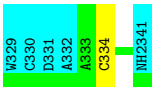
Chain A: 



4.2.43 Score per residue for model 43

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

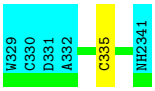
Chain A: 



4.2.44 Score per residue for model 44

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

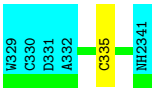
Chain A: 



4.2.45 Score per residue for model 45

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

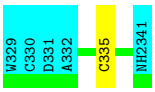
Chain A: 



4.2.46 Score per residue for model 46

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

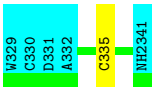
Chain A: 



4.2.47 Score per residue for model 47

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

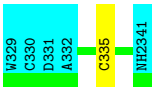
Chain A: 



4.2.48 Score per residue for model 48

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

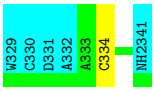
Chain A: 



4.2.49 Score per residue for model 49

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

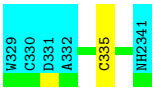
Chain A: 



4.2.50 Score per residue for model 50

• Molecule 1: TRP-CYS-ASP-ALA-ALA-CYS-CYS-ALA-ALA-ALA-LYS-ALA-NH2 peptide

Chain A: 


W329
C330
D331
A332
C335
NH2341

5 Refinement protocol and experimental data overview

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

Of the 5888 calculated structures, 50 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
MacroModel	structure calculation	

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	79
Number of shifts mapped to atoms	79
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZBR, NH2

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	2750	2750	2450	-

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 -.

There are no clashes.

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	8/13 (62%)	8±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	400/650 (62%)	400 (100%)	0 (0%)	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	3/6 (50%)	2±0 (64±9%)	1±0 (36±9%)	1 8
All	All	150/300 (50%)	96 (64%)	54 (36%)	1 8

All 3 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	335	CYS	44
1	A	334	CYS	6
1	A	339	LYS	4

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	ZBR	A	401	1	9,9,12	0.66±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	ZBR	A	401	1	12,12,15	0.84±0.04	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZBR	A	401	1	-	-	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 54% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	79
Number of shifts mapped to atoms	79
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 54%, i.e. 43 atoms were assigned a chemical shift out of a possible 79. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	16/40 (40%)	16/16 (100%)	0/16 (0%)	0/8 (0%)
Sidechain	27/39 (69%)	27/27 (100%)	0/11 (0%)	0/1 (0%)
Overall	43/79 (54%)	43/43 (100%)	0/27 (0%)	0/9 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 65 atoms were assigned a chemical shift out of a possible 125. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	23/60 (38%)	23/24 (96%)	0/24 (0%)	0/12 (0%)
Sidechain	36/53 (68%)	36/36 (100%)	0/16 (0%)	0/1 (0%)
Aromatic	6/12 (50%)	6/6 (100%)	0/5 (0%)	0/1 (0%)
Overall	65/125 (52%)	65/66 (98%)	0/45 (0%)	0/14 (0%)

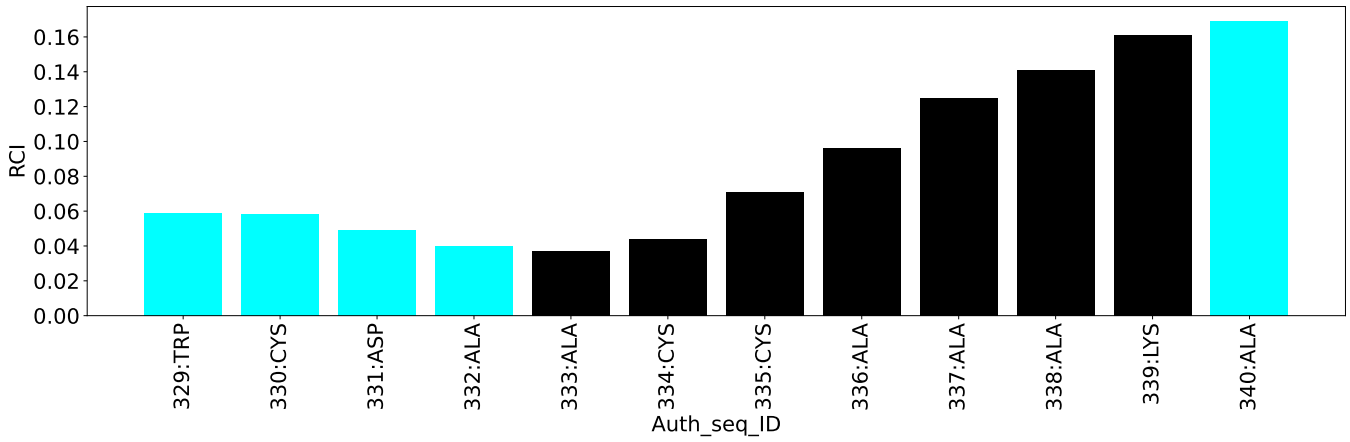
7.1.4 Statistically unusual chemical shifts (i)

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	115
Intra-residue (|i-j|=0)	57
Sequential (|i-j|=1)	24
Medium range (|i-j|>1 and |i-j|<5)	14
Long range (|i-j|≥5)	20
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	30
Number of restraints per residue	8.2
Number of long range restraints per residue[1]	1.4

[1]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)	1.8	0.2
0.2-0.5 (Medium)	2.8	0.46
>0.5 (Large)	1.7	1.43

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 (i)

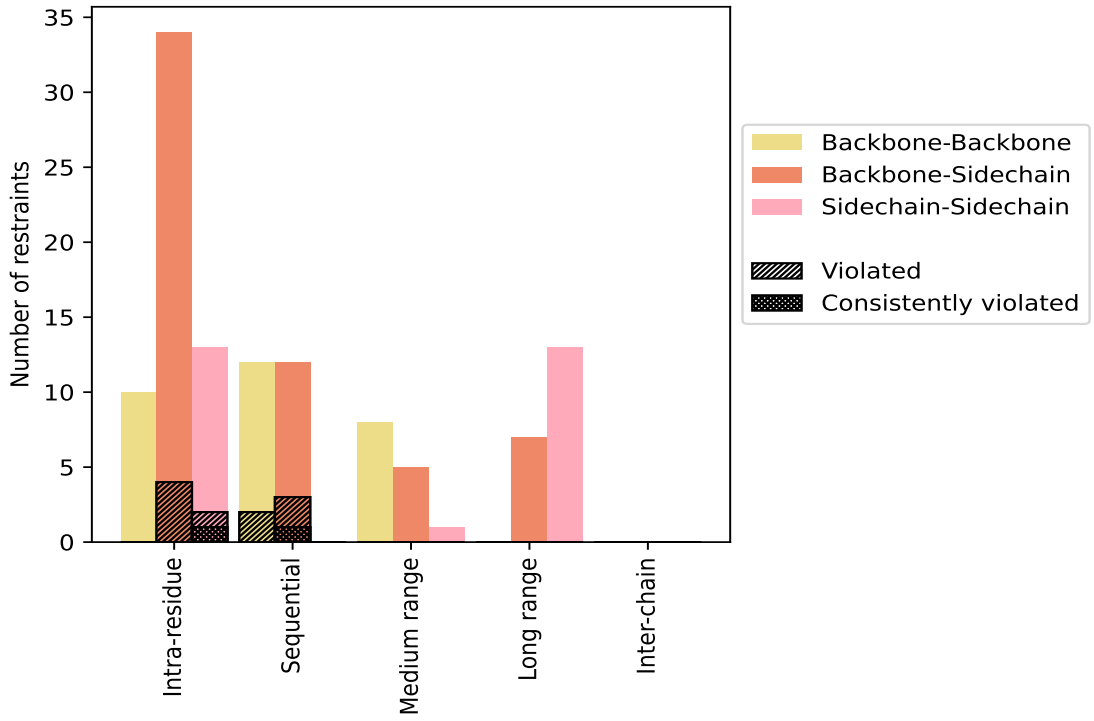
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	57	49.6	6	10.5	5.2	1	1.8	0.9
Backbone-Backbone	10	8.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	34	29.6	4	11.8	3.5	0	0.0	0.0
Sidechain-Sidechain	13	11.3	2	15.4	1.7	1	7.7	0.9
Sequential (|i-j|=1)	24	20.9	5	20.8	4.3	1	4.2	0.9
Backbone-Backbone	12	10.4	2	16.7	1.7	0	0.0	0.0
Backbone-Sidechain	12	10.4	3	25.0	2.6	1	8.3	0.9
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	14	12.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	8	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	4.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	0.9	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	20	17.4	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	7	6.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	13	11.3	0	0.0	0.0	0	0.0	0.0
Inter-chain	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
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	115	100.0	11	9.6	9.6	2	1.7	1.7
Backbone-Backbone	30	26.1	2	6.7	1.7	0	0.0	0.0
Backbone-Sidechain	58	50.4	7	12.1	6.1	1	1.7	0.9
Sidechain-Sidechain	27	23.5	2	7.4	1.7	1	3.7	0.9

[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



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

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	4	5	0	0	0	9	0.42	1.43	0.38	0.28
2	4	5	0	0	0	9	0.42	1.43	0.38	0.28
3	4	4	0	0	0	8	0.46	1.43	0.39	0.36
4	3	5	0	0	0	8	0.45	1.43	0.39	0.34
5	4	5	0	0	0	9	0.45	1.43	0.39	0.4
6	3	5	0	0	0	8	0.45	1.43	0.39	0.34
7	4	5	0	0	0	9	0.43	1.43	0.38	0.27
8	3	4	0	0	0	7	0.46	1.43	0.42	0.34
9	4	5	0	0	0	9	0.42	1.43	0.38	0.28
10	4	5	0	0	0	9	0.42	1.43	0.38	0.29

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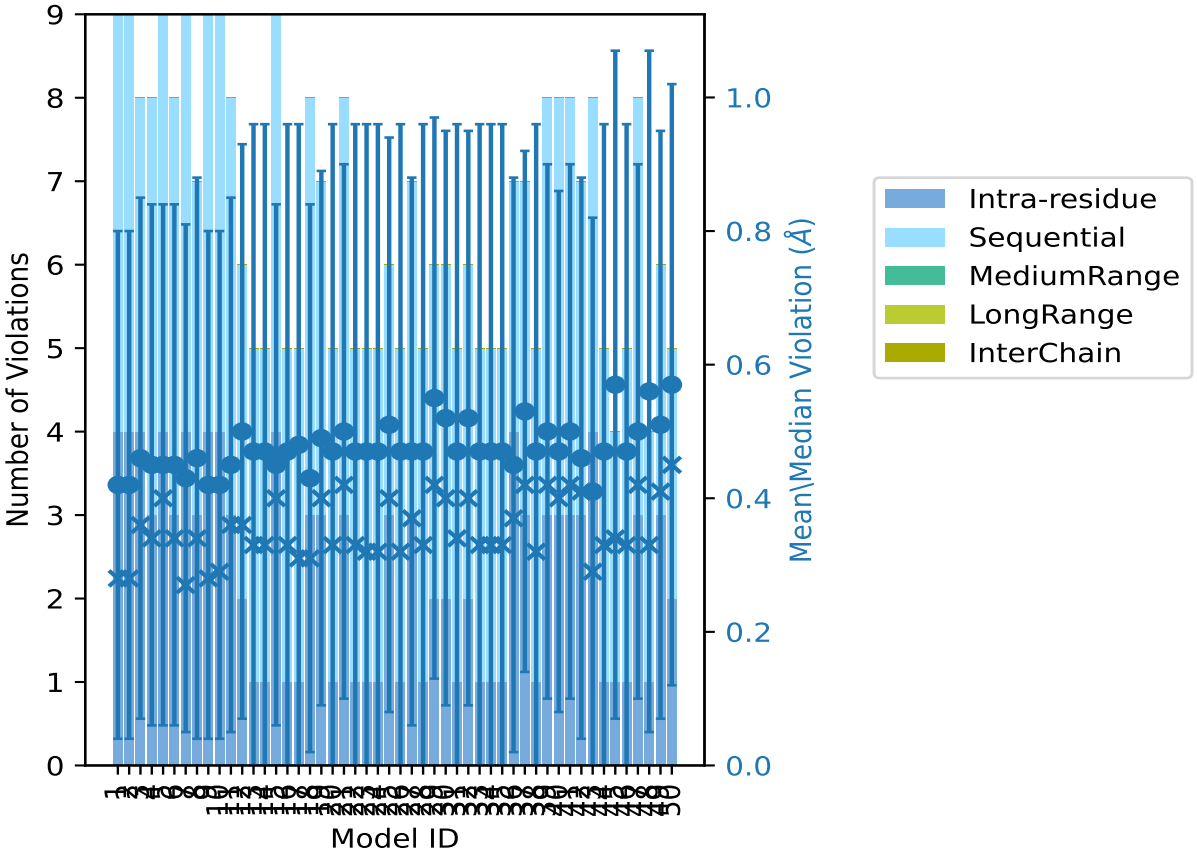
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	3	5	0	0	0	8	0.45	1.43	0.4	0.36
12	2	4	0	0	0	6	0.5	1.43	0.43	0.36
13	1	4	0	0	0	5	0.47	1.43	0.49	0.33
14	1	4	0	0	0	5	0.47	1.43	0.49	0.33
15	4	5	0	0	0	9	0.45	1.43	0.39	0.4
16	1	4	0	0	0	5	0.47	1.43	0.49	0.33
17	1	4	0	0	0	5	0.48	1.43	0.48	0.31
18	3	5	0	0	0	8	0.43	1.43	0.41	0.31
19	3	4	0	0	0	7	0.49	1.43	0.4	0.4
20	1	4	0	0	0	5	0.47	1.43	0.49	0.33
21	3	5	0	0	0	8	0.5	1.43	0.4	0.42
22	1	4	0	0	0	5	0.47	1.43	0.49	0.33
23	1	4	0	0	0	5	0.47	1.43	0.49	0.32
24	1	4	0	0	0	5	0.47	1.43	0.49	0.32
25	3	3	0	0	0	6	0.51	1.43	0.43	0.4
26	1	4	0	0	0	5	0.47	1.43	0.49	0.32
27	3	4	0	0	0	7	0.47	1.43	0.41	0.37
28	1	4	0	0	0	5	0.47	1.43	0.49	0.33
29	2	4	0	0	0	6	0.55	1.43	0.42	0.42
30	2	4	0	0	0	6	0.52	1.43	0.43	0.4
31	1	4	0	0	0	5	0.47	1.43	0.49	0.34
32	2	4	0	0	0	6	0.52	1.43	0.43	0.4
33	1	4	0	0	0	5	0.47	1.43	0.49	0.33
34	1	4	0	0	0	5	0.47	1.43	0.49	0.33
35	1	4	0	0	0	5	0.47	1.43	0.49	0.33
36	4	3	0	0	0	7	0.45	1.43	0.43	0.37
37	3	4	0	0	0	7	0.53	1.43	0.39	0.42
38	1	4	0	0	0	5	0.47	1.43	0.49	0.32
39	3	5	0	0	0	8	0.5	1.43	0.4	0.42
40	3	5	0	0	0	8	0.47	1.43	0.39	0.4
41	3	5	0	0	0	8	0.5	1.43	0.4	0.42
42	3	4	0	0	0	7	0.46	1.43	0.42	0.41
43	4	4	0	0	0	8	0.41	1.43	0.41	0.29
44	1	4	0	0	0	5	0.47	1.43	0.49	0.33
45	1	3	0	0	0	4	0.57	1.43	0.5	0.34
46	1	4	0	0	0	5	0.47	1.43	0.49	0.33
47	3	5	0	0	0	8	0.5	1.43	0.4	0.42
48	1	3	0	0	0	4	0.56	1.43	0.51	0.33
49	3	3	0	0	0	6	0.51	1.43	0.44	0.41
50	2	3	0	0	0	5	0.57	1.43	0.45	0.45

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

[5]Inter-chain restraints, [6]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, 104(IR:51, SQ:19, MR:14, LR:20, IC:0) 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]	%
1	0	0	0	0	1	1	2.0
1	0	0	0	0	1	2	4.0
0	0	0	0	0	0	3	6.0
0	0	0	0	0	0	4	8.0

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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	0	0	5	10.0
0	0	0	0	0	0	6	12.0
0	0	0	0	0	0	7	14.0
0	0	0	0	0	0	8	16.0
1	0	0	0	0	1	9	18.0
0	0	0	0	0	0	10	20.0
0	0	0	0	0	0	11	22.0
0	0	0	0	0	0	12	24.0
0	0	0	0	0	0	13	26.0
0	0	0	0	0	0	14	28.0
0	0	0	0	0	0	15	30.0
0	0	0	0	0	0	16	32.0
0	0	0	0	0	0	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	0	0	0	20	40.0
0	0	0	0	0	0	21	42.0
0	0	0	0	0	0	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
1	0	0	0	0	1	25	50.0
0	0	0	0	0	0	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	0	0	0	0	29	58.0
1	1	0	0	0	2	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	0	0	0	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	1	0	0	0	1	40	80.0
0	0	0	0	0	0	41	82.0
0	0	0	0	0	0	42	84.0
0	0	0	0	0	0	43	86.0
0	1	0	0	0	1	44	88.0
0	0	0	0	0	0	45	90.0

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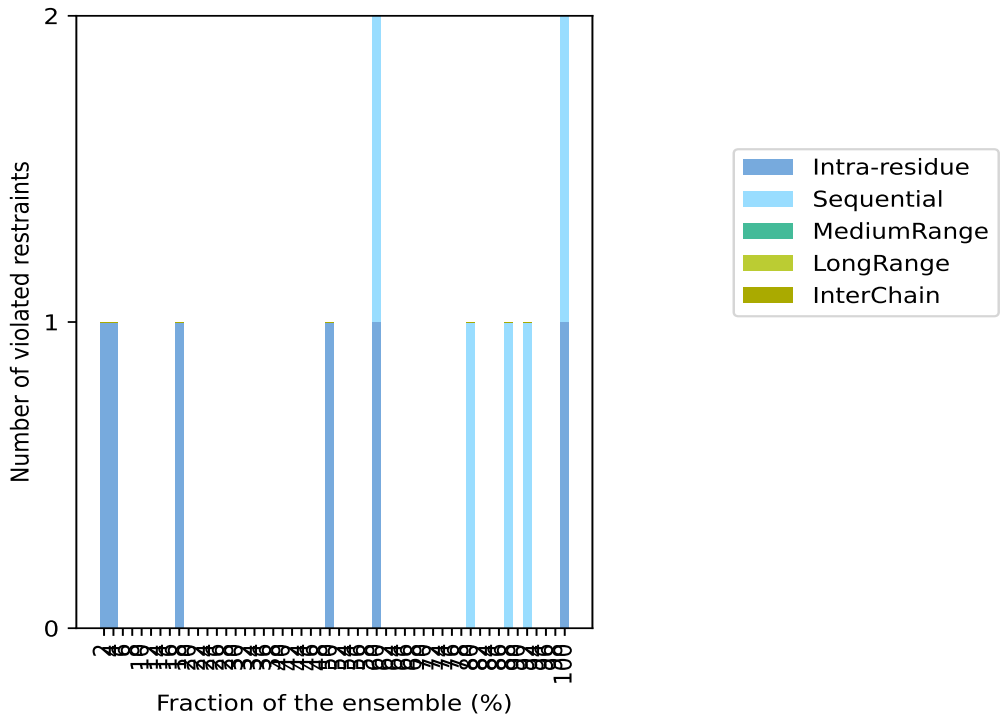
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	0	0	0	1	46	92.0
0	0	0	0	0	0	47	94.0
0	0	0	0	0	0	48	96.0
0	0	0	0	0	0	49	98.0
1	1	0	0	0	2	50	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

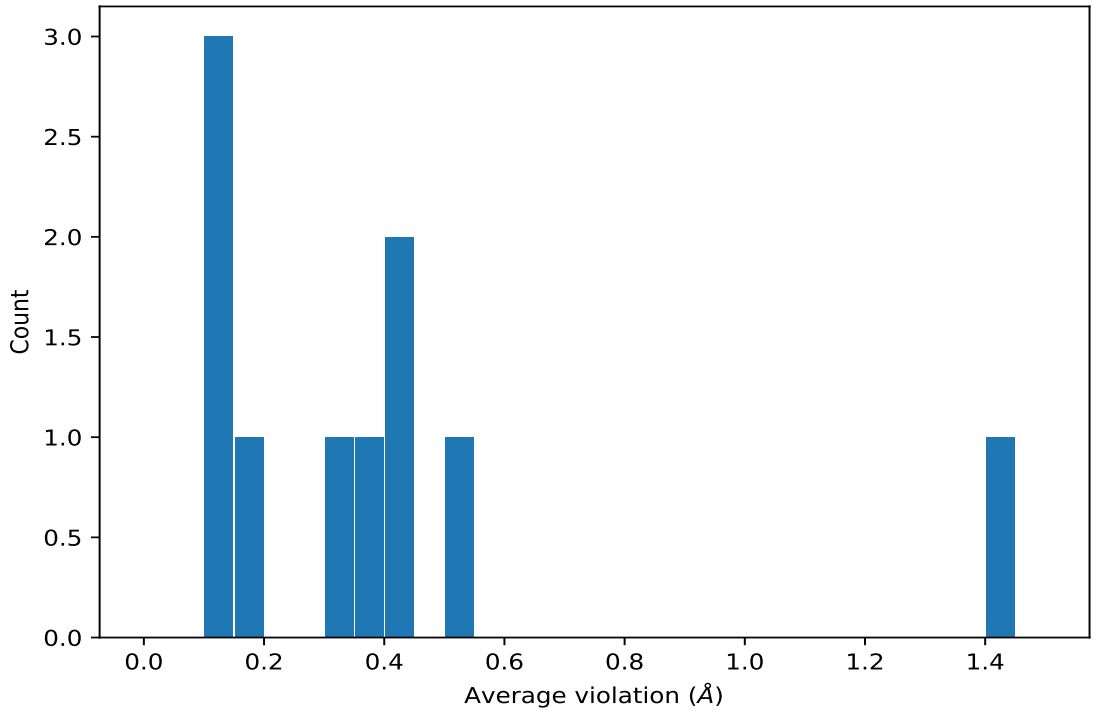
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

The following table provides the mean and the standard deviation of theviolation 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.

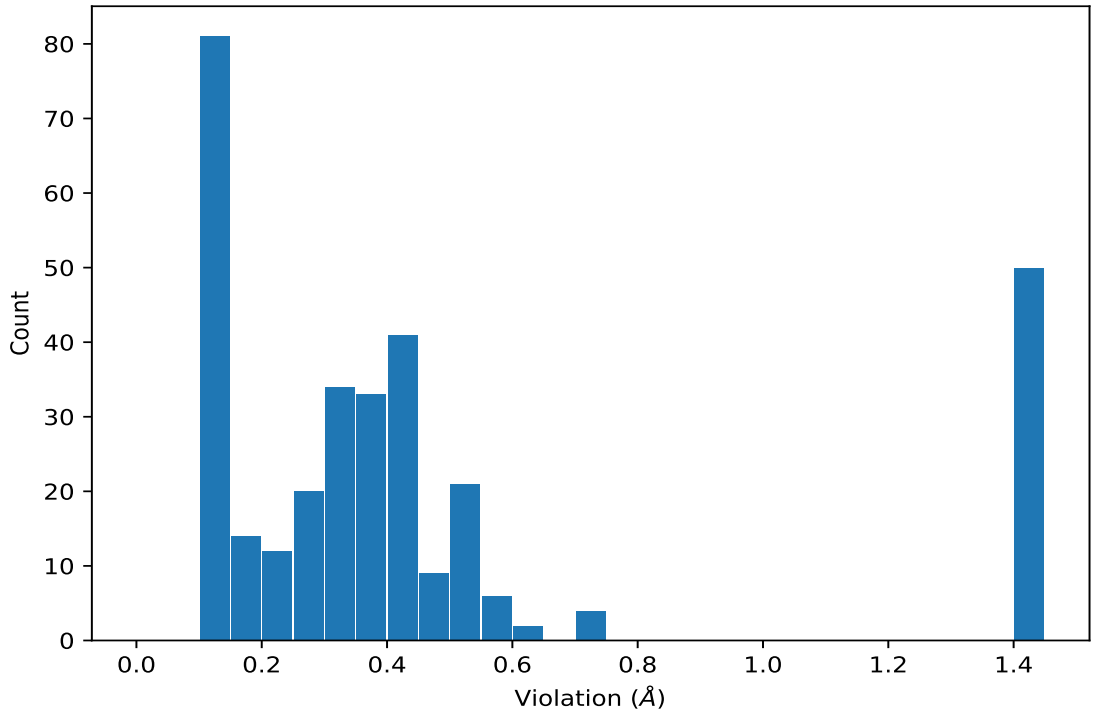
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	50	1.43	0.0	1.43
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	50	0.31	0.05	0.32
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	46	0.13	0.02	0.12
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	44	0.38	0.14	0.35
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	40	0.11	0.01	0.11
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	30	0.51	0.06	0.53
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	30	0.4	0.04	0.4
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	25	0.43	0.01	0.43
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	9	0.19	0.01	0.2
(1,27)	1:334:A:CYS:H	1:334:A:CYS:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]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)
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	1	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	2	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	3	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	4	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	5	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	6	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	7	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	8	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	9	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	10	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	11	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	12	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	13	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	14	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	15	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	16	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	17	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	18	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	19	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	20	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	21	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	22	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	23	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	24	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	25	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	26	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	27	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	28	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	29	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	30	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	31	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	32	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	33	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	34	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	35	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	36	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	37	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	38	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	39	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	40	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	41	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	42	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	43	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	44	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	45	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	46	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	47	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	48	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	49	1.43
(1,2)	1:329:A:TRP:HE1	1:329:A:TRP:HZ3	50	1.43
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	21	0.71
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	39	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	41	0.71
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	47	0.71
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	5	0.61
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	15	0.61
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	29	0.57
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	5	0.56
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	15	0.56
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	6	0.55
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	37	0.55
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	40	0.55
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	1	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	2	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	4	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	7	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	9	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	10	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	11	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	36	0.54
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	3	0.53
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	12	0.53
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	19	0.53
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	25	0.53
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	27	0.53
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	50	0.52
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	8	0.52
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	18	0.52
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	42	0.52
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	43	0.52
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	49	0.52
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	30	0.51
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	32	0.51
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	21	0.46
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	39	0.46
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	41	0.46
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	47	0.46
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	21	0.45
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	39	0.45
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	41	0.45
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	47	0.45
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	50	0.45
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	37	0.44
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	40	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	18	0.44
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	25	0.44
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	29	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	1	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	2	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	3	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	4	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	6	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	7	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	9	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	10	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	11	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	19	0.43
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	36	0.43
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	32	0.42
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	3	0.42
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	37	0.42
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	40	0.42
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	42	0.42
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	43	0.42
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	49	0.42
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	30	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	1	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	2	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	5	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	7	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	9	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	10	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	15	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	42	0.41
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	4	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	6	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	11	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	19	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	29	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	43	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	49	0.4
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	5	0.4
(1,10)	1:330:A:CYS:H	1:330:A:CYS:HB3	15	0.4
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	18	0.39
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	41	0.39
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	40	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	8	0.38
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	21	0.38
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	30	0.38
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	32	0.38
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	39	0.38
(1,17)	1:331:A:ASP:H	1:331:A:ASP:HB2	47	0.38
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	27	0.37
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	29	0.37
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	37	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	12	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	25	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	27	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	36	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	37	0.37
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	40	0.37
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	12	0.36
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	13	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	14	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	16	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	17	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	20	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	22	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	28	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	31	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	33	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	35	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	44	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	45	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	46	0.35
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	48	0.35
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	8	0.34
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	31	0.34
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	45	0.34
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	23	0.34
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	24	0.34
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	26	0.34
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	34	0.34
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	38	0.34
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	13	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	14	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	16	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	21	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	22	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	28	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	33	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	34	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	35	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	39	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	41	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	44	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	46	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	47	0.33
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	19	0.32
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	23	0.32
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	24	0.32
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	26	0.32
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	38	0.32
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	11	0.31
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	17	0.31
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	48	0.31
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	3	0.3
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	50	0.3
(1,45)	1:339:A:LYS:H	1:339:A:LYS:HB2	8	0.3
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	4	0.29
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	5	0.29
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	6	0.29
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	10	0.29
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	15	0.29
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	1	0.28
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	2	0.28
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	9	0.28
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	30	0.28
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	7	0.27
(1,70)	1:332:A:ALA:H	1:331:A:ASP:HB3	32	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	1	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	2	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	3	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	7	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	9	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	10	0.27
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	6	0.26
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	27	0.26
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	11	0.24
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	12	0.23
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	18	0.23
(1,69)	1:330:A:CYS:H	1:329:A:TRP:HB2	19	0.23
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	18	0.21
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	1	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	2	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	3	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	7	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	9	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	10	0.2
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	27	0.2
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	25	0.19
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	42	0.18
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	43	0.18
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	49	0.18
(1,74)	1:335:A:CYS:H	1:334:A:CYS:HB2	36	0.17
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	17	0.17
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	5	0.17
(1,5)	1:329:A:TRP:HD1	1:329:A:TRP:HB2	15	0.17
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	4	0.15
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	6	0.15
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	7	0.15
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	24	0.15
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	38	0.15
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	45	0.15
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	48	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	13	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	22	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	23	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	26	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	33	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	34	0.14
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	44	0.14
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	4	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	6	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	7	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	8	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	17	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	50	0.13
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	8	0.13
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	31	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	35	0.13
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	42	0.13
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	43	0.13
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	13	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	22	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	25	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	33	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	34	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	36	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	42	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	43	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	44	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	3	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	11	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	14	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	16	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	20	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	21	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	28	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	39	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	41	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	46	0.12
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	47	0.12
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	1	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	2	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	9	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	11	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	14	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	16	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	21	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	23	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	24	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	26	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	28	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	31	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	35	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	38	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	39	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	41	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	46	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	47	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	2	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	5	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	9	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	10	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	12	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	15	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	19	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	27	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	29	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	30	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	37	0.11
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	49	0.11
(1,27)	1:334:A:CYS:H	1:334:A:CYS:HB3	36	0.11
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	5	0.1
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	10	0.1
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	15	0.1
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	18	0.1
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	20	0.1
(1,53)	1:338:A:ALA:H	1:339:A:LYS:H	40	0.1
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	18	0.1
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	32	0.1
(1,51)	1:337:A:ALA:H	1:336:A:ALA:H	40	0.1
(1,27)	1:334:A:CYS:H	1:334:A:CYS:HB3	43	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found